Full title:

Models for Assessing and Forecasting the Impact of Environmental Key Pollutants on Marine and Freshwater Ecosystems and Biodiversity

Acronym: MODELKEY

Sub-Priority 1.1.6.3 Global Change and Ecosystems

Research Area III.4. Risk assessment, management, conservation and rehabilitation options to terrestrial and marine ecosystems
Topic III.4.2: Develop model(s) for assessing and forecasting the impact of environmental pollution on freshwater and marine ecosystems and their biological diversity

Integrated Project

Co-ordinator: Dr. Werner Brack
Co-ordinator organisation: UFZ Centre for Environmental Research Leipzig, Germany

Participants:

1.	**UFZ Centre for Environmental Research Leipzig (D)**	**UFZ**
2.	**University of Antwerp (B)**	**UA**
3.	**Centre for Environment, Fisheries, and Agriculture (UK)**	**CEFAS**
4.	**Delft Hydraulics (NL)**	**DELFT**
5.	**Consorzio Venezia Ricerche (I)**	**CVR**
6.	**Vrije Universiteit Amsterdam (NL)**	**VUA**
7.	**Centre National de Recherche Scientifique (F)**	**CNRS**
8.	**Instituto de Investigaciones Quimicas y Ambientales J.P. Vila Consejo Superior de Investigaciones Cientificas (E)**	**CSIC**
9.	**Universitat de Girona (E)**	**UdG**
10.	**University of Bern (CH)**	**UB**
11.	**Veterinary Research Institute (CZ)**	**VRI**
12.	**Institute of Vertebrate Biology (CZ)**	**IVB**
13.	**University of Joensuu (FIN)**	**UJOE**
14.	**Elbe Water Quality Monitoring Agency (D)**	**EWQMA**
15.	**National Institute for Coastal and Marine Management (NL)**	**RIKZ**
16.	**Netherlands Institute for Fisheries Research (NL)**	**RIVO**
17.	**National Research Centre for Dioxins and Related Compounds (SK)**	**SZU**
18.	**Rijksinstituut voor Volksgezondheid en Milieu (NL)**	**RIVM**
19.	**University of Stuttgart (D)**	**UoS**
20.	**St. Petersburg University (RUS)**	**SPbU**
21.	**Agencia Catalana de l'Aigua (E)**	**CWA**
22.	**University of Barcelona (E)**	**UdB**
23.	**ECT Ökotoxikologie GmbH (D)**	**ECT**
24.	**Xenometrics GmbH (CH)**	**XEN**
25.	**Donabaum & Wolfram OEG Technisches Büro für Ökologie (A)**	**DW**

Summary

Proposal full title: Models for Assessing and Forecasting the Impact of Environmental Key Pollutants on Marine and Freshwater Ecosystems and Biodiversity

Proposal acronym: MODELKEY

Call Identifier: FP6-2003-Global-2

Research Area III.4. Risk assessment, management, conservation and rehabilitation options to terrestrial and marine ecosystems

Topic III.4.2: Develop model(s) for assessing and forecasting the impact of environmental pollution on freshwater and marine ecosystems and their biological diversity

Proposal abstract:

MODELKEY comprises a mulitdisciplinary approach aiming at developing interlinked and verified predictive modelling tools as well as state-of-the-art effect-assessment and analytical methods generally applicable to European freshwater and marine ecosystems:
- to assess, forecast, and mitigate the risks of traditional and recently evolving pollutants on fresh water and marine ecosystems and their biodiversity at a river basin and adjacent marine environment scale,
- to provide early warning strategies on the basis of sub-lethal effects *in vitro* and *in vivo*,
- to provide a better understanding of cause-effect-relationships between changes in biodiversity and the ecological status, as addressed by the Water Framework Directive (WFD), and the impact of environmental pollution as causative factor,
- to provide methods for state-of-the-art risk assessment and decision support systems for the selection of the most efficient management options to prevent effects on biodiversity and to prioritise contamination sources and contaminated sites,
- to strengthen the scientific knowledge on an European level in the field of impact assessment of environmental pollution on aquatic ecosystems and their biodiversity by extensive training activities and knowledge dissemination to stakeholders and the scientific community.

This goal shall be achieved by combining innovative predictive tools for modelling exposure on a river basin scale including the estuary and the coastal zone, for modelling effects on higher levels of biological organisation with powerful assessment tools for the identification of key modes of action, key toxicants and key parameters determining exposure. The developed tools will be verified in case studies representing European key areas including Mediterranean, Western and Central European river basins. An end-user-directed decision support system will be provided for cost-effective tool selection and appropriate risk and site prioritisation.

Content List

Full title:
Models for Assessing and Forecasting the Impact of Environmental Key Pollutants on Marine and Freshwater Ecosystems and Biodiversity

Acronym: MODELKEY

B.1 Scientific and technological objectives of the project and state of the art

Scientific and technological objectives:

MODELKEY comprises a multidisciplinary approach aimed at developing **interlinked and verified diagnostic and predictive modelling tools** as well as **state-of-the-art effect-assessment and analytical methods** generally applicable to European freshwater and marine ecosystems:

- to **assess, forecast, and mitigate the risks** of traditional and recently evolving pollutants **on fresh water and marine ecosystems and their biodiversity at a river basin and adjacent marine environment scale**,

- to **identify site- and basin-specific key toxicants**, which are not necessarily currently monitored "priority pollutants",

- to provide a better understanding of **cause-effect relationships** between the impact of environmental pollution as a causative factor and changes in **biodiversity** and the ecological status, as addressed by the Water Framework Directive (WFD),

- to provide **early warning strategies** on the basis of sub-lethal effects measured *in vitro* and *in vivo* and provide links to effects on community health and biodiversity,

- to provide methods for **state-of-the-art risk assessment** and **decision support systems** for the selection of the most efficient management options to **prevent adverse effects on biodiversity** and to prioritise contamination sources and contaminated sites,

- to **strengthen the scientific knowledge on an European level** in the field of impact assessment of environmental pollution in aquatic ecosystems and **biodiversity** by extensive training activities and knowledge dissemination to stakeholders and the scientific community.

In order to successfully achieve these objectives, MODELKEY is organized in **7 subprojects** which specifically address the following **aims**:

KEYTOX will aim at **tool development** and application for **effect-directed identification of site- and basin-specific key toxicants** (including state-of-the-art effect assessment and analytical methods) for the establishment of cause-effect relationships and improved risk assessment.

BASIN is designed to **compile** existing data and insert new **monitoring data** created during the duration of MODELKEY by the agencies or the project itself, for database establishment and linking to other databases providing the basis for site selection and basin-directed impact assessment.

EXPO will focus on the establishment of **easy-to-use exposure models** for the prediction of **risks of toxic pollution in river basins and adjacent coastal areas** including modules on most relevant processes including sediment erosion and sedimentation, transport and fate, and bioavailability and food web accumulation.

EFFECT aims to develop deterministic and stochastic models for **understanding, diagnosis and prediction of effects on populations, communities and ecosystems and their biodiversity.**

SITE is designed to deliver and apply site-directed experimental and field tools for a **characterisation of processes, cause-effect relationships and effect propagation** focusing on providing a better understanding of the toxic impact on aquatic ecosystems and a calibration and verification of modelling tools. SITE will apply innovative **early warning systems** such as *in vitro* assays and biomarkers and provide **links to effects on communities and biodiversity**.

DECIS aims to develop **integrated risk indexes** and **decision support systems** for an exploitation of MODELKEY results for better management options, preventive policies and cost-efficient remedial activities.

DIS/TRAIN aims to disseminate results and to organise training programmes for MODELKEY participants, external scientists and end-users.

The deliverables arising from MODELKEY will include

- **exposure models** to forecast exposure of communities to priority and newly identified key toxicants.
- **effect models** to anticipate effects by key toxicants at different levels of biological organisation and biodiversity.
- **predictive risk assessment verified in case studies in river basins and marine areas**.
- **decision support system**, as an **end-user framework** choosing **the most efficient way to spend limited resources on remediation, prevention and optimal protection of ecosystem function and biodiversity (sustainable management).**

Specific tools provided by MODELKEY to increase the power of the models are

- a **diagnostic toolbox** to identify sources and sites posing a risk to freshwater and marine ecosystem function and biodiversity.
- *In situ* biomarkers and *in vitro* assays serving as **early-warning tools**.

- an **identification toolbox** to identify **key *viz.* effect-priority toxicants**, based on *in vitro* (Effect Directed Analysis) and *in vivo* (Toxicity Identification Evaluation) biotests.
- a **key *viz.* effect-priority compound database**, accessible by internet, holding *a.o.* sources, physico-chemical and toxicological data of compounds, affecting structure and function of ecosystem components throughout Europe.

State of the Art and Advancement by MODELKEY:

The **Water Framework Directive** (WFD) demands a good ecological status of European surface waters by 2015. Although the WFD focuses on **freshwater ecosystems** its implementation is also considered a major contribution to the protection of **marine ecosystems**, which was decided e.g. in the OSPAR Convention for the North-East-Atlantic and the Barcelona Convention on the Protection of the Mediterranean Sea, since contaminated rivers are considered as major sources of marine pollution. The protection of **biodiversity** (good ecological status) plays a key role in international and European efforts to protect aquatic environments and is the major goal of the **Convention on Biological Diversity**.

One of the driving forces for changes in biodiversity is chemical stress due to environmental pollutants. The WFD qualifies the quality status of aquatic ecosystems based on traditional hydromorphological, physico-chemical, biological parameters and priority pollutant (PP) concentrations. This procedure allows a rough quality assessment. However, open questions impede a scientifically sound diagnosis and forecasting of the impact of environmental pollution on freshwater and marine ecosystems and exploitation for the development of management options, preventive policies and remedial activities. These questions will be addressed by **MODELKEY**.

Chemical pollution is well known as one factor, which may cause a decline in biodiversity in freshwater and marine ecosystems. However, the diagnosis, prediction and forecasting of toxic impacts demands for a discrimination from other stresses and for reliable cause-effect relationships between chemical pollution and biodiversity decline. To date, no generally accepted approach exists to establish this link between exposure of freshwater and marine ecosystems to environmental toxicants and observable effects on these ecosystems. There are basically two approaches to establish this link: (I) the **deterministic approach** that focuses on an understanding of functions, processes and mechanisms and (II) the **stochastic approach** focusing on an identification of relationships by statistical means. For both approaches **MODELKEY** will develop innovative and integrative models and experimental tools:

(I) Deterministic approach.

There are still big gaps in understanding links (i) between chemical quality of sediments and surface waters and measurable toxic effects, (ii) between measurable toxicity in *in vivo* and *in vitro* biotests and effects on higher levels of biological organisation including population, community and ecosystem and (iii) between the exposure to toxicants at a contaminated site and the exposure on a basin and adjacent coastal area scale.

(i) Link between chemical quality and toxicity.

Effect analysis. There is increasing evidence that effect analysis using well designed **batteries of *in vitro* and *in vivo* assays** could be a powerful tool to discriminate toxicity from other possible causes for biodiversity decline, to identify modes of action, to establish concentration-response relationships, and to serve as an **early warning** that identifies potential hazards before a decline of biodiversity is observed. **MODELKEY** will strengthen this approach by the development, advancement, standardisation and compilation of biotest batteries designed for the detection of major effect types and optimised with respect to their ecotoxicological and analytical significance, discriminative power, throughput, reproducibility, minimised test volumes and costs. These test batteries serve not only as early warning tools, but also for primary site characterisation and for toxicity identification.

Effect-based identification of key toxicants. To date, chemical quality assessment is based on chemical analysis of priority pollutants as laid down in the WFD. About 60 compounds were selected as priority pollutants in different priority categories. The discrepancy between the number of compounds potentially present in the environment and the number of regularly monitored priority pollutants is evident. To date, about 16 million compounds are known and registered in the Chemical Abstracts (CAS). Numerous studies combining chemical and biological approaches for hazard assessment of complex environmental mixtures indicate that priority pollutant concentrations are a poor indicator of toxicity. Thus, it is evident that the aim identified in FP6 to assess and forecast the impact of chemical pollution cannot be met on the basis of priority pollutant analysis alone but demands an **effect-based identification of key toxicants**, that are responsible for measurable effects. **MODELKEY** will address this demand by (a) providing a **toolbox for effect-directed analysis (EDA)** including a basic set of generally accessible, standardised or intercomparable EDA methods for European-wide use, (b) developing **innovative and tailored tools** for addressing those problems which cannot be solved by existing EDA methods, e.g. the fractionation and identification of compounds generally occurring in very complex mixtures of isomers such as polyaromatic compounds, the fractionation and identification of very polar compounds or effect detection and EDA of pharmaceuticals, (c) establishing a comprehensive and generally accessible **key toxicant database** including toxicological, physico-chemical, and spectroscopical properties that help to facilitate EDA on an European scale, (d) **training** of scientists from different parts of Europe and disseminating tools and results in order to promote EDA for a better impact assessment in European basins and (e) **identifying key toxicants** in basins selected for case studies in MODELKEY.

Assessment of bioavailability and food chain accumulation. There is increasing evidence that bioavailable fractions rather than total concentrations of chemicals in aquatic ecosystems determine the exposure of biota to toxicants. For persistent lipophilic organic toxicants and heavy metals the accumulation in the food web also plays an important role. Thus, **MODELKEY** will provide innovative and powerful tools and approaches for addressing bioavailability and food chain accumulation including (a) properly calibrated and verified **state-of-the-art food chain models**, (b) **tissue extraction and analysis of internal concentrations** in test and field organisms and relating them to observed effects, and (c) **identification of key factors determining the bioavailability** of sediment- and suspended matter-associated toxicants. (d) **derive the primary target species** of those toxicants. The food chain model will be integrated as innovative modul into integrated exposure models.

***(ii) Link between in vitro and in vivo toxicity and effects on higher levels of biological organisation*.**

While biotests are powerful tools for diagnostic purposes on a cellular and organism level our understanding of **effect propagation** on populations, communities and ecosystems is still rather limited. **MODELKEY** addresses this problem with innovative theoretical concepts supported by modelling tools and with powerful diagnostic laboratory and field tools for assessing effects on species, populations, and communities. A modelling approach based on the concept of dynamic energy budgets (DEBs) using canonical communities and simplified food chains will be used for a better understanding of effects on communities and trophic levels. The model will be calibrated and verified in well-designed laboratory experiments and field assessment, which focus on the same endpoints relevant to DEBs such as reproduction, growth and feeding rates. Experimental assessment of effect propagation will focus on finding **links between toxicity** to cells and organisms **and community effects**. State-of-the-art concepts focused on in **MODELKEY** include **pollution induced community tolerance** (PICT), **micro-** and **mesocosm** approaches, and *in situ* **biomarkers**. Effects on biodiversity are assessed on the basis of **metabolic profiling**, **taxonomic analysis** and integrative ecological indexes on the one hand and important **functional parameters** such as reproduction and growth rates on the other.

(iii) Link between sites and basins.

While at a site scale exposure to key toxicants may be experimentally determined, at a basin scale exposure modelling is believed to be the most efficient way to predict the large scale chemodynamics of contaminants. **Easy to use generic exposure models** for risk assessment of contaminated sediments, which provide good predictions with a limited number of input parameters and which take into account the major processes relevant for risks to downstream ecosystems are still to be developed. This will be done by **MODELKEY** with specific focus on erosion and sedimentation processes, transport and fate of contaminants and food chain accumulation. Extensive model calibration and verification by innovative experimental tools will further their value.

(II) Stochastic approach.

With respect to the development of management strategies for safeguarding of biotic integrity there is a big demand for tools allowing an **attribution of most probable causes to overall effects** even without fully understanding the highly complex interactions within an ecosystem and between an ecosystem and environmental pollution. Thus, **MODELKEY** wants to provide new stochastic approaches for the identification of probable cause-effect relationships on the basis of large data sets on chemical pollution, habitat, toxicity and biological inventories. This will include **integrated diagnostic models** for the identification of probable causes as well as **predictive component models** for the prediction of effects of individual toxicants and mixtures on biodiversity. Both models will be based on existing monitoring data. New monitoring activities by environmental agencies are to be expected within the duration of **MODELKEY** for WFD implementation. The integration of the most relevant agencies as full partners and the close contact to many other ones will ensure the availability of these data to **MODELKEY** and the possibility to influence monitoring designs.

MODELKEY will **significantly advance the state of the art** by

- **improved risk assessment concepts**: closely interlinking innovative deterministic and stochastic approaches for a better impact assessment of environmental pollution on marine and freshwater ecosystems. This includes comprehensive effect analysis, effect-directed key toxicant identification, bioavailability and food chain accumulation assessment, effect propagation analysis, basin-scale exposure modelling and stochastic diagnostic and predictive effect models.

- **validated risk assessment concepts**: comparison and mutual verification of both approaches at common sites,

- **enhanced scientific basis for risk assessment:** introduction of new knowledge on key toxicants, processes and community effects into running and future monitoring programs enhancing the significance of these data for stochastic effect modelling, risk assessment on a basin scale and better decision making, and

- **advanced exploitation of monitoring data**: a demand-driven evaluation, integration and exploitation of monitoring data as well as of new knowledge on key toxicants, processes and cause-effect relationships for risk assessment and decision making based on powerful weight-of-evidence approaches, integrated risk indexes,

- **improved basis for decision making**: development of end-user friendly GIS-based decision-support systems (DSS) to help environmental managers prioritise risks and measures with respect to the development of cost-efficient management options, remedial action strategies, and preventive policies for the mitigation of harmful effects on ecosystems and their biodiversity.

B.2 Relevance to the objectives of the Global Change and Ecosystems Sub-Priority

The **MODELKEY** Integrated Project addresses the general EU objectives of thematic sub-priority "Global Change and Ecosystems" (1.1.6.3) in area III: "Biodiversity and Ecosystems". The project focuses on task III.4.2 ("*Develop model(s) for assessing and forecasting the impact of environmental pollution on freshwater and marine ecosystems and their biological diversity*").

The sub-priority "Global Change and Ecosystems" was designed to **strengthen** the necessary **scientific knowledge** for the future orientation of the sustainable development strategy. According to the Brundtland Report (1987) "sustainable development meets the needs of the present without comprising the ability of future generations to meet their own needs". In agreement to this concept **MODELKEY** aims to provide powerful and innovative tools for risk assessment and forecasting with respect to the long-term protection of freshwater and marine ecosystems and their biodiversity as a crucial natural basis for human life. Scientific highlights are (1) powerful approaches for effect-directed identification of key toxicants, (2) innovative models for diagnosis, prediction and understanding effects on biodiversity and approaches to calibrate and verify these models, (3) exposure models for risk assessment of sediment-associated toxicants integrating sediment erosion and sedimentation, transport and fate, and bioavailability and food chain accumulation, (4) early warning test systems based on *in vitro* effects, (5) well designed experimental and field approaches for linking early warning with a better understanding of effect propagation in the ecosystem and (6) an end-user-friendly decision-support system to exploit this knowledge for a better management of toxicants in river basins and adjacent coastal areas. This integration of state-of-the-art diagnostic, predictive, process- and mechanism-oriented and decision supporting scientific approaches and the outstanding expertise of the leading European groups involved in **MODELKEY** are the specific strength of this project.

Since sustainable development also means sustainable economic development, MODELKEY aims to achieve maximum improvement of environmental quality with limited resources. It wants a) to focus on the development of models to assess and forecast risks to aquatic ecosystems, b) to reduce the costs involved with monitoring, c) to develop a toolbox to prioritise and prevent risks by compounds and sites based on a database of bioeffect directed key toxicants, d) to provide a decision support system to select effective and efficient tools in risk management.

The choice of the **"Integrated Project" instrument**, which was designed to generate new knowledge by **federating scientific and technological resources up to a critical mass**, is particularly relevant to the scientific objectives of MODELKEY:

- MODELKEY is a demand-driven research program focusing on the demands of site and risk managers and policy makers. This is achieved by integrating the governmental water quality monitoring agencies.

- MODELKEY addresses current societal needs, making the use of our aquatic resources sustainable by assessing adverse effects of human activities on freshwater and marine ecosystems.

- In order to achieve the challenging objectives of MODELKEY a multidisciplinary collaboration of the leading European institutes in the fields of assessment and modelling effects on all levels of biological organisation, exposure assessment and modelling and key toxicant identification was brought together.

- The overall implementation of MODELKEY covers (a) **a wide range of scientific disciplines** including ecology, ecotoxicology, environmental and analytical chemistry, hydraulics, geomorphology, mathematics, management, and economy (b) the **integration of scientist and stakeholders perspectives**, and (c) the **integration of academic and applied research** to disseminate results and training activities.

- The integration of scientists and a case study from **European associated countries** in research and training activities is undertaken to **disseminate end-user friendly tools** also to those countries who will have to implement European directives in near future to protect their biodiversity. **Training of the scientific public** outside the consortium will be provided by hands-on training in laboratories and in the field as well as in specific **training seminaries**.

MODELKEY directly addresses the objectives of topic **III.4.2 by developing models for assessing and forecasting the impact of environmental pollution on fresh water and marine ecosystems and their biological diversity**. The multidisciplinary approach is designed to provide **major breakthroughs and innovation** with respect to the assessment and forecasting of the impact of environmental pollution on freshwater and marine biodiversity by:

- a set of **highly innovative modelling** tools for diagnosis, prediction and functional understanding of **effects on ecosystems and biodiversity** anchored on combined ecological, ecotoxicological and chemical monitoring as well as specifically designed laboratory testing and field assessment

- easy to use integrated **exposure modelling** on a river basin and adjacent coastal area scale integrating models for the key processes for risks due to chemical contamination including erosion and sedimentation processes, transport and fate, and bioavailability and food chain accumulation.

- **extensive calibration and verification** of **exposure and effect models** *in situ* and in laboratory experiments

- **early warning strategy** based on *in vitro* testing of sublethal effects and *in situ* biomarker assessment.

- a comprehensive toolbox including generally applicable easy-to-use methods as well as highly innovative tools for specific site- and basin **key toxicants identification** by effect-directed analysis (EDA) as well as a general accessible database on key toxicants that will promote the use of EDA on an European scale.

MODELKEY focuses on an advanced risk assessment combining classical PEC/PNEC approaches for priority pollutants and newly identified key toxicants with extensive effect assessment and modelling, innovative approaches on toxicant accumulation and effects in food webs, and *in situ* assessment of microbial, invertebrate and fish communities for integrated risk indexes based on a weight-of-evidence approach. By establishing missing links between biodiversity and the chemical status MODELKEY will help to implement the EU Water Framework Directive and the 2010 targets of the Convention on Biological Diversity by providing decision tools for improved management options, remedial action strategies and preventive policies for the mitigation of harmful effects.

B.3 Potential impact

Strategic Impact

The sustainable use of water resources and the protection of European freshwater and marine ecosystems are crucial for a competitive economic development and vital to ensure the quality of life in Europe. The health status of aquatic ecosystems and biodiversity is threatened by environmental pollution with traditional and emerging toxicants. There is a global concern about species loss and the role of toxicants herein. **MODELKEY** addresses this concern by improving our understanding of ecosystem responses to such perturbations, contributing to the mitigation and sustainable use of natural resources. Innovative diagnostic and predictive tools for an improved understanding and forecasting of effects on different levels of biological organisation and a proper identification of those toxicants responsible for observable effects will help to improve risk assessment and prioritisation significantly and will allow a better allocation of limited resources for management, remedial activities and preventive policies.

MODELKEY will integrate for the first time highly innovative and state-of-the-art approaches from several different scientific disciplines including theoretical and practical freshwater and marine ecology, *in vitro* and *in vivo* biotesting, environmental chemistry and analysis, exposure and effect modelling, hydraulics and sediment physics, and risk assessment and prioritisation. The synergies produced by this interdisciplinary approach and the effective translation of science into applied decision-support systems will be of outstanding significance for the enhancement of **European competitiveness in environmental science** and for the building of the **European Research Area.**

MODELKEY aims at the integration of the novel approaches developed in the project into **environmental regulatory and management frameworks** and will help to further promote the enormous potential of Europe to play a leading role not only in international environmental sciences but also in international environmental policies and the sustainable use of resources.

A **unique consortium** has been assembled to address the ambitious objectives of this project involving the leading European scientists in all key disciplines relevant to **MODELKEY**, important end-users as full partners (EWQMA, CEFAS, RIKZ and ACA), and several experienced and innovative SMEs. Several project partners are among the world leaders in the development of ecological exposure and effects research, models and applications. Innovative approaches of key toxicant identification, the development of dynamic energy budget population models, food web models and species sensitivity distributions for assessing risks on biodiversity, and the use of Decision Support Systems (DSS) to implement management decision, are all examples of European innovation in this field.

The distribution of the partners over 13 different countries across Europe including candidate and other associated countries and the extensive training activities for scientists from inside and outside the consortium will further enhance the scientific, technical, and societal capacity to implement the sustainable utilisation of freshwater and marine ecosystems all over Europe.

Dissemination and exploitation

Dissemination and exploitation of **MODELKEY** results and developed tools are high priorities in the implementation plan. An entire subproject – DIS/TRAIN (see B4.3) **-** is dedicated to dissemination and training activities guaranteeing best use of MODELKEY results. Wide communication, high awareness and optimised exploitation of results is recognised through:

- A yearly updated project flyer and a newsletter
- The project web-site including links to the meta-database as well as the specific databases for the case studies and the key toxicant database
- Both project and partner-based press releases,
- Summary of annual reports for end-users and stakeholders
- High-quality peer-reviewed publications and popular-science articles
- Regular workshops and two conferences
- Generally accessible protocols for tools developed in MODELKEY, and training courses on application of these tools
- A wide range of training activities with a specific focus on young researchers, scientists and stakeholders from candidate countries, and end-users
- Co-operation with European research networks and water management networks
- Communication to international conventions
- Consulting of local managers by MODELKEY case study team leaders

The practical application of MODELKEY tools and results and the engagement of end-users will be ensured by:

- The integration of key end-users for the three case studies as full partners in the project. This includes (1) the **Elbe Water Quality Monitoring Agency (EWQMA)** as the governmental institution in charge for monitoring in the river Elbe basin for many years, (2) the **National Institute for Coastal and Marine Management (RIKZ)** that is together with its closely collaborating sister organisation RIZA a part of the **Ministry of Public Transport and Water Management of The Netherlands** and responsible for implementing the Water Framework Directive (WFD)**,** and the **Catalan Water Agency (ACA)** responsible for monitoring activities in the Llobregat and in charge for the implementation of the Water framework Directive (WFD) The establishment, maintenance of the databases required for exposure and effect modelling as well as the input of MODELKEY results are lead by these partners. This will optimise the benefit of these data and results for end-users.

- The close contact to a number of other end-users, which are not directly involved into the project. The following end-users have already expressed their intent to use the MODELKEY results and accompany the project or have been contacted for collaboration.

- the Landesumweltamt Brandenburg

- the Sächsisches Umweltamt für Umwelt und Geologie

- the Landesamt für Umwelt, Naturschutz und Geologie (Sachsen-Anhalt)

as co-ordinators of the implementation of the WFD in the river Elbe basin in the respective countries.

- the Flemish Environmental Agency (VMM)

as an agency responsible for the implementation of the WFD in the river Scheldt

- Aigües Ter-Llobregat (ATLL)

as the agency in charge for water depuration from the Llobregat for drinking purposes serving water to Barcelona and neighbouring cities

- Aguas de Barcelona (AGBAR)

as the company providing Barcelona with drinking water.

- the Flussgebietsgemeinschaft Elbe and the Elberat,

as the newly founded umbrella organization responsible for the implication of the WFD in the Elbe basin,

- the Referat Gewässerschutz of the Bundesministerium für Umwelt, Naturschutz und Reaktorsicherheit

as the representative of the German Government in the Elberat

- the Länderarbeitsgemeinschaft Wasser (LAWA)

as the union of German ministries responsible for water supply and distribution

- The Internationale Kommission zum Schutz der Elbe (IKSE)

as the German/Czech institution organising the protection of the river Elbe

Within the first three months of MODELKEY together with the start-up meeting a **end-user communication board** will be established including (1) the Project Co-ordinator, (2) the heads of the subprojects most relevant for direct transfer of knowledge and demands between end-users and science (DECIS, designed for the development of end-user friendly decision support systems and DIS/TRAIN designed for the dissemination of results and training activities with particular focus on end-users), (3) the key end-users for the case studies in MODELKEY as full partners, as well as (4) an assembly of external end-users as listed above that will be invited to join the board. The board is designed to optimise the communication between science and end-users, to advice all MODELKEY subprojects with respect to an optimised design of scientific approaches with respect to their exploitation by end-users and to guarantee that new knowledge flows directly in current and future monitoring programs, risk assessment and prioritisation and decision making by environmental agencies and authorities.

European added value

Carrying out the work at a European level is essential since:

- The expertise required is spread across a number of countries. MODELKEY will energise and restructure current research and will increase this competitive advantage and knowledge base. Carrying out the project at a European level will allow the participants to share resources and expertise in a resource-intensive, technically- and intellectually-challenging field, in which strong synergies are anticipated.

- The integration of state-of-the art key toxicant identification, innovative models, experimental and field assessment tools for the assessment and forecasting of the impact on freshwater and marine ecosystems is an ambitious goal which requires a critical scientific and financial mass that can be provided only on a European scale.

- The toxic impact on freshwater and marine ecosystems is a problem occurring on a river basin and a European scale. Thus, as intended by the Water Framework Directive the problem of toxic pollution has to be addressed also at this scale.

- MODELKEY provides a set of generally applicable tools, which are designed to help scientists and end-users all over Europe to make impact assessment of toxicants in European freshwater and marine ecosystems more reliable, comparable, and cost-effective.

- A methodology as developed by MODELKEY, which is designed to be generally applicable in European freshwater and marine ecosystems, has to be calibrated and verified in different European ecoregions such as the Central European, Western European and Mediterranean.

International and national research programmes

MODELKEY will take into account a large number of international and national research programmes, which contribute to the assessment, understanding and prediction of the effects of environmental toxicants on biological systems on different levels of organisation (from cell to ecosystem), to the assessment and management of contaminated sediments, to the development of exposure and effect models, and to risk assessment on different scales. The UFZ as the co-ordinator of MODELKEY and many other participants play key roles in European Scientific networks and in international and national research projects. A close collaboration within the networks and with the other projects will ensure that existing data and results will be seriously taken into account and that new tools, data and knowledge developed by MODELKEY will be disseminated.

The UFZ initiated the European **Partnership for European Environmental Research (PEER),** which was established to develop and promote joint strategies in environmental research in support of both EC and national policies. The PEER secretariat is located at the UFZ in Leipzig. Several MODELKEY partners including RIKZ, CSIC, VUA, UA, and UFZ are also members of the core group of EU FP5 **SedNet**, a demand-driven European Sediment Research Network. **SedNet** is designed to provide a European platform where organisations responsible for the sustainable management of river basin/fresh water body related sediments and dredged material (problem owners) can meet and communicate with organisations (problems solvers) that help to provide solutions to their problems, in the form of tools, knowledge, technologies and expertise needed for that management. The close collaboration between **MODELKEY** and **SedNet** will support, catalyse, optimise and facilitate: (1) demand driven research activities, (2) exchange of information between these activities, (3) co-operation between problem solvers and problem owners, (4) dissemination to, and exploitation of knowledge by problem owners, (5) publication of research results and (6) inform public and decision-makers.

A list of recently completed and ongoing EU and national projects of direct relevance to MODELKEY is given below. Several MODELKEY partners play a key role in these projects ensuring that MODELKEY can directly build on the relevant knowledge available in Europe.

EU FP5 **BEAM**: Bridging effect assessment of mixtures to ecosystem situations and regulation (UFZ)

EU FP5 **IMAGETOX**: Intelligent Modelling Algorithms for General Evaluation of toxicities (UFZ)

EU FP5 **CELL ECOTOX**: Application of *in vitro* cellular approaches in aquatic ecotoxicology (UFZ)

EU FP5 **BIOFORUM**: European Biodiversity Forum - Implementing the Ecosystem Approach

EU FP5 **WELCOME**: Water, Environment, Landscape Management of Contaminated Megasites; Development of Integrated Management Systems (IMS) for Prevention and Reduction of Pollution of Waterbodies at Contaminated Megasites (UFZ)

EUFP5 **EUFRAM**: Concerted Action to develop a European Framework for probabilistic risk assessment of the environmental impacts of pesticides (UFZ, RIVM)

EU FP5 **PHOBIA**: Phototrophic biofilms and their potential applications: towards the development of a unifying concept (UFZ)

EU FP5 **EDEN: E**ndocrine disruptors: exploring novel enpoints, exposure, low dose- and mixture effects in humans, aquatic wildlife and laboratory animals (UB)

EU FP5 **AWACSS**: Automated water analyser computer supported system (CSIC)

EU FP5 **WATCH**: Water catchment areas: tools for management and control of hazardous compounds (CSIC)

EU FP5 **EXPRESS-IMMUNOTECH**: Development of new express enzyme immunotechniques for pesticides and surfactants monitoring in water (CSIC)

EU FP5 **FATEALLCHEM**: Fate and toxicity of allelochemicals (natural plant toxins) in relation to environment and consumer (CSIC)

EU FP5 **P-THREE**: Removal of Persistent Polar Pollutants Through Improved Treatment of Wastewater Effluents (CSIC)

EU FP5 **ARTDEMO**: Artificial recharge demonstration project (CSIC):

EU FP5 **STAMPS**: Standarised aquatic moniotring of priority pollutants uisng passive sampling (CSIC)

EU FP5 **SOWA**: European Community. Integrated Soil and Water Protection (CSIC)

EU FP5 **PHYTOHEALTH**: Improving health through dietary phytoestrogens: A pan-European network on consumer issues and opportunities for producers (CSIC)

EU FP5 **COMPARE**: Comparison of Exposure-Effect Pathways to Improve the Assessment of Human Health Risks of Complex Environmental Mixtures of Organohalogens (VUA).

EU FP5 **FIRE**: Risk assessment of brominated flame retardants as suspected endocrine disruptors for human and wildlife health (VUA).

EU FP5 **ACE**: Analysing combination effects of mixtures of estrogenic chemicals in marine and freshwater organisms (VUA)

EU FP5: **EUROCAT**: European catchments: catchment changes and their impact on the coast (VUA)

EU FP5: **DINAS-COAST**: Dynamic and interactive assessment of national, regional and global vulnerability of coastal zones to climate change and sea-level rise (VUA, DELFT)

EU FP5 **PAEQANN**: Predicting aquatic ecosystem quality using artificial neural networks: Impact of environmental characteristics on the structure of aquatic communities (CNRS)

EU FP5 **BIOFILMS**: Natural biofilms as high-tech conditioners for drinking water (UdG)

EU FP5 **NICOLAS**: Nitrogen control by landscapes structures in agricultural landscapes (UdG)

EU-FP5: **Eloise** Coordination Consortium and Secretariat; for (EVK1-CT-2002-70001) with NILU, NIOO-CEME, UEA-CSERGE; http://www.nilu.no/projects/eloise/)

EU FP6 **SustainabilityA-Test**: Advanced Techniques for Evaluation of Suatainability Assessment Tools (VUA)

EU FP6 **ALARM**: Assessing large-scale environmental risks with tested methods (UFZ, UB)

EU FP6 **EUROLIMPACS**: Integrated project to evaluate the impacts of global change on European freshwater ecosystems (CNRS, UFZ, CSIC)

EU FP6 **AQUATERRA**: Understanding river-sediment-soil-groundwater interactions for support of management of waterbodies (river basin & catchment areas) (UFZ, CSIC, CWA, VUA)

EU FP6 **ELME**: European Lifestyles and Marine Ecosystems (CEFAS, CSIC)

EU FP6 **FLOODSite**: Integrated flood risk analysis and management methodologies (UFZ)

EU FP6 **HAIR**: Harmonised environmental indicators for pesticide risk (UFZ)

EU FP6 **REBECCA**: Relationships between ecological and chemical status of surface waters (DELFT, UA).

CHEMSTRESS: Chemical key stressors and their scale dependent distribution and transformation in rivers (UFZ)

EXPECT: Extrapolation practice for ecological effects and exposure characterization of chemicals. An international project funded by the American Chemistry Council LRI program. This project will lead to a SETAC publication on available state-of-the-art risk assessment methodologies (RIVM)

Structure and function of fluvial biofilms: effect of the riparian forest and implications for water quality (UdG)

AQEM: Development and testing of an integrated assessment system for the ecological quality of streams and rivers throughout Europe using benthic macroinvertebrates (5^{th} Framework Programme of the European Union – module chemistry (DW)

STAR: Standardisation of river classifications: Framework method for calibrating different biological survey results against ecological quality classifications to be developed for the Water Framework Directive of the EU – modules chemistry and phytobenthos (DW)

B3.1 Contributions to standards/policies/regulations

The tools and the knowledge provided by MODELKEY will contribute to a wide range of European and International policies, international agreements and conventions (see below) by providing tools for assessing and forecasting the impact of environmental pollution on freshwater and marine ecosystems and biodiversity.
In recent years, the international community has initiated a myriad of initiatives on regional and global scale to assess the state of freshwater and marine ecosystems, many of them with the support of the European Union. Some of the more prominent of such initiatives are the Global International Waters Assessment (GIWA), the assessments of the North and Baltic seas completed by OSPARCOM and HELCOM respectively, and the report of the UN Joint Group of Experts on the Scientific Aspects of Marine Environmental Protection (GESAMP) on land-based sources of pollution affecting the quality and uses of the marine, coastal and associated freshwater environment. There has even been a recent effort to establish a Global Marine Assessment as a means of harnessing the scientific knowledge being generated from scientific activities for the purpose of formulating action strategies and preventative policies. A recurring theme within these efforts is the need to better understand the impact of pollutants on freshwater and marine ecosystems, and to offer support to decision-making processes on the basis of this understanding.

For Europe, the Sixth Environmental Action Programme emphasizes “Ensuring the sustainable use and high quality of our water resources” and the implementation of the Water Framework Directive as well as the “protection of nature and biodiversity” as objectives of highst priority. Thus, MODELKEY will contribute to the implementation of sustainable development in Europe. The European Council recognises the importance of the **Sixth Environmental Action Programme** as a key instrument for progress towards sustainable development and this was endorsed by the participation at the **World Summit on Sustainable Development (WSSD)** in Johannesburg.

One of the objectives of this project will be to provide a clear conceptual framework linking levels of both priority pollutants and novel/emerging toxicants with their impacts on ecological structure and function. Such an approach will help define regulatory criteria for sediments, soils and waters that should allow for management decisions focused on net improvement of ecological health and biodiversity. However, to do this effectively with limited resources, it is important to have both the scientific, modelling and decision tools in order to evaluate, prioritise and manage individual emissions or sites based upon their relative impact on ecosystem health. The goal of this programme is to develop, interlock and validate predictive modelling tools in support of the above needs. The developments from MODELKEY will allow for an unprecedented insight into the controlling factors, dynamics and sensitivity of ecosystems to previously ignored toxicants. A better understanding of these processes will result in more focused, proactive and effective implementation of EU and national guidelines. Results from the MODELKEY work programme will directly contribute to guidelines for implementing

- The **Water Framework Directive (WFD)**, aiming at a the establishment of a good ecological status of European surface waters by 2015
- The **Convention on Biological Diversity (CBD),** aiming at a conservation of biodiversity
- The **European Habitats Directive**, focusing on the conservation of natural habitats
- The **Espoo (EIA) Convention on Environmental Impact Assessment in a Transboundary Context,** and
- The **Protocol on Strategic Environmental Assessment (SEA),** which will require to evaluate the environmental consequences of official draft plans and programmes such as regional development concepts, specific industrial productions, and transport plans.

In addition, the regional conventions on the protection of European seas rivers will also largely benefit from increased understanding of toxicant effects on ecosystem functioning and structure. These include:

- The Barcelona Convention on the Protection of the Mediterranean Sea
- The Convention for the Protection of the Marine Environment of the North-East Atlantic (OSPAR)
- The Convention of the Black Sea Against Pollution
- The Convention on the Protection of the Marine Environment of the Baltic Sea Area (Helsinki Commission)

- The Convention on the Protection and Use of Transboundary Watercourses and International Lakes (Helsinki Commission)
- The Convention on Co-operation and Protection and Sustainable Use of the Danube River
- The Convention for the Protection of the Rhine
- The Convention for the Protection of the Meuse

B.4 Outline Implementation Plan

General Approach

MODELKEY comprises a mulitdisciplinary approach aiming at developing **interlinked and verified diagnostic and predictive modelling tools** as well as **innovative field and laboratory methods** generally applicable to European freshwater and marine ecosystems (Figure B.4.1):

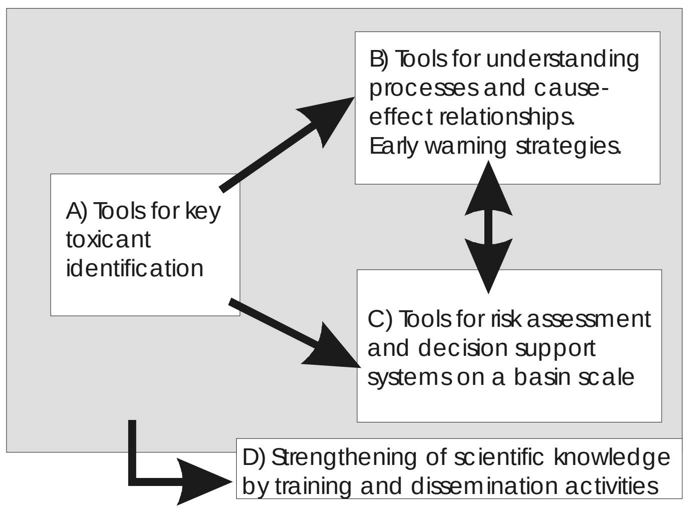

Fig. B.4.1: MODELKEY approach

A) to **identify the key toxicants** impacting marine and freshwater ecosystems on a site and basin scale as a crucial basis for scientifically sound risk assessment and decision support on risk management, remedial action strategies and preventive policies for the mitigation of harmful effects. Subproject **KEYTOX** is designed to meet this task.

B) to provide a better understanding **of toxic impacts** on aquatic ecosystems, **cause-effect-relationships** between changes in **biodiversity** and the impact of environmental pollution as causative factor as well as the underlying processes. This will include the assessment of sub-lethal effects *in vitro* and *in vivo* as **early warning strategies** and of their strength to predict potential hazards to the ecosystem. These tasks are addressed in the subprojects **SITE** (experimental approaches) and **EFFECT** (effect models) and **EXPO** (exposure models).

C) to **assess, forecast, and mitigate the risks** of key toxicants on fresh water and marine ecosystems and their biodiversity **at a river basin and adjacent marine**

environment scale focusing on **decision support systems** for the selection of the most efficient management options to **prevent effects on biodiversity** and to prioritise contamination sources and contaminated sites. These tasks are addressed by the subprojects **BASIN** (providing the database) as well as the modelling subprojects **EFFECT** and **EXPO**.

D) to **strengthen the scientific knowledge on an European level** in the field of impact assessment of environmental pollution on aquatic ecosystems and their **biodiversity** by extensive training activities and knowledge dissemination to stake-holders and the scientific community. Subproject DIS/TRAIN will fulfil this task.

Overall structure and integration

MODELKEY is highly innovative by integration of highly advanced diagnostic, predictive and mechanistic approaches for the assessment of risks of the impact of environmental pollution on freshwater and marine ecosystems with state-of-the-art key toxicant identification and easy-to-use enduser-oriented decision support systems for advanced river basin and coastal area management. In order to meet this task MODELKEY is structured through highly integrated sub-projects including **KEYTOX** (key toxicant identification), **BASIN** (establishment and interlink of basin-specific data bases), **EXPO** (exposure modelling), **EFFECT** (effect modelling), **SITE** (site assessment and model verification), and **DECIS** (decision support system) (Fig.B.4.2). In order to keep the figure clear only most important links between and within subprojects are shown, not between work packages of different subprojects. The **scientific co-ordination** is a task penetrating and guiding the whole scientific process in MODELKEY. It will be explained in detail in B6. The prospective time schedule is given in the gantt chart (Fig. B4.3)

BASIN, where the environmental agencies that are involved in MODELKEY play a crucial role, will provide data on a basin scale from past and continuing monitoring programs in selected river basins and adjacent coastal areas. This will be the basis for all other subprojects delivering hydrological, chemical and biological together with geographic data as a prerequisite for hot spot identification to select sites for key toxicant identification (**KEYTOX**) and site assessment (**SITE**), effect, exposure and risk modelling and assessment (**EFFECT, EXPO, DECIS**).

KEYTOX will provide tool development and application for effect-based key toxicant identification as an input to **BASIN** for inclusion into current and future monitoring programs. This is ensured by the direct involvement of the respective monitoring agencies in **MODELKEY**. Key toxicant identification in **KEYTOX** will also direct exposure (**EXPO**) and effect (**EFFECT**) modeling to those compounds that predominate the true risk to the ecosystems as assessed and used for decision support and risk prioritisation in **DECIS**.

EXPO is designed to provide and apply modelling tools to predict the distribution and the transport of priority pollutants as included in **BASIN** databases and key toxicants (**KEYTOX**) between different environmental compartments as well as along the rivers and into the marine environment. Thus, **EXPO** provides exposure prediction on different scales from organism-sediment interactions upto exposure on a basin scale as a prerequisite for sound risk assessment and prioritisation (**DECIS**).

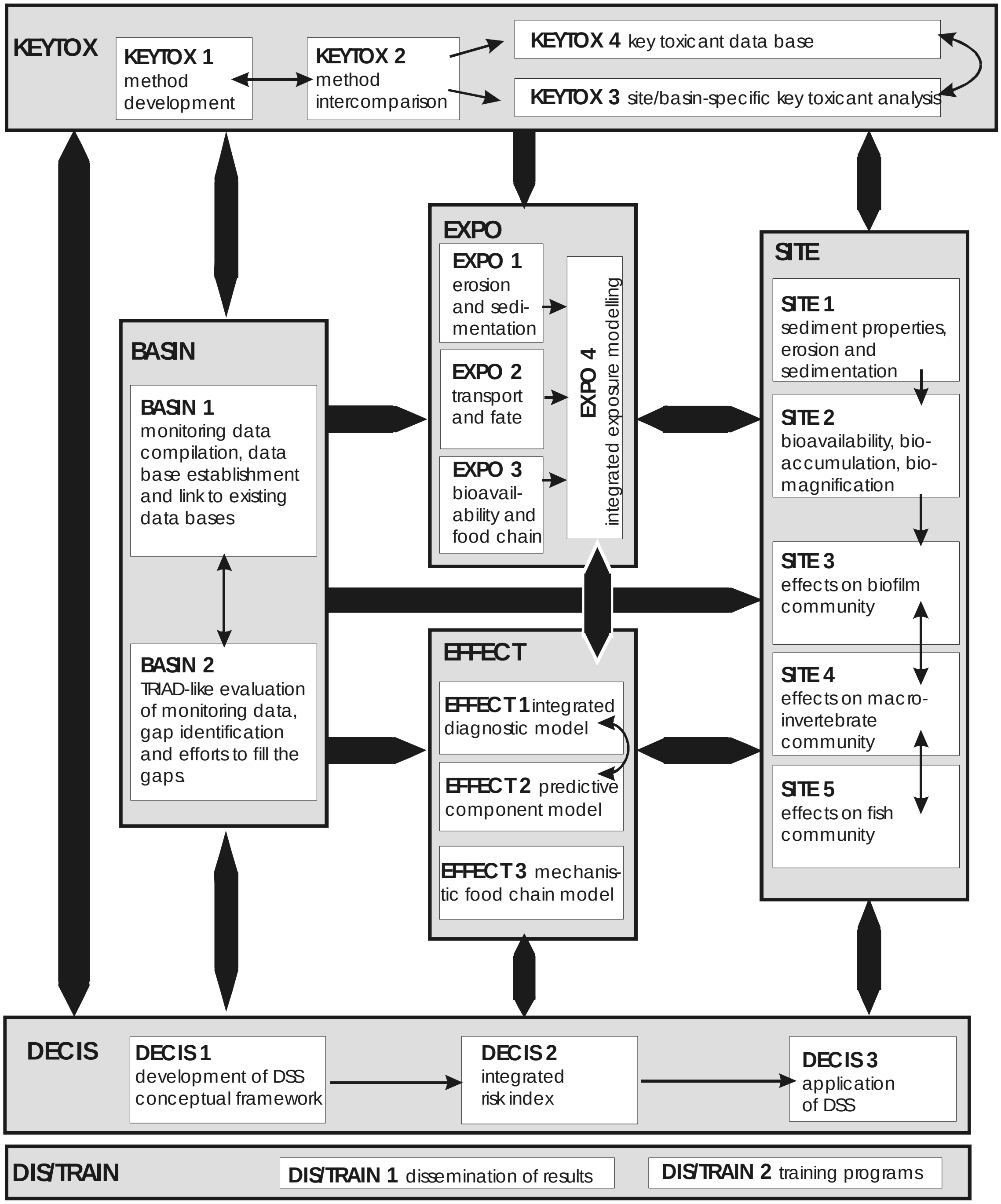

Figure B.4.2: MODELKEY pert chart

EFFECT is designed to model and predict effects of key toxicants (**KEYTOX**) to freshwater and marine communities and thus to biodiversity on the basis of biological monitoring data (**BASIN**) as well as toxicity data and innovative theoretical concepts.

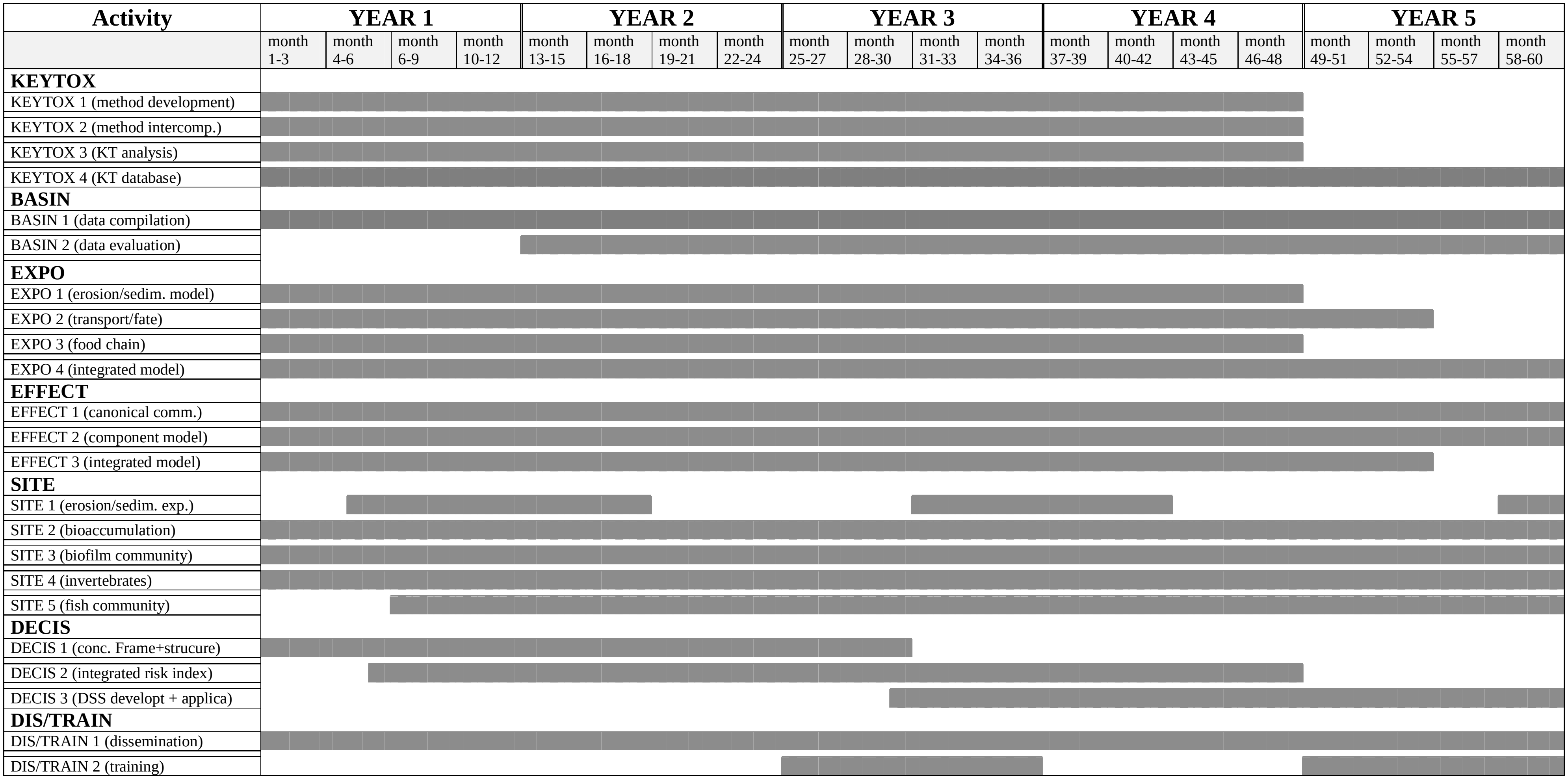

Fig. B 4.3: Time schedule for the work packages of the subprojects of MODELKEY

The modelling results of **EXPO** and **EFFECT** are verified in in-depth investigations at selected sites in **SITE** and are used together for integrated risk assessment and prioritisation in **DECIS**.

SITE is designed to provide a better understanding of exposure and effects on different levels of biological organisation and on biodiversity by in-depth physical chemical and biological investigations at selected sites. By this end early warning systems on the basis of *in vitro* assays and *in situ* biomarkers will be provided and verified for their relevance for biodiversity, exposure (**EXPO**) and effect (**EFFECT**) models will be calibrated and verified, the relevance of key toxicants (**KEYTOX**) will be confirmed, and risk assessment and prioritisation (**DECIS**) will be put on a scientifically sound basis.

DECIS is designed to integrate all other subprojects for integrated risk assessment and to transform scientific innovation into improved risk prioritisation and management by supplying an end-user friendly decision support system and by integration of end-users, socio-economists and scientists for decisions on optimised management options and preventive policies with limited budgets.

The MODELKEY tools will be developed and applied in three case studies in the basins of the rivers Elbe, Scheldt and Llobregat including estuaries and adjacent coastal areas in order to cover freshwater and marine ecosystems. A specific focus of MODELKEY is on toxic risks due to contaminated sediments as a long term accumulator and important source of many key toxicants in freshwater and marine ecosystems. The links between the workpackages will be described in the following.

There is increasing evidence that scientifically sound risk assessment and prioritisation at a basin scale as well as a true understanding of processes and cause-effect-relationships in a specific ecosystem cannot be achieved on the basis of the analysis of toxicants that have been selected *a priori* as priority pollutants alone. A site- and basin-specific identification of key toxicants on the basis of measurable effects is required and basically available on the basis of the effect-directed analysis (EDA) approach. The MODELKEY subproject **KEYTOX** is designed to significantly promote this approach in Europe. The leading European groups in this field are involved in **KEYTOX** bringing together their expertise in order to provide an effect-directed analysis (EDA) tool box of innovative, standardised and intercomparable methods generally applicable across Europe for the identification of key toxicants in freshwater and marine ecosystems (KEYTOX 1 and 2). This aim will be further promoted by **KEYTOX** by providing a generally accessible key toxicant data base compiling existing and collecting new data on their occurrence, environmental concentrations, physico-chemical, chromatographic, spectrometric and toxic properties (KEYTOX 4). Key toxicants at the sites and basins under investigation in MODELKEY are identified (KEYTOX 3), introduced into the key toxicant data base (KEYTOX 4) and delivered (i) to BASIN in order to allow an inclusion in further monitoring programs, (ii) to EXPO and EFFECT for exposure and effect modelling, to SITE for in-depth assessment of their partitioning in different compartments and their effects to community health and biodiversity, and (iii) to DECIS for basing decision making on true key toxicants rather than *a priori* selected priority pollutants.

Sub-project **BASIN** is designed to compile (BASIN 1) and evaluate (BASIN 2) existing monitoring data on chemical concentrations of heavy metals and organic pollutants, ecotoxicological monitoring data and community and biodiversity data as well as hydrological and physico-chemical data from the basins of the rivers Elbe, Scheldt, and Llobregat, the adjacent coastal areas as well as from additional basins including lowly contaminated ones such as the river Ems for comparison. In close collaboration with other projects such as REBECCA existing databases are interlinked and made accessible to the MODELKEY sub-projects. Thus, BASIN provides a crucial input to (i) EXPO by delivering toxicant concentrations in water, sediment and biota on a basin scale, (ii) EFFECT by delivering TRIAD-like data for diagnostic and predictive effect modelling on a basin scale (EFFECT 2 and 3), (iii) KEYTOX and SITE by selecting sites for in depth investigation and by delivering initial data on contamination, toxicity and community health at these sites, and (iv) DECIS by delivering input data for an integrated risk index and a decision support system for the identification and prioritisation of hot spots in a river basin and the adjacent coastal area with respect to an optimised risk management and mitigation with limited resources. BASIN receives input from KEYTOX suggesting additional key toxicants for involving in running and future monitoring programs and from DECIS by critically reviewing these programs with respect to their value for decision making. In BASIN the water agencies EWQMA, RIKZ, and CWA for the rivers Elbe, Scheldt, and Llobregat, respectively will play a decisive role as providers, compilers and end-users of monitoring data.

In sub-project **EXPO** easy to use exposure models with a special focus on risk assessment of contaminated sediments in freshwater and estuarine ecosystems are developed. EXPO provides and integrates valuable tools for risk assessment on a basin scale as well as for general understanding of the impact of toxicants on aquatic ecosystems. The integrated exposure modelling proceeded in EXPO 4 will integrate sedimentation and erosion processes (EXPO 1), transport and fate of sediments and contaminants (EXPO 2), and bioavailability and foodweb accumulation (EXPO 3) in a basin-directed approach. All EXPO work packages support diagnostic and predictive effect modelling, risk assessment and decision supporting on a basin scale (EFFECT 2 and 3, DECIS), while EXPO 3 is also closely interlinked with experimental bioavailability and bioaccumulation assessment in SITE 2 that delivers the key factors affecting bioavailability and bioaccumulation and verifies the models developed in EXPO 3. Food chain accumulation modelling in EXPO 3 is also closely interlinked with effect modelling in canonical communities and food chains (EFFECT 3). Both models will be developed in close collaboration using the same set of chemicals. Erosion and sedimentation models in EXPO 1 designed for predicting the chance that a contaminated site will erode as well as for forecasting the sediment retention in riverbasin and estuary are closely interlinked with experimental work *in situ* and in the laboratory for model calibration and verification at selected sites (SITE 1).

Sub-project **EFFECT** is designed to develop, integrate, apply and verify models for the diagnosis, prediction and functional understanding of effects on higher levels of biological organisation such as populations and communities in order to protect functional and structural biodiversity. Highly innovative approaches by worldwide leading groups in this field are involved in order to meet this goal. Integrated diagnostic models (EFFECT 1) are designed to attribute the observed effects in species composition to the underlying causes. Predictive model development (EFFECT 2) will provide advanced tools to predict effects of toxic exposures on aquatic communities. Both models are based on basin- (and European-) scale data as delivered from BASIN and are designed to support decision making and management in river basins and adjacent coastal areas (DECIS). Functional-based models providing a better understanding of processes and their dynamic change in communities on the basis of dynamic energy budgets in canonical communities and simplified food chains are provided in EFFECT 3. The models are based on laboratory testing of population-related toxicological parameters and rely experimental toxico-kinetic data on toxicant uptake and elimination provided in SITE 2, which will be used in both EXPO 3 and EFFECT 1.

Subproject **SITE** focuses on experimental and field work with focus on a better understanding of processes, effect propagation and cause-effect-relationships relevant for the impact of toxicants on ecosystems on a site scale. SITE is closely linked to KEYTOX that provides information on key toxicants and DECIS and BASIN for site selection, and is designed to calibrate and verify effect and exposure models in EFFECT and KEYTOX *in situ*. SITE is composed on (i) one mainly physical WP (SITE 1) on erosion, sedimentation and other processes related to grain size and physical properties of sediments in close connection to EXPO 1, (ii) one WP (SITE 2) providing a better understanding of factors determining bioavailability and bioaccumulation and will support EFFECT 3 and EXPO 3, which focus on food chain modelling, and SITE 3 to 5 by measuring internal concentrations in laboratory and field collected organisms, (iii) and three WPs (SITE 3 to 4) focusing on a better understanding of effect propagation in biofilm, macroinvertebrate, and fish communities. This will include *in vitro* and *in vivo* biotesting of water, sediments and extracts thereof, mesocosm studies and *in situ* biomarkers as a link between biotesting and community effects and in depth community health assessment including species richness, pollution induced community tolerance and funcional parameters.

Subproject **DECIS** is designed to integrate the MODELKEY deliverables in a framework to manage impacts of key pollutants on ecosystems and biodiversity. Thus, it will be based on the input from BASIN, KEYTOX, EXPO, EFFECT, and SITE. DECIS will provide a common framework to integrate project deliverables and a decision support system (DSS) to use them for risk prioritisation and decision making. For risk prioritisation integrated risk indexes (IRI) based on a weight of evidence approach will be developed. IRI and DSS will be applied to the three case studies Llobregat, Elbe and Scheldt.

There is a strong focus of MODELKEY not only on the development of innovative approaches for the assessment and forecasting the impact on freshwater and marine ecosystems but also on an optimised dissemination and exploitation of results and tools across Europe. This will be provided for all parts of the developed methodology by **DISS/TRAIN** in two work packages including DISS/TRAIN 1, that focuses on optimised dissemination of results by internet, peer reviewed papers and conferences and DIIS/TRAIN 2 responsible for training activities with a special focus on young researchers, researchers from candidate countries and end-users e.g. from environmental agencies.

All subprojects are implemented in three case studies at different river basins including the estuary and coastal zone of typical regions of Europe including the **River Llobregat** (Spain) as a typical Mediterranean river basin, the **River Elbe** (Czech, Germany) and its catchment area, representing a large central European river basin, the **River Scheldt** (France, Belgium, The Netherlands), both representing highly impacted river basins with a strong interaction with the coastal zone. These freshwater ecosystems receive significant pollution from point and diffuse sources including present and former industrial production, municipal wastewater treatment plants and agricultural production. Reference sites will be included for all cases (e.g. River Ems). The basins are characterised below.

River Elbe

The River Elbe is situated in the Czech Republic and Germany. It is approximately 1100 km long and covers a catchment area of about 150,000 km^2 that is inhabited by 25,000,000 persons. Heavily industrialised areas are spread along the River Elbe and its tributaries. Within the last years many industrial plants have been closed down, so aquatic ecosystems are supposed to recover. Extensive monitoring programs have been established, to study ecosystem health and recovery of the aquatic communities as well as for hot spot identification. The EWQMA as German governmental environmental agency responsible for monitoring programs in the river Elbe basin that is involved in MODELKEY as full partner will make these data available and organise them in a database.

River Scheldt

The River Scheldt is situated in France; Belgium and the Netherlands. It is 350 km long and covers a catchment area of about 21,000 km^2 which is inhabited by 10,000,000 persons (477 persons/km^2). The Scheldt is known as one of the most polluted systems within Western Europe, but quality is improving by the installation of waste water treatment plants in Belgium during the last and current decade. Extensive monitoring programs have been established especially in the Flemish and Dutch areas. In Flanders there are monitoring programs for water quality, sediment quality based on a Triad like approach and for body burdens in eels, which are carried out by the Flemish Environment Agency (FEA). The FEA is also responsible for the implementation of the monitoring programs for the WFD. Monitoring data of the Scheldt estuary are collected by UoA for the watercolumn in the Flemish part and by RIKZ/Rijkswaterstaat for all compartments (physical/chemical and biological) in the Dutch part.

River Llobregat

The River Llobregat is situated in Catalonia, Spain. During the last decades, the river Llobregat and its tributaries has been highly polluted by industrial and urban wastewaters, and by surface runoff from agricultural areas. This river experiences periodic floods and droughts which lead to frequent morphological variations in the river bed and to modifications in its banks. Previous studies carried out in these rivers have evidenced the presence of estrogenic compounds, coming from both industrial (surfactants) and municipal (estrogens) sources, and its correlation with important alterations (an abnormally high incidence of intersex and elevated levels of plasmatic vitellogenin) in carps inhabiting these rivers. Close to its mouth, the Llobregat river flows nearby the city of Barcelona, and its water is used for abstraction of the drinking water supplied to most of the districts in the province of Barcelona. At present, the watercourse of the river, close to its mouth, is being deviated and canalised, and one of the largest European sewage treatment plants (Depurbaix) is currently under construction. The Catalonian Water Agency (ACA) is in charge of the management and administration of all aspects related to the water cycle, including planning, execution and operation of hydraulic infrastructures and wastewater treatment plants, preservation of aquatic ecosystems, and water quality control.

B.4.1 Research, technological development and innovation activities

In this section the research to be carried out in each subproject will be described. Subproject (SP) heads are identified as well as lead participants for every work package (WP). For each WP the lead participant is underlined. Deliverables are given for every WP.

SP KEYTOX: Key Toxicant Identification (CEFAS)

Detailed description of each work component, partners involved in the component and contribution of each to the project as a whole

KEYTOX work components are structured into four work packages. KEYTOX 1 (Innovative Tool development) is a multidisciplinary thematic programme of work aimed at filling the gaps in techniques available for identifying toxicants, KEYTOX 2 is a package aimed at toolbox design, inter-laboratory comparison and validation of available techniques so that they can be used on a multinational level, KEYTOX 3 applies the developed and validated techniques to identify the key toxicants present in the three study sites in relation to SITE and KEYTOX 4 is focused on developing an Internet access database that will facilitate the identification of key toxicants through providing easily accessible data for their identification.

Work packages 1-4

Key toxicant identification - Introduction and five-year overview

KEYTOX 1

Participant	CEFAS	CSIC	RIKZ	RIVO	SPbU	VRI	VUA
Person Months	28	14	27	24	65	6	31
Participant	UFZ	XEN					
Person Months	62	16					

KEYTOX 2

Participant	CEFAS	CSIC	RIKZ	RIVO	SPbU	VRI	VUA
Person Months	10	13	8	22	20	6	20
Participant	UFZ	XEN					
Person Months	12	2					

KEYTOX 3

Participant	CEFAS	CSIC	RIKZ	RIVO	SPbU	VRI	VUA

Person Months	10	60	12	10	39	28	12
Participant	UFZ	XEN					
Person Months	12	7					

KEYTOX 4

Participant	CEFAS	CSIC	RIKZ	RIVO	SPbU	VRI	VUA
Person Months	2	5	23	2	20	1	2
Participant	UFZ	XEN					
Person Months	15	1					

Introduction

Human activities including industrial production, combustion processes, agriculture and private chemical application result in the contamination of freshwater and marine environments with complex mixtures of toxicants that are potentially hazardous to ecosystem and human health. These contaminants include the released substances as well as numerous unidentified by- and transformation products. Currently, the risk assessment of contaminated ecosystems is typically conducted on known chemicals (e.g. a priority pollutant approach estimating risks using individual compound toxicity and occurrence data). The priority pollutant list for the EU was established by combined monitoring-based and modelling-based priority setting (COMMPS) on the basis of 86 chemicals (including metals) for which monitoring data in at least three countries were available. About 60 compounds were selected as priority pollutants in different priority categories. Around 16 x 10^6 compounds are known and registered in the Chemical Abstracts Service (CAS) list. The discrepancy between the number of compounds potentially present in the environment and the number of regularly monitored priority pollutants is therefore quite evident.

Not knowing which key substances contaminate an ecosystem make the effectiveness of the existing priority pollutant based risk assessment approach limited (Ankley & Mount, 1996). This is supported by numerous studies, combining chemical and biological approaches for hazard assessment of complex environmental mixtures, that indicate priority pollutant concentrations to be a poor indicator of toxicity (Jacobs et al., 1993; Samoiloff et al., 1983). Ideally a broad-spectrum non-targeted approach to the analysis of complex environmental mixture would allow the detection and identification of a broader range of compounds. However, it is time-consuming, not routinely applicable and the results are often difficult to evaluate, since toxicological data of the compounds identified are missing (Reemtsma et al., 1999).

A scientifically sound approach to evaluating the effect of complex environmental samples is to use effects based monitoring employing bioassays. Toxicity assessment using bioassays provides an integrative parameter for the presence of compounds affecting the applied test system. Prior knowledge of key contaminants is not necessary and interactive toxicity among the components (*e.g.* additivity) is reported in the test results. A battery of bioassays can therefore provide a large amount of information on the harmful effects of compounds in complex environmental mixtures, however used alone bioassay tests do not provide information on the hazardous substances causing the measured effects.

Effect-directed fractionation/analysis (EDA) is the most cost- and time- effective approach currently available for the identification of unknown toxicants in complex environmental mixtures. Ecotoxicological and analytical chemistry techniques are integrated to identify specific groups of contaminants that are exerting measurable effects in the environment. This process is also often referred to as toxicity identification evaluation (TIE) and involves the bioassay-directed sequential fractionation of complex environmental mixtures in order to identify the compounds responsible for a measurable biological response. Typically, a bioassay or suite of bioassays is used to establish whether a sample exerts a particular effect(s) that is then used to direct the isolation of the substance(s) responsible for this effect. The isolation of the substances responsible can take the form of simple chemical manipulations, such as filtration, or can be more technologically advanced and use various chromatographic techniques. Analytical efforts are then focused on identifying the substances responsible in the significantly active fractions.

Having initially been reported over twenty years ago (Parkhurst et al., 1979), the EDA/TIE has become increasingly popular for the identification of unknown environmental contaminants. EDA/TIE is considered a scientifically sound concept for identifying unknown contaminants (Burgess, 2000). Although standardised techniques are available (USEPA REFS), bioassay-directed analysis is a philosophical concept comprising a number of different chemical and biological techniques and is not considered a specific method. This philosophy makes the approach extremely powerful as it allows the procedures used to be specifically tailored to the problem being addressed. Therefore EDA is best described as a ‘toolbox’ of techniques that are selected on a case-by-case basis to solve specific problems.

The true power of bioassay-directed analysis in identifying hazardous substances in the environment has been demonstrated in a number of key studies over the past decade (REFS + For full review see Brack, 2003a). European research groups have led the field in this area and made significant contributions to the success of the technique (*e.g.* Castillo & Barcelo, 1999; Thomas et al., 2002; Brack et al., 2003b). Although EDA has been successfully applied as a research tool to solve specific problems further development in a number of areas is required in order to make the tools available in the EDA ‘toolbox’ generally applicable across Europe for the identification of key toxicants in freshwater and marine ecosystems.

When compared to routine chemical and biological analysis, EDA is currently a costly and time-consuming approach requiring highly experienced and well-equipped research groups with relatively low throughput. In order to provide a scientifically robust approach for ecosystem protection there is a real need for EDA to be routinely applied in laboratories on a European scale. Before this can happen there are a number of methodological advancements with respect to throughput, ease of operation as well as a consequent exchange and dissemination of methods and results that are required. **KEYTOX** aims to provide these methodological developments.

KEYTOX focuses on a series of original work programmes designed to provide fully developed and validated techniques for identifying the key toxicants in freshwater and marine ecosystems. The fundamental philosophy of the sub-project is effect-directed analysis (EDA). The advancements that the **KEYTOX** partners have identified as requiring development fall into four objectives that will be addressed in the corresponding work packages:

Specific objectives:

- Development of methods for identifying the key toxicants present in freshwater and marine ecosystems: EDA 'toolbox' development: KEYTOX 1.
- Inter-laboratory comparison and validation of existing and developed techniques: KEYTOX 2.
- Site-specific key toxicant identification at the Scheldt, Elbe and Llobregat basins: KEYTOX 3.
- The development of an Internet based database to facilitate the information flow between European laboratories conducting EDA: KEYTOX 4.

Research, technological development and innovation activities

The research and development element of the sub-project is addressed in KEYTOX 1, concentrating on the gaps that currently exist in the EDA 'tool box'. Innovative approaches regarding 1) extraction, 2) fractionation, 3) EDA design for biota, 4) novel bioassays and 5) identification strategies are developed. These will allow important classes of key toxicants to be identified and address the limitations of throughput and the applicability of the techniques that the EDA concept current suffers. Consequently, for existing and developed techniques to be used on a Europe-wide level, methods will be validated during numerous inter-laboratory comparison exercises (KEYTOX 2). Guidelines will be prepared for the techniques considered suitable for widespread use and their performance monitored through inclusion in the BEQULAM[1] quality assurance scheme. In KEYTOX 3, in order to demonstrate the power of the EDA approach and provide information on the key toxicants to sub-projects BASIN, EXPO and SITE the techniques will be used to identify key toxicants in samples collected from the three study sites; the Elbe, Scheldt, and Llobregat estuary. This application of the EDA 'toolbox' is crucial in demonstrating the scientific robustness of the EDA approach and the distinct advantage of identifying the key toxicants that are actually responsible for the detrimental effects measured at the study sites as opposed to just attempting to correlate the effects of the concentrations of priority pollutants. To further facilitate the flow of knowledge and

[1] The Biological Effects Quality Assurance in Monitoring Programmes (BEQUALM) project, initiated in 1998, was funded by the European Union through the Standards, Measurements and Testing programme of the European Commission. It was set up as a direct response to the requirements of the Oslo and Paris Commission (OSPAR) to establish a European infrastructure for biological effects Quality Assurance/Quality Control, in order that laboratories contributing to national and international monitoring programmes, such as the OSPAR Joint Assessment and Monitoring programme (JAMP) and the Co-ordinated Environmental Monitoring Programme (CEMP) can attain defined quality standards.

data between European laboratories a KEYTOX database will be established on the Internet (KEYTOX 4). The database will allow groups to share data and information on key toxicant identification therefore simplifying many of the procedures that are currently specialised and providing easy access to data on newly identified key toxicants.

Temporal sequence

For an overview on the temporal sequence of the tasks in KEYTOX see Fig. B4.4.

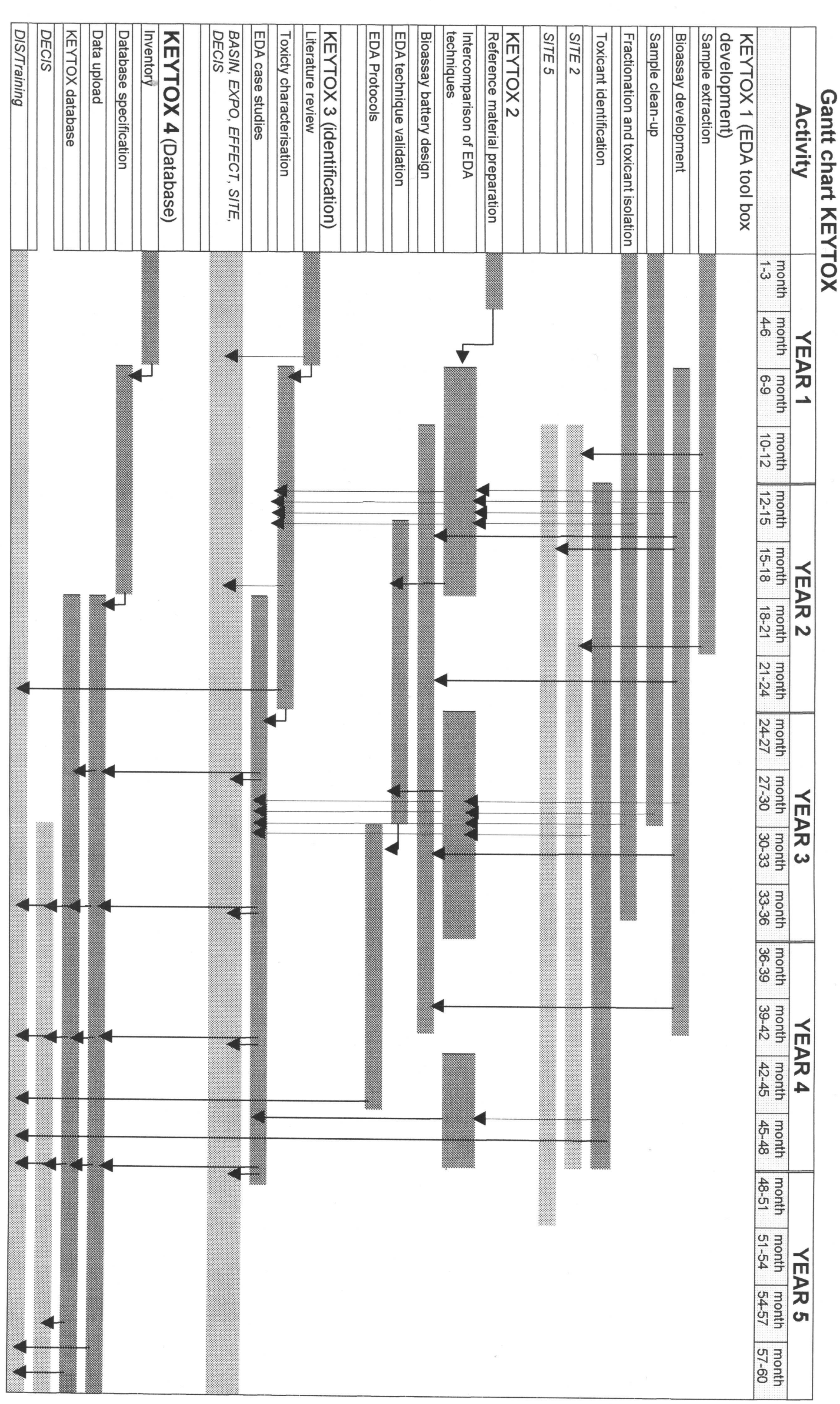

Fig. B4.4: Temporal sequence of the tasks in KEYTOX.

WP KEYTOX 1 (K1): Development of methods for identifying the key toxicants present in freshwater and marine ecosystems: EDA 'toolbox' development (VUA, CEFAS, CSIC, RIKZ, SPbU, VRI, UFZ)

In the following paragraphs the innovative approaches regarding 1) extraction, 2) fractionation, 3) EDA design for biota, 4) novel bioassays and 5) identification strategies will be presented.

1. Sample extraction

Valid techniques are required for the extraction of hazardous substances from water, sediment and tissue. With regard to sample extraction in EDA, there are two major gaps: extraction of polar compounds and targeted active extraction. Sampling of polar compounds from water can be performed using integrated sampling or grab sampling. Grab water samples have been the norm, but one of the drawbacks of this approach is that discrete grab samples may not be representative of the water body being sampled (Thomas et al., 1999). Suitable techniques that do offer an integrated sample are semi-permeable membrane devices (SPMDs), polar organic contaminant integrative samplers (POCIS), silicon sheets and transposed biota (Huckins et al., 1990; Jones-Lepp et al., 2001; Smedes and Luszezanec, 2003).

SPMDs, silicon sheet samplers and transposed biota focus on bioaccumulative, hydrophobic substances, are developed areas and will be assessed and validated in KEYTOX 2. There is however a research need to develop a system for the integrated sampling of polar organic contaminants.

Integrated sampling of polar organic contaminants
Polar Organic Chemical Integrative Sampler (POCIS) is a technique that can passively accumulate hydrophilic compounds (Jones-Lepp et al., 2001). POCIS devices consist of a mixture of polymeric resins within a hydrophilic membrane enclosure. Using organic solvent elution, near quantitative recoveries can be obtained. To date these devices have only been used for a very limited number of targeted contaminants.

In KEYTOX1, the current POCIS configuration will be evaluated for a broad range of polar organic contaminants. It will be established whether the system is quantitative and reproducible and it is suitable for use with in vitro bioassay systems or if alternatives should be investigated. Successful evaluation of POCIS will result in the pertinent procedure being validated and tested in KEYTOX 2.

Off-line extraction of polar organic contaminants
Some key classes of contaminants, such as compounds that are very hydrophilic (i.e. polar organics with a log K_{OW} < 3), are currently omitted from standard extraction procedures, mainly because they are not easy to extract or analyse. Important classes of novel contaminants fall into this category, for example certain antibiotics and pharmaceuticals.

Solid Phase Extraction (SPE) has been successfully used in EDA to extract mid- to non-polar organic compounds from surface waters and effluents, but only with some success to extract polar organics from estuary water samples. Recently developed polymeric SPE sorbents are capable of extracting compounds that have a wide range of polarities, including compounds with log $K_{OW} < 0.5$.

In KEYTOX, an SPE method will be developed for the quantitative extraction of polar unknowns from effluent, freshwater and marine water samples. Following development the method will be fully validated using a suite of compounds covering a wide range of polarities (KEYTOX 2) and be used to extract water samples collected as part of KEYTOX 3 from the three case study sites.

Targeted active extraction (e.g. immunoaffinity SPE and HPLC)
Immunoaffinity extraction (IAE) allows the extraction of specific groups of compounds (e.g. oestrogen receptor (ER) agonists or aryl hydrocarbon receptor (AhR) agonists; Weller, 2000; Huwe et al., 2001). This is possible since the extraction media have unique molecules on their surface that have the ability to attract and to bind specific molecules. The technique is used to selectively extract target molecules from a heterogeneous solution. After the extraction the target compound(s) can be washed away from the surface and collected.
IAE systems would be very useful in the context of EDA, as they would for example allow compounds with similar affinities for the oestrogen receptor to be selectively extracted from complex environmental matrices, pre- or post- assay. Pre-assay extraction of a complex extract would give a clean extract for in vitro assay testing, whilst post-assay extraction would make the identification process easier as many of the interfering non-active compounds would have been removed. Within KEYTOX1 androgen and oestrogen IAE will be developed, and validated in KEYTOX 2.

2. Fractionation and toxicant isolation

Once it has been established that a sample is toxic then EDA focuses on isolating the substances responsible for the measured responses. Chromatographic techniques such as SPE and high performance liquid chromatography (HPLC) have been used most often for isolating toxicants (REFS). Reverse phase and normal phase HPLC (for isolation from water extracts and more lipophilic extracts, respectively), will be validated in KEYTOX 2. Certain classes of compounds may be difficult to isolate and new fractionation methods will then be required. Gaps exist on methods for pre-mutagenicity testing clean up, fractionation of compound classes including big numbers of isomers with different biological activities such as polyaromatic compounds, and hydrophilic toxicants. Innovative method developments for these gaps are presented in the next paragraphs.

Rapid pre-mutagenicity testing clean up and fractionation method.
A major unresolved problem of mutagenicity EDA is the recognition, evaluation, and elimination of matrix and mixture effects, which may suppress genotoxic and mutagenic effects e.g. in crude extracts almost completely despite high contents of mutagens. Thus, a selection of hazardous samples on the basis of mutagenicity of crude extracts seems to be questionable. After clean up and fractionation mutagenicity often significantly increases. However, to date there is no generally accepted pre-

assay clean up and fractionation procedure of complex environmental samples. KEYTOX wants to fill this gap in order to enable a comparison and ranking of mutagenic potency with respect to hot spot and subsequent mutagenicity identification. Thus, simple and rapid initial clean up and fractionation procedures will be evaluated for their potency to provide a realistic picture of the mutagenic potency of complex mixtures.

The problems of mutagenicity suppression in complex environmental samples are closely related to a general lack of knowledge on joint effects of mutagenic and non-mutagenic compounds. KEYTOX aims to better understand the mutagenicity of complex mixtures is based on the outstanding experience of UFZ in mixture toxicity and in close collaboration with national projects run at UFZ.

Establishment of fractionation procedures for polyaromatic compounds (PAC) based on multi-step HPLC separation and preparative GC-MS.

Polyaromatic compounds including polycyclic aromatic hydrocarbons (PAHs) and alkyl, halogen, nitro, oxy, hydroxy, and amino derivatives thereof as well as nitrogen-, oxygen-, and sulphur-containing heterocycles represent a fraction, which is believed to predetermine to a great extent the mutagenic, tumour promoting, and Ah-receptor-mediated potency of sediment- and suspended matter-associated contamination in surface waters (Myers et al., 1991). To date, mostly a set of 16 PAHs, which was selected by USEPA as priority pollutants, together with selected PCBs and PCDD/Fs are analysed for hazard assessment of contaminated sediments. It is of increasing evidence that non-priority PAC derivatives may contribute significantly to the toxic and genotoxic potency of the mixture (Brack et al., 2003b).

The isolation of individual toxicants from complex environmental PAC mixtures is a challenging task that requires high-efficiency multi-step fractionation procedures. Current procedures, however, are based on offline combinations of preparative HPLC techniques (e.g. Durant et al., 1998; Brack et al., 2003c), and are costly, time consuming and have only limited resolution due to the exclusive use of HPLC methods. There are at least two promising approaches to advance these procedures with respect to efficiency, throughput, and resolution. Both of them will be addressed in KEYTOX:

- The development of robust **automated multistep- and multicolumn HPLC fractionation procedures** designed to avoid off-line solvent exchange and pre-concentration steps, which are laborious, time consuming and bears the risk of contamination and toxicant losses. The development will be based on existing experience with available automated two-step (Zebühr et al., 1993) and off-line multi step fractionation procedures (Brack et al., 2003b).
- The development of high-resolution fractionation procedures with quasi-online toxicant identification using preparative GC/MS. GC on capillary columns has superior efficiency compared to HPLC but is, however, almost exclusively applied for analytical purposes. Preparative GC fractionation procedures may provide an enormous advancement in EDA, especially as post-HPLC fractionation, when the complexity of the mixtures is already reduced to few individual compounds that cannot be further separated by HPLC methods. Preparative GC/MS will be developed at the example of PAC isomer

separation but is also open for other demands evolving during the term of MODELKEY.

The development of powerful effect-directed fractionation procedures for PACs demands for a close collaboration between groups with outstanding experience in fractionation (*UFZ*), synthesis of standard compounds, which are not commercially available (*SPbU*), and biological detection (*XENO, VRI*).

Fractionation of hydrophilic toxicants (HPLC and GPC)
As stated above, hydrophilic organic toxicants are a group of toxicants that have received little attention. Following the development of suitable extraction techniques there is an obvious requirement for fractionation techniques to isolate the biologically active compounds. Existing HPLC fractionation techniques for non-polar organic compounds do not provide adequate separation of hydrophilic compounds (log K_{OW} < 3). A preparative HPLC fractionation procedure for polar organic contaminants will be developed and made suitable for preparative LC-MS^n.

3. Novel EDA design of biota

The EDA of biota is an area where very little work has been conducted. Being able to establish which active substances are bioaccumulating in different organisms is very important as it allows compounds that are both toxic and bioaccumulative to be identified whilst also allowing an assessment of how these substances move through food chains to be made. A large data gap, therefore, exists on the identification of unknown toxicants in biological samples, which is highly interesting with regard to bioaccumulation and metabilism. Due to the limited work that has been conducted in this area there is a need to develop extraction techniques for a broad range of substances from tissues and pre-treatment steps that will be required before these extracts can be bioassay tested. Sample extraction and pre-treatment methods for the bioassay testing and identification of unknown environmental toxicants in biological samples are very limited due to a number of knowledge gaps that exists:

i) Pre-fractionation of the bulk of matrix compounds (e.g. triglycerids, cholesterol, steroids) from the unknown environmental toxicants.
ii) Separation of active endogenous compounds (e.g. natural hormones) from the active unknown environmental toxicants (e.g. xeno-estrogenic compounds).
iii) Cytotoxicity of tissue extracts for bioassays
iv) Deconjugation of bound active metabolites

Without pre-fractionation step to remove endogenous compounds, which are normally present at much higher levels than the toxicants, bioassay testing and identification of unknown environmental toxicants in tissues is not possible.
An identified research need for KEYTOX 1 is therefore the development of a generic extraction technique and pre-treatment methods for biologically active compounds from biota using generally applicable laboratory extraction procedures, including the deconjugation of bound active metabolites. KEYTOX 1 will develop tailored and robust maximum efficiency extraction and pre-treatment methods for important links in the food web including algae, invertebrates and fish applied for EDA in biota and delivered to SITE 2 for the analysis of internal concentrations in food chain and effect-related investigations. For the development of the methods the biological

reference materials (marine and fresh water mussel and fish samples) from KEYTOX 2 that are spiked with a large number of compounds that have a broad range of physical-chemical properties, and different modes of action (e.g. AhR- and ER-based toxicity, genotoxicity, narcotic toxicity, immuno toxicity) will be used. New extraction methods (e.g. pressurised liquid extraction) will be evaluated for a broad range of toxicants. For the pre-fractionation step, to remove endogenous compounds (e.g. triglycerides, cholesterol, steroids, lipophilic vitamins) from the environmental toxicants, several analytical techniques will be developed (HPLC, GPC, SPE, immunoaffinity SPE/HPLC and receptor columns). Once these techniques have been developed they will be validated in KEYTOX 2 in the intercomparison exercise using other reference materials. In the next paragraph the development of methods for the deconjugation of bound actives in biota samples, which was the last gap in the EDA for biota, is presented.

Deconjugation of bound actives in biota samples
In organisms, many compounds are eliminated from the body by metabolic conversion to water-soluble metabolites. For example in fish, conjugates of many estrogenic chemicals, endogenous as well as xenobiotic, are excreted via bile into the intestine. For conjugation of hydroxylated metabolites of steroids as well as xenobiotics, glucuronidation is likely to be the dominant pathway for biliary excretion. Once in the intestines, intestinal bacteria may deconjugate estrogens, thereby forming a new source of the active parent compound. In the environment, estrogens are mostly found in their biologically active, parent forms, probably due to bacterial hydrolysis of excreted conjugates. Measurement of estrogenic activity in fish bile could yield useful information about the animal’s internal exposure to (xeno-)estrogens. Enzymatic deglucuronidation of bile samples will be applied for the preparation of suitable extracts for bioassays that determine oestrogenicity (YES, ER-CALUX) as well as for chemical analysis for elucidation of the identity of the compounds responsible for the estrogenic response.

4. Bioassay testing

Bioassay tests are the crucial first step in any EDA study. Typically, EDA requires high-throughput, micro-scale, cost-effective and biologically significant bioassays. Some of the bioassays suitable for EDA have already been approved for use in monitoring programmes (e.g. by OSPAR), whilst others are emerging techniques or merely developmental. For simplicity the bioassays available in this sub-project are divided into a number of categories in vitro and in vivo bioassays (Table B4.1.).

Table B4.1 Development *in vitro* and *in vivo* bioassays

Toxicity syndrome	Assay	References
In vitro assays:		
Genotoxicity	Accumulation of p53 protein	Machala
	UmuC	Hamers et al., 2000a
	Mutatox	Klamer
Hormonal disruption		
Androgenicity	AR-CALUX	Sonneveld et al., in preparation
Thyroid hormone	T4-TTR binding competition	Meerts et al., 2000
Neurotoxicity	esterase inhibition	Hamers et al., 2000b
Tumour promotion	gap junction intercellular inhibition, cell proliferation	
Antibiotic resistance	antibiotic challenge assay	
In vivo assays:		
Species specific overall toxicity	*Tisbe battagliai*[M]	
	Mytilus edulis larvae [M]	
	Corophium volutator [M]	
	Fish embryo toxicity [M]	
Multiple endpoints	*C. elegans*	

M=Marine species

Assessment of genotoxicity by p53 protein accumulation and tumour promotion is innovative assays measuring important endpoints. The UmuC and Mutatox assays will be further adapted for environmental matrices. Measurement of novel endocrine disruption parameters such as androgenicity and thyroid hormone displacement will add to the understanding of different endocrine influences from the environment. Neurotoxicity as determined by esterase inhibition is a novel but relevant endpoint for incorporation in EDA.

In vitro assays will be also applied to determine relative toxic potencies of individual key toxicants identified by the EDA approach. These data should be included in the database.
Typically *in vitro* bioassays are used as early warning tools, whilst *in vivo* tests show that there are effects currently occurring. *In vitro* tests also tend to be used on extracts and therefore can be used on samples collected from both freshwater and marine ecosystems. *In vivo* tests can be used on both neat samples and extracts, however in order to keep the study relevant they are only used with samples relevant to where the organisms are found. Ideally, sample preparation and/or fractionation results in

extracts that can be tested without further adjustments in different bioassays that provide complementary information. Depending on the characteristics of the sample, innovative dosing techniques such as application of polymer films that ensure more accurate, realistic exposure of test systems (*in vitro* as well as *in vivo*) will be developed.

This part of the work package focus on two major gaps that exists for bioassay for EDA: high throughput EDA *in vivo* bioassays, and the development for an antibiotic challenge bioassay.

Development, standardisation and validation of high throughput EDA compatible in vivo bioassays

For bioassays to be suitable for use in EDA studies they need to be sensitive, cost effective, environmentally relevant, use low sample volumes and have good quality control data. A large number of *in vitro* bioassays fulfil these criterions, however very few *in vivo* test systems do. As a first step in establishing suitable *in vivo* bioassays for EDA a number of standardised and internationally accepted bioassays already used for monitoring and assessment will be miniaturised. Marine algae, copepod and bivalve embryo tests will be miniaturised to reduce the sample volume required and increase the throughput of the techniques. These will then be assessed against the performance of the full size test in order to establish that they are just as robust and effective.

In addition, EDA does not utilise assays at the higher trophic levels for a number of reasons. Firstly, the *in vivo* assays using fish are expensive, time consuming and fall under the legislation covering licensed animal testing along with the associated ethical issues. Secondly, *in vivo* fish bioassays require large sample volumes and this has made their use in EDA impossible with current methodologies. An alternative is to utilise the nematode, *Caenorhabditis elegans* as a model system using transgenic strains with analogous fish/mammalian biomarker proteins with easily quantifiable reporter genes. These strains could produce the powerful, small-scale and high throughput bioassays required for the advancement of EDA. A number of biomarker proteins have been identified for potential for development in the *in vivo C. elegans* bioassay. Feasibility studies for six different biomarkers will be conducted initially. These include: 1) Vitellogenin (VTG) marker of endocrine disruption, 2) Glutathione S-transferase (GST) and/or other markers of oxidative stress; 3) Adenosine Triphosphate (ATP) indicative of interference of metabolic rate; 4) Arylhydrocarbon receptor (AhR) indicator of exposure to planar aromatic hydrocarbons; 5+6) Two Nuclear Hormone Receptors (NHR) of which some constitute important targets for pharmaceuticals and pesticides and so could potentially be markers for environmental pharmaceutical and pesticide contaminants. The feasibility studies will evaluate the strains available and the biomarker response after exposure to relevant chemical standards. After these initial studies, further standardisation and validation studies will be conducted to produce bioassays capable of repeatable, reproducible application to environmental samples.

Development, standardisation and validation of antibiotic challenge bioassay

Antibiotic resistance is an emerging concern, particularly since the occurrence of antibiotics is being frequently reported in discharges from wastewater treatment plants and in surface waters. Antibiotic resistant bacteria are a real problem to the environment, animal and human health. To date only targeted chemical analysis of parent antibiotics has been conducted following prioritisation procedures. No assessment has been made of the metabolites or transformation products of antibiotics and in particular whether they may be antibiotic resistant and contribute to the potential antibiotic resistance of bacteria. Following the KEYTOX philosophy then an effect based screening procedure to assess whether antibiotic compounds are present in both freshwater and marine ecosystems is required. It is proposed that an antibiotic challenge bioassay developed for use in pharmaceutical quality assurance laboratories is assessed for its suitability with environmental samples.

The suitability for use in EDA of all bioassays that are either developed or adapted for application to environmental matrices in this work package will be evaluated and considered for further validation in KEYTOX 2.

5. Toxicant identification

One of the last steps in the EDA approach is the identification of the toxicants. The identification task in KEYTOX 1 aims to develop techniques for identification of unknown contaminants using modern analytical instrumentation such as HPLC, GC, two-dimensional comprehensive GC coupled to time-of-flight mass spectrometry (MS), and tandem MS as well as spectroscopic methods. Validation of the methods will take place in KEYTOX 2. In KEYTOX complementary techniques (GC-(EI)MS, GC-(NCI)MS, GC-FTIR, GC-ToF-MS, GCxGC-ToF-MS, LC-MS, LC-MS/MS, LC-ToF-MS, LC-DAD) are use for the structure elucidation of unknown compounds in the environment. GC-MS and LC-MS techniques can provide information about structural fragments and molecular mass of the unknown compound. GCxGC can give group-type information since compounds with similar properties form clusters. GC-FTIR can provide valuable information regarding functional groups in the molecule. For tentatively identified key toxicants that are not commercially available yet, standards will be synthesised. In addition to the analytical identification computer tools for toxicant identification based on estimation and interlocking of chromatographic, spectrometric and toxicological properties from molecular structure will be developed in order to provide cost effective identification options.

Development and validation of novel identification techniques for unknown toxicants (GCxGC-ToF-MS, GC-FTIR, LC-MS^n, LC-ToF-MS)
Comprehensive two-dimensional GC (GCxGC) is a novel technique with a tremendous capability to separate and identify organic compounds in complex environmental samples. Impressive results have been obtained in terms of separation efficiency and, also, compound classification of (classes of) structurally related compounds. Examples are the group separation of paraffins, naphthenes, and mono-, di- and triaromatics in petrochemical products (Shoenmaker et al., 2000), and the separation of toxic from non-toxic PCBs (Korytar et al., 2002). The grouping or ordering of the peaks in the GCxGC chromatogram facilitates the identification of unknown compounds and the comparison of complex environmental samples. GC x GC combined with time-of-flight mass spectrometry (ToF-MS) permits the rapid screening of groups of compounds and other unknown contaminants (Frysinger et al., 2002).

For decades, the identification of unknown environmental pollutants has been largely limited to compounds amenable to GC-MS analysis (i.e., non-polar, thermally stable, and volatile compounds) (Bobeldijk et al., 2001). However, technological progress over the past few years in the field of LC-MS have significantly changed this picture, by allowing the identification and analysis of many polar, thermolabile, and/or non-volatile compounds that before the advent of LC-MS were difficult and sometimes impossible to measure (López de Alda et al., 2003). Nevertheless, most of the research activities conducted in this area have focused on the determination of target analytes rather than on screening for unknown contaminants. The use of LC-MS and LC-MS-MS in the various possible scan modes (full scan, precursor-ion, product-ion, and neutral loss) for compound identification has been scarce; basically because of the low sensitivity, low mass resolution, and limited structural information achieved, and because of the lack of standards and LC-MS libraries. Recently, new techniques are commercially available that combine time-of-flight mass spectrometers (TOF-MS) with LC, which are much more sensitive than the standard LC-MS instruments. The possibilities of these advanced techniques for polar and semi-polar pollutants identification are notable, but up until now, they have not been yet employed for this purpose on the routine basis, probably due to the high cost of the instruments.

In KEYTOX 1, the GCxGC-ToF-MS, LC-MS, LC-MS-MS, and LC-TOF-MS techniques will be evaluated for identification of unknown toxicants by using environmental samples/fractions that have shown to present measurable biological effects in previously performed bioassay/effect-directed fractionation and analysis (EDA) from samples of KEYTOX 3 and SITE 2. Parallel to this, libraries containing mass spectra characteristic of the compounds identified will be created and made freely available to facilitate the identification of key toxicants. Also, simple LC-MS and LC-MS-MS methods will be optimised and published for the target determination of the identified compounds (by using these two relatively wide implemented techniques).

Innovative computer tools for key toxicant identification

In EDA studies toxicant identification is typically done by GC/MS techniques. For many compounds including PACs mass spectra provide the molecular weight and information on present heteroatoms but are not indicative for distinct isomers. Thus, KEYTOX will establish innovative computer tools for key toxicant identification. These will be based on structured evaluation procedures combining automated mass spectral deconvolution & identification systems (AMDIS) with mass spectra data bases, retention index data bases, programs for boiling point calculation, substructure recognition from mass spectra, and generation of molecular structure (e.g. MOLGEN). The application of multivariate statistics including principle component analysis and cluster analysis helps to structure and sort GC/MS data.

The exploitation and exchange of complete GC/MS profiles of properly defined fractions rather than mass spectra alone will help to identify toxicants particularly for compound classes, which occur in source-type-characteristic mixtures of isomers and congeners which may be found all over Europe. That is the case e.g. for most PACs emitted by combustion, oil spills or applied in technical mixtures. The availability of source-type-characteristic patterns will facilitate the recognition of site-specific compounds emitted by specific sources. For data exchange the transformation of producer-specific data to compatible data formats represents a serious problem that has to be solved in KEYTOX.

In addition to mass spectra often additional parameters for toxicant characterisation are available including HPLC capacity factors on different columns, UV-, FTIR- and fluorescence spectra and toxicity data. Combined spectra similarity analysis, quantum chemical methods, quantitative structure retention relationships (QSRR), quantitative structure activity relationships (QSAR) together with multivariate statistics will be established for exploiting these data together with GC/MS data for compound identification. Links to the key toxicant data base that will be established in KEYTOX 3 further enhance the analytical power of computer-based compound identification and will reduce the expense for standard synthesis.

Strength of KEYTOX 1:

The key strength of KEYTOX 1 is that the package of research is pragmatically focused on developing the key tools required to successfully apply EDA to vast range of complex environmental problems. The techniques proposed for development address all of the current flaws and limitations that EDA has when being applied on a broad-scale. The techniques in isolation may appear to be a list of methods but it is the philosophy behind the application of the techniques within the context of EDA that is the great strength of the approach. When integrated with existing EDA methods the newly developed procedures will allow for a greater range of key toxicants to be identified and make the data generated more ecologically significant.

Deliverables:

Month 1-18

KD1.1 Pre-mutagenicity testing clean up method for crude sediment extracts (month 6).
KD1.2 Selection, development and evaluation of individual fractionation steps for subsequent development of automated multi-step fractionation method for sediment-associated PACs (month 12).
KD1.3 Tailored protocols for high-efficiency accelerated solvent extraction (ASE) of toxicants with selected physico-chemical properties from biota tissues (month 15).
KD1.4 Off-line extraction method for polar organic compounds (month 15).
KD1.5 Identification and optimisation of injection, separation and trapping parameters for the development of preparative GC/MS fractionation (month 18).
KD1.6 Synthesis of alkylated and heterocyclic PAC standards with MW>250 (month 18)
KD1.7 Passive integrated sampling method for polar organic compounds (month18).
KD1.8 Initial selection of test species for high-throughput *in vivo* bioassays (month 18).

Month 19-36

KD1.9 Protocols for preparative GC/MS fractionation methods for PAC fractions with different physico-chemical properties (month 24)

KD1.10 Protocols for the automated multi-step fractionation method for sediment-associated PACs on the basis of preparative HPLC with coupled columns (month 30)

KD1.11 Integrated computer tools for efficient evaluation of GC/MS data based on AMDIS, retention index data bases, programs for boiling point calculation and structure generation, and multivariate statistics (month 36)

KD1.12 Protocols for the pre-bioassay testing clean-up of biota extracts (month 36)

KD1.13 Protocols for in vivo/high-throughput in vivo bioassays (month 36).

KD1.14 Developed antibiotic challenge bioassay (month 36).

KD1.15 Procedures for the separation of hydrophilic toxicants (month 36).

KD1.16 Protocols for the immunoaffinity extraction of ER and AhR agonists (month 36).

KD1.17 Procedure for use of comprehensive GC x GC ToF MS for the identification of unknowns (month 36).

KD1.18 Procedure for the use of HPLC-(ToF) MS^n for the identification of unknowns (month 36).

Month 37-48

KD1.19 Integration of HPLC capacity factors, spectroscopic evaluations, QSRR and QSAR into the integrated computer tools for key toxicant identification (month 42).

WP KEYTOX 2 (K2): Toolbox composition and inter-laboratory comparison and validation of existing and developed techniques and preparation of reference materials (RIVO, CEFAS, CSIC, RIKZ, SPbU, VRI, VUA, UFZ)

The objectives of KEYTOX 2 are i) the preparation of suitable reference materials that will be used for validation of the EDA methods in KEYTOX 1, ii) the organization of a inter-laboratory study to further validate the methods between the

KEYTOX laboratories, and (iii) to deliver a generally applicable toolbox and recommendations for a problem-directed tool selection. This will be the first EDA inter-laboratory comparison study in the world.

KEYTOX 2 will start with the preparation of ten reference materials (three water, three sediments, two mussel, and two fish samples) from fresh water and marine environments. These materials will be used for the validation of the different existing and developing EDA techniques (extraction, clean-up, fractionation, bioassays, identification) in KEYTOX 1, and for the inter-laboratory study of KEYTOX 2. All materials will be spiked with various key toxicants with a broad range of physical-chemical properties (e.g. log K_{ow}, vapour pressure) and toxic endpoints (e.g. genotoxicity, hormonal disruption, AhR-base toxicity, growth/immuno toxicity, neurotoxicity). Endpoints will be based on the *in vitro* and *in vivo* bioassays from KEYTOX 1. Deuterated, 13C-labelled, or native compounds will be used for spiking. All candidate materials will be tested for homogeneity. Five reference materials (two waters, two sediments, one mussel and one fish sample) will be used for chemical validation of the sample pre-treatment step in KEYTOX 1, providing information on the recoveries of the key toxicants, repeatability, and ruggedness of the sample pre-treatment techniques. In addition, the reference materials will also be used for bioassay validation in KEYTOX 1, providing information on the suitability of the sample pre-treatment techniques (e.g. cytotoxicity), ruggedness, and the link with the chemical data.

After the EDA techniques have been validated with the reference materials in KEYTOX 1, an inter-laboratory study to compare the validate EDA techniques between the KEYTOX laboratories will be organised in KEYTOX 2. The inter-laboratory tests will be built-up in the following stepwise approach. Three EDA levels will be validated: i) sample pre-treatment, ii) bioassay response, and iii) identification techniques. In the first step the sample pre-treatment method and the bioassay response will be validated using four reference materials (water, sediment, mussel, fish) with unknown solutions of a number of selected key toxicants. In this step standardised extraction, clean-up and general fractionation methods will be validated, and all KEYTOX laboratories will chemically determine the key toxicants. Validation of the specific fractionation techniques will take place by the laboratories that developed these methods only. These laboratories will fractionate the reference materials, and will send the fractions to the laboratories that perform the bioassays. This will confirm i) the performance of the specific fractionation method, and ii) the evaluation of the various performance criteria of the bioassays will form the basis of the assessment of the suitability of bioassays for EDA and eventually recommendation for use in routine monitoring programs. The bioassays that are validated are given in Table 2. Some of these bioassays can be regarded as established tools for assessment of biological or toxicological response. In addition to these, there are a few bioassays that are currently being developed (see B4.2), which will be evaluated for application to environmental matrices.

In the next step the identification techniques will be validated. For this validation so-called 'hot-fractions' from the Scheldt, Elbe and/or Llobregat samples (e.g. water, sediment, biota) from KEYTOX 3 will be used. The hot-fractions will be analysed with i) a standard identification technique (GC-MS with EI mode) by all laboratories, and ii) more specific and hyphenated techniques GC-MS NCI, GC-ToF-MS, GCxGC-

ToF-MS, LC-MS^n, LC-ToF-MS) by a limited number of partners. The GC-MS EI will show the ruggedness of this standard technique.

Each interlaboratory step is immediately followed by an evaluation including statistical treatment of the data at workshops for the KEYTOX partners**.** Important questions are: i) what are the performance characteristics (e.g. recoveries, repeatability etc.) of the standardised EDA methods, ii) is there a general sample pre-treatment method for various bioassays possible, iii) what are the limits of chemical and bioassays methods, iv) what is the relation between chemical and bioassay data, v) which overlap in identified compounds exists between the various techniques, vi) are there differences in the list of identified compounds by using GC-EI/MS between the laboratories?

Strength of KEYTOX 2:

- This will be the first intercomparison exercise on the validation of EDA methods in the world. The total chain from sample to bioassay response and key toxicant identification will be validated.
- Information on the ruggedness and performance characteristics of the EDA method will be provided.
- Standardised validated EDA protocols will be provided that will be part of the decision support system developed in DECIS.

Deliverables:

Month 1-18

KD2.1 Reference materials of key toxicants in water, sediment, mussel and fish for KEYTOX 1 and 2 (month 3).

KD2.2 Validation report on sample pre-treatment and bioassay response of EDA method, including performance characteristics (month 18).

KD2.3 Evaluation of relative performance of applied EDA techniques at different laboratories. (18 Months)

Month 19-48

KD2.4 Validation report on identification methods of key toxicants.

KD2.5 Validated standardised protocol for complete EDA methods, including performance characteristics.

KD2.6 Recommended list of EDA compatible bioassays .

Table B4.2 Bioassays to be selected for validation purposes.

Toxicity syndrome		**Assay**
In vitro assays:		
Genotoxicity		Mutatox
		Ames test
AhR-based toxicity		EROD fish hepatocyte DR-CALUX (dioxin-like response)
Hormonal disruption		
	Estrogenicity	ER-CALUX
		YES Yeast Androgen Screen
	Androgenicity	YAS Yeast Androgen Screen
Cell toxicity		Microtox
Narcotic/bioaccumulation	SPME	RIVO
In vivo assays		
Species specific overall toxicity marine		*Tisbe battagliai*
		Mytilus edulis larvae
		Corophium volutator
Species specific overall freshwater		*Hyalella azteca*
		Chironimus
		Daphnia magna
		MSP
Primary production toxicity marine		*Skeletonema costatum*

WP KEYTOX 3 (K3): Site-specific key toxicant identification (VRI, CEFAS, CSIC, RIKZ, SPbU, VUA, UFZ)

In KEYTOX 3, the Scheldt, Elbe and Llobregat study sites will be investigated using an array of validated techniques from the KEYTOX EDA ‘toolbox’. The EDA/TIE techniques will be applied to identify the key toxicants that occur at the ‘hot-spots’ of activity that occur in the study river basins and will provide these data to BASIN, EXPO, SITE and DECIS.

Depending on the outcome of BASIN 1 and 2, a range of water, sediment and biota samples will be collected from the three study sites and screened using the battery of bioassay tests selected in KEYTOX 1 on three separate occasions. EDA/TIE techniques from the KEYTOX 'toolbox' will then be applied to identify the key toxicants responsible for the effects seen during the bioassay screening. At this stage it is not possible to say which bioassays and techniques will be specifically used for KEYTOX 3 since technique and bioassay selection will depend on the problems being observed at the sites following BASIN and SITE investigations. The key output of this will be a wide range of data on the responsible compounds for the KEYTOX 4 database and the identity of hazardous substances that may be responsible for the observed effects.

An important area during any EDA analysis of samples is scientifically robust confirmation that substances tentatively identified as responsible for the observed effects are indeed responsible. Where it is agreed that the pertinent compound is an important key toxicant and when authentic reference material is unavailable, it will be synthesised by St. Petersburg University.

Synthesis of authentic reference compounds in parallel with their identification in the environment and development of analytical methods
MODELKEY provides a unique opportunity for an innovative approach in development of analytical methods for new classes of toxicants.
Previously, attempts of a *de novo* synthesis were done stepwise, not parallel (e.g., detection of a new class of toxicants, development of general synthetic methods for the class, synthesis of few congeners and unequivocal structure elucidation by NMR and X-ray spectrophotometry, broad toxicological research on pure synthetic compounds).

As a result, the time between the first identification and development of analytical method for routine monitoring was 10 years or more (examples – PAHs, PCDD/Fs, PCBs, PCNs, Toxaphene congeners).
Within KEYTOX, the time between identification of a problem and finding a solution can be shortened to 1-2 years by using innovative approaches.

Innovation

The suggested improvement in the procedure is to prepare and test mixtures of congeners, not pure compounds, of the new class with fixed structural elements, which is faster. When structure elucidation is successful, pertinent compounds are synthesized and used for preparation of reference materials and for toxicological research. It is of utmost importance for the success of this approach that every synthetic mixture is compared against environmental samples and/or examined in the same biotests, immediately after preparation.

One of the goals of WP KEYTOX 3 – TOXICANT IDENTIFICATION is to develop and test criteria for selection of the first or the novel approach to synthetic work, depending on the analytical data and biotests. After selection of a model class of new toxicants, both approaches will be explored in parallel, results compared and recommendations made. During the whole project, for each new class of toxicants, the same scheme will be used.

Strength of KEYTOX 3:
KEYTOX 3 is the scientifically sound integration of analytical and ecotoxicological techniques to identify key toxicants at the three study sites. The strength of the approach is that compounds responsible for the effects measured will be identified and used to inform an assessment of the risk of contaminants to the aquatic environment. Within KEYTOX, KEYTOX 3 is an applied work package that sees the demonstration of the tools developed and validated in KEYTOX 1 and 2 and will provide valuable data to KEYTOX 4, EFFECT, EXPO and SITE.

Deliverables:

Month 1-18

KD3.1 Literature review on previous EDA studies in the basins of interest. Key toxicant suggestion on this basis (month 6).
KD3.2 Toxicity characterisation at selected hotspots in the basins of Elbe, Scheldt and Llobregat (month 18).

Month 19-48

KD3.3 Identity of key toxicants at selected hot spots in the basins of Elbe, Scheldt and Llobregat (month 36)

KEYTOX 4 (K4): The development of an Internet based database to facilitate the information flow between European laboratories conducting EDA (RIKZ, CEFAS, CSIC, RIVO, SPbU, VRI, VUA, UFZ)

The database concept is to offer, in one portal, a complete overview of all existing data, o.a. via linking, and the storage of project data. The database is the primary medium where policy makers, managers and scientists "search & find" data, including modelling parameters, on key toxicants, specific sites with respect to toxicity, chemicals and biota (TRIAD).

The basic idea of **KEYTOX DATABASE** is to use as much as possible all existing databases. It will begin with an inventory of existing Internet databases offering site specific (water, sediment, biota, key toxicants, etc.), toxicity, physico-chemical, production, and application etc. data on individual chemical compounds, including known synergistic/antagonistic mixtures.

The second phase is the development of the database specifics, using the QPID system developed by RIKZ (NL) as a starting system. This further development and harmonisation (upgrade) is primarily tuned with the needs and available data of **KEYTOX** partners.

The database will allow the following data to be accessible:

- Sample specific data (locations, GIS coordinates etc, chemo- and bio analytical worksheets, analytes, responses, TRIAD, biotic indices, etc.)
- (synonym) name, CAS and other basic data (e.g. http://chemfinder.cambridgesoft.com/)
- Physico-chemical data (several INTERNET databases)
- Analytical specific data (system specific, e.g. Kovats retention index for GC-MS)
- Toxicity data (several INTERNET databases)
- Bioassay specific response data (INTERNET, literature search, own research data)
- Integrated software (like AMDIS, toxicity calculation and key toxicant prioritizing modules)
- Site, toxicant, source etc. searching facilities
- Generation of DSS essential parameters (DECIS)

Strength of KEYTOX 4

Numerous databases are used throughout Europe offering a strong variety of information on compounds. No database can be found however, where specific data on key toxicants, biology and geography are combined in such a way that search & find entries (queries) can be done for such combinations as: "Where in Europe is TCDD still considered a problem, shown by which bioassays or 'on site' biodiversity? What are the suspect sources? Are the levels suspect of ecological effects? Are other priority key toxicants acting at this site?, etc.". The queries are intended to be versatile, supporting the information need of many (end-) users, but specifically institutes dealing with EDA and environmental Risk Assessment.

Since the MODELKEY/KEYTOX database is also dedicated to supply input data to the EXPO and EFFECT models, other modellers would benefit from this database.

Deliverables:

Month 1-18

KD4.1 Inventory of existing databases and their specifics (month 1-6)
KD4.2 Specification of the final **MODELKEY** database (platform, parameter list, features), including **SITE** data, based on existing databases (month 6-18)

Month 19-36

KD4.3 1st version of the **MODELKEY** database
KD4.4 Uploading of data into **MODELKEY** database

Month 37-60

KD4.5 (Continued) Uploading of data into **MODELKEY** database

KD4.6 Compound and Site specific **KEYTOX** data, as comparison for data generated by **KEYTOX** and **SITE**

KD4.7 DSS (DECIS) supportive data

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SP BASIN: Basin-specific database (UA)

Detailed description of each work component, partners involved in the component and contribution of each to the project as a whole

In sub-project **BASIN** an inventory will be made of the state of art of monitoring and data-evaluation. Monitoring efforts are increasing in function of the requirements for the Water Frame work directive, but often these efforts focus mainly on physico-chemical and biological quality elements. For a good understanding of the relation between physico-chemical aspects and the biological status, more information is needed such as toxicological effects, bioaccumulation, water current, discharge, sediment transport etc. In BASIN 1 a meta database will be compiled of all existing data of three river basins. Based on the requirements of the other sub-projects available data will be collected in existing river basin – specific databases. In BASIN 2 an evaluation will be made of the collected data based on a triad-like approach. A causal analysis of effects of toxicants will be revealed to improve understanding of relationships between exposure and effects on aquatic communities. Hot spots will be selected and additional information will be gathered if necessary.

Work packages 1-2

Basin-specific database - Introduction and five-year overview

BASIN 1

Participant	UA	CSIC	UdG	VRI	IVB	EWQ MA	RIKZ	RIVO	ACA
Person Months	24	17	6	2	18	40	6.9	2	2.8

BASIN 2

Participant	UA	CVR	CSIC	UdG	VRI	IVB	EWQ MA	RIKZ	RIVO	ACA
Person Months	22	4	3	2	2	17	5	7.7	1	0.7

Participant	SZU
Person Months	10

General Introduction

BASIN will provide a data distribution platform for the MODELKEY project. Data are needed for the development and validation of tools and models within the other sub projects. Because a lot of data are already available, a database with existing data will be established instead of collecting new data within the project (BASIN 1). However additional data will be collected if necessary (BASIN 2). Dependent on the individual data sources the data will be stored in a central database(s) or remain in situ and connected via a high-speed data link.

Investigations within MODELKEY will be performed in **three case studies**, covering different eco-regions of Europe. The Scheldt river basin and estuary represents a marine aquatic ecosystem, the River Elbe a central Europe river basin. The River Llobregat has been chosen as a mediterranean case study. All river basins are situated in landscapes, heavily modified by anthropogenic influence. They are polluted by effluents of industrial activities and diffuse drainage from agriculture during the last decades. A short description of the river basins is given in BASIN 1.
BASIN will mainly focus on the integration of existing data, evaluation of the data, selection of hot spots and collection of lacking data into river-basin specific (meta) databases. These are amongst the basic data within the other subprojects EFFECT, EXPO and SITE. KEYTOX will supply the basic data on key toxicants to those subprojects. TRIAD evaluation (BASIN 2) of existing monitoring data will be done based on: (1) physico-chemical parameters, (2) chemical pollutants including heavy metals, PAHs, PCBs, PCDD/Fs, (3) toxicological data (e.g. sediment contact tests or *in vitro* testing on genotoxicity, dioxin-like activity or estrogenicity) and (4) in situ assessment of aquatic communities and biodiversity (algae, macroinvertebrates and fish).

Specific objectives

- to compile a meta database including monitoring data and site specific data
- to link modelling and assessment tools to a database
- to provide data for the other sub projects
- to reveal hot spots and lacking information on the case study river basins and their marine coastal areas.
- to apply and improve TRIAD-like environmental quality assessment tools, as input into the decision support system of DECIS

Research, technological development and innovation activities

The main effort will be to create a complete overview of all existing monitoring data and the originating sources of the original data, being an innovative aspect.

The central idea of collecting data suitable for a TRIAD approach defines the main research aspect: to identify the gaps in data. This will be the input to BASIN 2, where the lacking data will be generated and added to the existing to compile a TRIAD-proof data set on all three basins.

Temporal sequence
For an overview on the temporal sequence of the tasks in BASIN see Fig.. B4.5.

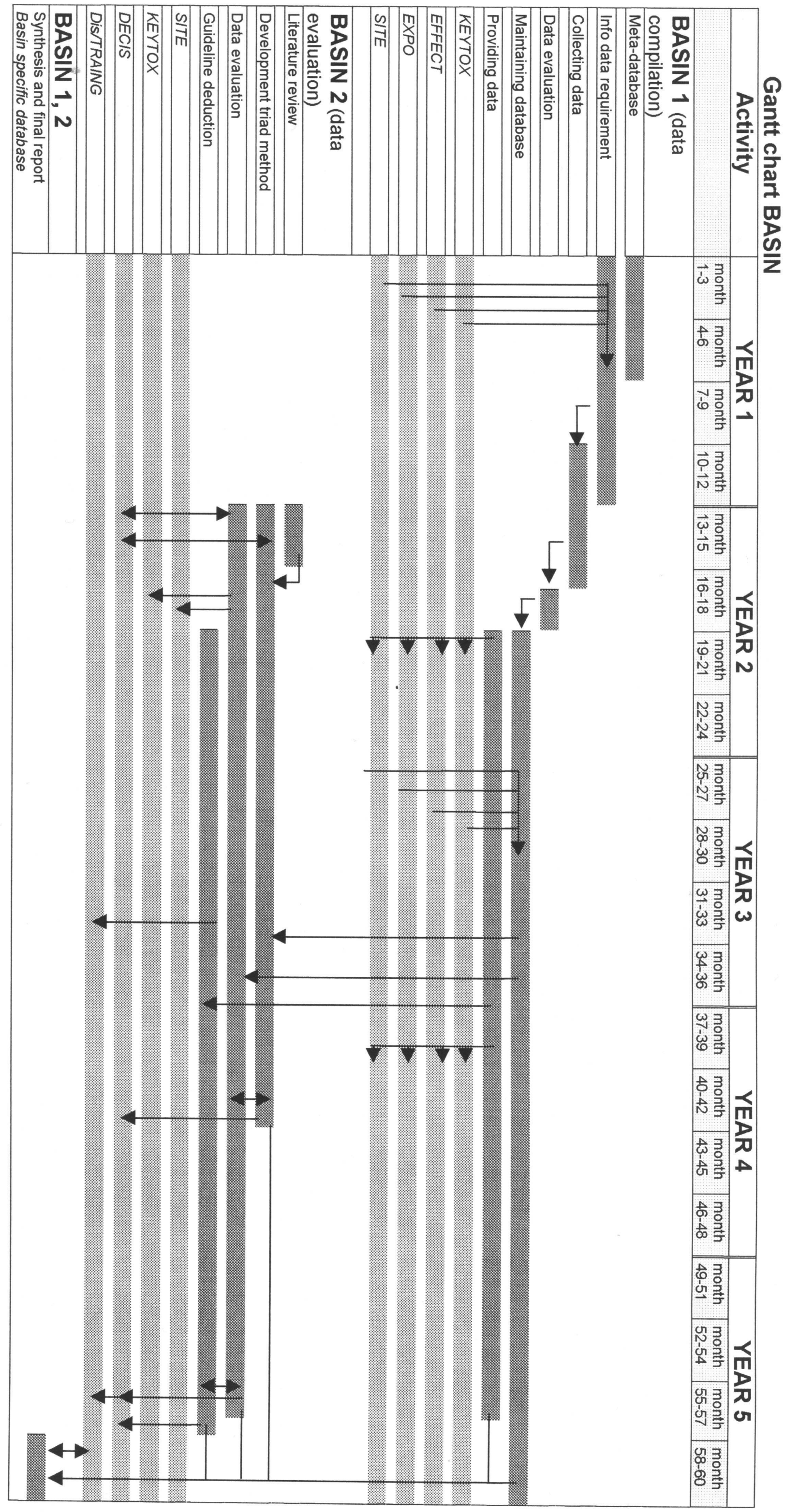


Fig. B4.5 Temporal sequence of the tasks in BASIN

WP BASIN 1 (B1): Establishment of river basin specific (meta) data bases (<u>EWQMA</u>, UA, ACA, CSIC, UdG, VRI, IVB, RIKZ, RIVO)

Tools for the assessment of ecological risk are developed and validated in the subprojects EFFECT, EXPO and SITE. A lot of data are needed to do this, but gathering data is time and cost consuming. However monitoring projects and research programs are carried out a lot in all river basins. The integration of the collected data is often lacking because the Environment Agencies, who are responsible for the monitoring, and scientific groups who carry out the research programs, have different objectives. In BASIN a meta-database will be compiled to get an overview of the data that are available in the specific river basins. This will be done in close cooperation with the FP6 project REBECCA, in which a meta-database is developed for a number of river basins. BASIN 1 will then start up a databank of field data. During the first 18 months the MODELKEY employees working at the EWQMA, UA and CSIC will gather data related to respectively the river Elbe, river Scheldt and the river Llobregat provided by local institutions. The data will be stored in river-specific databases or links will be established to the data sources. The objective is to make the data available and accessible to the modellers. This will be done via the internet, using internal parts of the MODELKEY's website. Data gaps will be identified and potential hot spots will be identified. The data gaps will be filled for a limited number of sampling locations within BASIN 2. The hot spots will be locations were more detailed studies will be carried out within KEYTOX, EXPO, EFFECT and SITE. The data in the databases will be continuously updated during the rest of the project.
At the beginning of the project the work consists mainly of sifting through existing data on the three river basins, checking their accessibility- and compiling a (meta-data) catalogue of available monitoring and research data, which helps the modellers to select what they need. In doing so the persons collecting the data will of course also use existing metadatabases and descriptions. For instance, the currently project German research project NOKIS+ will enlarge data of Schleswig-Holsein existing data collection on water framework relevant aspects of the Elbe estuary. In addition to collating and collecting data, tasks to be performed will also include inquiries e.g. via the Internet as well as maintaining contact with data providers, including arranging meetings with them as required.
The data are to be stored in an SQL database on a system operating under Windows 2000 and using the open-source product MySQL in connection with MS-Access 2003 as a front-end and temporary/partial data storage system. The data model will be designed and set up to meet the demands of data storage and distribution within MODELKEY. A MySQL database can be posted on the Internet, which will require close coordination with the MODELKEY website manager at the UFZ, Leipzig. It can serve as a database for the geograhic information systems ArcGIS and ArcView supplied by ESRI, Inc. (ODBC).
An important aspect of BASIN 1 is that the modellers will specify how exactly their needs for data will be covered. This has to be done in close cooperation with the MODELKEY employee at the EWQMA so that she/he can subsequently provide appropriately edited data.
The MODELKEY database and the links to external data sources have to be maintained throughout the project as well as the provision of permanent access to the

data. Therefore the person working at EWQMA has to be employed during the whole project period.

The three case study river basins are described separately. One coordinator per river basin coordinates the exchange of information and data for the three river basins.

River Elbe

Responsible group: EWQMA

The River Elbe is situated in the Czech Republic and Germany. It is approximately 1100 km long and covers a catchment area of about 150000 km² that is inhabited by 25000 persons. Heavily industrialised areas are spread along the River Elbe and its tributaries. Within the last years many industrial plants have been closed down, so aquatic ecosystems are supposed to recover. However in the Czech part biological diversity decreased substantially in the main stream during the nineties, which might be do to other pressures then chemical pollution, such as the hydrological characteristics.

Extensive monitoring programs have been established in the German part of the system, to study ecosystem health and recovery of the aquatic communities as well as for hot spot identification. EWQMA as the German governmental organisation responsible for these monitoring programs will make this data available and organise them in a database. QWMA plays a key role as stakeholder and end-user of the results at this project.

Monitoring data in the Czech part are collected on an irregular basis. Periodic monitoring is done by the “Czech Research Institute of Hydrology” at seven sites and additional data exist from more than 30 sampling sites. The data at the seven sites contain information over biological data such as fish (biomass, diversity and bioaccumulation), macrozoobenthos (species composition, diversity and bioaccumulation) and phytoplankton (biomass), and chemical data of sediments.

River Scheldt

Responsible group: UA

The River Scheldt is situated in France; Belgium and the Netherlands. It is 350 km long and covers a catchment area of about 21,000km^2 which is inhabited by 10,000,000 persons (477 persons/km^2). The Scheldt is known as one of the most polluted systems within Western Europe, but quality is improving by the installation of waste water treatment plants in Belgium during the last and current decade. Extensive monitoring programs have been established especially in the Flemish and Dutch areas.

In Flanders monitoring programs for water quality, sediment quality are based on a Triad like approach, including chemical analysis, macroinvertebrate composition and bioassays. The methodology for sediment quality assessment is developed by the UA in close cooperation with the Flemish Environment Agency (FEA). The FEA is also responsible for the implementation of the monitoring programs for the WFD. Currently the collected dataset contains data of more than 1200 sampling locations where all parameters have been sampled. The data are stored in a central database and is accessible by the internet (http://www.vmm.be) Beside this a monitoring program exist for body burdens in eels. This program is lead by the Institute of Forestry and Game Management. Currently they are trying to link this network to the sediment monitoring network.

In the Dutch part of the Scheldt and its North Sea coastal area the monitoring program carried out bij Rijkswaterstaat (RIKZ) includes water, SPM , sediment and biota quality parameters at variable frequencies. They imply chemical compounds in all matrices, nutrients in water, algal blooms, macro-zoobenthos communities and health indices of Flounder and Mussels. Bioassay data, as part of the TRIAD, are scarce and available only as project results. Rijkswaterstaat (RIKZ and RIZA) is responsible for the implementation of the monitoring programs of the WFD and reporting data to OSPAR and ICES. RIVO carries out the DYFS (Demersal Young Fish Survey) annually. 1970-1986 twice a year (April and September/October). Since 1987 only in autumn. On average 28 - 45 hauls are carried out per year. Parameters are abundance, length-frequency of all collected species and data on age, mass, maturity and sex of all flatfish species. The numbers caught are generally presented in catch per unit of effort (CPUE). Chemical, physical and biological data are stored in the DONAR central database of Rijkswaterstaat and all freely available by INTERNET (http://www.waterbase.nl). The RIKZ participants of BASIN have relevant project data on bioassays. DYFS data are stored in the data base system of the RIVO institute.

River Llobregat

Responsible group: CSIC
River Llobregat is situated in the NE part of Spain. It is 156.5 km long and covers a catchment area of about 4948 km2 which is inhabitated by 3.089.465 persons (in year 1999) During the last decades, the river Llobregat has been highly polluted by industrial and urban wastewaters, and by surface runoff from agricultural areas. This river experiences periodic floods and droughts which lead to frequent morphological variations in the river bed and to modifications in its banks. The river Llobregat has two main tributaries, the river Cardener and the river Anoia, and all three rivers receive the input of various sewage treatment plants effluents. Furthermore, the occurrence of natural salt formations and the corresponding mining exploitations in the basin (Cardona, Suria and Sallent mining sites), have caused an increase in the salinity of the water.
Previous studies carried out in these rivers have evidenced the presence of estrogenic compounds, coming from both industrial (surfactants) and municipal (estrogens) sources, and its correlation with important alterations (an abnormally high incidence of intersex and elevated levels of plasmatic vitellogenin) in carps inhabiting these rivers. Close to its mouth, the Llobregat river flows nearby the city of Barcelona, and its water is used for abstraction of the drinking water supplied to most of the districts in the province of Barcelona. In those periods when the quality or the quantity of the surface water is low, groundwater from the aquifers located in the lower valley and the delta of the Llobregat river is used for drinking water production. These aquifers are subject to artificial recharge. Close to its mouth, the watercourse of the river is currently being deviated and one of the largest European sewage treatment plants

treating the wastewater of the southern part of the Barcelona area, has been recently constructed.

The Catalonian Water Agency (ACA) is in charge of the management and administration of all aspects related to the water cycle, including planning, execution and operation of hydraulic infrastructures and wastewater treatment plants, preservation of aquatic ecosystems, and water quality control. The ACA, thus, keeps historic records and databases of quality monitoring results for both continental (surface and ground) and littoral waters, including biota and sediments. Data available cover chemical (general chemistry, heavy metals and organic micro-contaminants), microbiological and biological aspects required by the existing EU Directives. The ACA also operates an automatic quality control network constituted by 11 points located in the Llobregat basin, that monitorizes the water quality continuously and at real-time, helping to prevent contamination episodes, and preserving the quality of the water supply to the Barcelona area. As water authority, the ACA also keeps inventories of the industrial and urban wastewater discharges, water intake permits etc. Additional required studies previous to the implementation of the new WFD are currently under way, such as the ecological classification of water bodies, the identification of anthropogenic pressures etc., as well as, those necessary to adapt the existing monitoring networks to the new requirements of the WFD (mainly on ecological aspects).

Strength of BASIN 1:

The development and validation of new tools by MODELKEY must be supported by actual field input and validation data. BASIN 1 will collect existing data and identify gaps, which are crucial as input into EXPO and EFFECT and should be collectd by BASIN 2.
The institutes involved in MODELKEY/BASIN are also strongly related to the monitoring programmes for the specific river basins. Beside this the UA, RIKZ and EWQMA are involved in (the coordination of) joint or national research programmes in respectively the Scheldt and Elbe. The accessibility of the data is ensured in this way.

Deliverables:

Month 1-18

BD 1.1 Status report on monitoring programmes (month 6)
BD 1.2 First meta database on available data with links to data originating databases (month 6)
BD 1.3 TRIAD database and identification of missing data for each case study river basin as input to the research items of BASIN 2 (month 16)
BD 1.4 First selection (on limited data set) of potentially hazardous sites and respective key effects as a crucial input to SP **SITE** and **KEYTOX**. (month 18)

Month 19-36

BD 1.5 A complete (meta) data set for a limited number of sites in the three river basins.

BD1.6 Input Datasets to the other subprojects in the format they require.

Month 37-60

BD1.7 An overview of application of the in MODELKEY developed assessment tools on the specific river basin datasets

WP BASIN 2 (B2): Data collection, quality assessment and guideline deduction (UA, EWQMA, ACA, CVR, CSIC, UdG, VRI, IVB, RIKZ, RIVO)

The objectives of the Water Framework Directive (2000/60/C) are that for all community waters covered by the Directive there should be no deterioration in their quality, and that good status should be achieved by 2015. For the assessment of the ecological status physico-chemical and biological monitoring programs are under development, often based on experiences of previous national monitoring programs. These monitoring programs focus mainly on a limited number of well-known chemical compounds and in a lesser content also on the biodiversity of macroinvertebrates. The measured concentrations were compared with existing sediment or water quality guidelines and based on this the potential risk was estimated. There are two main objectives against this approach. First of all there are quality guidelines derived for only a limited number of chemical compounds, even less than one percent of the compounds known to be present in the environment due to human activities (Van Wezel, 1999). Secondly there is no direct link between the concentration of a compound and the ecological quality. An important aspect in the risk caused by sediment-bound chemicals is the degree of exposure encountered by sediment-dwelling organisms. Bioavailability, bioaccumulation and additive and synergistic effects of mixtures of compounds play in important role in this. For these reasons, and because of the large number of unknown contaminants, ecological risk assessment has received much attention in the last decades (Den Besten et al., 2003). The basic principle of ecological risk assessment is the use of multiple lines of evidence (Burton et al., 2002). Important lines of evidence are:

- Assessment of the condition of the benthic macroinvertebrate community
- Assessment of sediment toxicity by using bioassays
- Assessment of the potential effect occurring through foodchain poisoning.

Biological effects-based assessment of the in situ risks focuses on location-specific conditions with respect to the bioavailability of contaminants and the assessment of the damage to the ecosystem. Biological effects-based assessment can be done by the integration of information from large numbers of parameters that use different lines of evidence (Ingersoll et al., 1997). The TRIAD assessment method developed for sediments is such an approach that can be applied in integrated or tiered approaches. The collected dataset within BASIN 1 will result in a huge data set of physico-chemical, biological and ecotoxicological data.

In BASIN 2 a triad assessment tool will be developed, based on the Flemish triad assessment methodology. Available and collected information in BASIN 1 will be used as much as possible for this. This tool will be developed in the first 18 months and applied on the collected data to select the potential hot spots and to identify data gaps. Additional data collection will be limited to fill in the gaps for a TRIAD evaluation at a number of locations in the three river basins. The goal is to collect a complete data set for a number of locations per river basin to ensure the possibility to apply and validate the tools that are developed in SITE, EXPO and EFFECT. The entire field work is planned in close cooperation with the local Environment Agencies.

Finally the large data set gives the opportunity to derive No Observed Effect Concentrations (NOEC) based on the biological community, bioassay results and bioaccumulation results. These NOECS can be compared and used to develop Predicted No Effect Concentrations (PNEC). These values will be extracted and can be used as a scientific base for the deduction of sediment quality guidelines.

Strength of BASIN 2:
The institutes involved in MODELKEY/BASIN are also strongly related to the monitoring programmes for the specific river basins. The available dataset will contain an enormous amount of integrated datasets, which has never been used before. Beside this the UA, RIKZ and EWQMA are involved in (the coordination of) joint or national research programmes in respectively the Scheldt and Elbe. They have experience in the integration of data from different fields. Experts of physico-chemical analyses, bioassays and biotic communities are all involved in BASIN 2. This ensures a good expert-judgement of the different steps, which will be established in this WP, such as hot spot selection and deduction of guidelines. BASIN 2 will be done in close cooperation with the subproject DECIS.

Deliverables:

Month 1-18

BD 2.1 Report on the use of integrated biological-effect based assessment methods (month 15)
BD 2.2 A triad assessment methodology that will be used after month 18 for evaluation of the sediment quality based on the available data (month 18)
BD 2.3 Revision and Identification of potentially hazardous sites and respective key effects as a crucial follow up to SP SITE and KEYTOX (month 18)
BD 2.4 Survey data of in vitro and chemical analysis in the Czech part of the river elbe basin (month 18)

Month 19-36

BD2.5 Report containing the missing information which are reported in BASIN 1 as data gaps
BD2.6 An evaluation of the sediment quality in the three river basins, based on the proposed triad assessment methodology.

Month 37-60

BD2.7 Guidelines for contaminants in sediments based on biological effect-based assessment

BD2.8 Report with recommendations for the improvement of integrated monitoring and assessment programmes

Burton G.A. Jr., G.E. Batley, P.. Chapman, V.E. Forbes, E.P. Smith, T. Reynoldson, C.E. Schlekat, P.J. Den Besten, J. Bailer, A.S. Green, R.L. Dwyer (2002). A weight-of-evidence framework for assessing ecosystem impairment: improving certainty in the decision-making process. Human and Ecological risk assessment 8: 1675-1696.

Den Besten P.J., E. de Deckere, M.P. Babut, B. Power, T. Angel DelValls, C. Zago, A.M.P. Oen, S. Heise (2003). Biological effects-based sediment quality in ecological risk assessment for European waters. J. Soils & Sediments 3: 144-162.

Ingersoll C.G., T. Dillon, G.R. Biddinger (1997). Ecological risk assessment of contaminated sediments – Proceedings of the Pellston workshop on sediment ecological risk assessment, 1995. SETAC Special publications series, 389 pp

Van Wezel A.P. (1999). Overview of international programmes on the assessment of existing chemicals. Institute for studies on Human Health and the Environment (RIVM) report 601503 015, Bilthoven.

SP EXPO: Exposure modelling of contaminants (DELFT)

Detailed description of each work component, partners involved in the component and contribution of each to the project as a whole

EXPO work components are structured into four work packages. Work package 1 (sedimentation and erosion) contains the analysis and evaluation of sedimentation and erosion processes. Work package 2 (transport and processes) is a package aimed at the understanding and modelling of the transport and bio-chemical processes of contaminated sediments in the Elbe river and Scheldt estuary. Work package 3 (bio-availability and foodweb) focuses on the review and summary of knowledge on bioavailability and food chain transfer. Work packages 1,2 and 3 will jointly develop suitable paramerisations to be applied in a generic users-friendly exposure assessment model on a basin scale to be develop in work package 4. The figure B4.6 shows the overall structure of sub-project EXPO.

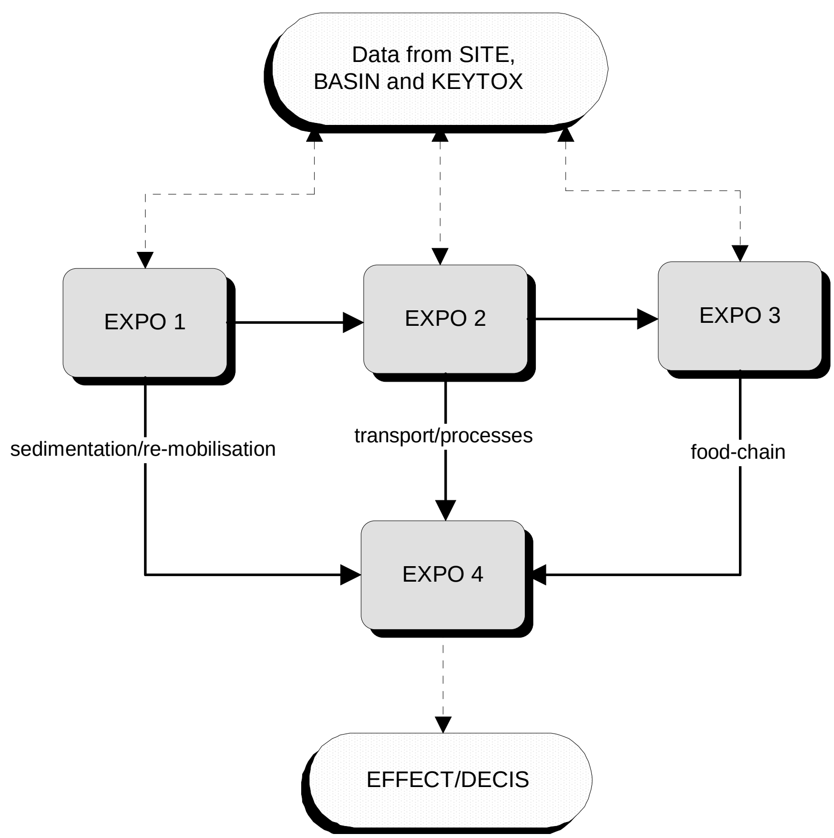


Fig. B4.6 : Overview of the EXPO structure

Work packages 1-4
Introduction and five-year overview (RTD)

EXPO 1

Participant	Delft	UoS	UA
Person Months	2	23	2

EXPO 2

Participant	Delft	UoS
Person Months	10	17

EXPO 3

Participant	Delft	VUA	UA	UJOE	RIKZ	UdG	VRI
Person Months	2	8	2	2	13.5	2	2

EXPO 4

Participant	Delft	UoS	VUA
Person Months	33	1	1

Introduction

In the past decades most of the European river basins have been polluted severely with a wide range of toxic substances, by a large number of industrial and domestic discharges. In addition, the pressure on the environment has recently increased by new evolving substances. In view of the growing social and economic interest in preserving a good water quality and healthy eco-system, a proper understanding of the behaviour of these contaminants is required to assess, control and mitigate anthropogenic effects. The transport and fate of these contaminants in river basins and coastal systems is determined by a intricate interaction between various natural physical and bio-chemical processes and/or human activities. To accommodate for the assessment of the exposure risk of traditional and recently evolving pollutants in river basins, this sub-project provides improved understanding of processes and the response to changes in the environment and its impact on the water system, either by natural cause or by human activity. This understanding will be translated in a set of sub-models that will be implemented and applied for the river Elbe and the Scheldt estuary. As such, EXPO will use a combination of state-of-the-art water quality and sediment models to integrate site data with current scientific understanding of the physical, chemical and biological processes governing the transport and fate of the contaminants.

To facilitate the use by local and regional authorities, the formulations of the sub-models will be integrated and transferred in a parameterised form to develop a generic “easy-to-use” exposure assessment model applicable for a wide range of European river basins and estuaries with minimal requirements for model steering and use. The model will be able to predict the risks of mobilistation of contaminated sites, resulting environmental abiotic and biotic concentrations, transport fluxes and mass balances to forecast the risk and effectiveness of remedial (emission) measures and new technologies. The model tool will be adaptable to comprehend the differences in environmental conditions within the European river basins. The model will account for the effects of natural physical, chemical and biological processes such as tidal motion, flooding, temperature, salinity, sedimentation, emission, rates of degradation and complexation in water, sediment and biota. In the final generic model the upper river network will be linked to an estuary and adjacent marine coastal zone in a schematic way. The risk of remobilisation of contaminated sites can be quantified and visualised throughout the basin. The well-known and defined physical and bio-chemical transport and fate processes will be translated and transferred into simplified rules and formulations.

Temporal sequence
For an overview on the temporal sequence of the tasks in Expo see Fig.. B4.7.

WP EXPO 1 (EX1): Sedimentation and erosion processes (UoS, DELFT, UA)

All the data collected in BASIN 1 and SITE 1 on hydraulics and sediment, in particular at the hotspots must be evaluated to model the relationship between the flow field, erosion and sedimentation processes. Focusing on hotspots mobilized by erosive hydraulic conditions and their impact on the river ecosystem the critical flow parameters for the onset of erosion must be specified as well as the rate of contaminated sediment release (Witt, Westrich 2003). The sediment erosion mass flux plays an important role because it controls the source strength of pollutants and therefore, determines the concentration field not only of the resuspended particulate contaminants but also of the dissolved pollutants associated with the pore water. The erosion is the triggering mechanism followed up by the hydrodynamic transport, desorption and remobilization of sediment bound contaminants and, finally results in sedimentation of remaining polluted fractions downstream in headwaters and stagnant water bodies like groyne fields or harbors and flood plains . The combined effect of physical (grain size), chemical and biological (EPS) factors on the sediment erosion stability is not at all fully understood as to formulate the respective model terms (Haag, Westrich 2001). Therefore, a geostatistical evaluation of erosion relevant sediment parameters in terms of averaged values, spatial variance and uncertainty is required which allows to account for the probabilistic component of erosion and sedimentation processes and the resulting exposure (Li, Westrich 2001; Li 2004). Special interest will be given to the contaminated sediment depth profile which in combination with the duration of an erosive event and the rate of erosion controls the contaminant source strength. In addition, the hydraulic conditions at the hotspots will be derived from hydrological data for a rough erosion potential estimation. By multiple regression analysis of the hydraulic and sediment data a preliminary general parameterized description of erosion processes applicable to the three river basins (Elbe, Scheldt, Llobregat) can be delivered. This enables to describe different hydrological scenarios with variable flow field and site specific erosion related sediment parameters (Witt 2004).

The modeling of sedimentation processes requires detailed information on suspended sediment parameters, in particular on the settling velocity of the contaminated fraction because of its model key function. Those parameters can only roughly be estimated from the existing data and hence, actual measurements in SITE 1 and particle size measurements must be performed (UfZ, Leipzig) . Further gaps in the data set, e.g.

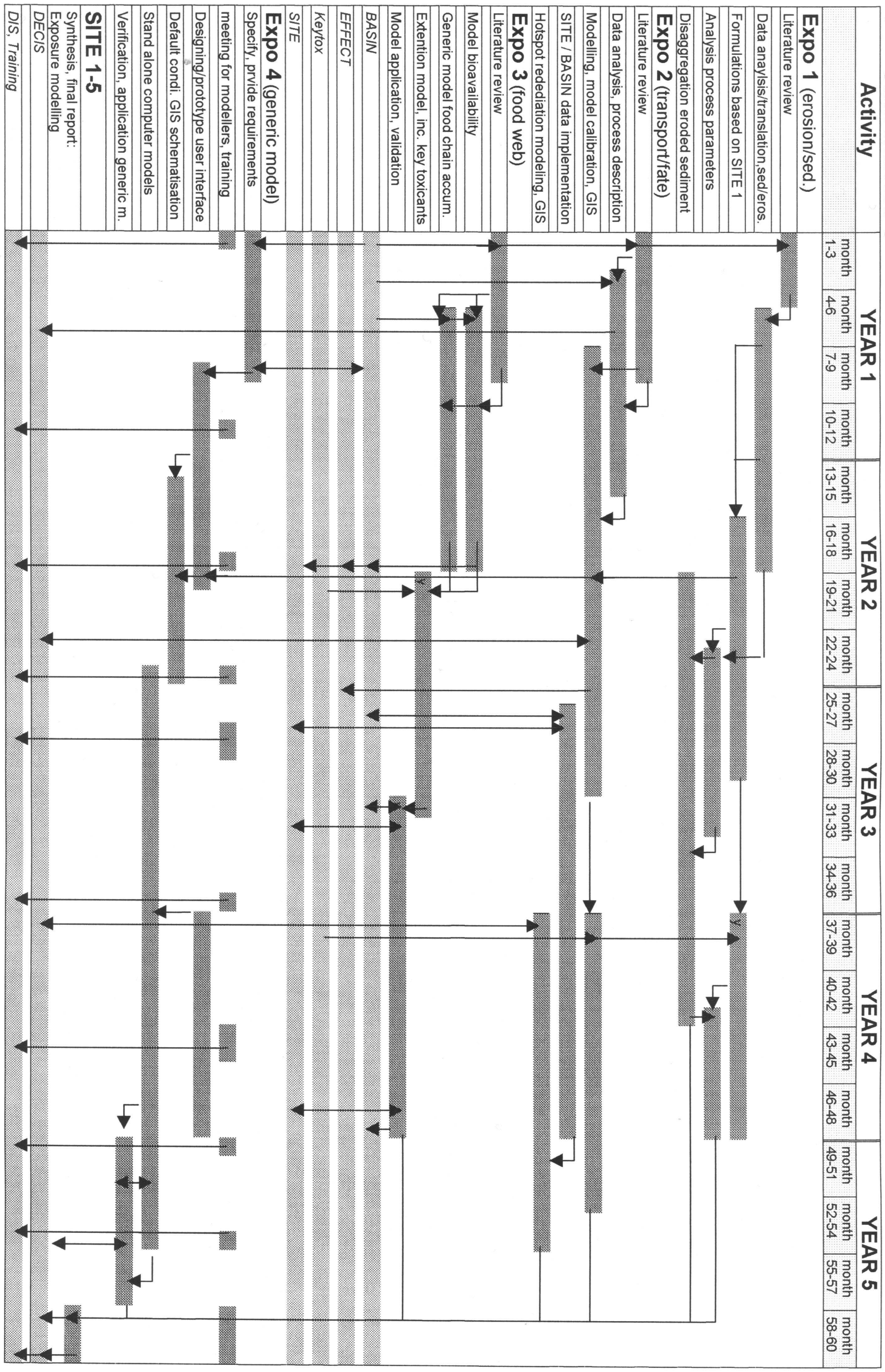


Fig. B4.7: Temporal sequence of the tasks in Expo temporal sequence of the tasks in Expo

partitioning coefficient K_d, will be identified and filled by the experiments in SITE 1. The model approach will be validated by targeted experiments performed in SITE 1. The evaluation of the Elbe flood data towards a pollutant mass balance is expected to facilitate the formulation of a parameterized relationship for erosion processes.

Besides the physical aspects, the sedimentation and erosion behaviour of sediments is also determined by benthic organisms. Benthic organisms such as macrofauna, microphytobenthos and higher plants are organisms that live in or are attached to the bed. The presence of benthic organisms affect the (de)stabilisation of sediment in many different ways. These organisms are very much dependent on the physical and chemical properties of sediments. However, the presence and activity of benthic organisms can also reversely influence the physical and chemical properties and processes that take place within the sediment (Reise, 2002). Benthic organisms can change the sediment stability and thus have effect on erosion/deposition processes by their potential effect on both the bed shear stress and the shear strength of the sediment. The bed shear stress is a combined effect of hydrodynamic conditions near the sediment and the bottom roughness. Higher plants such as seagrass decrease the current velocities thereby reducing the local erosion. Other organisms increase the bottom roughness by creating elevations and depressions at the sediment surface. This greater bottom roughness will increase the shear stress and thus has a negative effect on bottom stability. The shear strength of the sediment bed is increased by the excretion of polymeric substances by organisms such as epipellic diatoms, sticking the sediment particles together and stabilising the sediment. Not only physical, but also chemical composition and processes in the sediment are influences by benthic organisms. This is both a direct result of their metabolic processes (production and respiration) and their behaviour (tube building, sediment reworking). Suspension feeders remove particles from the overlying water an deposit them to the sediment. Deposit feeders ingest sediment and return it to a different location in the sediment. This mixing of sediment by the activity of macrofauna is termed bioturbation.

Literature overviews of (de)stabilisation mechanisms for main groups of benthic organisms were presented in WL research reports (2002a/b). These typical populations seem to be controlled and organised by a relatively small set of key species and abiotic processes. In case of inter-tidal estuarine systems, the development of the typical populations is closely connected with the development of mudflats and sandflats. (Widdows and Brinsley, 2002; Herman et al., 2001; de Brouwer et al., 2000). Figure B4.8 provides an overview of typical species in an inter-tidal zone.

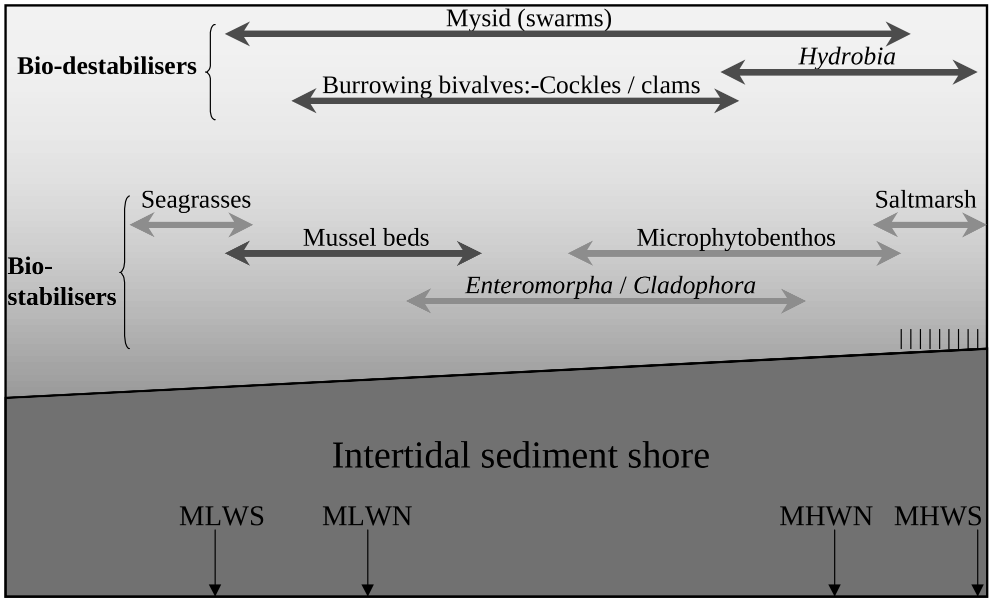


Fig. B4.8: Benthic organisms in the inter-tidal zone

This work package will provide an overview of the various processes and controlling mechanisms for sediment stability to be implemented and applied in the detailed basin models of work package 2. In addition, appropriate parameterization and rules for local sedimentation and erosion will be derived to be applied in the generic model of work package 4

Strength of the EXPO 1:

The data-analysis and literature overview will compile a set of state-of the art formulations related to the sedimentation and erosion of sediments in river basins and estuaries, that will be applied both fresh and saline systems. Besides the chemo-physical properties the linkage with biological benthic organisms affecting the sediment stability will be defined.

Deliverables

Months 1-18

EXD 1.1: Overview of processes: sedimentation, erosion, mixing and consolidation (month 18)

EXD 1.2: Analysis and evaluation of data on river morphology, flow velocity field and transport characteristics to identify sedimentation and erosion areas for Elbe, Scheldt and Llobregat (month 18)

EXD 1.3 Compilation, evaluation and synopsis of physical and chemical data of hotspot deposits (month 18)

EXD 1.4: Description of relations between benthic organism and the physical and chemical properties of the sediment (month 18)

EXD 1.5: Parameterised formulations and rules for the beginning and intensity of sediment erosion to be used in EXPO 2 and 4 based on master variables (month 18)

EXD 1.6 Parameterised formulations and rules of local transport conditions for the beginning of suspended contaminated particle sedimentation and their sedimentation rates for the EXPO 2 and 4 models (month 18).

EXD 1.7: Description and specification of additional necessary and actual data on sediments which must be provided by targeted field measurements in SITE 1 for the respective rivers: Elbe, Scheldt and Llobregat (months 6, 12 and 28)

EXD 1.8: Report overview Elbe flood 2002 (month 18)

Months 19-60

- Multivariate statistical analysis for the improvement and generic description of physical, chemical and biological effects on erosion and sedimentation processes to be used in the EXPO models
- Sensitivity analysis on erosion and sedimentation relevant physicochemical factors to define significant master variables
- Improving the modelling of the interaction of pore water and sediments quality , the non erosive diffusive release of toxicants
- Modelling the time depended dis-aggregation of eroded cohesive sediment aggregates as a controlling factor for adsorbed toxicant release.

WP EXPO 2 (EX2): Transport and fate of contaminants (DELFT, UoS)

Within this work package an improved understanding and forecasting of the transport and fate processes of contaminants within a river basin will be examined and applied in detailed sub-models for the river Elbe and the Scheldt estuary.

Transport processes

The behaviour of contaminants in the water and sediments in river basins cannot be studied without taking into account the relevant processes in the basins and the boundaries with the upstream river system and the coastal region. The rivers that flow into these coastal areas take a considerable amount of contaminated sediments which are stored for longer or shorter periods in these estuaries. Retention of sediments will take place in the low-energy areas such as the smaller tributaries in the river basin. Within this work package various empirical formulations and characteristics will be defined that typically determine the sediment retention (e.g. hydraulic load and specific runoff). The estuarine regions of a river basin represent a diverse and complex water system. The tidal motion and the density currents induced by the change from fresh to saltwater are of particular importance in describing the water quality of estuaries. In the estuary strong intrusion of saltwater landward and current reversal might occur. The coastal area is characterised by the typical oscillations of the tidal movement and has a complicated current structure resulting from the horizontal intrusion of saline water and vertical stratification due to density differences. It is obvious that the estimation of the time and spatial behaviour of the exposure of contaminants in estuaries is complicated by the effects of tidal motion and chemical behaviour. In order to have an accurate description of the fate and distribution of contaminants in estuarine regions, a carefully analysis of model concepts and implementation is needed in this work package to assess the degree of complexity and valid merging of process formulations.

Bio-chemical fate processes

Besides transport processes compounds are subject to many distribution and transformation processes or reactions which determine the exposure of contaminants within a river basin. Physico-chemical processes such as sorption, partitioning and evaporation determine the distribution between the water, air and particulate phases. Most compounds are subjected to transformation or degradation reactions, such as hydrolysis, photo-degradation, redox reactions and degradation by micro-organisms. The significance of degradation processes may vary with depth. For several compounds degradation is most prominent in the upper water layers, due to photo-degradation. Biodegradation rates in the lower water column are assumed to be lower. In anoxic sediments, biodegradation rates usually are much slower than in the water column. Many trace metals and persistent organic compounds are strongly bound to particulate phases or dissolved organic material or in the case of trace metals bound to inorganic and organic ligands. Usually only a limited fraction of a specific compound is present in a truly free dissolved state and available for uptake by aquatic organisms. Until 1995 the principle of linear equilibrium partitioning had been the main guiding principle in studying adsorption of hydrophobic pollutants onto sediments and soil. However, the literature of the nineties also showed that the partition coefficient increases at the progress of the ageing of sediment (Hatzinger and Alexander, 1995, Weber and Huang, 1996; Huang *et al*., 1997; Leboeuf and Weber, 1999; Kan *et al*., 1998; Jepsen and Lick, 1999; WL, 2003a).

The sediment and pollutant transport dynamics of the Elbe river upstream of the tidal range and the Llobregat river in Spain, is governed by the hydrological characteristics of the catchment and the subcatchments, respectively. The driving force for erosion, transport and sedimentation is the discharge and hence, the model input data must be chosen on a statistical basis in order to link the transport processes to the hydrological risk. This allows to investigate the ecological impact of representative discharge scenarios and to attribute a hydrological probability. In addition, the spatial variability and uncertainty of the sediment data must be taken into account, e.g. by applying the Monte Carlo method to come up with statistical model results, i.e. expected values and variance for pollutant load and concentration, sedimentation rate, residence time, exposure duration etc. (Li, 2004) which are useful and important results for the following ecological impact assessment in EXPO and EFFECT. Erosion and sedimentation, transport and mixing, residence time, sorption and 1-st order degradation can be described by the reactive model COSMOS (Kern, 1997) after calibration. The major hotspots in the Elbe river are located in the groyne fields which have a high trapping efficiency at low water level and become strong pollutant sources at higher erosive discharge. To account for the Elbe specific morphology a hierarchical model will be conceptualized consisting of a 2-dimensional model (TELEMAC- SUB2; Jacoub, Westrich, 2004) which can be coupled or nested in a 1-dimensional model (COSMOS). Representative river portions with critical hotspots or high ecological vulnerability are selected and modelled by the 2-d model with high spatial and temporal resolution to cover the dynamic process whereas the 1-dimensional model is applied to capture the whole river Elbe with its most important hotspots located in the tributaries, i.e. Bilina in Czechia and Mulde, Saale in Germany, and to allow long term simulation for future exposure and environmental impact assessment very efficiently. A sensitivity analysis will be performed for model parameter ranking to come up with a limited number of key parameters. The intention is to validate the 2-d pollutant transport model by recent actual data collected by specific measuring campaigns in SITE 1 which provides a data set independent from the former calibration data set.

Within this work package available state-of-the-art knowledge and formulations of transport and bio-chemical processes will be compiled and linked with the sedimentation and erosion processes from work package 1. These formulations will be implemented in detailed sub-models to be applied for the Scheldt estuary and river Elbe. The models will be verified with field data compiled from the Sub-projects BASIN and SITE. A thorough analysis of the model performance will be conducted comprising a sensitivity analysis of the various bio-chemical parameters and environmental conditions. The results will be used to derive generalised transport and fate formulations that will be applied in the generic exposure assessment model of work package 4. At a later stage the models can be used to predict the spatial distribution of deposited key toxicant (KEYTOX) for various hydrological scenarios and to evaluate alternative hotspot remediation strategies resulting from DECIS.

Strength of EXPO 2:

Most partitioning and risk assessment exposure models only includes a few of the aforementioned transport phenomena and bio-chemical fate processes. Since, non-equilibrium partitioning or salinity related environmental properties might be of significance, only more comprehensive numerical models (such as e.g. Delft-3D and derived linked models) are capable of simulating the detailed physico-chemical and biological processes and interactions. Especially for a sound comparison of the exposure of different compounds it will be of great importance that these processes and interaction-effects can be embedded directly or in a parameterised way in the model. The extensively studied Scheldt estuary and the river Elbe will be applied as case study for testing and demonstration of the detailed and parameterised formulations. The models will be able to predict the spatial distribution of key toxicitants within the river basins and to evaluate various hotspot remedial strategies.

Deliverables

Month 1-18
EXD2.1: Data analysis (of data collected in BASIN) (month 12)

EXD2.2: Preliminary results of detailed 2D/3D modelling of Scheldt estuary including the marine coastal zone (month 15)

EXD 2.3: Preliminary results of detailed 2D modelling of river Elbe (Tasks EX2.4, 2.10, 2.11), including erosion risk and impact assessment for identified hot spots in the rivers (Elbe etc.) and quantification of mobilized hotspots and contaminant mass balance caused by the Elbe flood 2002 (18 month)

EXD 2.4: Results of calibration of models on collected data (from BASIN) (18 month)

EXD 2.5: Sediment origin analysis (determining the origin and retention time of sediment) (18 month)

Description of proposed parameterisation of transport and fate processes including:

EXD 2.6: Review and description of the state-of-the art transport and bio-chemical processes that determines the behaviour of contaminants in riverine and estuarine systems (month 6)

EXD 2.7: Initial simplified parameterisation/generalisation of transport and sedimentation processes (month 12)

EXD 2.8: Sensitivity analysis parameters and processes (month 15)

EXD 2.9: Classification of river/estuary types and environmental conditions (month 18)

EXD 2.10: Model parameter sensitivity analysis by application of principle component method and/or Monte Carlo simulation (month 18)

EXD 2.11: Specification of characteristic hydrological discharge scenarios (low, medium, high discharge and flood) with significant impact of sediment bound toxicants on the ecosystem (month 18)

Month 19-60

- Further elaboration parameterisation of processes and model calibration and validation on an appropriate field data set from BASIN and SITE
- Exposure modelling aiming at the prediction of spatial distribution of deposited particulate key toxicants for different hydrological scenarios of he river Elbe and its tributaries (low, medium, high discharge; flood events) for the EFFECT subproject.
- Simulation of alternative hotspot remediation strategies resulting from DECIS on along term basis by local 2-d and large scale 1-d modelling
- Mapping of exposure model results (GIS) in terms of: Erosion risk; erosion mass; concentration and residence time of (dissolved and particulate) contaminants in the water column and in the deposits; location and intensity of sedimentation (Elbe river)

WP EXPO 3 (EX3): Bio-availiability and foodweb (VUA, DELFT, UA, UJOE, RIKZ, UdG, VRI)

Bioavailability, ecophysiological factors, and food web dynamics are key factors determining the extent to which exposure to contaminants way lead to accumulation in food webs. In the current European risk assessment frameworks (TGD, 1996) these complex exposure pathways are hardly addressed, or considered only in a simplified approach. Although existing approaches may have worked for classical neutral hydrophobic contaminants, there is increasing evidence, that this approach is insufficient for newly emerging contaminants or to protect aquatic life from sublethal effects such as endocrine disruption.

The main abiotic factors that determine the bioavailability of sediment-bound neutral persistent hydrophobic compounds include content and composition of organic carbon (Park et al., 1999), particle characteristics, ageing and contact time (Kukkonen and Landrum, 1998) and sequestration in less or non-bioavailable sediment fractions, such as e.g. soot (for PAHs; Gustafson et al, 1997). For trace metals factors such as grain size, mineral composition, acid volatile sulphides, cation exchange capacity, redox-conditions (Hummel et al, 1998), presence of iron or manganese hydroxides have been reported to affect the bioavailability (Chapman et al., 1998). For polar and ionized compounds, such as e.g. surfactants and pharmaceuticals, simple organic carbon partitioning models seem inadequate to describe the sorption processes, and the insight in the driving factors of bioavailability is much more restricted (Salloum et al, 2000; Tolls, 2001). Sediment ageing may have a severe impact on the bioavailability of contaminants (Kukkonen and Landrum, 1998).

Residue levels of contaminants in organisms are further determined by uptake from aqueous and dietary sources, internal distribution, passive and active elimination, growth and reproductional activity and transformation reactions such as (bio)degradation and (bio)transformation. Uptake of compounds may take place from aqueous systems, via gills or the skin, and from dietary sources via the gastro-intestinal tract. Epibenthic and sediment inhabiting invertebrates may have additional uptake from ingested sediments or from porewater. Bacteria and fungi, constituting a large fraction of the benthic bioass, have been reported to be a major vehicle in mass transfer of hydrophobic compounds between sediment and macrozoobenthos (Gunnarson et al., 1999). In pelagic organisms direct aqueous uptake of compounds (bioconcentration) seems to be dominant in most invertebrates and fish for compounds with a log K_{ow} < 4 (Thomann and Komlos (1992). The fraction of a contaminant concentration that is available for uptake by aquatic organisms, i.e. the bioavailable fraction, varies between species and depends on the relative significance of different uptake pathways (Gobas and Morrison, 2000). Following uptake, compounds may be subject to biotransformation, to internal distribution among tissues and organs, and to elimination of parent compounds or biotransformation products. Although generally metabolism leads to degradation, detoxification and elimination, products may be generated with enhanced endocrine potential. Especially in vertebrates the biotransformation route is more predominant in comparison to invertebrates and phytoplankton (Van der Linde et al., 2001) Elimination may be the result of redistribution at respiratory surfaces or in the gastro-intestinal tract or via excretion products. Most of the currently developed food web models are restricted to neutral hydrophobic compounds, such as PCBs, chlorinated pesticides, and dioxins.
Current risk assessment practices mainly rely on application of simple experimental or predicted bioconcentration factors (BCF), bioaccumulation factors (BAF) and biota/sediment accumulation factors (BSAF) factors to predict internal concentrations in food webs and do not take into account the many (and often species- and compound

specific) biological factors affecting toxicokinetics (e.g. feeding behaviour, lipid metabolism, biotransformation) and food web dynamics. Proper prediction of internal concentrations in food webs are required to estimate direct and indirect effects on biodiversity or secondary poisoning in (top)predatory species that., which will be addressed in EFFECT, SITE and DECIS.

Objectives

In this workpackage we will develop innovative approaches, supported by the experimental and field studies conducted in SITE-2, to generate model formulations and parameterizations that will allow a more appropriate handling of bioavailability and food web accumulation in the generic exposure assessment module to be developed in EXPO-4. The food web parameterization in EXPO-3 is closely interlinked with effect modelling in canonical communities and food chains in EFFECT 3. It is expected that improved treatment of bioavailability and food web accumulation in the exposure assessment model might lead to different risk prioritization and hence allocation of funds in risk assessment and management approaches.

The overall objective of this work package is to review and summarize current knowledge on bioavailability and food chain transfer of contaminants and to develop suitable parameterisation and formulations for the generic exposure assessment model of WP4

More detailed objectives:

- Comprehensive review of existing and innovative approaches for inclusion of bioavailability and food chain models in exposure assessment modelling
- Development and testing of parameters and formulations to predict bioavailability of waterborne and sediment-bound key contaminants from innovative *in-situ* assessment methods (desorption studies, biomimetic methods)
- Development of conceptual framework to derive components of generic freshwater and estuarine food webs
- Development and testing of a tiered approach for parameterisation and model formulations for food chain transfer and biomagnification
- Evaluate the impact of uncertainty in parameters and data on model outcome
- Validate the bioavailability food chain modules in the different case studies.

Parameterisation of bioavailability.
The work will start with a comprehensive review of current exposure assessment models and to what extent factors determining bioavailability of contaminants in sediments, pore water, suspended matter, and the water column are included in those models. Special attention will be paid to factors such organic matter composition and concentration (POM, DOM), pH, redox potential, sediment grain-size and specific area related parameters, and different classes of compounds. In cooperation with SITE-2 and KEYTOX-1 an evaluation will be made of currently available rapid in-situ assessment methods (tenax desorption studies, biometic techniques) and their

suitability to incorporate their endpoints in exposure assessment models. At this stage it is expected that the discrimination between slowly and rapidly exchanging sediment fractions, derived from sediment desorption experiments with Tenax (Kukkonen et al, 2003; Ten Hulscher et al., 2003), proper handling of sorption to DOC (Akkanen and Kukkonen, 2003), and biomimetic estimates of the freely dissolved water concentrations (KEYTOX-1, SITE-2) measurements) could lead to a more adequate description of bioavailability in exposure assessment models. Based on a critical evaluation of these approaches and the outcome of SITE-2 in which a number of these methods will be tested in experimental and field studies, parameters and model-formulations will be derived for inclusion in the prototype model. During the first 18 month period of the project, parameters estimates will be based on literature-derived relationships and data on main characteristics of sediments and overlying water (from BASIN and SITE-1 and 2). A database of factors, affecting bioavailability and distribution constants (Kd, Koc, Kdoc) in relation to compound characteristics and environmental conditions will be constructed and maintained. In the second phase of the project results from in-situ measurements and laboratory studies (executed in SITE-2) will be used for validation. The selection of compounds to be considered will be made in cooperation with other workpackages at an early stage in the project. In order to allow comparisons with results from related field or experimental studies we will include in the first 18 month period a limited set of standard priority compounds, such as selected PCB congeners (PCB 153) and some PAHs. In the second phase of the project, further selections of compound will be guided by the outcome of the TRIAD assessments in BASIN-2 and the effect directed approaches in KEYTOX-4. The bioaccumulation studies with oligochaetes and chironomids and the determination of residue concentrations in biota in the Scheldt, will provide an opportunity for calibration and validation. An analysis of the uncertainty of input-parameters and the effect on the model outcome will be executed in cooperation with the other workpackages and may include the application of Monte-Carlo simulations or other probabilistic methods.

Parameterization of food web accumulation

A critical review will be made of food web accumulation models reported in literature and internal dosage-based approaches in regulatory risk assessment frameworks. This will range from lower tier approaches, such as the application of simple experimental or predicted concentration factors (BCF, BAF, and biota/sediment accumulation factors (BSAF), as e.g. reported by Voutsas et al. (2002), Nendza et al. (1997), Traas et al. (2001), to more complex toxicokinetic and rate-constant bases approaches, which may include feeding behavior, lipid metabolism, food web dynamics. (Thomann et al., 1992; Hendriks 1995; Gobas and Morrison, 2000; Loizeau et al., 2001). As most of these models are location specific, special attention will be given to the possibilities to translate the basic concepts to a more generic modeling framework (Le Gall et al., 2003).

An inventory will be made of available databases and literature compilations of relevant toxicokinetic parameters (e.g. BCF, BAF, BSAF, rate constants for uptake, elimination, biotransformation) for different species and compound classes. Together with EFFECT-3 a joint database will be constructed and maintained. If available, specific data for the Elbe, Scheldt and Llobregat will be obtained from BASIN-1.

Based on input from BASIN, SITE 3-5, and EFFECT-1 on species and communities present, abundancies and other characteristics in the three catchments, a classification of dominant taxa, species guild structures, and food web relations will made in co-operation with EFFECT-3. Based on this analysis prototype generic food webs (freshwater, estuarine) will be constructed, that may be applied to all three catchments. The generic food web may include decomposers, primary production, benthic invertebrates, zooplankton, secondary producers, and as top predators a predatory fish and possibly a piscivoreous bird or mammal. The parameterization of biofilm-communities will be part of EFFECT-3.

During the first 18 months the focus will be on freshwater food webs, and on a limited selection of hydrophobic neutral compounds, such as e.g. PCBs for which biodegradation and biotransformation is expected to be low and for which monitoring data probably will be available from BASIN. As most food web modelling studies described in the literature have included PCBs, this facilitates a comparison with related studies. Estimates for biological and toxicokinetic parameters will be derived from the database, or in case of missing data, from extrapolations based on QSARs and/or scaling techniques (Hendriks et al., 2001; Kooiman, 2000).

In the second phase of the project the generic estuarine foodweb modules will be developed, which will in part be based on the classification of food webs in European waters by Le Gall et al. (2003), and supplemented with data from BASIN-1 and SITE 3-5. Formulations and parameterisations for biodegradation will be developed, based on a critical evaluation of current approaches. As for many compounds there is limited information on realistic degradation rates under field conditions, guidelines for the derivation of parameter estimates from experimental studies will be provided. Special attention will further be given to the possibility to include biotransformation in the food web model. For several PAHs experimental data on biotranformation rates are available for various invertebrate and fish species (Van Brummelen et al., 1998). Additionally, techniques for the analysis of metabolites of PAH metabolites are operational (Stroomberg et al.,2003) and will be applied for the Scheldt in SITE-2, which allows calibration and validation studies. At this stage there is limited experimental data for other compound classes to derive realistic parameter estimates for biotransformation rates under field conditions. The feasibility of approaches, such as e.g. proposed Van der Linde et al. (2001) will be investigated.

Based on the uncertainties of input-parameters a sensitivity analysis will be executed, using probabilistic methods. The optimised models wilt finally be applied to 1) a limited set of reference compounds for which validated analytical methods are available in SITE-2, 2) compounds identified in the TRIAD assessments in BASIN-2, and to 3) compounds assigned by KEYTOX-4. Depending on the availability of suitable methods of analysis in biota, the validation studies in SITE-2 will be extended to these compounds.

Strength of EXPO 3:

Compared to existing models, which to a large extent are based on simple equilibrium partitioning, the incorporation of new insights on bioavailability in a generic exposure assessment model is innovative, and expected to result in more realistic predictions for the field situation. Most food web models in literature are location specific and in many cases restricted to a limited set of classical priority compounds. The ambition to parameterize generic food webs, and to address biotransformation, will enhance the applicability of the model to other European catchments and a more broad spectrum of compounds. The fact that the work is embedded in and integrated with simultaneous field and experimental studies, allowing calibration and validation of model components and parameters, provides an unique opportunity for successful implementation.

Deliverables

Month 1-18

EXD 3.1 Review report on factors affecting bioavailability in aquatic systems and the current status of inclusion of bioavailability in exposure assessment and risk assessment models. Report will include evaluation of currently available rapid in-situ assessment methods (month 8)

EXD 3.2 Report with proposed parameterization and model formulations for sediment bioavailability, parameter estimates and uncertainties, to be used in the prototype model EXPO4 (month 18)

EXD 3.3 Report on current status of food chain transfer / biomagnification modelling and inclusion in regulatory risk assessment practices and potential for inclusion in the generic model (month 8)

EXD 3.4 Report on selection of food chain accumulation models, parameterization, and literature-based inventory of parameter estimates and uncertainties, to be used in the prototype model EXPO WP 3.4 and compatible with EFFECT and DECIS (month 18)

EXD 3.5 Joint database with EFFECT3 (month 8)

Month 19-60

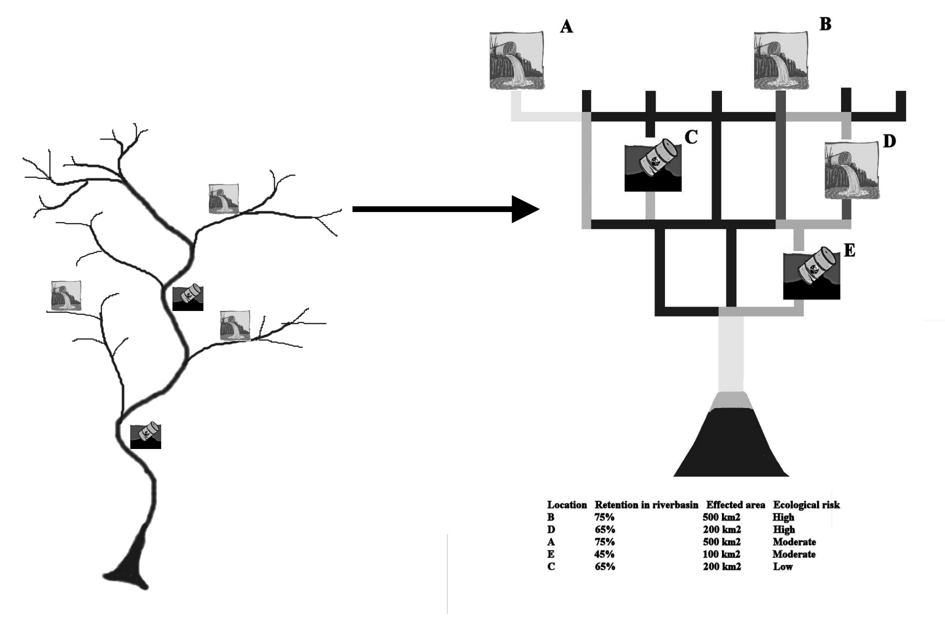
- Development of estuarine food web formulations
- Parameterisation of biodegradation and biotransformation
- Application to keypollutants identified by BASIN and KEYTOX
- Quantification of uncertainty in parameters, sensitivity analysis
- Validation of model
- Delivery of final formulations to EXPO-4

WP EXPO 4 (EX4): Generic exposure assessment model (DELFT, UoS, VUA)

Exposure assessment is an essential step in the risk assessment procedure. For contaminants bound to sediment, proper description chance of erosion at contaminated sites is essential. Once transported by water, a proper description of transport, sedimentation, mixing and other processes determine the accuracy of the predicted exposure concentrations and effected areas. Finally, the actual bio-availability and foodweb uptake determine the potential environmental impact. These three aspects are covered in detail in EXPO work packages 1-3. Work package EXPO 4 integrates existing knowledge and parameterizations obtained from work package 1-3 into a generic exposure assessment model.

Currently existing exposure models fall into two categories: detailed specific 2D/3D models (or model applications) like Sobek, Delft3D, Great-er, etc., and generic 1-box type models such as SimpleBox, Euses, etc.. The first category of models is spatially resolved but very "data-hungry", they require an enormous amounts of input data and often a detailed knowledge of the hydrology. The second category requires less data, but lacks the spatial resolution which leads to large uncertainty and safety ranges, which make proper inter-comparison of risks difficult. There are currently no tools available which integrate the aquatic environments from river basin, to estuary, to coastal zone with respect to spatially resolved exposure assessment in a simplified manner.

We will develop a generic, easy-to-use, exposure assessment model, based on parameterizations from existing detailed models and knowledge gained from specific field and laboratory experiments. Mathematical routines will be developed to derive a spatially resolved schematization of a river network including river basin, estuary and coastal zone using GIS oriented maps. Based on digital elevation maps (DEM) and digital topographic base maps, the path of the river will be structured in nodes and junctions to be compiled in a simplified schematic river network with a structured stream order. This "Candelabrum" shaped river network will be linked with a "Trumpet" shaped estuary (see an example in figure B4.9, WL, 2003b).



Location	Retention in riverbasin	Effected area	Ecological risk
B	75%	500 km2	High
D	65%	200 km2	High
A	75%	500 km2	Moderate
E	45%	100 km2	Moderate
C	65%	200 km2	Low

Fig B4.9 Automated conversion of GIS based river basin into a "candelabrum" shaped river network linked with a"trumpet" shaped estuary

Default values for environmental conditions and parameters will be derived from EXPO 1,2 and 3 and classified into databases. This results in a model that can be run with very limited data input from the user, while it will still give a spatially resolved exposure risk assessment. The model can be fine-tuned to specific conditions by changing the default values. In Figure B4.10 the various categories of data information is schematically outlined. The model will be able to visualise the risk of remobilisation of contaminant sediments and the distribution and contribution of contaminants throughout the river basin originated from various polluted sources (e.g. hot-spots and point sources). At the end this generic exposure assessment model might be used:

1. To assist local and regional authorities with an easy-to-use generic tool to provide insight in the behaviour of contaminated sites and to aid in prioritisation of clean-up strategies;
2. To assist in development and optimise future monitoring strategies for ungauged catchments in European river basins including the estuaries;
3. To provide information and guidelines to set-up and apply detailed modelling of contaminants in river basins.

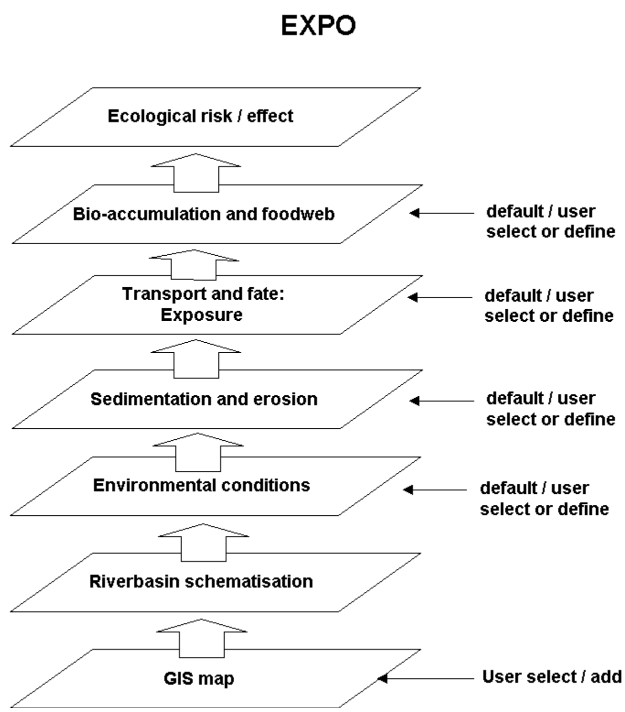


Figure B4.10 Overview of required information categories for the generic exposure model

The results of this model will be used in EFFECT to assess the impact on a population scale and in DECIS for further risk and economic assessment. Furthermore, the generic model will be applied for the Llobregat basin and tested against the detailed model results of Scheldt and river Elbe.

Strength of EXPO 4:

There are currently no risk assessment tools available that combine the ease of use of box-models with the spatial resolution of detailed 2D/3D models. In addition there are no tools available that link the upper river network to a estuary and adjacent marine coastal zone as proposed in this work package. The parameterization of the most important processes that determine exposure in aquatic environments, combined with GIS based automated network schematization, will enable spatially resolved exposure assessment without huge requirements on data input and user knowledge. With the final deliverable of this work package (a computer model), it will be possible to assess and compare the risk to the environment of each source or contaminated site in every European river basin/estuary/coastal zone with minimal requirements for model steering and use.

Deliverables

Month 1-18

EXD4.1: Specifications user requirements (month 8)
EXD4.2: Input data requirements (month 8)
EXD4.3: Output data requirements (month 8)
EXD4.4: Conceptual design of generic exposure model, including the procedures to obtain "candelabrum" and "trumpet" shaped river/estuary network from GIS maps (month 18)
EXD4.5: Classifications riverbasins/estuaries (month 18)
EXD4.6: Incorporation of transport and fate parameters from Expo 1,2,3 into design (month 18)
EXD4.7: Proposed default set for parameters. (month 18)
EXD4.8: Prototype of user interface of the generic exposure model (month 18)
EXD4.9: Modellers meetings (month 10, 18)

Month 19-60

- Stand alone computer model to assess exposure in aquatic environments (river basins/estuaries/coastal zones), applicable to European environments with minimal data requirement.
- Verification of the generic model against the detailed model results of the Scheldt and Elbe
- Application of the generic exposure model to the Llobregat basin
- Incorporation of the model in DECIS

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SP EFFECT: Modelling effects of toxic substances (CNRS)

Detailed description of each work component, partners involved in the component and contribution of each to the project as a whole

Sub-project EFFECT deals with the development of innovative models to diagnose, predict and mechanistically simulate the ecological effects of exposure to toxic substances on community composition and food chain propagation. EFFECT components consist of three work packages in a hierarchical structure. Work package EFFECT 1 (Integrated diagnosis of observed effects) aims to attribute the observed effects on species composition to the underlying causes in a multiple stressed environment, among which the combined risk of ecotoxic exposure. Work package EFFECT 2 (Predictive model development) will lead to the construction of models that reliably can predict the effects of toxic exposure on single species population and the community as a whole. Work package EFFECT 3 (Mechanistic modelling of toxic effects propagated through a simplified food chain) provides insight in the toxification mechanisms related to energy requirements that are underlying indirect effects. Modelling within a theoretical framework will be integrated with theory-driven experimentation to reveal the mechanisms and test them for realism.

Work packages 1-3

Modelling effects of toxic substances - Introduction and five-year overview

WP EFFECT 1

Participant	VUA	CNRS	RIVM
Person Months	3	5	15

WP EFFECT 2

Participant	VUA	CNRS	RIVM
Person Months	3	91	5

WP EFFECT 3

Participant	VUA	CNRS	RIVM	UFZ	ECT
Person Months	82	3	30	3	54

Introduction

The purposes of impact assessment are to evaluate whether or not a stress has changed the environment, to determine which components are adversely affected, and to estimate the magnitude of the effects. Thus toxic substance models are most often biogeochemical models, attempting to describe the mass flows of the toxic substances considered. Evaluating change in environmental conditions is often difficult, due to several factors. It is often not clear which environmental component will be affected by the stressor, what type of change will occur and what the exposure will be. Choices must be made about where and when the potential effect will occur (i.e. define the spatial and temporal extent), what organisms will be affected (fish, macroinvertebrates, diatoms, etc.), what the exposure will be (magnitude, duration), what any mitigating factors could be (what affects distribution of exposure) and how these factors may alter exposure and effect. Detailed answers to these questions may require models of the processes taking place in the organisms, and a translation of the concentrations in various parts of the organisms into effects.

The sub-project EFFECT deals with probabilistic and deterministic effect models of toxic substances, both of empirical and mechanistic nature. It is innovative because for the first time a tool kit will be developed that allows the simulation of a broad range of hydrological, chemical, toxicological and biological conditions with a single integrated water quality evaluation system, also addressing uncertainties. EFFECT has the following specific objectives:

1. to develop a state-of-the-art modelling tool-kit to analyse, understand and link habitat suitability models with exposure and effect models for toxic compounds in freshwater and marine ecosystems;
2. to apply this modelling tool-kit to a range of catchments being studied in sub-project BASIN;
3. to investigate the process interactions that occur within these catchment systems and to investigate the interactions occurring between toxic substances and other habitat characteristics;
4. to utilise the models to assess the impacts of toxic substances in European water bodies and deliver scenario results to sub-project DECIS;
5. to use the modelling tool-kit together with the socio-economic tools being developed in DECIS to evaluate the impacts of socio-economic driven change; and
6. to investigate methods of mitigating human impacts on freshwater and marine ecosystems across Europe.

Ecotoxicological models are increasingly applied for environmental risk assessment of the emission of chemicals to the environment. They are classified into two major categories: fate models and effect models. The former focuses on concentration of a chemical in one or more environmental compartments, while the later translates a concentration or body burden in a biological compartment to an effect either on an organism, a population, a community, an ecosystem, a landscape or the entire ecosphere (Forbes and Forbes 1993; Jørgensen and Vollenweider 1990).

The usefulness of water quality simulation models for environmental management is explored with a focus on prediction uncertainty. Scientific uncertainty is present in all ecological simulation modeling and risk assessments. Uncertainty does not prevent management and decision making; rather, it provides a basis for selecting among alternative actions and for deciding if (and what) additional information (experimentation and/or observation) is needed (Morgan and Henrion 1990; Reckhow 1994). Uncertainty can be used in this way because the magnitude of the uncertainty provides a measure of value of information: the smaller the uncertainty, the more confident (and valuable) is the assessment. Not only does this hold for formal environmental assessments, but it also reflects our day-to-day reasoning and decision making. Perhaps the best example of this is the response to probabilistic forecasts of rain. Many of us adjust our outdoor plans on the basis of these probabilities. A forecast of "it will rain" or "it will not rain" is unsatisfactory; we like to know the odds and act according to our attitude toward risk. This same reasoning should apply to uncertainty in environmental assessment and decision making. However, for these and other advantages of uncertainty analysis to be realized, the analysis of uncertainty must be complete. That is, all scientific uncertainties in an ecological risk assessment or in pollutant transport and fate modeling must be estimated and included in the analysis. Failure to be complete can result in decisions that are not only far from optimal but are far from satisfactory in outcome. This issue is of immediate concern because some of the models proposed for ecological risk assessments are large mechanistic models which have yet to be subjected to thorough uncertainty analyses

The accurate characterization of the probable causes to observed biological effects allows managers to identify appropriate management action to restore or protect biological condition. Once stressors are identified and management actions to control them are in place, the effectiveness of the stressor identification (SI) process (as demonstrated by improved conditions) can be monitored using appropriate monitoring tools and designs. The most important tools to bring to the SI process are experience in multiple disciplines (especially ecology); careful, deliberate critical thinking; and a strong desire to find the cause of biological impairment.

The core of the SI process consists of five steps:

1. listing candidate causes of the impairment
2. eliminating alternatives
3. employing diagnostic and predictive protocols and models
4. comparing strength of evidence for causes not identified through elimination, diagnosis or prediction
5. identifying probable causes

Eliminating causes, diagnosing causes, and comparing strength of evidence require that the investigator analyze new and existing data to generate evidence for each candidate cause. This evidence is used to produce a causal characterization that identifies the stressors most likely to have caused the impairment. The process may be iterated if there is insufficient confidence in the causal characterization.

Data and process-based understanding derived in SITE, BASIN & KEYTOX form the main inputs to EFFECT (Fig. B4.11) and these will be supplemented by data from other data-rich sites needed to drive forward model application and development. The availability of data on nested river and marine systems across Europe, with independent gradients from pristine to highly perturbed, is a key requirement for the development of these models. The nested river-marine approach together with the experimental data provided by sub-project SITE enables both the diagnostic and the predictive models to be rigorously tested and verified. EFFECT will be the primary tool for delivering scenario results that will serve as the main input to the development of the suite of management, assessment and training tools in DECIS.

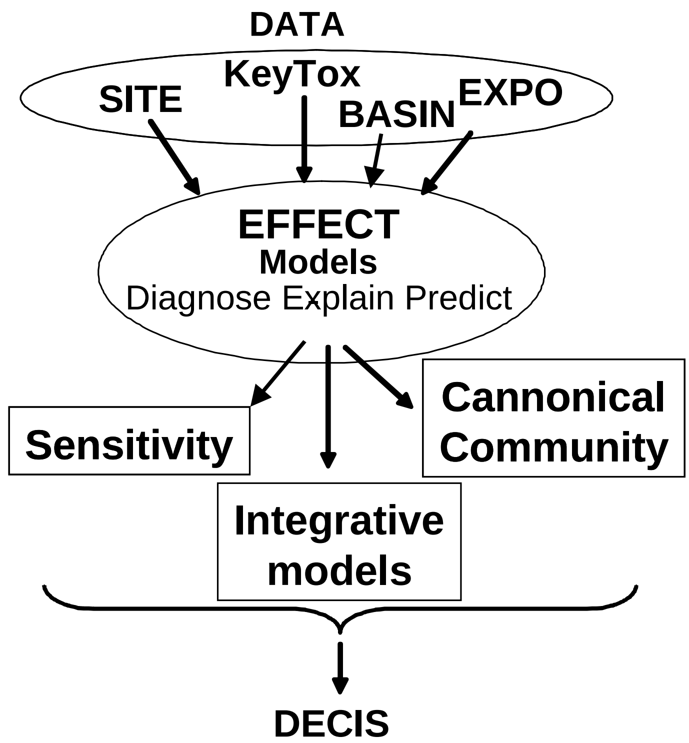

Fig. B4.11 Interactions and links between EFFECT and other SPs

The overall study procedures of EFFECT in the MODELKEY can be defined as a combination of following steps:

1. Focusing on the interpretation of collected data. Several types of data are required for ecological risk assessment and risk diagnosis: sensus data on local community composition, autoecological properties of end-point species (e.g., sensitivity profiles), ecotoxicological information (e.g., bioaccumulation factors and toxicity reference values), and information describing the spatial and temporal variability of environmental factors in the river and estuarine (e.g., topography, geological features, soil types, vegetation, point data on pollution as well as habitat degradation) (EFFECT 1 & 2).
2. Quantifying the spatial variability of pollutants by overlaying in GIS appropriate topographic and community maps and the application of state-of-the-art knowledge on focal species, resulting in the definition of homogeneous habitat patches and pollution concentration maps (EFFECT 1&2).
3. Giving an explicit statement of assessment endpoints and associated functions or qualities that have to be maintained or protected. This step results in the definition of a conceptual model in the form of a food web that identifies the endpoint species, exposure routes, and sources (EFFECT 3).

4. Using GIS to include spatial and temporal components of the exposed organisms of the food web (EFFECT 3). In their search for food, animals move through the heterogeneous contaminated area and are exposed to different levels of contamination. Currently, a simple home range model is used to model this behaviour but also more complex models are available that take into account species interaction and prey density. This step results in a set of area-weighted contamination concentration distributions for different foraging ranges in the evaluated areas that are used as input for the exposure model (EFFECT 2).
5. Giving an estimate of the exposure for the different components of the food web in the community. A probabilistic model calculates the exposure using the area-weighted concentrations in homogeneous habitat patches and species-specific regression coefficients for bioconcentration and accumulation of pollutants. The input parameters for the model are defined as probability distribution functions. Through the application of the Monte Carlo simulation technique and Artificial Neural Networks, the model takes into account pollutant variability within each homogeneous habitat patch. This step results in a geo-referenced set of predicted exposure concentration distributions that can be presented in river and estuary areas (EFFECT 2).
6. Evaluating the results of the ecological risk assessment. The site-specific risk maps will be used to identify potential high-risk areas in the current situation, while also risks for alternative management scenarios can be presented. Comparison of the resulting maps allows the river manager to choose the most efficient river management alternative.

The planned procedures illustrate the use of spatial modelling in the risk analysis of contaminated ecosystems. Site-specific risk maps allow the delineation of the high-risk areas and based on this information managers can make decisions that take into account both sanitation costs and environmental benefit. The modular structure of the presented procedure is an important advantage. It allows easy integration of advanced knowledge through the inclusion of state-of-the-art models, while specific needs of managers also can be taken into account. Research will focus on the integration of spatial models on habitat use and foraging behaviour of endpoint species, while also risks for future planning scenarios will be evaluated. In addition, the probabilistic treatment of the model parameters, coupled with sensitivity analyses, should provide the basic parameters that are important for making sound environmental decisions.

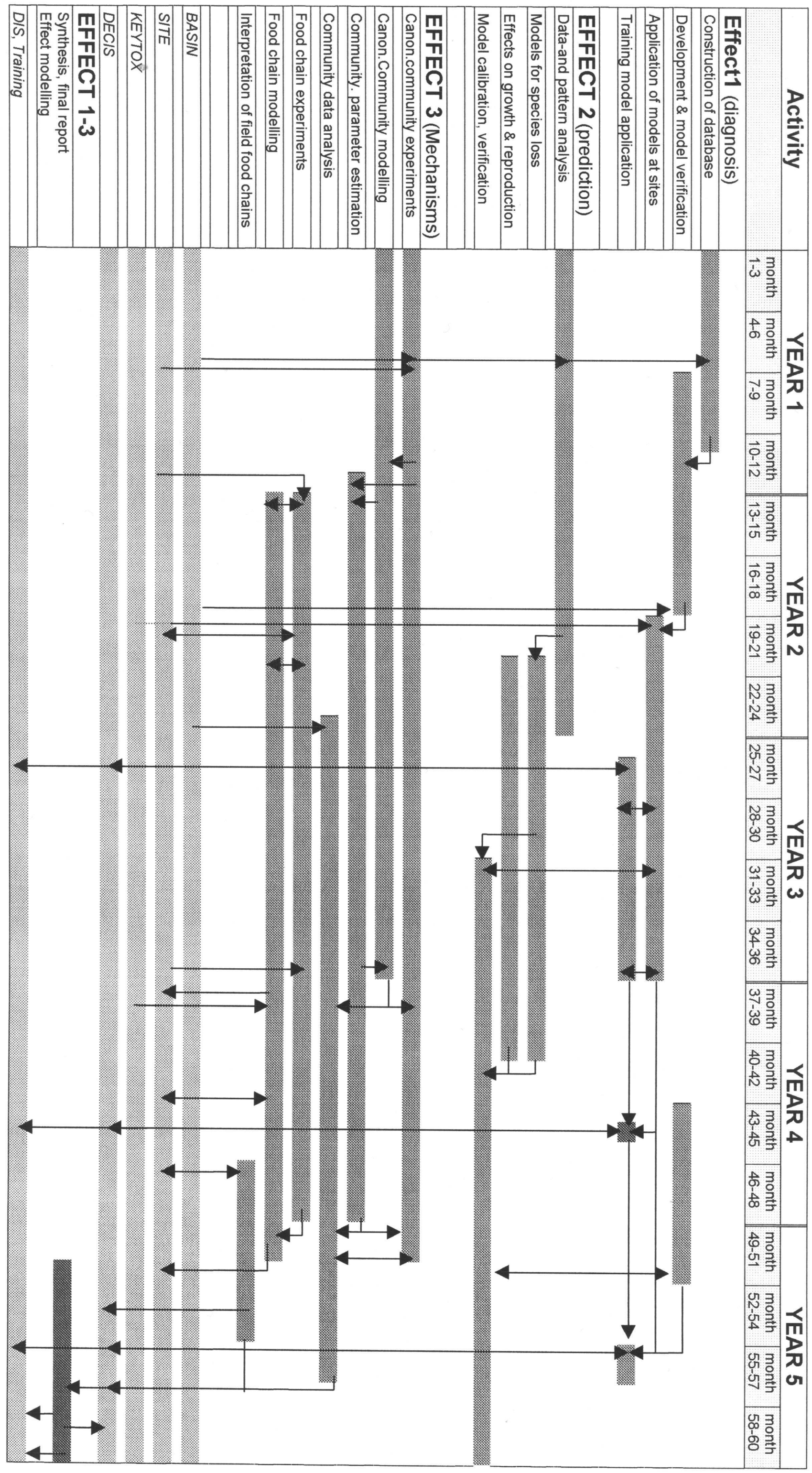

Fig. B4.12 The temporal sequence of the tasks in EFFECT.

***State-of-the-art of used models*:**
Sub-project EFFECT uses a combination of state-of-the-art water quality models to integrate site data with current scientific understanding of the physical, chemical and biological processes governing the fate and effect of pollutants in the environment. These models are used to assess contaminant sources, design management plans, estimate exposure for risk analysis, and evaluate the potential impacts of various remedial strategies on receiving water quality. According to the high complexity of relationship between pollutants and biota in the environment, several modern modelling techniques as well as advanced statistical and spatial presentation techniques will be used separately, sequentially and/or linked to each other, e.g. clustering and regression-tree analysis in combination with discriminant analysis (Hawkins and Carlisle 2001; Moss et al. 1987), generalized linear regression applications (McCullagh and Nelder 1989), artificial neural network models (Lek and Guegan 2000), dynamic energy budget models (Kooijman 2000), heuristic models (Downs and Ambrose 2001), GIS, etc.

The temporal sequence of the tasks in Expo temporal sequence of the tasks in Expo can be seen from Fig. B4.12.

WP EFFECT1 (EF1): Integrated diagnosis of observed effects on community patterns in a multiple stressed environment (RIVM, VU, CNRS).

Biotic integrity and declining biodiversity are not a stand-alone function of responses to toxic substances. Species diversity and abundance respond to a range of physico-chemical habitat characteristics (Baird and Burton 2001). The first problem in quantifying and attributing effects is to determine the deviation from species composition in a state of minimally disturbed condition. This requires the establishment of biological reference communities, either by expert judgement or ecological modelling. Then, the cause of the biotic integrity change can be pointed out on the basis of subsequent ecoepidemiological analyses, in which the change in species occurrence and/or density is explained with respect to the values of the local stress factors of various natures. To this end, models and meta-models linking prediction of reference state, exposure to toxic substances, effects in terms of loss of species and models to attribute the effects to underlying causes will be developed, optimised and validated. Modelling approaches to be used may include: bioavailability considerations, RIVPACS-type modelling (Barbour and Yoder 2000), species sensitivity distribution statistics (Posthuma et al. 2002), rules for mixture toxicity evaluation (Traas et al. 2002), regression techniques, classification techniques and regression trees.

A secondary objective of the work on WP EFFECT1 is the field verification of the community effects predicted by the application of a simple statistical model for estimating multi-substance toxic risk in terms of the potentially affected fraction of species. This model is based on site specific interpretation of species sensitivity distributions (SSD) for multiple toxicant exposure. When the SSDs are based on lethal concentrations, it is expected that the potentially affected fraction of species is corresponding to the loss of species richness that can be observed in the field.

The final outcome of this WP will be (1) a description of the input data and (2) a description of the models developed for estimating toxicity related effects on biodiversity, (3) a description of the model links constructed, and (4) elaboration of a limited number of case-studies for verification purposes. Once the models are constructed and validated, they most probably allow the execution of scenario studies: e.g. “What will happen to aquatic biodiverstity if we stop using the pesticides related to potato culture”?

This WP will provide the link between WPs in BASIN, KEYTOX, EXPO and SITE on the one hand, and WPs in DECIS on the other hand. The WPs of BASIN, KEYTOX and EXPO will largely provide the data needed for model development, whereas the present WP will provide the link between the different sub-models. The experimentation and gathering of additional data performed in the sub-project SITE will will provide the means for model verification. An overview of results, data gaps and recommendations for further testing will be provided as input for the other WPs. The results will be related to reference condition and targets. An assessment will be made of possible remediation strategies. The model outputs will provide data for input into the DSS to be constructed by DECIS, co-investigating the socio-economic consequences of toxins on ecosystem population and communities.

Data input from other SPs

Data from BASIN:
1. Species list and abundance of e.g. macroinvertebrates and/or fish
2. Physico-chemical habitat data, temporal and spatial associated with the biological inventory data
3. Expert judgement on reference conditions (included in monitoring programme)
4. Environmental concentrations of toxicants in rivers, temporal and spatial associated with the biological inventory data

Data from KEYTOX:
1. Identity of key toxicants
2. Information of intrinsic toxicity
3. Physico-chemical properties of toxicants

Data from EXPO:
1. Data on fate and bioavailability of key toxicants
2. Results of exposure modelling and bioavailability evaluation

Data from SITE:
In depth site-specific evaluation data that will be used in model verification

Strength of the WP EFFECT 1:
Epidemiological attribution of most probable causes to overall effects on biodiversity in the field is a new approach that ultimately will enable the development of management strategies for safeguarding of biotic integrity in the context of the EU

Water Framework Directive. Biological assessments should both estimate the condition of a biological resource (magnitude of alteration) and provide managers with a diagnosis of the potential causes of any observed impairment. Although methods of quantifying condition are well developed, identifying causes of impairment remains problematic in a situation with multiple stressors. Furthermore, analyses of both condition and cause have often been difficult to communicate to managers and policy makers because of the sophisticated multivariate statistical methods used and complicated output. We will use biological inventories, habitat, and chemistry data collected from streams and rivers to evaluate a method of linking assessment of biological condition with probable causes. We also will develop a way of presenting this information in a manner that should facilitate communication between researchers, managers, the public, and policy makers. Results will be mapped as simple pie-diagrams, with pie sizes corresponding to magnitude of impact, and slice sizes to the relative probable contributions of different stressors to the local impact.
The costs and complexity involved in assessment of toxic risk would reduce considerably if the loss of species attributable to toxic stress is consistently corresponding to the simple SSD prediction of community effects, only requiring the input of local toxicant concentrations and site specific quantification of sorption capacity as a regulator of bioavailability.

<u>Deliverables:</u>

Months 1-18

EFD1.1 Overview and interpretation of required data available and identification of data gaps in close collaboration with BASIN 1 (month 6)
EFD 1.2 Conversion of concentration data of individual toxicants to overall combined toxic risk also for the benefit of WP EFFECT 2 (month 12)
EFD 1.3 Construction of a site oriented MS Access database for model input data in collaboration with EFFECT 2 on the basis of the meta database from BASIN 1 (month 12)
EFD 1.4 Overview of existing modelling techniques and decision on modelling techniques to apply in the next stage of the WP (month 14)
EFD 1.5 Preprogramming of required models (months 18)

Months 19-36

EFD 1.6 Application of developed models to a limited number of well-documented case studies for validation purposes
EFD 1.7 Intercomparison of results with EFFECT 2
EFD 1.8 Preparation of courses on model application
EFD 1.9 Conversion of model results to DSS input data

Months 37-60

EFD 1.10 Model verification by comparison with SITE derived data
EFD 1.11 Execution of two courses in model application
EFD 1.12 Preparation of final report

WP EFFECT2 (EF2): Development of a component model, predicting effects of exposure to single and combined toxicants on species success and community composition (CNRS, VU, RIVM).

Modelling methods

A range of modelling approaches to simulate toxin dynamics and biota response (species sensitivity analysis), including classical statistics (CART, GAM, GLM …) as well as modern statistics like artificial neural networks (ANNs) (Lek and Gueguan 2000), will be used in this WP. These models were already successfully applied in the EU 5th FP (PAEQANN, EVK1-1999-00125, http://aquaeco.ups-tlse.fr, Lek et al. 2004) to predict aquatic ecosystem quality by using the biota community according to the changes of environmental factors. Two algorithms of ANNs will be used. Firstly, SOM (Self Organizing Map, Kohonen 1982) will be implemented to build models for patterning communities in ordination and classification of communities according to the effects of toxic substance. Secondly the MLP-BP (Multilayer Perceptron trained with backpropagation algorithm, Rumelhart et al. 1986) will be used to predict such population and community disturbed by anthropogenic impacts, especially toxic substances. ANN, the "black-box" type model, is power as predictive models to express the relationship between ecological response (i.e. biota) and chemical changes (i.e. environmental condition). However, by the use of the sensitivity analysis technique (Gevrey et al. 2003), it is possible to illuminate the cause-effect relationship between toxin and biota. A sophisticated second-order Monte Carlo will be used to project both natural temporal variability and measurement error, and expresses its results in risk-analytic outputs such as the risk of the population's declining to a given level.

Data input from other SPs

Data from BASIN and SITE temporally and spatially distributed:

- Species list and abundance of biota (periphytons, macroinvertebrates and fish)
- Environmental data including habitat data, physical, chemical (including toxin substances), associated with the biological inventory data
- Expert judgement on reference conditions (included in monitoring programme)

Data and information from KEYTOX

- Identification of key toxicants
- Information of intrinsic toxicity
- Physico-chemical properties of toxicants
- Environmental concentrations of toxicants in rivers, temporal and spatial associated with the biological inventory data

Data and information from EXPO

- Data on fate and bioavailability of key toxicants
- Results of exposure modelling and bioavailability evaluation for all organisms

Strength of EFFECT 2:

The component models developed in the previous EU projects (e.g. PAEQANN, TARGET) as well as project from USA and Canada (e.g. RAMAS Ecotoxicology & RAMAS Ecosystem) represent the state-of-the art in term of simulating of the effect of toxic substances. This WP argues for a complex modelling, multilevel conceptualization of ecotoxicology beyond the simple organism-level effects of toxin to the multi-species interaction in the community level. Such a concept embraces complex systems, ecotoxicology, ecoepidemiology, and ecosystem health and integrity. One way of thinking about the relative stability of ecosystems and their biological and non biological components is the conditional (Bayesian) probability of their coherent versus incoherent response to perturbation. Anthropogenic and natural stress may change the structure, function and/or organization of dissipative systems at any level, compromising self-regulation and making unstable incoherent responses of communities. Ecotoxicological researches argue for increased understanding of how ecotoxic agents or events may be disrupting self-regulating mechanisms at the organism, population, and/or community levels through their multilevel ecotoxico-dynamics (data from BASIN, SITE and EXPO). Stochastic population dynamic model will be constructed and simulated by developed models, using the dose-response parameters, survival rates and fecundity rate. Simulation results show the population-level risk of toxins on population in terms of abundance, quasi-extinction and apparent growth rate.

Bioassays for assessing the impact of toxins on natural systems are usually expressed in terms of individual-level assessment endpoints such as growth, survivorship and fecundity. Developed models translate such results into a forecast of their likely consequences at the level of the entire population. For instance, if there is an increase in mortality rate due to a contaminant, the meaning of this effect can only be determined by projecting the consequence in terms of the total population’s future abundance and vitality. It is generally important to do this projection to the population level because impacts at the organism level cannot be easily extrapolated to predict their population-level consequences. For instance, minor and inconspicuous impacts on individuals can sometimes cascade through population dynamics into significant effects at the level of the population. Conversely, seemingly major impacts on individuals may translate into only minor population-level consequences once the normal population feedbacks have been taken into account. Moreover, contradictory findings are possible at the level of the individual (e.g., decreased survival but increased fecundity) that must be resolved.

This WP will provide the link between WPs in BASIN, KEYTOX, EXPO and SITE on the one hand, and WPs in DECIS on the other hand. The WPs of BASIN, KEYTOX, EXPO and SITE will in part provide the data needed for model development, whereas the present WP will provide the link between the different sub-models. An overview of results, data gaps and recommendations for further testing will be provided as input for the other WPs. The results will be related to reference condition and targets. An assessment will be made of possible remediation strategies. The modelled outputs will provide data for input into the DSS to be constructed by DECIS, co-investigating the socio-economic consequences of toxins on ecosystem population and communities.

In parallel, and adaptive to new knowledge, interdisciplinary teams of scientists, policy makers, and other stakeholders (MODELKEY socio-economists) must collaborate effectively to mobilize and integrate human, material, and information resources to prevent and control existing priority deterministic stressors.

Deliverables

Month 1-18

EFD 2.1: MS Access database for the river basins Elbe, Scheldt & Llobrogat and corresponding dataset; (months 12) (task EF2.1)

EFD 2.2: Integrative datamatrix within GIS interface; (months 12) (task EF2.1)

EFD 2.3: Overview of modelling methods for component patterns of community; (months 12) (task EF2.3)

EFD 2.4: Patterns of community (ordination and clustering); (months 18) (task EF2.2)

EFD 2.5: Preliminary results on patterns of toxins and environmental factors vs community (with intercomparison to EFFECT 1 for diagnose); (months 18) (task EF2.2)

Month 19- 60

EFD 2.6: Component patterns of community relating to the environmental condition. The component models to be used in the integrated modelling tool-kit have been developed in the EU project (e.g. PAEQANN). Classical statistical tools and ANN including both algorithms (SOM & MLP-BP) will be used to pattern and predict community structure according to toxicants in environmental conditions.

EFD 2.7: Component models for understanding system function and prevent species lost: The effects of toxins on the richness and diversity will be established by the way of the Sensitivity analysis studies. Cause-effect models will be illuminated for each population and community.

EFD 2.8: Effect of toxins on species growth and reproduction: Results from SITE 3-5 will be used to model the effects of toxins on fish growth and reproduction. ANN and dynamic models can be applied to illustrate these effects.

EFD 2.9: **Models'** comparison and verification: Component models established for each of river basin will be cross-validated and tested. According to their patterning and predicting powers, these models will be tested used in other European area.

WP EFFECT3 (EF3): Mechanistic modelling of toxic effects in canonical communities and in simple food chains (VU, CNRS, RIVM, UFZ, ECT).

Introduction

The translation from observed effects in bioassays to predicted effects in the environment is vital to proper environmental management, while the theoretical/conceptual tools we have available are very limited indeed. This WP aims at contributing to the translation toolbox in two respects:
- the development of appropriate concepts to quantify effects in very simple theoretical communities; this knowledge will be helpful to recognize effects in the field, where feedbacks and species interactions complicate the recognition of small effects on integrated systems.
- the modelling of the flux of compounds through a realistic food chain, and the effects of these compounds; this knowledge will be helpful to interpret the field data that are colleted in the SITE WP's.

Within WP Effect 3 we have two related studies: the theoretical community and the more practical food chain study.

Community study

The purpose of this modelling study is to evaluate how effects in well-integrated ecosystems would show up. The study will deal with the problem how to translate toxic effects on individuals to that on ecosystems, including the compensating adaptations that will occur if one or more of the functional aspects of the ecosystem will be affected. To study these mechanisms in a systematic way, it is essential to simplify the ecosystem to an extend that is much simpler than the field situation. We will use a theoretical metaphor for this purpose: the canonical community; this is a theoretical community that consists of three groups of organisms (producers, consumers and decomposers) in a homogenous environment that is closed for mass, and open for energy (light comes in, and temperature is constant). The word canonical means "the simplest representative that still has all essential properties"; it is widely used in mathematics. Dynamic Energy Budget (DEB) theory will be used to structure the model and to quantify all rates (Kooijman, 2000, 2001; Kooijman et al., 2003). Much research is already invested in the theory of canonical communities (Kooijman & Nisbet, 2000; Kooijman et al., 2002), but the application to the evaluation of toxic effects will be new. The DEB theory relates effects of toxicants to internal concentrations via changes of appropriate parameter values; the time it takes for an organism to equilibrate its internal concentration of some compound with the environment increases with its body size.

Although the community study does not aim to mimic field situations, there is still a need for biological realism of the simplified system. Therefore we specify the species (although the DEB theory applies to all species), and select appropriate parameter values. Moreover we will try to understand the effects in the biofilms that are studied in SITE 2. To this end we will organize a close collaboration with ECT (Dr. Knacker, SME) and UFZ (Ms Dr. Schmidt, SITE 2) to link experimental and theoretical work, starting with a kick-off crash course in DEB theory in Amsterdam to ensure a sound theoretical foundation for experimental work, followed by working visits during the research.

The first choice of canonical communities is: nitrogen (as DIN, a frequently limiting nutrient), bacteria (as decomposers), alga (as producers), paramecium (a ciliate that consumes algae). After a analysis of the behaviour of this system in the blanc, an in response to toxic stress, we extend the system in two steps by introducing didinium (a ciliate that preys on paramecium), and/or a rotifer (Brachiones rubens, which competes with paramecium). These organisms are all of small body size, which allow to test model predictions at the ecosystem level in dynamic detail. It also means that the process of toxicokinetics is less important, because we can assume that the internal concentration is fast in equilibrium with the external one. This combination of species is well-studied in the literature (e.g. Holyoak, 2000; Doucet & Maly, 1990). We will extend the choice of species with dominant ones in biofilms and estimate the parameters on the basis of a series single-species toxicity tests that are generated in UFZ and ECT, judge the goodness of fit, and adjust modelling details where necessary, select the appropriate parameter values and compare computer simulations of the canonical communities with data from experimental communities. We aim at closed systems (with full nutrient recycling), but if these turn out to be experimentally too unstable, we will use chemostat setups.

We hope to find out in this study how integrated ecosystems will respond to toxic stress imposed by chemical compounds with a variety of modes of actions (such as an increase of maintenance requirements, or a reduction of growth rate, or of the nutrient/food uptake rate). In other words: we want to develop a search image for mild forms of toxic stress in ecosystems, that allows us to recognize such stress in real-world ecosystems. Functional aspects (i.e. nutrient recycling) depend on structural aspects (biomass amounts in the various trophic levels), but how mild toxic effects will show up in both aspects is presently not known. Complex feedback mechanisms in these integrated systems make application of a modelling framework essential.

Food chain study

The purpose of this study is to assist the interpretation of the food chain data generated in SITE 1, 3, 4 and 5, in the light of the qualitative results that come from the community study. We focus on a benthos-feeding fish as top predator, benthic macro-invertebrates, algae and bacteria. Since we here deal with organisms of larger body size, so toxico-dynamics is more important than in the canonical community study. The choice of the specific species and chemical compounds will be made consistent with choices in the SITE WP's. We will model the flux of compounds through the food chain in the framework of the DEB theory (Kooijman, 2000). This includes the incorporation of the various uptake and elimination routes for the compound, and how this is modified by the nutritional state of the organisms (lipid content; body size and lipid content tend to increase with food chain node); this effort will be linked to WP EXPO 3. We will intensively collaborate with setting up a shared data base for data from literature, field measurements and experimental data.

Our modelling effort has elements in common with EXPO 3, but here we will study dynamics aspects (changing population sizes, and species interactions). Moreover, toxic effects will be taken into account, that are based on internal concentrations. To this end, we will analyse a set of bioassay from ECT on toxico-kinetics and effects, using the Software package DEBtox (Kooijman & Bedaux, 1996) to extract the required parameter values. We still evaluate the goodness of fit, and adjust the model details if required. We will then use these parameters to interpret the data from the field, in the light of the results of the community study. In a later stage of the project we will try to link the biological effect module to the exposure module to be developed in EXPO 4.

One the basis of this study, we hope to be contribute to the interpretation of the field data, and evaluate the strength of the toxic stress.

Strength of the WP EFFECT 3:

- effects of toxicants on sublethal endpoints are weighed with respect to the overall effect on a (simple) community
- effect studied are fully integrated with biodegradation studies.
- effects are followed during exposure; this allows the evaluation of peak emissions versus dispersed continuous emissions

Deliverables

Month 1-18

EFD 3.1: Literature study on theory for and experiments with simple closed communities (8 months)

EFD 3.2: Standard Operational Procedure for the gnotobiotic aquatic microcosm (10 months) **EFD 3.3**: Standard Operational Procedure for specific effects testing with a benthic fish species under laboratory conditions (10 months)

EFD 3.4: Toxicity data for two or three key toxicants (selected by KEYTOX) derived from single species tests with organisms representing three trophic levels related to the theoretical concept of canonical communities. (18 months)

EFD 3.5: Collection of data for ecophysiology of relevant species and toxico-kinetics and effects of target toxicants; both from literature and from experiments at ECT (month 18

EFD 3.6: Joint database on relevant food chains with EFFECT3 (month 8)

EFD 3.7: Computer simulation of effects of toxicants with various modes of action in canonical communities (month 8)

EFD 3.8: Computer simulation of toxico-kinetics and effects in food chains, using parameter values of selected target organisms and toxicants in the SITE studies (month 12)

Month 19 - 36:

EFD 3.9 Parameter estimation via model application on experimental results of ECT and UFZ.

EFD 3.10 Model studies of extensions of canonical communities with (simple) food webs (predators), and competing producers.

EFD 3.11 Simulation of effects of target compounds in biofilm dynamics.

EFD 3.12 Creating theory that quantifies the effects of toxicants on the link between ecosystem structure (biomass distribution) and function (nutrient recycling).

EFD 3.13 Creating theory for effects of toxicants in food chain that is based on internal concentrations that can vary in time.

Month 37 - 60:

EFD 3.14 Linking a trimmed effect module to the exposure module developed in EXPO 4

EFD 3.15 Linking between theory and experimental and in situ data of SITE WP's.

EFD 3.16 Continuation of the systematic analysis of possible effects of toxicants in extensions of canonical communities. Comparison of results with dataand concepts in the literature.

EFD 3.17 Evaluation of our fundamental underdstanding of observed effects of toxicants on biologically integrated systems.

References

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SP SITE – Site assessment and model verification (UFZ)

The overall objectives of the sub-project SITE are: (i) to develop methodological and conceptual approaches to causal analysis of site-specific risks on biodiversity, including the assessment of the risk that contaminated sediments are eroded and remobilised, the analysis of bioavailability and biomagnification of toxicants and effect assessment of communities of different trophic levels, (ii) to develop a diagnostic toolbox for site assessment on communities, covering different trophic levels (iii) to provide early warning systems based on *in vitro* effects and biomarkers and link them to observable effects on the community level, and (iv) to provide a calibration and verification of effect and exposure models at a site scale. The sub-project is structured into five closely interlinked and interdependent work packages. SITE 1 assesses the remobilisation of contaminated sediments as determined by physical properties. SITE 2 will focus on the assessment of bioavailability, bioaccumulation and biomagnification of contaminants that determine the internal exposure of biota. Work packages SITE 3-5 will analyse effects on different trophic levels and different levels of biological organisation (from cell to community). SITE 3-5 will apply early warning systems on the basis of *in vitro* effects and *in situ* biomarkers and investigate links to functional and structural biodiversity in natural biofilms, composed of algae, fungi and bacteria (SITE 3), in macro- and meiozoobenthos (SITE 4) and in the fish community as the top predator of the food web (SITE 5).

Structure of subproject SITE, five years:

WP SITE1 sediment properties, erosion and sedimentation

Participant	UoS	CSIC	ACA	UA					
Personal month	22	10	0.6	10					

WP SITE2 bioavailability, bioaccumulation and biomagnification

Participant	VUA	UJOE	RIKZ	RIVO	UFZ	SZU	CSIC
Person Months	9	80	23	11	22	23	10
Participant	ACA	UdG	VRI	UA			
Person Months	0.6	2	4	6			

WP SITE3 effects on biofilm community

Participant	UFZ	UdG	UdB	DW					
Personal month	58	72	6	30					

WP SITE4 effects on macroinvertebrate community

Participant	UA	DW	UdB	RIKZ	UJOE	IVB			
Personal month	30	88	69	8	51	10			

WP SITE5 effects on fish community

Participant	UB	VRI	IVB	RIVO					
Personal month	50	20	38	17					

Introduction

It is one of Europe's strategic challenges for a sustainable management of aquatic ecosystems to minimise harmful impacts on biodiversity. One crucial driving force shaping the loss of biodiversity in aquatic ecosystems are toxicants, which induce disturbances across all trophic levels and levels of biological organisation. Thus, ecological risk assessments that allow a proper **diagnosis and prediction of adverse effects on aquatic ecosystems** have to address these different levels but also include a proper exposure assessment focusing on internal concentrations in biota in relation to surrounding environments. This is particularly important with respect to the fact that many key toxicants are associated to sediments and thus sediment remobilisation and bioavailability play an important role for environmental risk assessment.

Present impact and risk assessment procedures suffer the following short comings that will be addressed in SITE:

1) **Early warning concepts** are needed that indicate hazards to biodiversity well before species losses and functional changes in the communities get visible. *In vitro* assays, *in vivo* biomarkers and metabolic profiling as developed and applied by MODELKEY in the subprojects KEYTOX and SITE sensitively detect the exposure to hazardous compounds and indicate changes on a metabolic level long before the organism health is visibly affected. Thus, these tools are believed to be excellent early warning systems. However, to understand their predictive value for the impact of toxicants on ecosystem health and biodiversity a better understanding of the processes and effect chains that determine the risks to freshwater and marine communities is required. Work package SITE 3 and 5 are designed to link early warning systems to community health and biodiversity for the example of fish communities by a unique assembly of experts on *in vitro* tests (VRI, VUA, UB), *in vivo* biomarkers (UB) and fish population and community assessment (RIVO, UB, IVB).

2) A better understanding of **effect propagation** is required. Current risk assessment, based on single species toxicity data fails to predict effects on higher level of organisation, because current methodologies of effect translation from individuals to population and community level are limited (Altenburger & Schmitt-Jansen, 2003). This gap will be bridged by SITE by linking sublethal effects derived from molecular/cellular level investigations, using *in vitro* bioassays, *in vivo* biomarkers and metabolic profiling to effects on community level, by applying comprehensive approaches like pollution induced community tolerance (PICT) (SITE 3), *in situ* community structure analysis (SITE 3-5), *in vivo* biomarker application in fish tissue (SITE 5) and the use of higher tier test systems (micro-mesocosms).

3) An extensive assessment of effects on **biodiversity** focusing on **all key groups of aquatic organisms** including biofilms (bacteria, algae and fungi) (SITE3), macro- and meioinvertebrates (SITE4), and fish communities (SITE5) are very rare. The

complementary and outstanding taxonomic expertise assembled in the MODELKEY consortium together with innovative approaches of effect assessment on the community level such as the pollution induced community tolerance concept (PICT) make this extensive assessment of biodiversity effects possible. Effect assessment on all trophic levels and interlinked food chain experiments will help to understand indirect effects and interactions in aquatic food webs and are designed to verify food web effect models as provided in EFFECT3.

4) Modelling approaches are of increasing significance in environmental risk assessment. A decisive short coming in many modelling approaches is the missing link to the true situation in the ecosystem. Thus, MODELKEY closely interlinks modelling and experimental site assessment approaches. SITE is designed to **calibrate and verify exposure and field models** in real world situations. This will significantly enhance the value of both *in situ* impact assessment and exposure (EXPO), effect (EFFECT) and risk modelling (DECIS). SITE 1 will provide data for calibration and verification of erosion and sedimentation models (EXPO 1). SITE 2 will feed and verify food web models (EXPO 3). SITE 3 to 5 are designed to verify probabilistic and deterministic effect models (EFFECT 1 – 3).

5) Current state-of-the-art risk assessment is based on environmental concentrations as indication for the exposure of aquatic organisms. A better understanding of **bioavailability** particularly of sediment- and suspended matter-associated toxicants is crucial for proper risk assessment. Since many lipophilic toxicants as well as heavy metals are accumulated in aquatic food webs and pose a specific risk to higher trophic levels scientifically sound approaches for the prediction and analysis of **internal concentrations in biota** of different trophic levels and biomagnification are required. This problem will be addressed in MODELKEY with modelling (EXPO3) as well as with experimental (SITE 2) approaches, which are closely interlinked.

The overall objective of SITE is to improve methods and concepts for the assessment of toxicant action on communities and biodiversity. To study theses questions and to develop feasible approaches of ecological risk assessment, SITE will study selected contaminated field sites. Therefore, in the first phase of this project, a comprehensive diagnostic toolbox will be developed and evaluated, using site-specific contaminates of hotspots, analysed in previous investigations and identified by the activities of BASIN, and in a second phase of the project, the toolbox will be used, to assess effects of key toxicants, identified by the subproject KEYTOX. The site-specific data obtained from these field sites will feed into the more principal subprojects of MODELKY such as BASIN, EFECT and DECIS, and, at the same time will allow to verify their conclusions and predictions.
The novelty in the approach taken by SITE is a) to combine exposure with biological effects in a stepwise approach, i.e. by going from determinants of environmental exposure and exposure pathways over bioavailability and bioaccumulation to molecular, cellular and finally ecological effects at various trophic levels at the population and community levels; b) to integrate the broad taxonomic and ecotoxicological expertise being available within SITE with the expertise being available in other subprojects of MODELKEY on chemical-analytical, basin-oriented and modelling approaches to environmental risk assessment; c) to utilise the site-specific information generated in SITE to derive general principles to be transferred into strategic procedures on environmental risk assessment, as done in DECIS.

Research, technological development and innovation activities:

Current understanding of site-specific thresholds of key toxicants on ecosystem function and biodiversity has its limits because of the oversimplification of real ecosystems by current test-based approaches, not considering site-specific characteristics of affected ecosystems. To approach this problem, SITE goes clearly beyond the state-of-the-art by addressing following key innovative tasks :

(1) to provide diagnostic tools and early warning concepts, which are applicable to contaminated hotspots across Europe to assess impairments of the biological integrity of freshwater or marine sites
(2) to improve our understanding of principle rules and causal relationships, when extrapolating from simple to more complex systems under toxic pressure (effect propagation) considering a multi-species level, site specific ecosystem characteristics and bioavailability and
(3) to deliver data for input, parameterisation and validation of models, developed in EXPO and EFFECT.

The SP SITE is innovative, because for a first time it will provide a comprehensive approach for identification of toxic effects on communities in a multiple stressed environment. The overall implementation of SITE within the MODELKEY environment will ensure a close link of site – specific investigations to the basin scale (BASIN) and to effect assessment of basin relevant key toxicants (KEYTOX). The SP will support the overall goals of MODELKEY by establishing a scientific founded understanding of toxic impacts on biota and their biodiversity at contaminated sites and by validation of models, developed in EXPO and EFFECT. In co-operation with DECIS, SITE will provide a foundation for environmental risk assessment and management and priorisation of monitoring programs.

Specific objectives of SITE

- to closely interlink exposure of sediment- and suspended-matter associated toxicants to effects on exposed ecosystems, site – specific communities and biodiversity, considering sediment properties and internal doses in biota
- To provide a state-of-the-art diagnostic toolbox and early warning concepts for site-specific hazard assessment
- To improve our current understanding of causal relationships of effects of key toxicants on aquatic communities and biodiversity
- To identify essential indirect effects of key toxicants considering effect propagation and food web analysis
- To verify the general principles predicted by the modelling work of EXPO and EFFECT for real world conditions

Temporal sequence

For the temporal sequence of the tasks of SITE see Fig. B4.13.

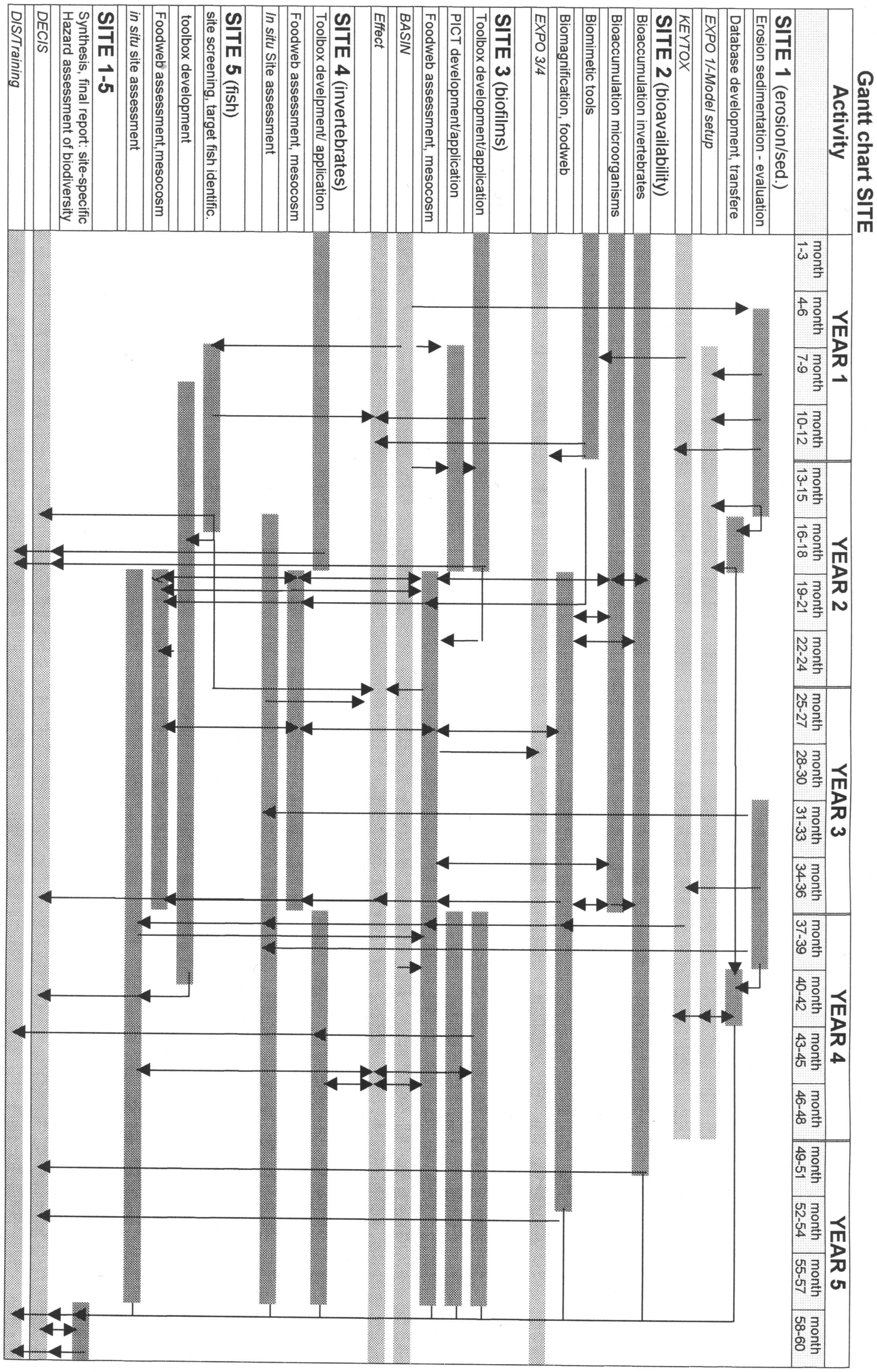

Fig. 4.13 Temporal sequence of the tasks of SITE.

SITE 1 (S1): Sediment properties, erosion and sedimentation (UoS, CSIC, ACA, UA)

Introduction

Contaminated sediments with particle size less than 20 micrometer show high sorption capacity reflected by the partitioning coefficient k_d. Those fine particles exhibit high sediment specific interparticle bounding forces which are enhanced by natural consolidation and influenced by diagenetic processes, ambient water chemistry and sediment biology**.** Older sediment deposits in the river Elbe and its tributaries Bilina, Mulde and Saale, as well as in the river Scheldt and Llobregat are known as highly contaminated hotspots which must be considered a severe latent hazard for the river ecosystem because of their high toxic potential. As for the contaminated sediment remobilization risk the sediment stability is the key issue because the hydrodynamic erosion triggers and controls the contaminant mass flux from the hotspots and therefore, directly effects the exposure conditions and the following chemical and biological processes in the water body. Despite of several research activities on sediment stability we have no understanding which physical, chemical and biological parameters are relevant and to what extent do they influence the sediment stability (Gerbersdorf et. al., 2004). The evaluation and comparison of experimental data on cohesive sediment erosion show that there is no conclusive correlation possible between sediment properties and hydrodynamic shear force. The very complex and unknown interaction of physical, chemical and biological factors does not allow a quantitative description of sediment erosion processes. Since there is no constitutive relationship or statistical correlation available for sediment erosion stability prediction experimental field investigation must be performed.

Beside the physical sediment properties the contamination level is subject to a great variability both in space and time which has to be taken into account when modelling and predicting the environmental impact of particulate contaminants in fluvial systems.

For erosion and sedimentation modelling many hydrological, morphological and sediment data of the river basin are required. Although there have been data collected in the past, that will be analyzed in BASIN 1 and EXPO1, one of the major tasks of the work package SITE 1 will be to identify and deliver specific data missing for modelling. Therefore, specific and targeted field measurements and experiments by application of new innovative techniques (Witt & Westrich, 2003) will be performed focusing on: sediment erosion stability, sedimentation rates, particulate contamination and contaminant load to fill the gap in the data list. In addition, monitoring is required at selected sites to observe future developments and to gain actual data for assessing the sediment erosion stability and establishing appropriate parameterized erosion and sedimentation terms as a function of the local sediment key parameters and hydraulic conditions. To provide the input data for a 1-dimention (COSMOS) or 2-dimention (SUB 2) numerical transport model field and laboratory measurements must be conducted. As not enough data are available neither for a geostatistical evaluation nor an accurate extra- or interpolation the contaminated sediment bodies must be explored in three dimensions (surface and depth) to get a complete picture of the hotspots which is necessary for modelling the total mass of contaminants resuspended by an erosive event.

The knowledge of the particle-size specific pollution and the sorption process caused by the interaction between the dissolved and particulate phase of micropllutants is necessary for determining the transport, fate, bioavailability and toxicity of such substances in river ecosystems. Thus SITE 1 will provide important information to the other SITE work packages. It is also of importance for assessing the actual situation and the future development of aquatic environments and for planning protection or remediation activities. The field-flow fractionation (FFF) techniques as a new analysis technique will provide size fractionated particle loads.

Sampling site selection

Elbe, Llobregat: As the river morphology strongly varies in space and time sediment and flow data must be taken from selected sites with hotspots which are representative for the main river basin and the tributaries, respectively. The investigation sites are chosen with regard to the local flow pattern (groyne fields in the Elbe, headwaters in the Llobregat), lateral mixing processes and contaminant inflow from municipal or industrial waste water systems (Llobregat) or tributaries like Bilina, Saale, Mulde and Spittelwasser which are the main pollution sources for the river Elbe.

Sedimentation rates will be investigated in the middle course of the Elbe river where large sediment depots with high pollution are known at different water levels. At the same sites sediment erosion stability tests will be performed, in particular after an erosive flood event has occurred.

Main investigations in the Elbe river groyne fields is near Steckby , Tangermünde and Lauenburg. Investigations will be performed in close co-peration with the European integrated project “Aqua Terra” (partners at UFZ).

Scheldt: One of the tributaries of the river Scheldt is the Grote Nete, which is very polluted with heavy metals, e.g. Zn and Cd, high chloride concentrations (CaCl) and inputs from the waste water of Tessenderlo Chemie. Several stations of water quality in the Nete basin are measured by the ecosystem management research group. In addition, on 6 sample sites sediment quality and fish stock assessments were carried out 5 years ago. The ecotoxicology studies showed only a minor acute impact on the benthic life community upstream the Grote Laak and an acute impact on the life communities in the Grote Laak. Downstream the Grote Laak no acute effects were measured possibly because of the lower bioavailability of toxicants.

Sampling and analysis methods

Undisturbed sediments samples will be taken in selected sedimentation zones, using core samplers and box samplers. The objective is to analyse physical sediment properties such as grain size spectrum (FFF- method), water and gas content (non intrusive high frequency capacity measurement method), TOC and bulk density (γ-ray), to specify the depth profile of critical erosion shear stress. In addition the erosion rate will be determined through laboratory experiments by the SETEG system

(Westrich et.al. 2001) and through the recently developed mobile in-situ erosion stability testing facility EROMOB. A further objective is to provide actual sediment samples from hotspots for chemical and eventually biological laboratory analysis which will be conducted by KEYTOX. In all three basins an further sediment stability testing method named Cohesive Strength Meter (CSM) will be applied and used for intercomparison (de Deckere et al., 2001), to correlate the sediment stability with the macrobenthos density which is a link to SITE 4.
Sedimentation rate measurements are conducted by a new developed sediment. Suspended particle matter concentration, particle size distribution and fall velocity spectrum will be measured by scooped samples in cross sections), to get model input data, if those are not available in BASIN 1 or EXPO 1. Bathymetric records must be taken in sedimentation zones to work out a sediment mass budget.

The field-flow fractionation (FFF) techniques at the UFZ provide new possibilities for the characterisation and reproducible separation of colloidal solutions and particle suspensions (Giddings, 1993 ; Beckett & Hart, 1993). The FFF- technique which works with a cross flow of carrier liquid is one of the most powerful sub-techniques (Gimbert et.al.,2003). It is usefully for separating particles of very different sizes (from about hundred microns to the submicron rage). A still existing problem is that FFF can only process very small quantities of sample (of the different fractions) and thus extremely sensitive analytical methods are required to detect the particle-size specific load of pollutants and to investigate sorption phenomena. For heavy metals such detection methods are available with the inductively coupled plasma - mass spectrometry, ICP-MS, (Taylor et al., 1992). With organic micro-pollutants it is necessary to combine FFF with another separation technique which allows to generate larger volumes of suspensions of definite particle size ranges, e. g. a centrifuging cascade.

Strength of SITE 1:
The sediment stability testing facilities are a unique triple set developed by innovative experimental laboratory and field research. The instrumental facilities allow to measure not only the beginning of erosion (critical bed shear stress) but also the erosion rate for different sediment layers. The mobile testing equipment facilitates to simulate a local erosive event. The combination of laboratory and in situ experiments enables to upscale and transfer sediment erosion and sedimentation criteria to the nature which is an essential prerequisite for numerical modelling of natural processes. In addition, it facilitates to collect freshly eroded particles on site for sedimentological (grain size etc.), geochemical and/or biological analysis.

Deliverables

Month 1-18

SD 1.1 Completion of the BASIN 1 and EXPO 1 data set and providing actual data for input in the EXPO 2 model. (10 months) (task S1.1)
SD1.2 Supply of undisturbed sediment cores from hotspots for key toxicant identification in KEYTOX (12 month) (task S1.1)
SD 1.3 Intercomparison of field and laboratory techniques for contaminated sediment sampling and erosion stability measurements (CSM, SETEG, EROMOB) using data from Elbe, Scheldt, Llobregat) (15 months) (task S1.1, S1.2)

SD 1.4 Mapping of the SITE 1 results for a comprehensive assessment in EXPO and DECIS (18 months)

Month 19-36

SD 1.5 Supplying sediment samples for chemical and biological analysis in KEYTOX and macrobenthos analysis in SITE 4

Month 37-42

SD 1.6 Comprehensive presentation of all laboratory and field experimental data for input into the data base to be used by EXPO and EFFECT

SITE 2 (S2): Bioavailability, bioaccumulation, biomagnification in food webs (VUA, UJOE, RIKZ, RIVO, UFZ, SZU, CSIS, ACA, UdG, VRI, UA)

Introduction

In current exposure assessment frameworks in OECD countries, the exposure assessment for new and existing chemicals and derivation of sediment quality criteria (Stronkhorst, 2003), is based to a large extent on the equilibrium partitioning (EqP) method (Di Toro et al., 2000). As large uncertainties still exist on the factors that determine the sorption to sediments, on species-specific uptake pathways, toxicokinetics and biotransformation, EqP method often fails to predict sediment and water exposure concentrations, as well as bioaccumulation in biota (Belfroid and Sijm, 1996; Van Brummelen et al., 1998), and the potency for biomagnification in predatory species (Nenzda et al., 1997; Traas, 2004). This holds especially for polar neutral compounds and ionized organic compounds, such as e.g. surfactants, modern agrochemicals, or pharmaceuticals (Salloum et al.,2000; Tolls, 1998, 2001). Even for neutral hydrophobic compounds, it may result in overprediction of the bioavailability of e.g. sediment bound PAHs to invertebrates (Van Hattum et al., 1998; Kukkonen et al, 2003), or the underprediction of risks due to biomagnification of toxic PCBs in fish eating birds and mammal (Traas et al., 2001). In many ongoing international monitoring programmes, the focus is on total water and sediment concentration, that do not allow extrapolations to bioavailable fractions. It has been recognised by many authors, that such data often are unsuitable for risk assessment and validation of exposure models (Holt et al., 2000). For field assessments the application of novel biomimetic extraction methods as presented in KEYTOX and residue based approaches at different trophic levels have been recommended (Nenzda et al., 1997; Sijm and Hermens, 2002; EPA, 1998) as a more adequate approach for risk assessment.

The main objective of this workpackage is to deliver improved exposure estimates to be used for input, parameterisation, and validation of the exposure and effect models to be developed in EXPO-3 and EFFECT-3, and for input to the community-based assessments (SITE 3-5) and integrated assessments in DECIS and BASIN. Novel empirical methods will be applied, resulting in an improved handling of bioavailability, bioaccumulation, and food web transfer in the exposure and effect models compared to tradition approaches in exposure assessment. It is expected that this will contribute to a better understanding and prediction of effects of contaminants on ecosystems.

The proposed activities include field studies in the 3 catchments and supporting experimental studies that will address the main factors that determine the extent to which

exposure to contaminants in the water column and sediments may result in increased bodyresidues at different trophic levels. In the field studies, biomimetic methods (including those from KEYTOX-1) will be used to determine *in-situ* the freely dissolved water concentrations, required as input in the exposure (EXPO) and effect models (EFFECT) and the field studies on communities of microorganisms, algae and meiofauna in biofilms, macro-invertebrates, and fish in this subproject (SITE 3-5). Further field and laboratory studies will provide insight in the role of properties of sediments, suspended particulate matter, colloidal phases, and sorption behaviour on the bioavailability to infaunal invertebrates and microorganisms. The outcome will be directly used for an improved and innovative parameterization of bioavailability the exposure assessment model (EXPO-3). Confirmation of the suitability of the descriptors for bioavailability will be obtained from measurements of internal dosage levels at different trophic levels in food webs in the different catchments, and exposed biofilm communities from field and experimental studies (SITE-3; EFFECT-3). Validated methods for extraction of biological material and chemical analysis from the KEYTOX subproject will be applied. The internal dosage based approach is vital input for the effect oriented studies (EFFECT 1-3, SITE 3-5), and for calibration and validation studies with the food web model (EXPO-3).

The key contaminants to be studied will be selected based on an effect oriented approach and will depend on the outcome of the assessments made in the KEYTOX, BASIN, SITE 3-5, and DECIS subprojects. For the purpose of calibration and validation of the exposure and effect models (EXPO-3; EFFECT-3), and to allow comparisons between the three catchments, a limited number of classical priority compounds will be applied, for which monitoring data and parameter estimates in related models are expected to be available, such as e.g. PCBs, PAHs and chlorinated pesticides. The selection of target compounds for the first period will be addressed in the first 6 months of the project in cooperation with other subprojects. Based on the review of known hotspots in the basins and preliminary assignment of key toxicants delivered by KEYTOX-3 (month 6-18), and fish biomarker studies in SITE-5, further compounds of concern will be selected. The tiered approach described in KEYTOX based on prescreening with the sequence of bioassays, will result in further assignment of key pollutants in the second phase of the project. Further compound selections will be based on the model compounds used in the bioaccumulation studies, the laboratory effect studies in SITE 3 and 5 in order to allow field-lab comparisons.

The activities are organized in 4 main themes: (1) bioavailability, desorption and bioaccumulation studies in invertebrates; (2) bioavailability and bioaccumulation in microorganisms and biofilm communities; (3) *in-situ* exposure assessment with biomimetic tools; and (4) food web transfer and biomagnification.

Bioavailability, desorption and bioaccumulation studies in invertebrates

Desorption studies

The sorption/desorption behaviour of contaminants in sediments, suspended matter and colloidal phases from the Elbe, Llobregat and Scheldt, will be investigated in relation to sediment composition, characteristics of particulate and dissolved organic mater, and to compound properties, in order to provide calibrated kinetic parameter estimates for the exposure model (EXPO-3). Desorption rates largely determine the flux of contaminants off the carrier-matrix into the organism. Desorption rates will be determined for contaminants sorbed to different particulate and dissolved organic matter fractions. Relationships between contaminant desorption kinetic parameters and carrier-matrices (organic matter, decomposition) will be investigated.

Desorption will be studied using the Tenax extraction method (Cornelissen et al. 1997, Kukkonen et al. 2003). In the experimental phase sediment samples are spiked with 14C-labelled model compounds. Sediment pore waters will be also analyzed for DOM-contaminant interactions (K_{oc} will be measured) using POM as SPME. The ^{14}C-labelled compounds are analyzed using liquid scintillation counting. HPLC/GC and GC-MS analyses for field samples will determine relevant contaminants.

The overall kinetics of desorption will be measured by determining the size of each kinetic fraction, taking into account the polarity of the pollutants, the mineral characteristics and the polarity of organic matter. Environmental factors (e.g. pH, temperature, ionic strength) that would be responsible for the mobilization of desorption-resistant fractions and pK-sensitive compounds will also be studied.

Results of these studies will be compared with existing experimental information using deuteriated model compounds (Smedes and Bakker, 1997).

Bioaccumulation studies:

The objective of the bioaccumulation studies is to verify the impact of abiotic factors on bioaccumulation and toxic risks. The results will be used for calibration and validation of the food web model (EXPO-3), the effect models (Effect 1,2,3) and as input to the macro-invertebrate field studies (SITE-4) and grazing pressure studies with biofilms (SITE-3).

The bioavailability of sorbed contaminants is generally considered to be related to the desorption rates of different fractions of the sorbed contaminants. However, specific biological mechanisms may be responsible for uptake rates higher than desorption rates measured in the absence of organisms. The bioavailability of sorbed contaminants will be investigated in terms of relationships between abiotic desorption rates and biological uptake rates for species representative of the biota in contaminated environments.

Bioaccumulation studies will be conducted with *Daphnia magna* in pore water samples, with *Lumbriculus variegatus* in freshwater sediments (Akkanen & Kukkonen 2003, Leppänen & Kukkonen 2004) and with *Nereis virens*/bacteria in marine sediments. The tests will be designed either to obtain the toxicokinetic data (uptake and depuration rates) or just to obtain the concentration factors (BCF, BAF or BSAF) to compare samples. Both laboratory- (phase 1) and field- (phase 2) contaminated sediments will be used. In all exposures ^{14}C-labelled or deuteriated model compounds will be used to minimize the number of the organisms used and the size of the exposure chambers. Similarly the analytical work will be quick and a large number of samples can be processed. The organic material in the samples will be characterized by spectroscopic methods (DOM) or by elemental composition (sediment OM/TOC). Also some other non-routine methods will be applied. Tenax resin in comparison with Silicone rubber will be used to respectively extract the "total" and "equilibrium" bioavailable fractions from the experimental waters or sediments. Results from these extractions will be compared to the true bioavailability measured with *D. magna, Lumbriculus variegatus, Nereis virens*.

Bioavailability and bioaccumulation in microorganisms and biofilm communities
(1) Role of bacteria in bioavailability
Bacteria have been reported to be the major vehicle in mass transfer of hydrophobic compounds between sediment and macro-zoobenthos (Gunarsson et al, 1999). It is hypothesized that the bacterial mass transfer is more important than transfer by water. Thus the feeding behaviour of bioassay species (zoobenthos) rather than the sediment-water exchange determines the mass transfer flux parameters to be used in the exposure models. The role of bacterial contaminant transfer in relation to compound specific parameters (like K_{ow} and K_{oc}) and feeding behaviour of (test) organisms will be investigated as a focus point in the bioavailability studies. The outcome will be used in EXPO-3 and EFFECT-3.
(2) Bioavailability and bioaccumulation in biofilms
Development of analytical tools to study matrix related changes in bioavailability and bioaccumulation of pollutants in biofilms by applying radiotracer techniques (EFFECT-3). (to be completed by Mechteld in the final version)

In-situ exposure assessment with biomimetic tools
An array of biomimetic methods, all based on Solid Phase Extraction (SPME, SPMD, SPE), but using different bio mimetic materials (TENAX, POM, Silicon rubber), tested and validated in KEYTOX-1, will be applied in the Scheldt basin. These methods will generate various estimates of the freely dissolved water concentration, assumed to be available for uptake by organisms. The range of estimates will be related to compound properties, salinity, exposure method (water, sediment slurry) and time, and compared with various data of field-collected biota and actively exposed biota, *i.c.* blue Mussel (*Mytilus edulis*). The output in the form of the bioavailable water concentrations and exposure-equilibrium ratios will be used in EXPO 3-4, EFFECT 1-2, SITE 3-5.

Food web transfer and biomagnification
The bioaccumulation and food web transfer of contaminants will provide information on internal dosage levels for dose-response linkages in the effect and community-based workpackages (EFFECT 1-3; SITE 3-5, DECIS), for field-lab validation of the results (SITE-2), and for parameter estimation and validation of the exposure and effect models (EXPO-3; EFFECT-3). The design of the studies (locations, organisms) will be tailored to the information needs of the end-users within the project. All end-users are represented in the workpackage.

The marine food web study in the Scheldt estuary will be executed in the first 18 month period in relation, and designed in line with the biomimetic exposure and sediment desorption studies. Protocols for sampling, sample treatment, chemical analysis are already available from ongoing monitoring programmes (ICES, JMP) in which local partners participate. For quality assurance of the chemical analysis the reference materials developed in Keytox-2 will be used.
The freshwater food web studies will be executed in the 2nd and 3rd phase of the project. During the first phase the freshwater studies will be prepared, and the focus during this period will be on species selection, program design, harmonisation of protocols, and feasibility analysis. Classes of organisms to be considered are: algae, biofim-communities, zooplankton, benthic invertebrates, predatory fish, and possibly a bird species foraging on fish (e.g. Common Tern; *Sterna hirundo*) and macro zoobenthos (.e.g. Oystercatcher; *Haematopus ostralegus*). Lung-breathing species have a much higher potency for bioaccumulation than gill-breathers. The output of BASIN-1 (responsive sites, information gaps in database), KEYTOX-3 (inventory of known hotspots, preliminary assignment of keypollutants) during the first 18 month will target the selection of compounds in the freshwater studies. Additional targeted food web studies will be addressed in the 4th year in response to the final assignment of key pollutants in KEYTOX-3. An innovative element will be the study of biotransformation of PAHs at different trophic levels in close co-operation with the biomarker related fish studies in SITE-5. Both parent PAHs and an indicator metabolite (1OH- pyrene) will be measured (Stroomberg et al. 2003) in tissues of lower tropic levels, and in liver and bile of fish. The results will be used for the parameterisation of PAHs in the food web model (EXPO-3).

Strength of SITE 2:

Current exposure assessment models do not properly address the bioavailability of contaminants or the risks of food web transfer. In SITE-2 field- and supporting laboratory studies are conducted that will provide insight in the role of key-determinants of bioavailability and bioaccumulation. The outcome will be used for parameterisation in the exposure and effect models, and as optimised exposure estimate in other workpackages. It is expected that the improved handling of bioavailability and food web transfer in KEYTOX will contribute to a better understanding and prediction of effects of contaminants on ecosystems.

Deliverables

Month 1-18

SD2.1 Detailed characteristics of sediment samples form the three catchments (Task S2.1) (month 10) (UJOE)
SD2.2 Desorption rate constants of model contaminants for different organic fractions (Task S2.1) (month 18) (UJOE)

SD2.3 Data on the structural parameters governing desorption rates of model contaminants.
(Task S2.1) (month 18)(UJOE)
SD2.4 Report on rapidly and slowly desorbing fractions of contaminants in field sediments in the Scheldt estuary (Task S2.2) (month18) (RIKZ, VUA)
SD2.5 Data on uptake of contaminants sorbed to organic matter by benthic invertebrates. (Task S2.3) (month 18) (UJOE)
SD2.6 Progress report on development of methods to study bioavailability and bioacumulation in micro-organsisms (Tasks S2.4) (month 18) (RIKZ, UFZ)
SD2.7 Biologically available concentrations in the Scheldt determined with biomimetic methods (Task S2.5) (month 12) (RIKZ, RIVO)
SD2.8 Internal concentrations of key toxicants in laboratory test organism in connection with canonical community modelling (EFFECT 3) (month 18) (UFZ)
SD2.9 Workshop report describing the organisation, planning, and protocols for the freshwater food web studies. (Task S2.6) (month 14) (all, coordin. VUA)
SD2.10 Report on the results of marine food web study in the Scheldt (Task S2.6) (month 18) (RIVO, RIKZ, VUA)

Month 18-36

SD 2.11 Mass transfer parameters of a range of compounds from sediment – bacteria zoobenthos (month 30) (RIKZ)

SD 2.12 Report summarising the results of the freshwater food web studies) (m 36) (all)

SD 2.13 Biotransformation of PAHs in a simple food chain (m 36) (VRI, IVB, VUA, UFZ)

Month 36-60

SD 2.14 Desorption rate constants of contaminants present in the field sediments to different organic matter fractions (month 36) (UJOE)

SD 2.15 Data on the structural parameters governing desorption rates of contaminants (month 40) (UJOE)

SD 2.16 Data on the bioavailability of contaminants present in the field sediments by benthic invertebrates (month 42) (UJOE)

SD 2.17 Data on the influence of organic matter decomposition and pollutant aging on bioavailable contaminant fractions (45) (UJOE)

SD 2.18 Data on the influence of sorbate aging and organic matter degradation on contaminant desorption rates (month 50) (UJOE)

SD 2.19 Final report on food web studies of keycontaminants selected by effect directed approaches (month 52) (all)

WP Site 3 (S3): Pollution induced effects on biofilm communities (UFZ, UdG, UdB, DW)

Introduction

Biofilms, mainly composed of algae, bacteria and fungi, enbedded in a complex matrix of extracellular polymer substances (EPS), occupy the sediment-water interface, thus integrate information across different temporal and spatial scales. Short generation times, strong linkage to their habitat, high species richness and widespread distribution are the reasons for their sensitivity to stressors of ecological quality. Periphyton, recommended for monitoring in the WFD are the basic primary producers of benthic food chains, fixing the main energy in their environment, thus toxic impacts on this group are essential for effect propagation through the food chain. Activities of bacteria and fungi are the fundament of several biogeochemical processes occurring in the river, and therefore their affection may interfere in the general functioning of the ecological system (e.g. organic and inorganic nutrient cycling). Meiofauna may find refuge and food within the biofilm, and its action may strongly affect the separate responses of algae and bacteria through grazing and disturbance of the biofilm structure.
The excellent indicator value of biofilm compartments has been recognised for long and several indices have been developed, using community changes of biofilms to detect changes in water quality (e.g. saprobic and trophic indication, acidity or Al-concentrations, Hofmann, 1996, Dokulil, 2003). However the development of suitable tools, using biofilm compartments for toxicity assessment is still an outstanding challenge and will be addressed within this WP. The overall objective of SITE 3 is the development of a scientifically sound approach to assess hazards of site specific contaminants on biofilm communities. This will include a mechanistic understanding of toxic effects on a multispecies level, by linking causal analytical tools like the concept of pollution induced community tolerance and food web analysis to structural and functional changes in communities and losses of biodiversity. There are four major tasks in WP SITE 3:

(1) to develop a state-of-the-art **diagnostic toolbox** for effect assessment of site specific key toxicants by combining structural, functional and physiological parameters of biofilm communities

The aim of the first phase of the WP will be, to identify bio-sensors that indicate toxic impacts on community level, to improve the monitoring methodology of changes in biofilm communities under toxic pressure and their biodiversity by translating basic ecological understanding into methods of a diagnostic toolbox.

Within the project, biofilm communities will be assessed, grown under multiple contamination *in situ* on surfaces (natural and standardised substrata) and sediments (epipsammon, epipelon) as well as artificial biofilms from micro- and mesocosms established under controlled conditions, to link toxicant exposure to effects on community level.

Structural community parameters (abundance of species) and metabolic profiling (changes of biochemical composition e.g. pigment and fatty acid profiles), using state-of-the-art analytical tools (HPLC, GC-MS) will be used to detect pollution induced changes in patterns of biomolecules under toxic pressure. Analysis of functional parameters, e.g. primary production will be used to directly link changes in biofilms to fundamental ecosystem functions.

Special emphasis will be the assessment of pollution induced changes of the microenvironment within biofilms by detecting changes in assembly structure (e.g. induction of EPS production) and the development of microgradiants e.g. of pH or redox. Further, biofilm sensitivity is directly linked to the succession status and exposure history of a biofilm (Ivorra (2002), thus one goal of our investigation will be in close collaboration with SITE 2 the quantification of matrix related changes in bioavailability and bioaccumulation of pollutants in biofilms.

(2) to give a **causal analysis** of toxic effects in a quantifiable, concentration dependent way by applying the concept of pollution induced community tolerance (**PICT)** as a diagnostic tool *in situ* and a prognostic tool to assess impacts of toxicants on an integrated community level

One of the key challenges of site specific effect assessment is, to derive a direct link of toxic effects on *in situ* communities next to other disturbances (e.g. eutrophication, structural degradation) in a multiple stressed environment. In general, changes of community structure and function in the field are difficult to link to a single stressor (abiotic and biotic stress including chemical exposure) of an ecosystem. One of the most innovative approaches, giving this causal link of community changes to toxicant exposure is the concept of pollution induced community tolerance (PICT). This method, initially been reported by Blank et al. (1984) has become an important technique in predictive and retrospective risk assessment and covers the issue of causality better than any ‘classical’ ecological community responses like community structure or function (Boivin et al., 2002).

The basis of PICT is the general concept that communities increase their overall tolerance during long-term exposure to a toxicant. It is based on the assumption that sensitive species within a community will be replaced by more tolerant species under toxicant exposure by the mechanisms of competition, adaptation and selection of species, thus PICT is directly linked to biodiversity (Schmitt-Jansen & Altenburger, submitted). PICT can be quantified by acute toxicity tests e.g. the inhibition of photosynthesis in a concentration dependent way, e.g. in shifts of EC50 (Dahl & Blanck, 1996), thus short term metabolic tests give the confirmation of the cause of toxicity.

The scientific robustness of this method was demonstrated several times, however, to apply the PICT-approach to an ‘easy-to-use’ tool in site toxicity assessment of multiple contaminated ecosystems, a selection of metabolic short-term tests need to be available, covering several mode of actions of site specific toxicants. One of the major aims of SITE 3 will be, to fill this gap by developing a toolbox of metabolic test systems addressing sensitive metabolic endpoints of biofilm organisms.

(3) to analyse **effect propagation** and **food web** interactions, to derive a mechanistic understanding of indirect effects of impacts of key toxicants on biofilm communities

The majority of toxicological studies address responses of target organisms, e.g. effects of a herbicide on algae. However, indirect effects on non-target organisms interacting with target organisms, translating toxic effects across different trophic levels have less been studies.

One major goal of the WP SITE 3 in the multi-disciplinary environment of MODELKY will be, to assess sensitive relationships between different trophic levels of biofilm components during toxicant exposure. Grazing pressure of relevant meio- and macrozoobenthic species will be evaluated in close co-operation with SITE 4. Chironomids and molluscs will be used as model organisms, however a final selection of this species will be done according the results within BAISN and SITE 4. Artificial food chains will be established in micro- and mesocosm systems, in order to analyse effect propagation of toxicants in systems with increasing complexity. Results of food chain analysis will be interlinked to biomagnification results from SITE 2, by determinating internal concentrations of toxicants in biofilm compartments. This investigations will be a close link to food chain modelling in EFFECT 3 by detecting sensitive biofilm species, providing data of population dynamics for modelling and by using the same endpoints (reproduction, growth, feeding rates).

(4) to use the developed tools *in situ* for **site assessment** and **model validation**

The tools and conceptual approaches, developed within the project, will be applied and validated at hotspots, determined by the other sub-projects during the project (BASIN; KEYTOX). Aim of this part of the WP is, to link experimental results from biofilm communities and food chain analysis to field observations, to give a proof of impacts of key toxicants on communities under field conditions. A further goal is the proof of the general applicability of the toolbox and the validation of modelling results for site assessment.

Strength of SITE 3:

The determination of field effects of toxicants on a community level is still an outstanding challenge in environmental research. The integrated approach, used in this WP goes essentially beyond the current state-of-the-art-site and effect assessment tools, by linking structural and functional changes of biofilm communities with ecotoxicological approaches, providing causal relationships of toxicant exposure in multiple stressed ecosystems to effects on biodiversity. The design of the WP will ensure interlinked and field validated research results, tools and conceptional approaches, that have the potential to give a causal analysis of observed impairments of the biological and chemical status of aquatic environments, addressed in the WFD.

Deliverables

Month 1-18

SD 3.1 Overview over approaches for the verification of cause-effect relationships between exposure to key pollutants (selected by KEYTOX) and effects on biofilm communities including their biodiversity (6 months)

SD 3.2 Effect assessment of key-toxicants on the structure, biodiversity and functioning of the biofilm communities (16 months).

SD 3.3 Establishment of standardised testsystems to measure pollution induced community tolerance of biofilms (16 months)

SD 3.4 *In-situ* application of the toolbox, developed within the project to derive a causal analysis of community disturbance at selected hotspots (regional scale) (18 months)

Month 19-36

SD 3.5 Identification of relevant benthic food chains from the database of BASIN and in co-operation with WP SITE 4 and SITE 5
SD 3.6 Establishment of experimental food chains to evaluate the implications for algae, bacteria and meiofauna, in co-operation with WP SITE 4 and SITE 5
SD 3.7 Effect assessment of site specific contaminants on biofilm compartment interaction under experimental conditions.
SD 3.8 Validation of biofilm analysis by chemical analysis (WP SITE 2)

Month 36-60

SD 3.9 Field validation of the PICT – approach and of benthic food chain assessment at contaminated sites
SD 3.10 model validation of models from EFFECT
SD 3.11 guidelines for approaches of toxicological and ecological site assessment; final reports, publications

WP SITE 4 (S4): Effects on invertebrate communities (UA, DW, UdB, RIKZ, UJOE, IVB)

Introduction

Macroinvertebrates are commonly used for water and sediment quality assessment both in freshwaters and in marine systems. Macroinvertebrates are included as an obligatory part in the monitoring programs that are developed for the implementation of the Water Framework Directive. The advantage of benthic macroinvertebrates in biological assessments lie in their abundance, sedentary nature, suitable lifespans, diversity of phyla and trophic levels, sensitivity and swift response to various pressure types and the many sampling methods available (Metcalfe-Smith, 1994). The organism group comprises a high number of species, which dwell all sorts of habitats of a water ecosystem. Macroinvertebrates connects the higher trophic level represented by fish to the lower trophic level represented by microalgae and bacteria. The linkage is highly important in terms of assessing the effects of a pollution (and remediation of a water body) on the scale between short time reaction (effects on the microbenthos) and long time reaction (e.g. effects on fish) of the ecosystem. The high number of species distributed in several functional groups does not only allow a taxonomic specification of the site regarded. The species communities represent the functioning and the trophic and morphological character of the water considered. A relevant change of the habitat factors causes a change of the functional community (e.g. from a collector-dominated to a filterfeeder-dominated community). Therefore, the macroinvertebrates present themselves as promising indicators in a toolbox for pollution assessment following the project goals. Benthic communities in rivers and estuaries are exposed to a diffuse flux of sediment-bound toxicants. The effects of contaminants such as trace metals, PCBs and PAHs are reflected on the community structure, both diversity and abundance (and community function: changes in biomass, growth, reproduction etc.). Quantification of these effects seems difficult, but an estimate in the Netherlands showed an effect of 6 up to 15%, dependent on river branch (Van Griethuysen, in press).

The requirements for an assessment toolbox based on the *in-situ* benthic community are (1) a good reproducibility, (2) a clear discernment, (3) good practicability and (4) a low cost price. All this topics will be addressed in the toolbox development of SITE 4.
Several methodologies are developed for biological effect-based sediment quality assessment including special macroinvertebrate groups as Oligochaeta, Chironomidae, Bivalvia and Nematoda.

The interpretation of the macrobenthic community can be done using biotic indices and certain profiles of the communities (feeding type character, dwelling type etc.), based on water type-specific references from unpolluted sites. For instance, a specific index for the sediment was developed in Flanders, namely the Biotic Sediment Index (BSI). The BSI is tested and evaluated in a large survey of the Flemish watercourses. However, based on the 620 sampling locations the determination level of the different taxa to calculate the BSI was restricted (de Pauw & Heylen, 2001). Indices like the BSI are to be optimized and linked directly to certain groups of certain contamination compounds. A problem not to be underestimated is the invasion of exotic species such as the current invasion of neozoans upstream the River Elbe. This may mask clear effects of pollution on the community and may be evited by using taxonomic groups (e.g. chironomids or nematodes) which are not affected by this phenomenon, as far as known today.

The species list does not only provide for a taxonomic community, but also a functional community (shares of feeding types, dwelling types etc.). A significant change of the functional community indicate that the whole foodweb becomes another structure caused by a more or less heavy influence of a disturbance compound in the ecosystem. The change of the taxonomic community is not necessarily linked to a strong change in the ecosystem functioning, but may well serve as an early warning system. The lack or invasion of a species may indicate an subtoxic change of the functioning.

Within SITE 4 we will try to establish a link of this type of indices to a certain type of contamination as is done with the Oligochaete index. The oligochaete community is used for sediment quality assessment, e.g. in France. The Oligochaete Index of Sediment Bioindication (IOBS) is developed and combined with total density and percentage of Tubificidae without setae. Prelimnary results showed that the results obtained with this index can indicate the groups of contaminants which most likely causes toxic effects (Prygiel et al., 2000).
The assessment method based on mentum deformities of Chironomidae was also applied during this survey. This method is based on the percentage of deformities of the fourth larval stage of the Chironomidae and mirror the physical or chemical disturbance of the sediment (Heylen & de Pauw, 2001). The mentum deformities of Chironomidae are significant to heavy metals (Martinez et. al, 2001) as well as to endocrin-disrupting chemicals (Watts et. al, 2003). Sometimes, the number of larvae in the sediment is low, and other pressures then contamination might also cause mentum deformities (de Deckere et al., 2002). However mentum deformities of Chironomidae used in *in-situ* mesocoms are a valuable indication for contamination (Meregalli et al., 2000).
Beside the macrobenthic species, sediment assessment can also be based on the meiobenthic community, especially nematodes. Representatives of nematodes are found in all environments examined so far, whether they may be extreme (hot or anoxic), clear and polluted sediments. The group includes sensitive, stress-intolerant species. Thus, changes throughout a wide spectrum of stress conditions can be assessed (Haitzer et al., 1999). Communities of meiofauna are continuously exposed to harmful materials that enter their environment, due to their limited ability to escape. Therefore, the community structure is very closely related to the physicochemistry of the habitat sampled. Based on the life strategy of the nematodes the Maturity Index (MI) is calculated (Bongers, 1990), but shall be extended and further developed.

Beside biological effect assessment based on the condition of the benthic macroinvertebrate community additional tools can be used to link the effect of pollutants to macroinvertebrates.

Mesocosms and artificial substrates are frequently used in the field or in the laboratory in order to estimate the influence of several factors of habitat morphology on the community structure. Even for studying the different degrees of pollutant-specific impacts, it is important to elaborate that a shifting of a community structure refers only to a smaller part to natural biotic or abiotic settings, but a higher to the pollutant. Thus, several studies, applying this approaches improved the understanding of e.g. the effect of biofilms on the community (Kiel, 1996), of substrate size on diversity (Wise & Molles, 1979), and spatial and temporal variations of species (Essafi et al., 1992). Therefore, a variety of artificial substrates have been used in the past to address different goals leading to a broad overview of experiences, limits and chances of this method, whether it may be researched on bottom or other compartments of the benthic habitat (Freedeen & Spurr, 1978, Thorp, 1982). However, in this project, it will be a task to design, adapt or optimize an artificial substrate for studies focussing questions relevant to certain site-specific pollutants.

A range of variables as well as different levels of biological structure must be taken into account to achieve a comprehensive ecotoxocological evaluation of natural systems. In this way, some field and laboratory experiments using mesocosms (artificial streams, Lamberti and Steinman, 1993) help us to elucidate secondary responses related with toxicant indirect effects on the macroinvertebrate community (van der Geest et al., 1999; Rosés et al. 1999). Some of these endpoints could be an important key for modelling.

The toxicity of collected sediment samples to sediment-dwelling organisms will be determined. This will be important explanatory information for field monitoring data.

Methodological approach

SITE 4 will focus on the application and development of biological effects-based quality assessment methods at the selected hot spots in the three river basins. The community will be studied both downstream and upstream of the pollution sources at those hot spots. The community upstream of the point will be regarded as a reference. The reference state will also be checked based on physico-chemical and ecotoxicological data that are available in the database of BASIN 1.

In general, four main strategies will be followed in SITE 4.

(1) **Quantitative sampling of species** from each relevant habitat of the river ecosystem. This process provides for the effects of a toxicant (or toxicant cocktail) on the biodiversity of a real *in situ* community. Oligochaeta, Chironomidae and Nematoda will be included.

(2) Surveying the communities from **artificial substrates** in field experiments. This sampling design excludes morphological factors which may cover the direct effects of the site specific toxicant in the water. However, this approach may, on the other hand, only represent a section of the real community and may not comprise those habitats which are dwelled by more sensible indicators than those which live on the artificial substrates. - This approach in combination with field studies will be used to supply each other.

(3) Surveying the effect of sediments contaminated with key toxicants to communities in laboratory **micro- and mescosm experiments**. This experimental design allows to make a direct link of certain key toxicants on the benthic community. The inclusion of other trophic levels (biofilms, fish) in these experimental studies in co-operation with the other community-based work packages of SITE (WP SITE 3/5) will further allow, to detect indirect effects and effect propagation in the food chain.

(4) Most standardised settings will be applied in **sediment contact tests**. The toxicity of collected sediment samples to sediment-dwelling organisms will be determined. This will be important explanatory information for field monitoring data. The benthic invertebrates to be used in this part of the project represent two common taxa of sediment-dwelling organisms: *Lumbriculus variegatus* (Oligochaeta) and *Chironomus riparius* (Insecta). They have different modes of feeding on detritus/microbes in and above sediment, and they appear to respond differently to

environmental contamination. Further, they also seem to have different capability to metabolise xenobiotics.

The data gained from the field work will be evaluated in respect to several metrics covering both the taxonomic and the functional parts of the communites. Taxonomic metrics (e.g. species composition, dominance and others) will be used to detect faunistic effects of the toxicant on one important part of biodiversity parameters. Functional metrics (e.g. distribution and development of feeding types, river continuum distribution and shifting, several indices and others) based on ecological specifications of the species recorded reflect the functional character of the system and shows how toxicants disturb the food web relations. Moreover, they filter biogeographic effects, which make it easier to adjust the tools at a continental scale.
In situ alterations of the benthic communities will be interlinked with *in vivo* effect assessment of sediments, bioavailability studies (WP SITE 2) and bioavailability-oriented extraction methods. Finally a link will be made with the results obtained for other trophic levels, studied in SITE 3 and SITE 5. And validated in food chain experiments.

Strength of SITE 4

A lot of tools for biological effect-based sediment quality assessment are available nowadays. However, each tool is developed based on the information of a specific site. Intercomparison of the developed methods is hardly done, often also because additional information about the physico-chemical and ecotoxicological information is lacking. On the other hand, bioavailability of contaminants and bioaccumulation within the food chains are often not considered. SITE 4 will develop a diagnostic toolbox, apply existing and newly developed methods on specific hot spots adapting them to site specific settings and toxicants. The overall environment of MODELKEY will ensure a close link of assessment tools to relevant site-specific key toxicants (KEYTOX) and the basin scale (BASIN). Using functional characters of a community enables the tool to be independent from biogeographic restrictions, which binds indicator species to a certain region, and makes it applicable on an European scale. SITE 4 links the indication on a small scale (biofilm, SITE 3) to a large scale (fish, SITE 5) and may help the model to assess the reaction time of pollution and remediation in freshwater and marine ecosystems. The methods are applied in three different geographical areas and also at both freshwater and a brackish site. This gives a unique opportunity to do an intercalibration of existing tools and to develop those tools based on the findings of the whole MODELKEY project.

Deliverables

Month 1-18

SD 4.1 overview of existing tools for biological effects-based sediment quality assessment (7 months)

SD 4.2 identification of suitable bio-indices to toxicity assessment (18 months)

SD 4.3 intercalibrated sampling strategy and design (7 months)

SD 4.4 evaluation of the role of invaders as indicators (12 months)

SD 4.5 overview of site – specific base line data, community structure and species diversity extracted from data collection in BASIN 1 (18 months)
SD 4.6 preliminary application of the toolbox at hotspots (18 months)

Month 19-36

SD 4.7 development of artificial substrate – sampling devices
SD 4.8 Adaptations in the existing assessment tools
SD 4.9 Community analysis of the macro-invertebrates at the selected hot spots
SD 4.10 food chain analysis in mico- and mesocosms
SD 4.11 River basin specific information on the impact of the environmental pollution on the macro-invertebrate communities (tolerance analysis for indicator species and communities)

Month 37-60

SD 4.12 risks (EXPO, EFFECT, DECIS) on macroinvertebrate communities Verification of modelled.
SD 4.13 adaptation of relevant bio-indices for toxicity assessment
SD 4.14 final toolbox for the identification and estimation of key toxicant (Keytox) effects on macroinvertebrate communities
SD 4.15 Final report on biological effects-based sediment quality assessment tools

WP Site 5 (S5): Effects on fish communities (UB, VRI, IVB, RIVO)

Introduction

The overall objectives of this workpackage are:

- Diagnostic toolbox: To explore the reponse of toxicological and ecological endpoints to basin- and site-specific contaminants (diagnostic toolbox)
- Site assessment: To assess site-specific toxic hazards at different levels of biological complexity: in vitro bioassays (toxic potentials), in vivo biomarkers (early warning signals) and population and community responses
- Effect propagation: To establish the relation between toxic hazards as measured by early warning signals (in vitro assays, in vivo biomarkers) and changes at the population and community level
- Model validation: To link experimental and in situ toxicological and ecological data to a modelling approach in order to derive generally applicable principles of deterministic and as well as diagnostic effects assessment (model validation)

A continuing problem in ecotoxicological hazard assessment is to link environmental toxic potencies, toxic responses in exposed biota and ecological responses (e.g., Downes et al. 2002). Establishing causal relationships will always be difficult in field situations, due to the presence of multiple stressors and confounding factors (e.g., Segner 2003). A major limiting factor to date in studying this problem has been the rather fragmented research. The large majority of existing studies on toxic impact on fish populations and communities investigated only part of the problem, i.e either the environmental exposure, or the toxic effects in organisms, or population and community responses. A further handicap to environmental hazard assessment is that theoretical concepts to provide predictions on the impact of toxicants on ecologically sensitive parameters are often not incorporated in field studies, so that only case-on-case observations, but no principal understanding is possible. Using fish as major components of aquatic ecosystems as target, SITE5 will go essentially beyond the current state of the art in ecotoxicological hazard assessment. Important to note that this will be successfully achievable only in the multifaceted MODELKEY environment: BASIN will link the site-specific approach, as used in SITE 5, to the overall processes within the river basins. KEYTOX will provide us with detailed chemical-analytical information on the exposure situation at the field study sites so that we can align the identified toxic hazards to specific chemicals. The other WPs within SITE will link our fish-focused view to other biological elements within the aquatic ecosystems site as well as to the questions of bioavailability and biomagnification. Finally, the interaction with the EFFECT models will allow to understand the underlying mechanisms of experimentally observed relations between exposure and effects, and by this, to extrapolate from the site-specific results as obtained in SITE 5 to principal responses, as it is essential for establishing site-independent, generally applicable strategies of ecotoxicological hazard assessment (e.g., Schmitt and Osenberg 1996). At the same time, the experimental data obtained at the field sites will help to validate the predictions generated by the EFFECT models.

To achieve the above mentioned goals, SITE 5 will rely on a broad array of conceptual and methodological approaches:

- ***in vitro* bioassay measurements**: Bioanalytical approaches are of increasing importance in environmental hazard assessment since they provide an integrative measure of toxic potencies. The value of in vitro bioassays for environmental hazard assessment has been recently reviewed (Eggen and Segner, 2003, Mothersill and Austin, 2003). In vitro assays to be included in SITE 5 will assess ER- and AhR mediated effects (CALUX assays), cytotoxicity and ATP contents, and, finally, genotoxicity (comet assay). As cell systems, we will use both recombinant yeast assays, since they enable us for high-throughput testing (an important testing in site assessment), but we will also use isolated fish cells, since their responses are expected to be more predictive of our target, the fish in vivo. The bioassays will be used for two purposes: Firstly, these assays will be applied to detect the presence of specific toxic potencies in sediments. This part of the work will be closely linked with the studies in KEYTOX in order to combine the bioanalytical with the chemical analytical data. At the same time, the in vitro assays will be applied on extracts from fish tissues. In this way, we will be able to estimate the internal exposure of the fish compared to the external exposure as present in the sediments, as it is generally agreed that one of the major shortcomings in linking toxicant exposure and toxicant effects is an insufficient knowledge on the actual bioavailability and bioaccumulation of the environmental contaminants, i.e. an insufficient knowledge on the internal exposure . For this reason, SITE5 will bridge external and internal exposure by the parallel application of in vitro sediments and fish tissue extracts.
- ***in vivo* biomarker measurements**: Biomarker measurements provide information on toxic exposure and effects (Segner and Braunbeck 1998). In order to make this part of SITE5 directly comparable to the in vitro bioassay part, the biomarkers measured in vivo will address the same endpoints as used in the bioassays in vitro. Thus, they will include ER- mediated effects (vitellogenin), AhR-mediated effects (CYP1A and glutathion-S-transferase), cytotoxicity and chronic toxicity (histopathology), and genotoxicity (micronuclei). Since biomarker usually are effective at the molecular and cellular level, they directly reflect toxicant exposure and effect. They are thus suitable as early warning tools. When biomarker responses are observed in the field, this may not immediately have consequences on the organism or population level. Therefore, SITE 5 includes as well organism, population and community measurements, and it uses the prediction models of EFFECT. In this way, the in vivo biomarker analyses will bridge the external exposure assessments with the ecological assessments.
- **Fish population and community measurements**: Ecological characteristics of fish populations and communities at the study sites will be assessed by measuring fish growth, survival, fecundity, fertility, abundance, age structure and species assemblage. Further, in order to assess expsoure pathways and the interaction of fish within its coenosis, we will intensively participate in the food chain studies and experiments within the SITE SP. To this end, we will anaylse stomach contents of our target fish species as a basis to establish trophic relationships. With the various approaches shortly indicated here, SITE

5 will perform a classical ecological assessment of the field sites, but, different to most fish populations studies, we will have the data to link those ecological parameters directly – via experimental measurements in SITE 5 and via theoretical models in EFFECT to toxic exposure and effect. Such a comparative approach is highly timely in order to explore when and under what circumstances population and community responses of fish are governed by toxicant impact, or when other environmental factors such as habitat structure or food availability may overlay the toxic factor (Newman, 1998). In this context it is important that MODELKEY does not only take the deterministic approach to study ecological impact of toxic substances, but also the stochastic approach, since fish population and community changes are greatly influenced by stochastic events. Thus, we do not naively expect a direct and linear relation between toxic exposure and ecological change, however, MODELKEY provides the scientific environment to establish when and how such relations may be detectable and relevant.

Practically, the work in SITE 5 will rely mainly on field studies at selected sites within the river basisn of Elbe and Westerscheldt. In addition to field work, we will employ mesocosm and laboratory experiments with key fish species selected from the fish communities being present at the field sites to complete the stepwise approach from toxicity tests to ecologcial consequences. Initially, we will perform laboratory experiments to establish the sensitivity and response profile of toxicological and ecological target parameters of the key fish species to chemical exposure. By this, we will validate the diagnostic toolbox for in situ assessment, and, at the same time, we will be able to feed data into the model development in EFFECT. In this initial run of experiments, the chemicals used for exposure will be selected on the basis of information generated in BASIN on relevant toxicants, while for a second run we will use those chemicals that meanhwile have been identified as major contaminants at the study sites. The knowledge obtained from laboratory experiments will be further validated in mesocosm studies and will be directly applied for *in situ* site assessment.

There are two important aspects to support successful site assessment in SITE5:

- the investigations will closely integrated with the chemical-analytical work of KEYTOX, the ecological modelling work of EFFECT, basin-wide information of BASIN and the bioavailability/biomagnification as well as ecological work done in the other SITE WPs
- we will not simply apply any available toxicological and ecological tools to the study sites, but in the step-wise approach described above (from laboratory experiment over mesocosm studies to the field work) we will carefully evaluate and validate the meaning and value of the assessment approach

Strength of the SITE 5

Strengths of SITE 5 are in three areas: Firstly this WP will exemplify how to link exposure, toxicological and ecological information. Although this sounds rather simple and basic, often it is exactly the missing link between these different pieces of data that is a major obstacle to successful site assessment. Secondly, SITE5 will develop innovative approaches to site-specific hazard assessment, since, as generally agree, currently available tools are not sufficient. We need to be able for high-throughput screening, but at the same for mechanism-based assessment and for integration of ecologically relevant parameters, both in terms of actual measurements and in terms of modelling. The latter point leads to the third strength of SITE 5, i.e. the fact that it will link experimental with theoretical modelling data. Up to now, approaches for site assessment have been by far too empirical. Combination of actual measurements with modelling approaches will help to extrapolate observations and to predict hazard.

Deliverables

Month 6-18

SD 5.1	toxicological and ecological screening of selected sites (15 months)
SD 5.2	selection of target species (15 months)
SD 5.3	method-oriented diagnostic toolbox for toxicological site assessment (18 months)
SD 5.4	Toxicological and ecological data to feed into EFFECT models (18 months)

Month 19-36

SD 5.5	ecological characterisation of target fish populations and communities at selected sites
SD 5.6	food chain evaluation (analysis of fish stomach content)
SD 5.7	Mesocosm experiments using target fish species
SD 5.8	In vitro assays of extracts of fish tissue

Month 37-60

SD 5.9	assessment of toxic and ecological hazard at the study sites in the Elbe and Westerscheldt basins
SD 5.10	validation of EFFECT models
SD 5.11	guidelines for approaches of toxicological and ecological site assessment *to be used by stakeholders*

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SP DECIS: Decision Making/Management (CVR)

Sub-project DECIS has the objective of developing a Decision Support System (DSS), which integrates the whole project deliverables in a framework to manage impacts of key pollutants on ecosystems and biodiversity. DECIS is structured into three work packages. Work package DECIS1 (Development of Conceptual Framework and hot spots prioritisation module) aims at providing a common framework to integrate project deliverables and at formulating DSS structure. Moreover, it develops the hot spots prioritisation module, in particular the socio-economic and economic analysis. Work package DECIS2 (Integrated Risk Index) aims at developing and applying a Weight of Evidence (WoE) based Integrated Risk Index (IRI), which provides the integrated estimation of ecological impacts of identified contaminants on biodiversity. The Integrated Risk Index will play a major role in the DSS. Work package DECIS3 (Development and evaluation of DECIS DSS) concerns the Decision Support System computer development and its evaluation through the application to the MODELKEY case-studies: Elbe, Scheldt and Llobregat.

Work packages 1-3

Decision Making/Management - Introduction and five-year overview

DECIS 1

Participant	CVR	UFZ	UA	CEFAS	DELFT	CNRS	CSIC
Person Months	30	3	1	1	1	1	5

DECIS 2

Participant	RIVM	CVR	CNRS	UA	CEFAS	DELFT	
Person Months	4	36	3	3	2	2	

DECIS 3

Participant	CVR	EWQMA	RIKZ	CSIC	UFZ	ACA	IVB	RIVO	UdB	UA
Person Months	59	1	1	3,5	9	1,3	1	1	1	4

Introduction

DECIS develops a Decision Support System for the assessment and management of biodiversity impacts at basin and site specific scale. For this purpose DECIS combines an integrated risk index based on a weight of evidence approach with socio-economic and economic assessment of biodiversity impacts. A brief introduction of state-of-the-art and role of DECIS with respect to Decision Support Systems, weight of evidence approaches for risk assessment and socio-economic evaluation of non-market goods is following presented.

Decision Support Systems

A decision support system (DSS) is an integrated, interactive computer system, consisting of analytical tools and information management capabilities, designed to assist decision making when management of critical, complex and unstructured environmental problems requires consensus building among different stakeholders (Watkins and McKinney, 1995; Newman et al., 2000).

Some DSSs have been designated and developed for specific water resource planning and management activities (Watkins and McKinney, 1995). They usually offer a **comprehensive approach to water management**, by encompassing land-use and socio-economic dynamics at catchments scale, water quality and quantity. Most of the existing DSS integrates socio-economic and environmental modelling techniques at catchment scale with a geographic information system (GIS), (e.g. MULINO, Giupponi *et al.*, 2000; Mysiack *et al.*, 2002). Many of them follow a **DPSIR (Driver-Pressure-State-Impact-Response) framework**, developed by the European Environmental Agency (OECD, 1994) in order to better frame analysis and management of complex natural systems subject to anthropological pressure (MULINO, Harmoni-CA). Referring to the DPSIR approach, the large scale concerted action Harmoni-CA (Harmonised Modelling Tools for Integrated Basin Management) is mainly centered on consensus building and aims at establishing a dialogue between science, policy and stakeholders, synthesizing available knowledge and transforming the DPSIR framework into a well structured, manageable assessment tool supporting stakeholder-based planning and decision processes (Arnold, 2003).
GIS-based DSSs can rely on a wide range of models and databases developed in support of water quality studies (Apitz and White, 2003). Available models support the prediction of water contamination from point sources and continuous discharges (e.g. GREAT-ER- Geography-referenced Regional Exposure Assessment Tool for European Rivers; Schroeder, 1997; Feijtel *et al.*, 1998) and from diffuse sources of chemicals (e.g. TERRACE-Terrestrial Runoff Modelling for Risk Assessment of Chemical Exposure; Beaudin *et al.*, 2002).
While a great deal of research work has been devoted to building general decision making frameworks for river basin management and for relating contaminant exposure to point and diffuse sources, **strategic spit-falls and lacks are still remaining** for relating chemical exposure to biodiversity and ecological impacts, and decision support tools are required for **ranking biodiversity impacts and selecting site specific interventions on hot spots**. Within existing DSSs, specific decision support tools to support the **assessment and management of pollutants impacts on ecosystems and biodiversity are still missing**. Moreover, with respect to existing models and tools, recent scientific literature indicates the need for a **further integration between catchments and local scale** (Apitz and White, 2003). While the environmental impairment can be appreciated at local scale, prioritisation should be performed at basin scale, actions usually require local specific assessment, and finally local interventions should be evaluated in the light of Basin Management Plans and benefits. For this purpose, there is the need for a DSS, which enables to find proper connections between impacts on biodiversity and socio-economic evaluation at the basin and local scale.
DECIS DSS addresses these lacks and pitfalls by assessing ecological risk for biodiversity and socio-economic demands at local and basin scale across Europe. A primary positive aspect characterizing DECIS system is the **effective integration and**

combination of innovative tools and methods developed within ModelKey. DECIS DSS offers the possibility to the potential end-user to have a complete and accessible system for impacts assessment and management of biodiversity at the basin scale. In a single system, analytical tools and decisional frameworks are present and interconnected in a **stepwise and guided procedure**. As an added value to the existing systems, **DECIS allows prioritisation of river hot spots**, based both on risk assessment procedures at basin and site-specific scales, and on socio-economic perspectives about biodiversity value. The prioritisation represents therefore the basis for intervention choices at the basin scale, taking into account general reference frameworks, such as the European DPSIR one. In fact, another relevant feature of DECIS is **the opportunity for the user to interlink the DECIS system with other existing tools and models and within other decisional frameworks**, in order to have a comprehensive and flexible basin management system for decision support.

Economic valuation and socio-economic analysis

In recent years, many studies on biodiversity and its loss have appeared, evaluating the notion of biodiversity value and the application of economic and monetary valuation methods for its assessment. **Economic valuation** of biodiversity leads to monetary indicators, regarded as a common unit for comparison and ranking of alternative biodiversity management policies. In general terms, the value of biodiversity can be assessed in terms of its impact on the provision of inputs to production processes, in terms of its direct impact on human welfare and in terms of its impact on the regulation of the nature-ecosystem-ecological functions relationships (Nunes and van de Bergh, 2001; Nijkamp *et al.*, 2001). Usually, market valuation mechanisms that price the value of biodiversity are lacking. Therefore, valuation of biodiversity requires the use of special valuation tools, which should address the following objectives: that a concrete biodiversity change scenario is formulated, that a multidisciplinary approach seeking the identification of direct and indirect effects of the biodiversity change on human welfare is used and, very importantly, that the change is well defined and not too large. **So far, relatively few valuations have met all these requirements**. Moreover, economic valuation methods have been usually applied for special cases, with relevant difficulties to extend the results to more general conditions.

In DECIS, a methodology of economic analysis for biodiversity valuing will be developed which **can be applied at the basin scale** and **addresses all the requirements mentioned above**. The aim is to combine and adapt state of the art economic valuation tools, in particular contingent valuation and travel costs methods, bearing in mind the available scientific information and also potentialities and lacks of each method. Moreover, the important feature of the socio-economic analysis is the relevance given to the stakeholders point of view, which allows to define priorities and to clarify conflicts of interest, in order to set up sustainable and long-term management strategies for the river basin.

Moreover, the monetary valuation of environmental goods should be combined with a wider assessment of socio-economic dynamics behind environmental conflicts. The socio-economic assessment has a wider consideration of social, economical and political factors which influence planning and choices at regional and sub-regional scale.

In DECIS, the **economic valuation** of biodiversity will be **combined with** a more comprehensive **assessment of socio-economic constraints and benefits** of ecological restoration objectives.

Weight of Evidence Approach

In the risk estimation process the measurement endpoints constitutes lines of evidence (LOE), and the process of analysing LOEs is generically defined as "Weight of Evidence" (WoE). A **WOE approach overcomes out spins of traditional approaches**, such as the PEC/PNEC quotient approach, reduces uncertainty associated with risk assessment and, thereby, improves management decisions (Burton et al, 2002). WoE does not estimate the risk simply on the basis of hazard quotients, dose-effect curves or biotic indexes, but integrates all these information in order to assure a better understanding of dynamics of the ecosystem especially when determination to population level are requested (Chapman, 2000).

According to the most recent definitions, the "Weight of Evidence" may be defined as: "*… the process of combining information from multiple lines of evidence to reach a conclusion about an environmental system or stressor*" (Chapman, 2002; Burton 2002), and "*…approach that combines analysis of field data (to determine patterns) with experimental hypothesis testing (to determine mechanisms) to make prediction of the future effects and provide appropriate management recommendations*." (Lowell, 2000).

The different types of implementation of the WOE have been organized in two main groups, according to Burton (2002) and Chapman (2002):

- **Qualitative combination**
- **Quantitative combination**.

The "qualitative combination" generally indicates a non-quantitative integration of Lines of Evidence (Burton, 2002), which means the interpretation of the experimental results in order to explain the consistency, or the inconsistency, of the lines of evidence indications (*e.g.* magnitude of harm, evidence of harm), between the various LoE. An example of this approach is the first formulation of the Sediment Quality Triad, proposed by Chapman, (1990). More recently, Diamond (2000), Loewengart (2001), and Shin and Lam (2001), proposed the qualitative approach in order to judge the effectiveness of dredging activities, to integrate monitoring data, to integrate literature and experimental ecotoxicological data, and to develop a pollution index for marine sediment. The qualitative approach was considered by Burton (2002) a simple method applicable to a wide range of ecosystems conditions; however, it is difficult to apply it to other environments except those for which it was developed (i.e., high site-specific); it has low sensitivity (i.e., discrimination capability between different levels of exposure or effects) and low coherence in results interpretation; it is not easily understandable by end users and stakeholders.

In order to prevail over the limits of the qualitative approach, a wide range of quantitative approaches were proposed. Generally, the quantitative approach integrates the lines of evidence in order to classify, rank or estimates risk, allowing a decision support. In fact, it connects the lines of evidence to management requirements in order to provide useful information for the decision-makers. The quantitative approaches may be classified in three groups: the ranking, the matrices and the quantitative likelihood approaches.

The ranking approach achieves a ranking of the sites along a gradient of risk or quality, and this system results are easy to understand, especially for non-technical or specialized stakeholders (e.g. the interested parts). Wildhaber and Schmitt (1996) and

Cherry et *al.* (2001) proposed a ranking approach in order to characterize sediments of Great Lakes and of Ely Creek, respectively, defining a quality scale between the best condition (i.e. the reference site) and the worst condition for exposure and effects, and assigning a intermediate value to others sites. The quality index was plotted by tri-axial plots (Canfield *et al.*, 1994), and by pie charts (Chapman, 1996), but there could be a substantial loss of information at wide spatial scale (Chapman, 2000).
The matrices approach concerns the representation of the LOE through a matrix of the responses, providing information about the test sites, the measurements results, the explanation of the combinations between the results and the proposed management solutions.
These matrices have been proposed for the first time by Chapman (1990) for explaining the three LoE that define Sediment Quality Triad (SQT), but their use has been remarkably widened in the number of LoE inquired and also in the type of inserted answers. Suter (2000) suggested a WoE based on both the predominant response and on the consideration of LoE reliability. Suter (2000) and Menzie (1995) propose a list of attributes in order to estimate the reliability of the LoE, assigning a qualitative judgment (high-medium-low) to each LoE. On the contrary, the "Massachusetts weight of evidence workgroup" proposed a quantitative procedure, implemented into the ecological risk assessment procedure, from the Problem Formulation phase to the Risk Characterization phase (Massachusetts weight of evidence workgroup, 1995). This method for the implementation of a WOE approach in the risk characterisation phase of the ERA has the benefit of being open because new LoE can easily be added in an iterative process (Suter, 2000). Moreover, according to Burton (2002), the main advantage of the process delineated from the "Massachusetts weight of evidence workgroup" is the elevated transparency that allows a high level of consensus between the stakeholders. On the other hand, the involvement of the best professional judgment in the qualitative approach and in the quantitative one (even if in smaller amount), requires a high degree of expertise of risk assessors.

In this work, **the Weight of Evidence approach will be applied to develop an Integrated Risk Index**, integrating different lines of evidence: literature data, field observations, laboratory tests, exposure and effect modelling results. The risk index will address **management objectives** at basin and site specific scale. The WoE approach will allow to make the **best use of the results of multiple approaches** developed in ModelKey, each one exploring different aspects of the ecological impairment caused by toxic substances. Since the complexity and the type of information widely vary among different experimental and modelling methods, the WoE procedure will have a **tiered structure**, moving **from basic to more accurate assessments**. In addition, the tiered structure will allow to **move from the basin to the site specific scale**. The consideration of different lines of evidence (i.e. experimental vs. modelling) along the tiered WoE procedure will also provide **an indication of the added value for management purposes** of further investigation and modelling.

The management purposes, the combination of experimental and modelling results, the tiered structure for multi-spatial and multi-purpose applications, these are all innovative features of the integrated index. Moreover, **state-of-the-art multi-criteria analysis methodologies** will be applied for the development of a robust structure of the index. The index will be suitable for being combined with the socio-economic indicators and will be flexible for being applied to different fresh water ecosystems. In addition, integrated index can support the definition of ***de minimi* approach** to a protective but cost-effective, tiered basin-scale management framework.

Research, technological development and innovation activities

Within MODELKEY, a significant amount of relevant research on the relation between toxic substances and biodiversity impacts is expected to be produced, encompassing interlinked and verified modelling and assessing tools. The scientific contribution of MODELKEY can be enhanced if all the research work is properly integrated into a Decisional Framework. **The Decisional Framework is intended to be the logic structure by which all the project deliverables are operationally interrelated** for management purposes. The Decisional Framework should define a specific role for each project deliverable, by highlighting limits and potentialities for applications and inter-linkage with other deliverables for diagnosis, understanding and prediction of impacts to biodiversity. The Decisional Framework will be also **a relevant reference of each research activity** to assure that significant scientific contributions are produced in the light of current and emerging models, decision frameworks, regulation and policies. Being a dynamic framework shaped by and guide of the ModelKey research activity, the **DECIS Decisional Framework will enhance the implicit originality and innovation of each project deliverable**. It will be an innovative user-friendly tool for managing biodiversity impacts, well integrated in the current legislation framework (DPSIR) and easy to combine with other systems.

The Decisional Framework is first developed as a conceptual model, and then implemented into a Decision Support System (DSS). The DSS will offer three type of instruments, (guidelines, “models and tools”, case studies demonstrations), in a web-based system. The end-user can use the web-based system as a laboratory on-line or can download the instruments of interest. Through the application of the system tools/models, it is possible to prioritise first risk sites at the basin scale and then to focus investigations at the site-specific scale. Management options can be therefore evaluated with respect of site objectives, always taking into account basin management objectives. Water uses objectives can be then valuated on the basis of the risk posed to biodiversity and management activities can be planned. Another relevant aspect which is provided by DECIS is the monitoring program. The proposed protocol facilitates the involved end-users in the definition of monitoring activities in order to meet modelling and policy requirements.

The main applied objective is to propose a set of tools for water management and water policies in order to allow to easily assessing ecological quality and perturbations of stream ecosystems. These tools (completely GUI based, i.e. graphical user interface) will provide information about water quality as well as community structure. The assessment tools will allow identifying measures which should be taken to restore biological integrity in waters. Hopefully, the study can be considered as a first step toward linking the improvement of water quality through specific management measures (e.g. waste water treatment, habitat restoration, etc.) with the expected improvement in ecological and biological value of water systems, including freshwater and marine waters.

Specific objectives

1. to develop a Decisional Framework to integrate project deliverables and support decision making;
2. to develop the integrate index defining water quality for diagnosis and management according to the EU directives;
3. to provide decision support tools for ranking hotspots at basin scale, based on both environmental risk and socio-economic factors;
4. to implement the Decisional Framework into a web-based Decision Support System (DSS);
5. to provide evaluation of the DSS through the application to three case-studies;
6. to provide the prioritisation of impacts at the basin scale;
7. to provide a monitoring program protocol for water biodiversity management.

Temporal sequence

For an overview on the temporal sequence of the tasks in DECIS work packages see Figures B.4.14.

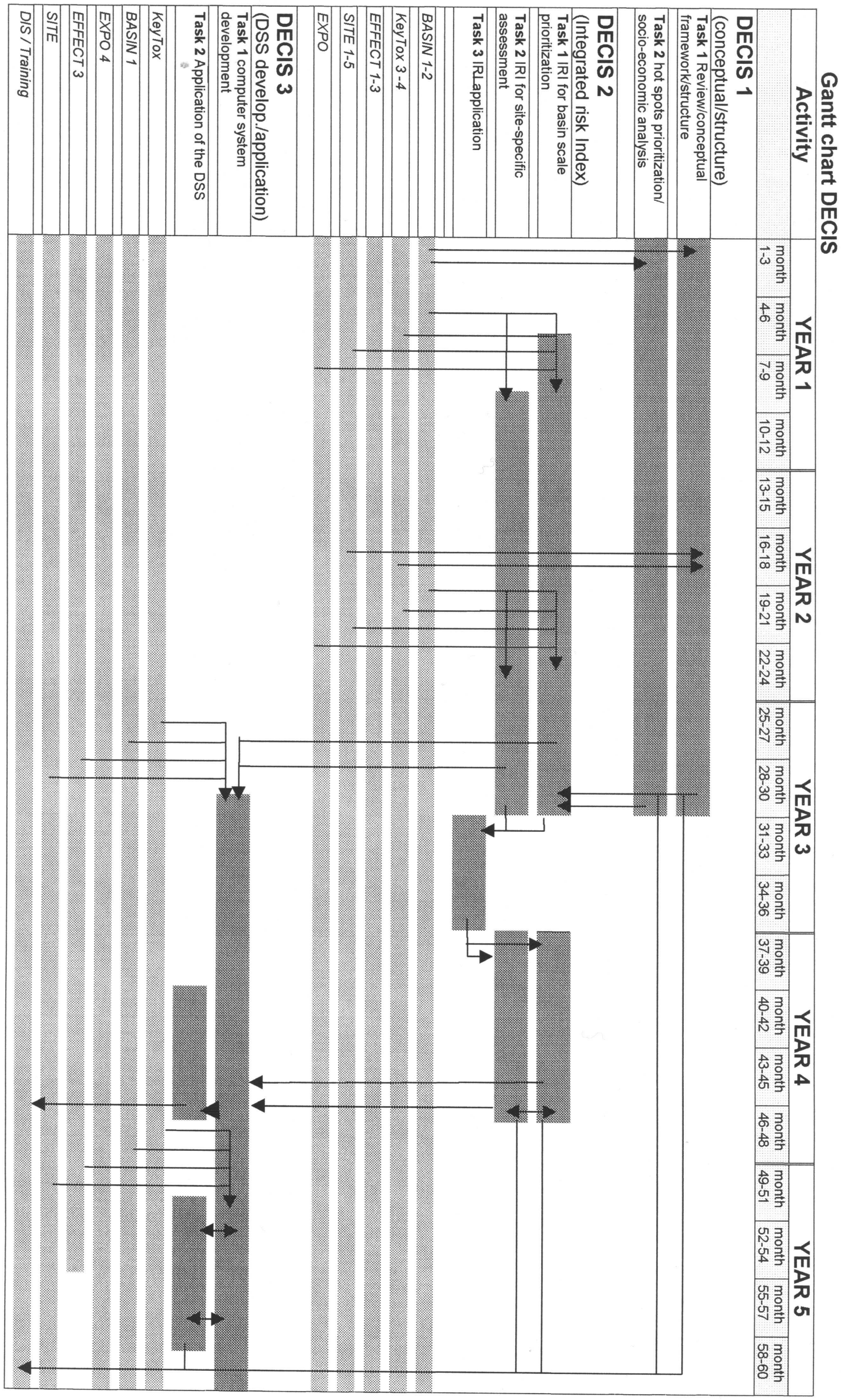

Fig. B4.14: Temporal sequence of the tasks in DECIS.

WP DECIS1 (D1): Development/Refinement of the conceptual framework and hot spots prioritisation module (CVR, UFZ, UA, CEFAS, DELFT, CNRS, CSIC).

DECIS main objective is the **integration of all MODELKEY deliverables in an operational system** for the assessment and management of river biodiversity and ecological status at basin and site scale. This operational system can be classified as a Decisional Support System (Watkins and McKinney, 1995; Newman et al., 2000) and is mainly **focused on the prioritisation of risk hot spots** where interventions are more urgently needed. Prioritisation is **based both on risk assessment and risk valuing taking economic and socio-economic perspectives into account**.

Risk assessment is performed in DECIS through the application of the Integrated Risk Index, which combines tools and models developed within KeyTox, SITE, EXPO, EFFECT and BASIN subprojects (see DECIS2). For evaluating conflicts and compatibility between the ecological risk and uses of the river, economic valuation and socio-economic assessment procedures are proposed in DECIS1 (Task 2). In fact, risk acceptance and social demand for environmental quality may vary depending on uses and public perception of the affected resource. The sustainable allocation of efforts and limited economic resources have to take into account socio-economic and economic drivers and constraints. The integration of risk index assessment and socio-economic analysis is then used for hot spots prioritisation and identification of sites where additional site-specific risk assessment should be performed.

In order to reach prioritisation objectives, **DECIS offers a decisional framework** that ensures a coherent organization of project deliverables, also in the light of existing frameworks (see Task 1), **and tools and models for analysis and application**, partly developed in the other MODELKEY subprojects and partly delivered within DECIS itself. **The proposed decisional framework relates the assessment and decision making at basin and local scale in a circular scheme**.

The Decisional framework is implemented into a Decision Support System. The overall structure of the DECIS Decision Support System is shown in Figure B4.15. The final product is a **Web-based system**, organized into four subsequent phases: **basin assessment**, **hot spots prioritisation**, **site-specific risk assessment** and **intervention protocol**. In the first phase, a basin assessment is performed by using SITE, EXPO and EFFECT tools and models. The second phase is mainly concerned with hot spots prioritisation. By calculating the Integrated Risk Index (developed in DECIS2 and based on results of EXPO and EFFECTS), a first risk prioritisation can be performed. The socio-economic and economic assessment of biodiversity and ecosystem conservation, developed in DECIS1, is integrated with the Integrated Risk Index to derive a prioritisation of hot spots for interventions. In the third phase, a site-specific risk assessment procedure is proposed (DECIS2) to deepen the analysis on specific identified hot spots and support the evaluation of local interventions. In the fourth phase, the integration of the proposed procedure within existing tools and frameworks for the selection of interventions is indicated.

For each phase, the DECIS DSS offers three types of instruments:

- Guidelines, supporting the user in the integrated application of experimental procedures and tools and in the interpretation of results;
- Models and tools, downloadable during the stepwise procedure;
- Case-studies demonstrations, showing how specific tools and models have been tested and implemented in the three MODELKEY case-studies, highlighting potentialities, limitations and practical problems and thus facilitating the user in the application of the tools/models package.

For the intervention phase, a guideline is provided to link the proposed ranking system to existing tools or frameworks for the selection of intervention options. In fact, a main feature of DECIS Web-system is **to provide tools and models for hot spots prioritisation which may be collected by the user in a personal DSS** with other tools/models, in order to support decision making for a whole basin-scale management. It is correct to say that general DSSs are usually not valuable for different basins, because they expect the European-wide strict harmonisation of methods, tools and data formats and assume the applicability to very different cases. While recommending for a general harmonisation of approaches and methods, DECIS assumes different DSSs can be built **by integrating ModelKey deliverables with different databases and models already in use for each basin**. In many cases, this approach is expected to enhance the capability of local expertise and knowledge and to fit better with basin specific features.
The activity of DECIS1 is structured in two tasks. The first one concerns the development of the decisional framework and the definition of the general structure of the DSS. The second task is focused on the hot spots prioritisation, in particular on the socio-economic and economic analysis. The programming of the web-based system will be performed in DECIS 3.

Task 1 - Development of decisional framework and Decision Support System (DSS) structure

The primary objectives of this task are:

- to develop a common decisional framework to integrate project deliverables for management purposes
- to ensure a coherent development of projects deliverables to be integrated within the DSS
- to formulate a structure for the DSS in order to provide an integrated system for decision making.

A critical review of the project conceptual framework in the light of current and emerging models, decision frameworks, regulations and policy will be performed. Potentialities and gaps for management purposes will be investigated. The integration of project deliverables within a DPSIR based fresh and marine water management will be addressed, as well as integration of the developed system with existing tools and models. A necessary part of this task is the building of a strong and fruitful collaboration with research groups and projects managers working on the same topics at the European level, such as SedNet, REBECCA, AQUATERRA and ALARM participants. Their contributions will be essential in order to better refine the proposed conceptual framework on the basis of recent experiences and research developments. A co-ordinated and regular basis for collaborating with these research groups will be established by the SubProject DIS/TRAIN.

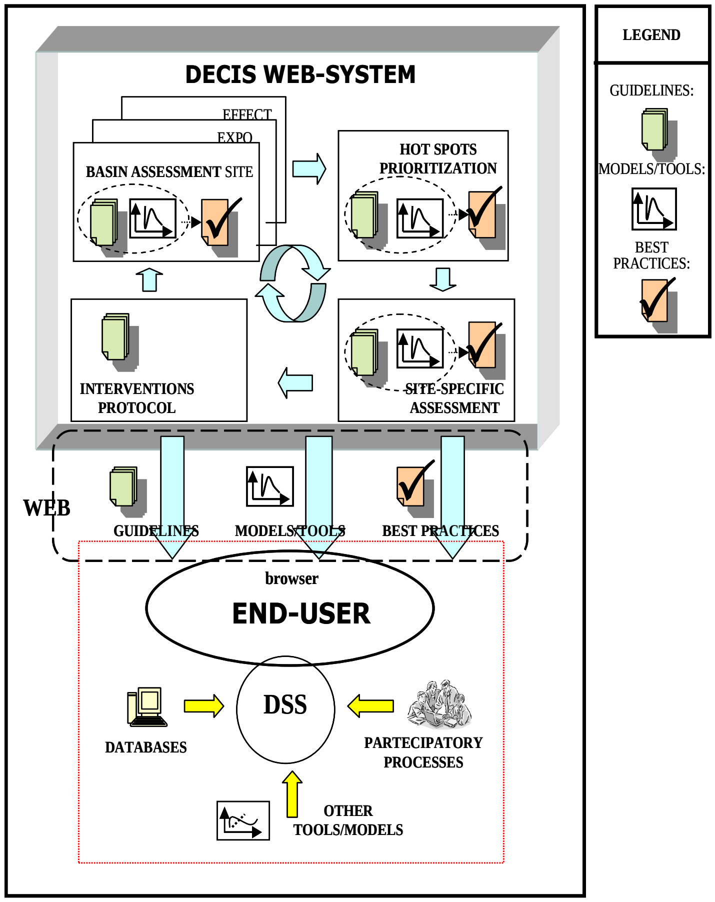

Figure B4.15: Scheme of the DECIS web-based Decision Support System

Based on the integration of ModelKey deliverables, a preliminary list of recommendations for the design of **monitoring programs** of biodiversity impacts at basin and local scale can be delivered at the 18th months deadline.

In the light of the proposed decisional framework, **a structure of the DSS will be developed**. In the first phase DECIS end-users will be clearly identified (Environmental Protection Agencies, Water management authorities, Ministries of Agriculture and Environment, as well as the European Commission for more general purposes) and involved in the process. The general structure and potential applications of the system will be discussed with a selected group of end-users in a meeting. Principal requirements, flow diagrams, general contents, efficient links to tools and models packages will be defined. Type and way of integration with tools and models developed outside the project will be also defined at this stage.

An important task to be performed is the collection and integration of tools and models developed within the project: SITE/BASIN TRIAD database and diagnostic tools, KEYTOX analytical tools, EXPO models, EFFECT models, integrated index calculation and socio-economic assessment. This apparatus, composed of GIS-based applications and protocols, is combined with guideline information and case-studies demonstration and offered via WEB-based system. The information system will be

engineered (hardware, software, data, databases and people responsibilities). A feasibility study will be carried out. Finally, properties and system functionalities needed for the system to better perform its requirements will be identified. The DSS structure design phase will be linked to DECIS 2 and other subprojects deliverables.
This task requires a close communication and collaboration with all partners involved in the project, with special regards for project leaders of BASIN (UA), DECIS (CVR), EXPO (Delft) and EFFECT (CNRS).

Task 2 – Hot Spots Prioritisation Module
The Module aims at the prioritisation of hot spots derived by the combination of the Integrated Risk Index with the economic and socio-economic valuation. The Integrated Risk Index is developed in DECIS 2. Socio-economic analysis is instead part of this DECIS1 second task, as described below.

The aim of the socio-economic analysis is as follows:
- **to assess how environmental problems affect economic uses** (e.g. quality of water, quality of sediments) and the planning framework
- **to investigate and to assess the stakeholders' strategy** with respect to the environment (pollution, quality of water) in order to stress possible environmental conflicts
- **to assess the economic value of biodiversity** in different situations and to consider how this can inspire environmental policies.

On the basis of the environmental characterisation of the different sub-systems, the research group will consider elements such as:
- economic uses involved
- the current planning framework, in order to stress some potential conflicts between uses' demand and the state of the environment
- how the environmental quality can affect the relationships between different economic uses
- the economic costs related to the gap between the current environmental state and the environmental standard goals (also requested by the WFD)

To do this, the research group will gather data related to: the economic uses (census, reports, direct investigation), the planning system, indexes of environmental quality.
The research group will focus on the **stakeholders' point of view**, with regard to the current situation and possible scenarios (to be evaluated with multicriteria analysis), and **economic methods** to evaluate the costs of environmental degradation in some particular contexts.
In concrete terms, once defined some critical hotspots, the analysis proposes to give an answer to the following questions:

a) Which biodiversity values need to be valued and evaluated?

To answer this question, **an interdisciplinary scientific Panel** will be established so as to identify, describe and conceptually model the complex network of human-ecological relationships present in the river ecosystem under consideration. The Panel will be composed by representatives of different partners involved in DECIS 1 plus representatives of EWQMA, RIKZ and CSIC with solid working experience in the study of the river ecosystems under consideration. The underlying idea for the creation of the Panel is that the economic valuation exercise is not an isolated application; it is necessary to establish ex ante an operational framework to allow interpretation of the valuation results.

For this purpose, it is important to discuss concepts relevant to the analysis and review models with the panel of experts. Such a discussion will help to better understand the relationships between the river ecosystem under consideration, river biodiversity, economic activity and human welfare.

b) What methods can be applied?
Various economic methods are available for valuation of the social benefits of projects targeted at the protection of ecosystem natural environment and resources. The aim is **to combine and adapt state of the art economic valuation tools**, in particular contingent valuation and travel cost methods, bearing in mind the available scientific information and the pros and cons of each method. The choice of the valuation method will be motivated in terms of its **originality and suitability to the ecosystem and biodiversity values under consideration**, or in terms of qualitative methodological and econometric developments (e.g. combine contingent valuation with con-joint analysis so as to compute marginal willingness-to-pay values for the set of survey described management policy changes). In addition, the proposed project also proposes to provide non-monetary indicators, based on ecological valuation methods such as biotic-richness and ecosystem health approaches.

c) What socio-economic groups need to be targeted?
Different stakeholders, such as fishery industry, tourism industry, transportation industry and environmental conservation groups, have different concerns and will value the same river management option differently. An economic valuation exercise is viewed as a means for dialogue between different stakeholders and policy makers. Special attention will be given to the fields identified as “crucial” in the environmental policy agenda for the river ecosystem under consideration, namely the evaluation of the effects of different practices and associated regulations. The primary motivation for the execution of a stakeholder valuation study is **to help defining priorities and to clarify conflicts of interest**, so as to assist in the design of an effective and robust long-term development strategy for the ecosystem under consideration.

The combination of the integrated risk index with criteria and valuation from the socio-economic and economic analysis (biodiversity values under different conditions, conflicts between socio-economic pressures and environmental quality) will be achieved by using multi-criteria analytical methodologies to derive hotspot prioritisation.

Strength of DECIS 1:

By integrating all models, tools and application practices within an operational decisional framework, **DECIS enhances the overall value of all project deliverables**. At the same time, **it assures that significant and coherent scientific contributions are produced**.
To set up intervention strategies for biodiversity preservation, a clear definition of impacts posed by released contaminants is strategic, and it can not be separated by the

social and economic consideration about the current and potential resource uses. DECIS1 provides a system in which **tools and models for assessing hot spots prioritisation are well combined and integrated in a decisional framework** which highlights the strong relationship between basin and site-specific scales. The system is characterized by **a very positive openness to other tools and models**, allowing different end users to integrate it within existing frameworks and facilities.

Deliverables

Months 1-18

DD1.1: Review of models/tools/decision frameworks and conceptual framework, Report (month 10)
DD1.2: Preliminary list of recommendations for the design of monitoring programs of biodiversity impacts at basin scale (month 10)
DD1.3: Socio-economic characterisation of three case studies (month 16)
DD1.4: DSS Structure Interim Report (month 18)
DD1.5: Review and preliminary proposal for prioritisation of hot spots based on risk and economic assessment of biodiversity and ecological impairment (month 18)
DD1.6: Design of investigation on biodiversity value (month 18)

Months 19-36

DD 1.7 DSS Structure Final Report (month 30)
DD 1.8 Economic and socio-economic factors influencing the biodiversity value at basin scale – final report (month 30)
DD 1.9 Procedure for prioritisation of hot spots based on risk and economic assessment of biodiversity and ecological impairment (month 30)

Months 37-60

No deliverables

WP DECIS2 (D2): Integrated Risk Index (<u>RIVM</u>, CVR, CNRS, UA, CEFAS, DELFT)

The main objective of DECIS2 is **the development of an Integrated Risk Index (IRI)** for the definition of sediment and water quality for management purposes at basin and site-specific scales. IRI is **based on a stepwise Weight of Evidence (WoE) methodology to integrate ecological, chemical and ecotoxicological data** (Burton, 2002). The proposed WoE methodology will include specific multi-criteria analytical procedures and tools. The integration of ecological, chemical and ecotoxicological data (*i.e.* lines of evidence) will be accomplished in a weight of evidence tiered analysis, taking into account **4 tiers: first (i.e., screening analysis) and second tier at basin scale, third and fourth tiers at site-specific scale (i.e., high priority sites)**. Thus IRI can be used for ranking hot spots sites at basin scale and for risk assessment of specific sites. River stretches will be classified, according to what is defined in BASIN1, and "hot spots" will be ranked at basin scale (tier 1 and 2). Based on this ranking, sites that need further investigation ("high priority sites") can be selected

(due to time constraints, in ModelKey the selection of sites to be considered in SITE is performed in BASIN). In these sites, IRI can be calculated (tier 3 and 4) to evaluate the site-specific ecological quality and intervention alternatives supporting the management process.
IRI will assess the ecological quality in term of impacts on biodiversity and specific ecological functions associated with the priority pollutants identified in KEYTOX 3.

According to the WFD (i.e. Annex II), the basin area will be classified in water body typology (i.e. river, lake, transitional waters, coastal waters, and artificial or heavily modified water body) characterized by specific hydro-morphological, biological and geographical parameters. For each water body typology a "type-specific reference site" will be selected. **IRI assesses the ecological quality alteration of investigated sites from the related reference conditions**. To do this, IRI integrates the results obtained from both experimental activities, such as those conducted in SITE, and models application (*i.e.* EXPO, EFFECT and KEYTOX models). Taking into account the WFD annex V, at least four classes of ecological quality will be identified (i.e., high, good, sufficient, and insufficient).
Moreover, **IRI will include two components of overall ecological quality: one related to sediment quality and one related to water quality**. Lines-of-evidence (*i.e.* experimental and models results obtained in other SPs) for water and sediments will be considered separately and assessed along the four tiers of analysis.
DECIS 2 activities will be structured into three tasks, the first two concerning the development of integrated risk index for basin and site-specific scale respectively, and the last one focusing on the index application in the three ModelKey case-studies.

Task 1 – *Integrated Risk Index for basin scale hot spot prioritisation*
The main objective of task 1 will be **the ranking at basin scale of water body stretches** identified in BASIN1 and **the identification of risk-based hot spots**. Tier1 and tier 2 of the WoE procedure will be defined.
In accordance with the WFD annex V, the screening analysis at basin scale (tier 1) will concern the estimation of the PEC/PNEC ratio on the basis of the BASIN1 database and international environmental quality criteria. Subsequently, based on the previous WoE framework, IRI tier 2 will integrate databases and results of predictive models at basin scale, such as those provided by BASIN 1, KEYTOX 3, EFFECTS 2 and 3, and EXPO 1 to 3.

Task 2 - *Integrated Risk Index for site specific assessment*
Task 2 will develop **the site-specific IRI**, assessing the site-specific ecological quality of water and sediment at "high priority sites".
The tiers 3 and 4 of WoE will be carried out at site-specific level in the high priority sites selected by BASIN 2, taking into account the results of the site-specific experimental activities conducted in SITE 1 to 5 (*i.e.* fate and transport, bioaccumulation, biodiversity at different trophic levels) and in KEYTOX 4 (*i.e.* bioassays), and the diagnostic models results provided in EFFECT 1 and EXPO. These third and fourth levels of analysis could include also lines of evidence from the first and second tiers.
A GIS-based spatial analysis of the Integrated Risk Indexes at different spatial scales and tiers of analysis will be performed (link to Task 3).

Task 3 – *Integrated Risk Index Experimental Application*
This task concerns the **experimental application of IRI for testing and refining of the proposed methodology**. Due to the timing of the site specific monitoring and testing programme in SITE and of the modelling in EXPO and EFFECT, the experimental application of IRI will be performed with preliminary and intermediate results, while the application with monitoring and modelling definitive results will be accomplished in DECIS 3.
The **application of IRI will follow a stepwise procedure**, moving from available monitoring data and further measurements to the inclusion of modelling results. The comparison of results obtained from different steps will highlight the additional value at management level of monitoring and modelling improvements. Different clusterisation of the river network and estuarine environment will be compared. The experimental application of different clusterisation and spatial estimation of IRI will highlight potentialities and limits of alternative options.
By the month 46, a preparation and execution of a course on IRI application will be performed as part of the DIS/TRAIN subproject activities.

Strength of DECIS 2:

The main strength of DECIS 2 is that **different experimental and modelling approaches proposed by ModelKey are evaluated in a Weight of Evidence approach** for the definition of an integrated risk index.
A flexible index is proposed to assess the ecological quality of water and sediments at different spatial scales (i.e., basin and site-specific scales), at different tiers and complexity levels (i.e., screening to site-specific analysis).
Moreover, **the application of multi-criteria analysis allows the definition of robust and transparent procedures**, which can be easily applied to other basins.

Deliverables:

Months 1-18
DD 2.1 Report of critical review of Weight of Evidence approaches and tools (month 10)
DD 2.2 Proposed preliminary Weight of Evidence procedures for Basin scale IRI, Interim Report (month 18)
DD 2.3 Proposed preliminary Weight of Evidence procedures for Site Specific IRI, Interim Report (month 18)

Months 19-36
DD 2.4 Programming of IRI and WoE procedures. Beta prototype (month 30)

Months 37-60
DD 2.5 Experimental application of IRI and WoE procedures to ModelKey basins and sites (month 40)
DD 2.6 Programming of IRI and WoE procedures. Definitive prototype (month 43)
DD 2.7 Weight of Evidence procedures for Basin scale IRI, Theory and application. Definitive Report (month 43)

DD 2.8 Weight of Evidence procedures for Site Specific IRI, Theory and application. Definitive Report (month 43)

WP3 DECIS3 (D3): Development and evaluation of the DECIS DSS (CVR, EWQMA, RIKZ, CSIC, UFZ, ACA, IVB, RIVO, UdB, UA)

DECIS3 concerns the computer development and application of the Decision Support System. Therefore, two tasks are identified: Task 1 concerns the DECIS computer system development, based on DECIS 1 design and engineering phase. Task 2 is focused on the evaluation of the whole system through the application in the three ModelKey case-studies: river Elbe, Scheldt estuary and river Llobregat.

Task 1 – DECIS Computer system development
This activity is based on the design and engineering phase previously performed in DECIS 1, when structure and organisation of the decision system were defined. At this step, **the system is implemented**: databases and information contents of the DSS are created and application programs codex developed.
The software tools developed by MODELKEY subprojects are made available to the user in subsequent steps, for **stand-alone elaboration** and for **creation of sets of results**, not necessarily needing Internet connection. Databases structure, to be referred to on-line or to be downloadable during the decision process, are provided. Links to alternative sources, to enhance the assessment capabilities, such as other tools available on the Web (e.g. GREAT-ER, TERRACE, MULINO, PAEQANN, AQEM), are provided. For the technological development of the system, different software extensions and server technologies can be evaluated (MatLab, Surfer, ArcMap, *Active Server Page*, XLM pages, etc.). The MODELKEY tool will be developed as graphical user interface (GUI) to allow an easy access to the selected models for inexperienced end-users and to provide a common platform for database queries, ordination of existing data and prediction of the biota community according to the environmental characteristics.
For the spatial representation of deliverables, such as thematic cartography of river and basin and visualization of hot spots, **the GIS applications** (ESRI ArcMap for example) may be used. The cartographic presentation of the geographic data are vector-based, and monitored sites are GIS elements identified by a codex and related databases.

Task 2 – Application and evaluation of DECIS DSS
This second task concerns the evaluation of the DECIS DSS through the application in the three case-studies.
In the first phase, the application of all the individual tools and models in the three case studies should be reported in specific format and included in the best practise sections of the DSS. The reporting activity should be performed by the end-users partners (involved in DECIS 3), supported by the developer of the model/tool. At this stage of the project, most of the tools and models developed in ModelKey should be already tested and evaluated in case studies. Only **the IRI index and the prioritisation procedure developed by DECIS still need to be applied**. The

reporting should also highlight limits, requirements for applicability, potentialities and practical difficulties encountered during the application.
In the second phase, the evaluation will mainly concern the functionalities of the overall DSS system. The users will be asked to apply the system and comment on the basis of a predefined questionnaire.
Methodological support will be provided by CVR.

Based on the overall results of ModelKey, the list of recommendations for monitoring biodiversity impacts at basin scale (deliverable of DECIS1) will be revised and completed.

Strength of DECIS 3:

DECIS DSS provides a system in which tools and models for assessing hot spots prioritisation are well combined and integrated, allowing the end-user to easily access analytical tools and models and therefore to assess ecological quality and management objectives at the basin scale.
The application of DECIS DSS in the three case studies will highlight potentialities and limits of the system and applicability to different environments, providing validation to the whole system. **The application of models and tools will guide the development of the DSS based on a learning-by-doing approach**.

Deliverables:

Months 1-18
No deliverables

Months 19-36
DD 3.1 DECIS B prototype release (month 40)

Months 37-60
DD 3.2 DECIS definitive prototype (month 54)
DD 3.3 B prototype end-user evaluation report (month 46)
DD 3.4 Definitive prototype end-user evaluation report (month 58)
DD 3.5 Basin scale IRI application to the three basins (month 51)
DD 3.6 Hot spot prioritisation in three case studies (month 54)
DD 3.7 Site specific IRI application to specific sites (month 54)
DD 3.8 Evaluation of possible interventions on site specific hot spots (month 60)
DD 3.9 Definitive list of recommendations for monitoring biodiversity impacts at basin scale (month 60)

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B.4.2 Demonstration activities

There will be no demonstration activities in MODELKEY in the sense of the EU guidelines for project funding. Nevertheless several key outputs will actually serve as “demonstrations” such as:

- innovative methodologies for key toxicant identification and impact assessment
- integrated exposure and effect models
- GIS-based decision support systems

The tools are designed to assist end-users and scientists in risk prioritisation and decision making. The demonstrations will be incorporated into the training programs.

B.4.3 SP DIS/TRAIN: Dissemination and Training (RIKZ)

DIS/TRAIN work components are structured into two work packages. **DIS/TRAIN 1** focuses on the dissemination of MODELKEY concepts and results to the scientific community, end-users and the public while **DIS/TRAIN 2** is designed to provide training and education programs for a wide variety of participants. A particular focus DIS/TRAIN 2 is on the training of members of environmental agencies and scientists from associated countries ("end users") and the introduction of the MODELKEY Decision Support possibilities to existing networks and institutes of policy makers and environmental management.
Close contacts to end-users of the river basin case studies are embedded as MODELKEY partners by the (1) the Elbe Water Quality Monitoring Agency (EWQMA), (2) the National Institute for Coastal and Marine Management (RIKZ) and its closely collaborating sister organisation RIZA a part of the Ministry of Public Transport and Water Management of The Netherlands and responsible for implementing the Water Framework Directive (WFD), and (3) the Catalan Water Agency (ACA) responsible for monitoring activities in the Llobregat and in charge for the implementation of the Water framework Directive (WFD)
The DIS/TRAIN tasks are excplitly focussed to transfer knowledge to outside of MODELKEY.

Work packages 1-2

DIS/TRAIN 1

Participant	CEFAS	CSIC	RIKZ	RIVO	SPbU	VRI	VUA
Person Months	0.5	1.5	0.5	1	1	0.5	1
Participant	CVR	RIVM	UdG	UFZ			
Person Months	3		0.5	4			

DIS/TRAIN 2

Participant	CEFAS	CSIC	RIKZ	RIVO	SPbU	VRI	VUA
Person Months	0.5	1.5	0.5	2	1	0.5	1
Participant	CVR	RIVM	UdG	DELFT	UFZ		
Person Months	14	2	0.5	4	2		

Introduction

The achievement of a good ecological status of surface waters as demanded in the Water Framework Directive (WFD) and the protection of aquatic biodiversity according to the Convention on Biological Diversity (CBD) at an European scale, requires particular focus on dissemination of knowledge and introduction into the MODELKEY tools towards policy makers, environmental managers and agencies. The WFD obligation to reach the ecological goals, to assess the "good ecological status" or "good ecological potential" are the fields, where the MODELKEY outcome is highly fit to support their decisions and solve their problems.

The developments in MODELKEY are also highly interesting to the scientific communities all over Europe. Because of the regional approach by river basin case studies, both the EU accession countries and the specific interest of northern European and Mediterranean European communities are being addressed.

To achieve this transfer of knowledge to both the excutive and scientific communities, DIS/TRAIN will focus on various lines of communication:

1) Internet site, brochure and concise yearly flyers describing the activities and progres of MODELKEY
2) Dissemination / Publication of results in both international scientific and (national) environmental management journals and 6-monthly news letters.
3) organisation of yearly workshops and two major conferences
4) close contacts with European networks, integrated projects
5) contacts with scientific networks, stakeholders, NGO's, conventions and inter-governmental agreements

Specific objectives

1) To share knowledge with European and world-wide stakeholders in the field of assessing and forecasting the impact of environmental pollutants on marine and fresh water ecosystems and biodiversity
2) To address and to offer environmental agencies and policy makers the fruits of MODELKEY to support their decision-making and problem- solving processes.
3) To optimise communication with end-users

Temporal sequence

Both dissemination and training programs run throughout the course of MODELKEY.

Specific courses and workshops are logically more fruitful when approaching the harvesting time of MODELKEY. Workshops to update interested stakeholders are, however, necessary to get attention and increasing awareness towards the potential of the MODELKEY outcome with respect to more effective environmental management.

WP DIS/TRAIN1 (DT1): Dissemination (CEFAS, CSIC, RIKZ, RIVO, SPbU, VRI, VUA, UFZ, CVR, RIVM, UdG)

Scientific community

Dissemination of concepts and frameworks for risk assessment and consequent decision support, assisted by modelling tools for exposure and effect assessment, and actual experimental and field assessment tools is powerful in strengthening the European Research Area.

Scientists will use all conventional means of dissemination like journals, conferences, workshops and books summarising the results of MODELKEY, as well as Internet-sites as general platforms for dissemination and communication of knowledge. This latter procedure is of specific importance for the dissemination of knowledge to scientific communities in candidate countries, because many scientific journals may not be readily accessible there.

MODELKEY is designed to create generally accessible and closely interlinked databases on key toxicants (KEYTOX) and on the toxic pressure in important European river basins and adjacent coastal zones (BASIN) with links to other European databases (see below). This will provide high quality information for general use at a pan-European scale.

MODELKEY is strongly linked to other European (Research) Networks and Integrated Projects providing a dissemination and exchange of approaches and results over a significant share of the European scientific communities. Examples for interlinked projects are:

- **EU FP5 SedNet**, a demand-driven European Sediment research Network designed to support, catalyse, optimise or facilitate demand-driven research activities, exchange of information between these activities, co-operation between problem solvers and problem owners, dissemination to, and exploitation of knowledge by problem owners, publication of research results and inform public and decision-makers. Several core group members and contractors of SedNet play an important role in **MODELKEY** ensuring that this platform can be used for the dissemination of approaches and results.
- **EU FP6 REBECCA**, a STREP focusing on compilation and analysis of existing information of experimental and field studies with respect to relationships between the ecological and chemical status of surface waters. An intensive data exchange between **MODELKEY** and **REBECCA** will be established for optimised dissemination of results and exploitation of existing knowledge on a European scale. This ensures thatthe innovative outcome of **MODELKEY** will be integrated in data compilation and dissemination by **REBECCA**, while **MODELKEY** will profit from **REBECCA** databases. The co-ordinators of the **MODELKEY** subproject **BASIN**, which focuses on database establishment, and of subproject **EXPO -** focusing on exposure modelling - are also key participants in **REBECCA.**
- **EU FP6 AQUATERRA** is an Integrated Project on understanding river-sediment-soil-groundwater interactions for support of management of water bodies. With respect to the common case study in the river Elbe, **MODELKEY** will help **AQUATERRA** to consider the impact of environmental pollution on the freshwater ecosystem, while **MODELKEY** will profit from **AQUATERRA** results on interactions with adjacent environmental compartments. The co-ordinating institute of **MODELKEY** and several other partners are also engaged in **AQUATERRA**.
- **EU FP6 ALARM**, which was designed to assess large-scale environmental risks with tested methods. The exchange of data and concepts on risk assessment between **MODELKEY** and **ALARM** will stimulate both projects and will promote dissemination of new knowledge. The co-ordination of MODELKEY will be situated in the same research centre as ALARM co-ordination. Thus, an optimal data exchange can be established.

Executive community

The executive community is considered as a "stake holder" in environmental policies. It consists of gouvernmental bodies, which develope policies, and gouvernmental and non-gouvernmental bodies, which have to implement or are faced with these policies.

At a European and world scale this community is organised in international cooperations and conventions. The outcome of MODELKEY is highly relevant to many of these international bodies. The dissemination of knowledge to this community will be organised by thematic and river basin specific outcome of MODELKEY.

The three main communication tasks of DIS/TRAIN1 are:

1) Public communication
    a. One central MODELKEY contact point at the UFZ (coordinators office), stated at the MODELKEY website, E-mails and communication products. This central contact point will alert the specific person(s), workpackage or national contactpersons to elaborate the action asked for (anwering a question, giving a talk to a specific group, organising a specific workshop etc.)
    b. Flyers and a (Internet and E-mail) newsletter on specific results or questions asked (MODELKEY contact point and website, E-mail, personal contacts).
2) Scientific and End-user communication
    a. Yearly, specific workshops, where representatives of the river basin case study areas are invited to discuss the problems and the solutions MODELKEY approach might offer. The items of those workshops will be focused on the project resultas at first and more elaborated in the later stages of MODELKEY. These workshops are explicitly focussing at the communication of MODELKEY with the end-users. The proceedings of the workshops will be published on the MODELKEY website, as concise flyers and more comprehensive newsletters. The first three proceedings wil also contribute to the mid-term review. *The technical workshops of MODELKEY workpackages are <u>not</u> in DIS/TRAIN, but in the individual work packages.*
    b. Two MODELKEY conferences, where the knowledge development will be presented and discussed in relaton to the management problems specific to the river basin case studies (Elbe, Scheldt, Llobregat) and more general with respect to other European river basins. The 1st MODELKEY conference (Month 30) is also the moment of the mid-term review. The 2nd MODELKEY conference (Month 60) presents the over-all outcome of MODELKEY. The proceedings of the conferences are to be published in both scientific and management issues international journals and newsletters.
    c. Case study river basin specific highlights, tuned to the demands of executive community (*e.g.* current status, encountered key toxicants, modelled solutions), in the MODELKEY reports.

3) Networking

   a. setting up close contacts of MODELKEY to other Networks, Ips

   b. contacts with scientific networks, stakeholders, NGO's, conventions and inter-gouvernmental agreements

   c. establishment of end-user communication board

   d. mid-term review organised by the communication board and EU Commission

workshops, conferences and networking

The following, not yet extensively explored list of organisations will be approached specifically to be informed on the outcome, workshops and conferences of MODELKEY:

scientific networks

- **SETAC** (www.setac.org), a worldwide stake holder research network on pollution, life time and effects by chemical compounds, contributed to by both the scientific and executive community. This platform would be ideal to organize specific thematic workshops
- **SEDNET** (www.sednet.org), as mentioned above.
- **ICES (**http://www.ices.dk **)**

international conventions

- **International Commission for the Protection of the Elbe**
- **International Scheldt Commissie** (ISC)
- **Emscommission**
- **International Rhine Commission ICPR (**www.iksr.org**)**
- **International Commission for the Protection of the Meuse (ICBM)**
- **International Commission for the Protection of the Danube River (ICPDR;** www.icpdr.org**)**
- **HELCOM - Baltic Marine Environment Protection Commission**
- **The Convention for the Protection of the Marine Environment of the North-East Atlantic** (**OSPAR;** http://www.ospar.org)
- **International Maritime Organization (IMO;**http://www.londonconvention.org**)**
- **North Sea Ministers Conference**, the cooperation and protection against pollution of the North Sea.
- **The Trilateral Wadden Sea Ministers Conference**, the cooperation and protection against pollution of the Wadden Sea, via the Common Wadden Sea Secretariat (http://www.waddensea-secretariat.org).

(inter)national watersystem management networks

- **EurAqua (the network of European Freshwater Organizations;** www.euraqua.org**)**
- **European Water Association EWA (former European Water Pollution Control Association) (**www.ewaonline.de**)**
- **EurOcean (European Centre for Information on Marine Science and Technology;** www.eurocean.org**)**

- **GLOBWINET - Global Water Information Network; (**www.globwinet.org)
- **European Sea Ports Organisation** (http://www.espo.be), the network of European sea port managers, who are facing the implementation of guidelines and regulations.

industries

- **European Chemical Industry Council** (CEFIC; http://www.cefic.be)

NGO's

- **World Wildlife Fund (WWF,** http://www.wwf.org)

Deliverables

DTD 1.1	M4: MODELKEY Website launch
DTD 1.2	M6/12/18/24/30/36/42/48/54/60: MODELKEY Newsletter
DTD 1.3	M12/22/34/46/56: full scope workshops on MODELKEY progress, open to scientific and executive communities. Progres reports at the MODELKEY website + concise flyers.
DTD 1.4	M30/60: MODELKEY conferences, presenting results, discussing progress and evaluate to remaining time. M30: mid-term review by peers and EU-commission. M60: Conclusive MODELKEY conference. Publication of dedicated proceedings in international scientific and management journals.
DTD 1.5	M3-12: End-user communication board.
DTD 1.6	M30: mid-term review

WP DIS/TRAIN2 (DT2): Training and Education (CEFAS, CSIC,RIKZ, RIVO, SpbU, VRI, VUA, CVR, RIVM, UdG, DELFT, UFZ)

Training and education of scientists and stakeholders (policy makers, environmental managers etc.) from inside and outside the consortium will help to strengthen and integrate both the European Research Area and European conceptual development of decision making on water system management. The anticipated program towards scientific and executive communities is described seperately.

scientific community

The scientific training activities aim typically at

1. young researchers (trainees, student exchange)
2. researchers from candidate countries
3. advisors involved in environmental policy making (environment agencies).

In collaboration with academic teachers **young researchers** will be involved in all subprojects resulting in a hands-on training process and practical experience with scientific reflection. Temporary exchanges of young researchers such as PhD students and postdocs between the partner groups throughout the MODELKEY course will further strengthen their scientific skills as well as their experience in international collaboration. In addition, they are particularly encouraged to participate in specialised MODELKEY courses.

The transfer of know-how in this innovative experimental and field assessment work can be done most effectively by hands-on training in MODELKEY laboratories. Thus, scientists and experts from outside the consortium and particularly from **candidate countries** will be strongly encouraged to participate during certain periods in the laboratory and fieldwork in MODELKEY.

Policy making is usually strongly depending on the knowledge available in **environment agencies**. The researchers and consultants involved represent an excellent transfer route of MODELKEY knowledge towards end-users. They will be notified explicitly on courses introducing the new techniques and decision support models of MODELKEY.

Training stays of one week up to several months can be organised. Possible subjects of these training stays are:

1. Conventional and innovative extraction and fractionation methods,
2. Chemical identification methods,
3. *In vitro* and *in vivo* bioassays,
4. *In vivo* biomarkers– a tool for detecting fish exposure to toxicants,
5. Erosion and sedimentation – experimental and modelling tools,
6. Bioavailability and bioaccumulation,
7. Modern tools in assessment of fish, macroinvertebrate and microphytobenthic communities.
8. Effect modelling

executive community

Education towards policy and decision making is targeted at two major tasks:

1. at the environmental agencies, implementing policies, to elucidate the know-how, practices and possibilities of MODELKEY tools and to assist in particular cases.
2. at the policy making proces, to create awareness of the MODELKEY possibilities to think of both preventive measures and effective problem solving measures.

Training and education will typically be as course or as trainee. Educational MODELKEY guest talks, courses and workshops for scientists and members of environmental agencies will be organised to elucidate the potentials of the MODELKEY toolbox and models in problem solving and decision taking processes. Training subjects are:

1. Application of MODELKEY models in risk assessment
2. Introduction into MODELKEY toolbox

Courses and workshops

Courses will open for general application. They may include those shown below, but also workshops on request, dealing with specific items or solving a particular environmental management problem.

MODELKEY will get in touch with SETAC to organise courses or workshops together with SETAC meetings.

The chouce of courses and workshops will address subjects ranging from purely technical to overall assessments and prognosis.

1. Toolbox and databases

a. The methods of TRIAD-type field assessment and key toxicant identification will be elucidated in discrete courses on either subject. The course is designed for environmental researchers and monitopring authorities, who want to either put the MODELKEY toolbox into practice or need to know the ins and outs of the Toolbox to be able to assess monitoring data, they retrieved from the database.
b. The MODELKEY database query model is subject of the database course. The course will introduce the specifics and (application) possibilities of the database. It is intended for a broad range: researchers to policy makers. The course will be adapted to the discipline of the participants.

2. Effect models – from species to communities

This course will give an overview of innovative modelling tools for the prediction of community effects on the basis of single species toxicity data. The course is designed for ecotoxicologists.

3. Basic and Advanced Exposure Models

An overview on tools will be provided for modelling processes related to the exposure of aquatic ecosystems to environmental pollutants with a specific focus on contaminated sediments. Subjects will be: erosion and sedimentation , transport and fate, transfer between sedimentand biota and food chain accumulation, and integrated exposure modelling on a river basin scale. The course is designed for researchers and modellers in either of the fields, with the intention to bring the different expertises together and to learn from each other, thus strengthening the European research ambition.

4. Integrated risk assessment and decision support systems

This course will focus on the evaluation of biological, toxicological and chemical monitoring data for an integrated risk assessment and the application of decision support systems for better prioritisation of risks and management activities with limited budgets. The course focuses specifically on environmental agencies and decision makers with respect to the DSS tool (IRI application) of DECIS. By the month 46, the preparation and execution of the try-out course on IRI application will be performed.

Deliverable

DTD 2.1: Training stays of young scientists (month 18 – 50)
DTD 2.2: Course on toolbox and databases for scientists and end users (month 36)

DTD 2.3: Course on effect models for ecotoxicologists (month 40)

DTD 2.4: Course on basic and advanced exposure models for scientists and end users (month 45)

DTD 2.5: Course on integrated risk assessment and decision support systems for end users (month 40, month 50)

B4.4 Management activities

The management structure for MODELKEY is described in detail in section B.6. MODELKEY will be co-ordinated at UFZ, where a project office (PO) consisting of the Project Co-ordinator, on part-time (50%) scientific co-ordinator and one part time (50%) project manager. Both positions might be held be the same person. The PO is supported by an administrative group at the UFZ exclusively entrusted with the financial and administrative management of EU projects consisting of three experienced officers.

The second pillar of MODELKEY management is the Project Co-ordination Committee (PCC) which is also headed by the Project Co-ordinator and includes all subproject heads and case study team leaders. This committee assembles a unique group of experienced scientists from all relevant scientific disciplines and with longstanding experience in the co-ordination and participation in large interdisciplinary EU-projects.

To guarantee an **optimised dissemination** of results and a **close integration of the end-users** into the entire scientific, training and dissemination process an **end-user communication board** will be established within the first months of the duration of the project assembling the end-users that are full members of the consortium (EWQMA, CEFAS, RIKZ, and ACA), the Project Co-ordinator and the heads of the subproject DECIS and DIS/TRAIN, which are responsible for the integration and dissemination of MODELKEY scientific results and their translation into an end-user friendly decision support system, as well as external end-users, particularly environmental and water agencies as listed in B3. This end-user communication board will advice all subprojects but particularly DECIS and DIS/TRAIN with respect to dissemination and training programs for end-users and will ensure that new knowledge developed by MODELKEY will directly flow in current and future monitoring programs, risk prioritisation and management options.

B.5 Description of the Consortium

B.5.1 General description of the consortium

We have assembled a unique consortium of 25 partners with outstanding international reputations and proven records in delivering research of highest quality. They all together form the necessary critical mass to realise the Integrated Project MODELKEY. The critical mass, multidisciplinarity, complementary and integrated demand-driven research is guaranteed by a tailored composition of the consortium, which includes

- all scientific and technical disciplines required for the fulfilling of the project objectives, including environmental and analytical chemistry, ecotoxicology, cellular toxicology, freshwater- and marine ecology, fish, invertebrate and algae taxonomy, theoretical biology, hydraulics and sediment physics, exposure and effect modelling, risk assessment and management, and socio-economy.
- partners with complementary skills including field and laboratory science, numerical analysis, modelling, social sciences and management.
- partners highly experienced in managing or participating in international and multi-disciplinary projects
- the leading European institutes in all key issues of the project.
- partners from all European regions including Central and Western Europe and the Mediterranean region, where the case studies will be run but also Eastern and Northern Europe for an optimal dissemination of tools and results.
- partners from 13 European countries including 9 EU Member States (Germany, Austria, Belgium, United Kingdom, Netherlands, France, Italy, Spain, Finland), 3 candidate countries (Switzerland, Czech Republic and Slovakia) and one INCO target country (Russia)
- the governmental authorities responsible for the implementation of the waterframework directive (WFD) in the river basins under investigations in the case studies
- 3 experienced SMEs as full partners and one more as subcontractor.

B5.2 Participant description, suitability and commitment of key personal to assigned tasks

A consise summary of all MODELKEY participants is given in Table B5.1. Their expertise and contribution is summarised in Table B5.2. For detailed participant descriptions see Annex B5.

Table B5.1: General information on MODELKEY participants

No	Acronym	Institute	Country	Key persons in the project
1	UFZ	UFZ Centre for Environmental Research Leipzig, Department of Chemical Ecotoxicology	D	W. Brack, M. Schmitt, K.-D. Wenzel, A. Paschke, G. Schüürmann, R. Altenburger

2	UA	University of Antwerp, Department of Biology - Ecosystem Management Research Group	B	P. Meire, E. de Deckere
3	CEFAS	Centre for Environment, Fisheries, and Agriculture	UK	K.V. Thomas
4	DELFT	Delft Hydraulics	NL	A. Baart, J. Boon
5	CVR	Consorzio Venezia Ricerche	I	C. Carlon
6	VUA	Vrije Universiteit Amsterdam Faculty of Earth and Life Sciences, Department of Theoretical Biology and Institute for Environmental Studies	NL	S. Kooijman, T. Jager, B. v. Hattum, M. Lamoree
7	CNRS	Centre National de Recherche Scientifique	F	S. Lek, S. Brosse, G. Loot, M. Gevrey
8	CSIC	Instituto de Investigaciones Quimicas y Ambientals J.P. Vila Consejo Superior de Investigaciones cientificas	E	M. Lopez de Alda, D. Barcelo
9	UdG	Universitat de Girona Department of Environmental Science and Institute of Freshwater Ecology	E	S. Sabater
10	UB	University of Bern, Centre for Fish and Wildlife Health	CH	H. Segner
11	VRI	Veterinary Research Institute	CZ	M. Machala, J. Vondráček
12	IVB	Institute of Vertebrate Biology, Academy of sciences of the Czech Republic , Department of Fish Ecology	CZ	P. Jurajda
13	UJOE	University of Joensuu, Department of Biology	FIN	J. Kokkonen, M. Leppänen, T. Ristola
14	EWQMA	Elbe Water Quality Monitoring Agency	D	B. Frank, B. Stachel
15	RIKZ	National Institute for Coastal and Marine Management	NL	J.F. Bakker
16	RIVO	Netherlands Institute for Fishery Research	NL	P. Leonards, E. Winter
17	SZU	National Reference Centre for Dioxins and Related Compounds Institute for Preventive and Clinical Medicine Slovak Medical University	SK	A. Kočan, J. Petrik
18	RIVM	Rijksinstituut voor Volksgezondheid en Milieu	NL	D. de Zwart, L. Posthuma
19	UoS	University of Stuttgart Hydraulic Laboratory Department Institut of Hydraulics Faculty of Civil Engineering and Environmental Science	D	B. Westrich
20	SPbU	St. Petersburg University Department of Chemistry	RUS	V. Nikiforov
21	UdB	University of Barcelona	E	Isabel Muñoz
22	ACA	Agencia Catalana de l'Aigua	E	A. Gibreda
23	ECT	ECT Oekotoxikologie GmbH	D	T. Knacker
24	XEN	Xenometrics GmbH	CH	S. Flückiger
25	DW	Donabaum&Wolfram OEG, Technisches Büro für Ökologie	A	C. Orendt, G. Hofmann, K. Donabaum, G. Wolfram, S. Höß

Consortium Expertise

MODELKEY brings together the leading European groups in (1) **effect-directed analysis (EDA)** including experts in *in vitro* and *in vivo* biological detectors, physico-chemical fractionation procedures and chemical analysis, (2) **fish, invertebrate and microbial ecology and ecotoxicology**, (3) **exposure assessment of sediment-associated toxicants**, (4) **effect modeling**, (5) **exposure and risk models and (6) decision support systems**. Here we describe their expertise and complementary skills.

(1) Effect-directed analysis (EDA). The MODELKEY consortium assembles all leading European groups in the field of EDA. Subproject KEYTOX, which is responsible for EDA is designed in order to provide a toolbox of standardized, generally applicable and inter-compared methods as well as highly innovative and sophisticated methods for answering specific questions. This is reflected also by the expertise of the consortium. While a number of basic methods and skills are available for most or several KEYTOX participants allowing the establishment of standardized or intercompared protocols for EDA application all over Europe, each participant has also unique and outstanding expertise in specific methods. Experts in the development and application of specific high throughput *in vitro* test systems as biological detectors in EDA are **VRI (M. Machala)** (tumor promotion, inhibition of gap junctional intercellular communication, Ah-receptor-mediated effects, hormonal disruption), **XENO (Sini Flückiger)** (high throughput AMES test), **VUA** (Marja Lamoree) (neural and immuno toxicity, hormonal disruption), and **CEFAS (K. Thomas)** (estrogenic and androgenic effects). **CEFAS** and **RIKZ (J. Bakker)** are experienced in marine and freshwater *in vivo* tests for EDA. **UFZ (W. Brack)** and **CEFAS** have outstanding experience in the development of tailored fractionation procedures based on preparative HPLC and GC methods. Receptor- and immunoaffinity SPE and HPLC will be provided by **RIKZ** and **CEFAS**. For chemical analytical identification of so far unknown toxicants most groups are experienced in GC-(EI)MS and LC-DAD. Specific expertise is provided by **RIVO (P. Leonards)** (GC*GC-ToF MS), **CEFAS** (GC-(NCI)MS, LC-MSMS), **CSIC (D. Barcelo)** (LC-APCI-MS, LC-IP-ESI-MS), and **UFZ (G. Schüürmann)** (computer tools). **SpbU (V. Nikiforov)** contributes its unique expertise in the synthesis of commercially non-available standards and structure elucidation by NMR. **RIKZ** will be responsible for the establishment of the key toxicant database.

(2) Fish, invertebrate and microbial ecology and ecotoxicology. The MODELKEY consortium assembles outstanding experts in freshwater and marine ecology and ecotoxicology with focus (i) on an expertise in the specific river basin, where the case studies are run, (ii) on taxonomy and community assessment for the major groups of organisms in the focus of MODELKEY including microbenthos, benthic invertebrates and fish, and (iii) on innovative concepts for linking laboratory toxicity testing to community effects in the field including *in situ* biomarker analysis, *in situ* functional parameter assessment such as reproduction and growth and pollution induced community tolerance (PICT).

(i) Specific river basins. The MODELKEY consortium involves experts with longstanding experience with the ecosystems in the basin of the Llobregat (**UdG (S. Sabater)** and **UdB (I. Munoz)**), the Scheldt (**UA (E. de Deckere)** and **RIVO (E. Winter)**), and the Elbe (**DW (C** and **IVB**).

(ii) Taxonomy and community assessment. Outstanding taxonomic expertise for phytoplankton and microbenthic communities are contributed by **DW (G. Hofmann, C. Orendt)** and **UdG**. For benthic macroinvertebrates, **DW**, **UA**, and **UdB (I, Munoz)** contribute taxonomic expertise and longstanding experience in community assessment. **IVB (P. Jurajda)** and **RIVO (E. Winter)** contribute their expertise in fish taxonomy and fish community assessment.

(iii) Innovative concepts. Since it is evident that there is a gap between toxicity as measured in laboratory *in vitro* and *in vivo* assays and alterations of communities *in situ* and since an establishment of cause-effect relationships between biodiversity decline *in situ* and toxic contamination seems to be impossible MODELKEY develops and applies innovative concepts to fill this gap. This includes *in situ* biomarker assessment and the *in situ* measurement of functional parameters related to reproduction and growth for fish run by the **UB (H. Segner)**, the application of the PICT concept by experts from **UFZ (M. Schmitt-Jansen)** and **UdG (S. Sabater)**, and micro- and mesocosm studies by **DW**, **UA** and **UFZ**.

In vitro and *in vivo* testing is contributed by KEYTOX participants (see above) **UJOE (J. Kokkonen)** with experience in sediment contact tests and **ECT (T. Knacker)** contributing their experience in testing toxicity on feeding rates, growth, reproduction, and development of organisms of different trophic levels. This expertise will ensure a calibration and verification of canonical community and food chain effect models run by **VUA (B. van Hattum)**.

(3) Exposure assessment of sediment-associated toxicants. MODELKEY assembles groups with longstanding and internationally recognized experience in (i) sediment hydraulics that provide powerful methods for the analysis of erosion and sedimentation processes (**UoS, B. Westrich)**), (ii) bioavailability of sediment-associated toxicants (**UJOE**), biomimetic tools for passive sampling of bioavailable compounds (**RIKZ, CEFAS, UFZ**) and food chain accumulation assessment (**VUA**). This excellent group is supplemented by experienced chemical analytical groups including **SZU, RIVO, CSIC, CEFAS, UFZ** and others.

(4) Effect modelling. Worldwide unique expertise in modelling effects on populations, communities and ecosystems is involved in MODELKEY. This includes (i) the inventor of the concept of dynamic energy budgets (DEBs) (**VUA**, **B. Kooijman**) contributing his outstanding expertise for the development of functional-based models for a better understanding of community effects on the basis of canonical communities and simplified food webs, (ii) the world leading group standing for the concept of species sensitivity distributions (SSDs) (**RIVM, D. de Zwart, L. Posthuma)**) and for international experience in the integrated diagnosis of observed effects on community patterns, and (iii) **CNRS (S. Lek)**, who invented neural artificial networks as a powerful tool for the prediction of toxic effects to communities on the basis of existing monitoring data sets.

(5) Exposure and risk models Highest quality state-of-the-art exposure modelling in MODELKEY is ensured by **DELFT (A. Baart)**, that is one of the leading European institutes in this field and will lead the subproject EXPO. The following groups with outstanding and internationally recognized expertise in their specific fields will contribute: **UoS**, as an expert in erosion and sedimentation modelling and **VUA**, that is highly experienced in food chain accumulation modelling. The responsibility of two closely collaborating departments of **VUA (B. van Hattum)** for food web effect and for food web accumulation modelling ensures maximal synergies and significant added values for both approaches.

(6) Decision support systems. Innovative decision support systems will be delivered by **CVR (C. Carlon)**, a very experienced interdisciplinary group assembling environmental scientists, risk assessors and managers and socio-economists. This expertise is further increased by integrating the Interdepartmental Centre for Sustainable Development at the University Ca' Foscari of Venice (IDEAS) as a subcontractor with outstanding economic and socioeconomic expertise. An optimal exploitation of the results for decision making and management is achieved by the involvement of end-users from every river basin and adjacent coastal area in the focus of MODELKEY including **EWQMA**, **RIKZ**, and **ACA** as full partners and several environmental agencies and companies in close contact with MODELKEY as end-users and advisors. **EWQMA (B. Frank)** and **RIKZ (J. Bakker)** will contribute their outstanding expertise in database building, which is crucial to the success of MODELKEY.

Table 5.2: Summary of expertise and tasks of MODELKEY participants

Acronym	Areas of expertise relevant for the role in MODELKEY	Main contribution to MODELKEY
UFZ	National research centre exclusively devoted to environmental research Co-ordination of large national and international projects Effect-directed analysis Computional toxicology and probabilistic risk assessment Biomimetic passive sampling, bioavailability assessment and extraction and analysis of complex biological matrixes Effect propagation on higher levels of biological organisation,	Project co-ordination and management KEYTOX: HPLC- and GC-based fractionation procedures and computer tools for toxicant identification. SITE: Subproject head SITE 2: Analysis of internal toxicant concentrations in biota and application of biomimetic passive samplers. SITE 3: Microbenthic community assessment and application of the pollution induced community tolerance (PICT) concept. Special focus on algae. Food web assessment on the basis of biofilms and grazers.
UA	Methodologies for quality and risk assessment of sediments. Biotic indices for water- and sediment quality. Impact of pollution on nature development in floodplains, marshes, streams and lakes. Bioavailability of pollutants.	BASIN: Subproject head, data compiling for Scheldt case study SITE 1: Assessment of erosion stability SITE 4: *In-situ* assessment of communities at the Scheldt estuary. Biotic indices for water- and sediment quality
CEFAS	Multidisciplinary scientific research and consultancy centre specialising in fisheries science, environmental management and marine monitoring and assessment Environmental management Monitoring and assessment of hazardous substances and effects in marine environment. Effect-directed analysis.	KEYTOX: Subproject head KEYTOX: Development and standardisation of sampling, extraction, fractionation and identification tools
DELFT	Research institute and specialist consultancy Dynamical numerical, deterministic and expert modelling approaches used for linking water quality and hydrological parameters to biological groups and habitat requirements.	EXPO: Subproject head EXPO: Exposure and risk modelling using the models E-USES, MamPec, REMA, GEMCO. Uncertainty assessment.
CVR	Research organization including the two Universities of Venice and the Municipality of Venice Research on risk assessment/management GIS-based decision support systems for the rehabilitation of contaminated sites (sediments and industrial megasites)	DECIS: Subproject head DECIS: Decision support systems and integrated risk index
VUA	Mechanistic community models based on dynamic energy budget (DEB) theory and DEBtox software package Chemical analytical and biological *in vitro* methods for trace pollutants. Effect-directed analysis. Experimental and modeling expertise on chemical fate, bioaccumulation and food chain transfer.	EFFECT 3: Modelling of effects on canonical communities and artificial foodwebs KEYTOX: *In vitro* biotest development and application. Development of fractionation techniques. EXPO 3: Foodweb accumulation modelling SITE 2: Experimental assessment of bioavailability and bioaccumulation
CNRS	Research on biodiversity and ecosystem functioning. Structure of biodiversity and ecological communities at global, regional and local scales of fish and macroinvertebrate in freshwater systems. Modelling techniques. Machine learning methodology, especially artificial neural networks (ANN).	EFFECT: Subproject head EFFECT 2: Component models for predicting effects on species success and community composition applying ANN

CSIC	Advanced analytical chemistry based on mass spectrometric analysis and biosensors, Effect-directed analysis Evaluation of the sources and distribution of pollutants by chemometric analysis and modelling. LC-MS integrated systems is the main tool of the research group	KEYTOX1: Development and application of innovative LC-MS/MS methods for the identification of polar compounds. BASIN, SITE: Responsibility for collection of monitoring data and site investigations in the Llobregat
UdG	Stream ecology and ecotoxicology with focus on biofilms (algae, bacteria, fungi). Indicators of biofilm structure and functioning. Diagnosis of effects on natural communities. Studies in the River Llobregat on algal (diatom) and cyanobacterial communities.	SITE 3: Investigation of toxic effects on structure and function of microbenthic communities in the River Llobregat. Special focus on bacteria and funghi. Application of the PICT concept.
UB	Pathology and toxicology of fish. Biomarker responses as indicators of environmental pollution. Ecoepidemiological studies on the impact of endocrine-disrupting chemicals on fish populations	SITE 5: Biomarkers in fish. *In situ* fish growth and reproduction assessment including fecundity and fertilisation success, and population structure analysis.
VRI	Toxicological and ecotoxicological assessment of xenobiotics using specific biochemical and cellular *in vivo* and *in vitro* biomarkers of toxicity mechanisms. Trace chemical analyses, bioassay-directed analysis.	KEYTOX: Development of innovative *in vitro* biotests and application for key toxicant identification SITE 5: *In vitro* testing of sediment, biota and water extracts for dioxin-like activity, estrogenicity, mutagenicity, and tumor promotion. SITE 2: Chemical analysis of key toxicants.
IVB	Fish biology, taxonomy and ecology Early life stages and reproduction of fish Revitalisation of rivers. Local knowledge of sites and communities in the River Elbe.	SITE 5: *In situ* assessment of fish communities in the River Elbe case study. Coordination of sampling activities in the Czech part of the River Elbe basin.
UJOE	Aquatic ecology and ecotoxicology. Bioavailability assessment and sediment toxicology. Fate and effects of xenobiotics in aquatic systems (water phase and sediment).	SITE 2: Bioavailability of sediment-associated compounds in relation to sediment properties. SITE 4: Sediment contact tests with invertebrates.
EWQMA	Collection, assessment, and publication of monitoring data in co-operation with the seven countries Saxonia, Sachsen-Anhalt, Lower Saxony, Brandenburg, Mecklenburg-Vorpommern, Hamburg and Schleswig-Holstein. Close co-operation with Czech authorities Povodi Labe and Povodi Vlatavy since 1993.	BASIN: Establishment and maintenance of the MODELKEY database. BASIN: Collection of chemical, biological and toxicological monitoring data and integration in modelling approach. DECIS: Enduser of results of the Elbe case study
RIKZ	National knowledge and consultation centre in the proces of policy decision making and management of the marine and estaurine areas. Advisory and Management, Development and Strategy, Monitoring and Information management. Environmental risk assessment. Identification of "unknown" compounds with detrimental effects (effect-priority compounds).	KEYTOX1-3: Various tools for key toxicant identification KEYTOX 4: Establishment of the key toxicant database. BASIN: Monitoring data from the Scheldt river basin, estuary and adjacent coastal area. DECIS: End-user of results of the Scheldt case study

RIVO	Multidisciplinary research and consultancy organisation on fish and the environment, fate and occurrence of contaminants in the aquatic environment, health of fish, and risk assessment. Anthropogenic and naturally induced changes in annual fish population/community and impacts on the coastal zone. Monitoring of hazardous substances in the aquatic environments for a variety of chemicals. Novel analytical methods for the identification of "unknown" compounds in the environment.	KEYTOX: Innovative analytical methods for key toxicant identification SITE 2: Bioavailability assessment using biomimetic tools. Chemical analysis of heavy metals, PCBs, PAHs as well as of novel compounds such as flame retardants, pharmaceuticals, fluorinated compounds. Scheldt case study SITE 5: Assessment of fish community in Scheldt estuary.
SZU	Incorporated in the EU Centre of Excellence in Environmental Health Research at IPCM since 2002 Outstanding analytical experience. Analysis of dioxins and Related Compounds.	SITE 2: Analysis of dioxins, PCBs and related compounds. HRGC/HRMS analysis.
RIVM	Probabilistic risk assessment Effect modelling on the basis of species sensitivity distributions (SSDs). Eco-epidemiology	EFFECT 1: Integrated diagnosis of observed effects on community patterns DECIS 2: Integrated risk indexes
UoS	Contaminated sediment issues in water resources engineering and management. Transport dynamics of dissolved and particulate contaminants. Combined stochastic and deterministic approach for assessing flood erosion potential and risk of environmental impact . Physical, geochemical and biological factors influencing erosion stability of cohesive fluvial sediments.	EXPO 1/2: Modelling of erosion, transport and retention of contaminated sediments. Risks of sediment remobilisation. Fuzzy logic modelling SITE 1: Experimental assessment of sediment stability, erosion and sediomentation processes.
SPbU	Synthesis of a wide variety of organic chemicals. Structure-property relationships NMR applications for structure analysis.	KEYTOX: Synthesis of key toxicants. Special focus on polyaromatic isomers, which are commercially not available..
UdB	Stream and river ecology. Nutrient dynamics, riparian influences, ecotoxicology, river water quality, and dynamics of biological communities. Biology and ecology of invertebrates (micro, meio and macrofauna) and their interactions with natural biofilms	SITE 3: Effects on food chains based on biofilms and interacting meiofauna SITE 4: In situ assessment of invertebrate communities. Ecological indexes. Case study leader for the Llobregat
ACA	Environmental agency responsible for WFD implementation at the river Llobregat	BASIN: Monitoring data for the Llobregat river basin DECIS: End-user of results from the Llobregat case study
ECT	SME for ecotoxicological services for industry and governmental authorities including environmental risk assessments. Development of new ecotoxicological testing methods under laboratory and field conditions, e.g. bio-accumulation and toxicity in sediment dwelling organisms, biodegradation of chemicals in surface water and sediment, biodegradation of organic matter under field conditions, determination of endocrine effects in fish and determination of fate and effects of chemicals in terrestrial and aquatic mesocosms.	EFFECT 3: Analysis of effects of key pollutants on feeding rates, reproduction and growth of bacteria, algae, invertebrates and fish as input to canonical and food chain effect models. Mesocosm studies.

XEN	SME developing and applying high-throughput mutagenicity tests	KEYTOX: Mutagenicity testing with high-throughput Ames II test
DW	SME for limnological and water quality assessment focused on *in situ* bioindication based on aquatic algae and invertebrates including special groups (e.g. chironomids). Outstanding taxonomic expertise for algae and invertebrates Development of biological water assessment methods for the purpose of the EU-WFD.	SITE 3: Assessment of algae communities and species composition SITE 4: In situ effects on macroinvertebrate communities. Ecological indexes.

B.6 Description of Project Management

Project Management and Decision-Making Structures

The Project Management structure of MODELKEY is summarised in Fig. B.6.1. It contains all central elements of management and decision-making.

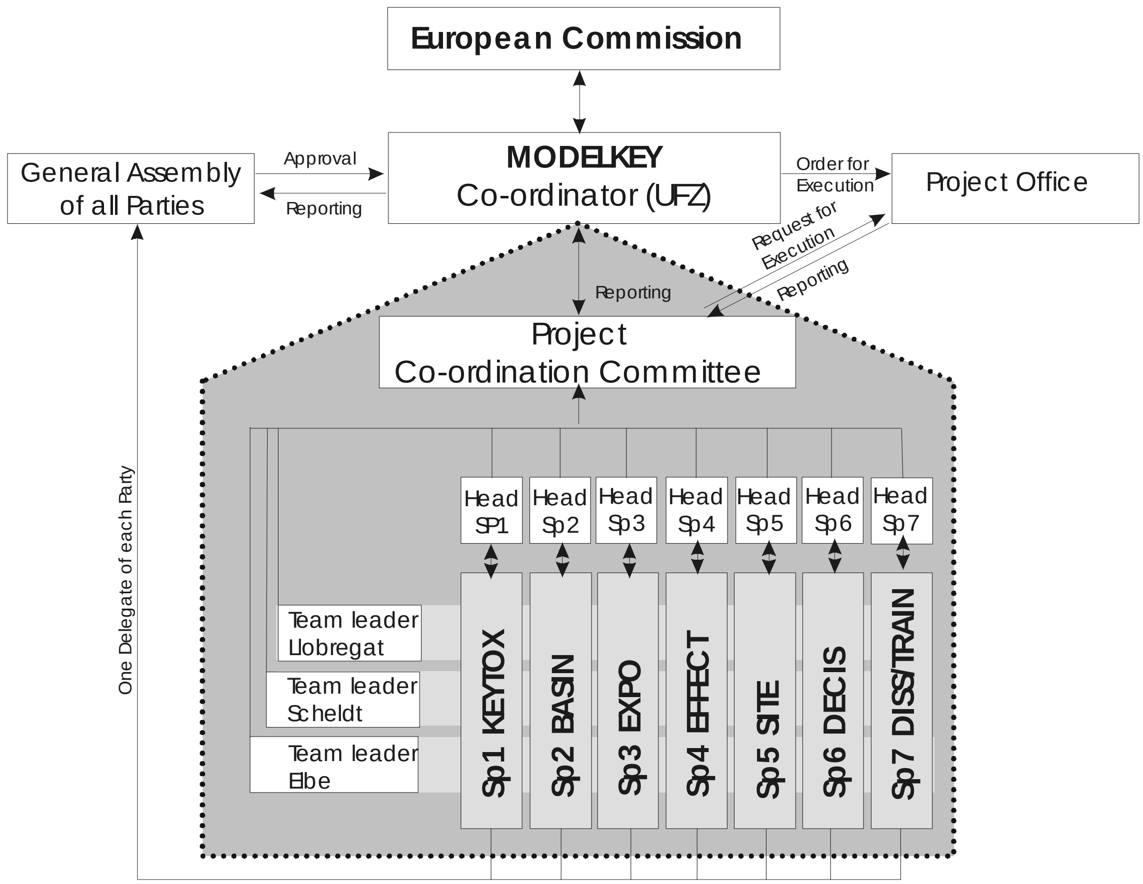


Figure B.6.1: Management structure of MODELKEY

Organisation Structure

MODELKEY requires very close integration across subprojects and thematic work packages as well as across different research sites/areas, and this has been carefully considered in the proposed organisation structure. The co-ordination structure of MODELKEY is based on experience gained from managing other major research projects with similarly rigorous requirements.

The Co-ordinator

The Project Co-ordinator, Werner Brack, will be the overall scientific and administrative co-ordinator of the project and will be the responsible contact person for the European Commission. He will supervise the scientific objectives of the project and organise the work of the Project Co-ordination Committee (PCC) and of the Project Office (PO). Werner Brack will be assisted by a highly qualified research team of the Department of Chemical Ecotoxicology. This team is very experienced in the scientific co-ordination of large interdisciplinary research projects and has been involved in many international projects, including EU – projects within the 4th, 5th and 6th framework programme (e.g. EUFRAM, BEAM, HAIR), co-ordinating several of them (CELLECOTOX, TUBERCOLOSIS).

The Project Co-ordination Committee (PCC)

The central body responsible for monitoring and evaluating project progress and supervising project objectives is the Project Co-ordination Committee (PCC), which takes the necessary decisions in scientific co-ordination and administration of the project. The PCC prepares the annual reports and updates of the implementation plan that have to be decided by the General Assembly. The PCC consists of the Project Co-ordinator, one part time (50%) scientific co-ordinator (PostDoc level, funded by the UFZ) and the heads (and deputies) of the subprojects who take major responsibility for overseeing their respective subproject and the case study leaders. The Project Co-ordinator (Werner Brack) heads both the PCC and the Project Office (PO).

The Project Office (PO)

The Project Office supports the co-ordinator in the day-to-day operational management of the project and handles the administrative management. The PO consists of the project management team, comprising of a part-time (50%) position of a project manager (potentially the other 50% part time position in the scientific project co-ordination might be held by the same person) and a part time (50%) position for the daily technical administration business (in total 0.5 position funded by the EC). A full time secretary is employed at the Department of the co-ordinator and will provide additional administrative support for the PO if needed for correspondence, project organisation, workshops, and meetings. Furthermore administrative staff of the UFZ is member of the PO, including representatives of the following departments: finance department, legal department, EU office, public relations and personnel office. Members of these departments contribute to the work of the PO as required during the course of the project. The work effort comprises approximately the equivalent of about 0.5 persons (or 6 PM per year). Experiences staff of these departments will work closely with the designated other Project Office staff and the MODELKEY co-ordinator.

Especially, the PO members

- guarantee adequate administrative project controlling and
- take care of financial and budgetary matters.

As a large research institute, the UFZ administration is highly experienced in all aspects of the management of major research projects. Since its foundation in 1992 UFZ has participated in 53 EU projects, co-ordinating 15 of them. 22 of these projects (7 co-ordinated by UFZ) were funded under the fifth framework programme. In the sixth framework programme, UFZ is up to now involved in 9 projects, co-ordinating ALARM, an Integrated Project of 53 partners from 26 countries which has just started. Hence, UFZ is experienced in all means necessary for managing an Integrated Project such as e.g. communication and decision making involving all participants and negotiating the consortium agreement.

The General Assembly

The General Assembly (GA) is the highest decision-making body in the consortium and comprises all project partners, who are also eligible to vote on propositions presented to the GA. The GA takes decisions on the following:

- Annual implementation plan
- Expansion of the consortium or exclusion of partners from the consortium
- Premature end of the project
- Modifications of the Consortium Agreement
- All matters of fundamental importance to the consortium

Decisions of the GA on the above matters requires a two-third majority of the project partners based on the principle "one partner – one vote". Partners have to be in the project at the meeting date of the GA. Partners which have left the project already or are not yet partners have no vote. The requirement of a two-third majority ensures a fair distribution of interests within the consortium.

The end-user communication board

An end-user communication board will accompany the project. The board will consist of the Project Co-ordinator (UFZ), the heads of the subprojects DECIS (CVR) and DIS/TRAIN (RIKZ), the end-users that are full members of the MODELKEY consortium (EWQMA, ACA, CEFAS and RIKZ) as well as a group of external end-users such as listed in section B3. (As this is an open board, it is not included in Fig B6.1 presenting the formal management structure.)

Progress Monitoring, Decision-Making Structures, Conflict Solution and Quality Control

The **main element of scientific project controlling and decision-making** is the PCC. The **PCC** takes all decisions about project progress, distribution of tasks, monitoring and re-organising of specific tasks if necessary and in all cases that do not require the voting of the General Assembly. In case of disputes about allocation of tasks which cannot be solved on the level of the work package or subproject, the MODELKEY co-ordinator and the PCC will immediately be informed and will be responsible for solving the issue taking into account the most effective solution for achieving the MODELKEY objectives. On the yearly update of the implementation plan or major issues of the work plan like exchange of participants, the General Assembly will decide. The work plan of MODELKEY has already been developed in detail by all partners, as can be seen in B4.

The PCC is composed of the MODELKEY co-ordinator, the scientific co-ordinator, the heads of the subprojects and the case study team leaders including 12 members from 8 European countries (Table B6.1). For each subproject head a deputy is appointed standing in for him in the PCC in the case of unavailability.

The PCC meets twice a year: one meeting connected with the main workshop and an additional one. The PCC makes decisions, based on a simple majority, on all matters pertaining to the scientific and administrative management of the project. It also decides on propositions to be voted on by the General Assembly (GA) (see below), in particular the annual implementation plan to be submitted to the Commission and the acceptance or elimination of partners.
In close co-operation with the Project Co-ordinator, the PCC is responsible for the overall supervision of the scientific content and budget as well as the co-ordination of all activities carried out by the MODELKEY partners within the various subprojects.

The **subproject level** is based on scientific tasks or areas of specialisation and ensures efficient management of the project. Research will be conducted within work packages which will be headed by partners with long-term research and co-ordination experience in the relevant fields.
The project will consist of 7 subprojects, with 5 subproject focusing on the scientific key issues of MODELKEY and 2 cross-cutting subprojects of highly integrative character. The head of each subproject and his deputy co-ordinate the activities of the project partners within that particular subproject and ensure that assigned scientific tasks and budget matters are effectively controlled.

The work within the **case studies** in the basins Elbe, Scheldt and Llobregat (data gathering, logistics, permits, local users) will be co-ordinated by a case study team leader with a tradition in research in the particular sites and strong links to local land users and managers. All of these case study team leaders will be members of the PCC (Table B.6.1).
If unforeseen difficulties arise, a case study team leader will consult at the earliest possible time with all teams co-ordinated by him. Decisions will be made in the same way as within the subprojects. If there are implications beyond his co-ordination responsibility, he will also consult immediately with the subproject head to raise the matter within the PCC and/or consult the co-ordinator.

The head (and deputy head) of the **subproject** collects all audits, reports and other information generated within the subproject and ensures that the subproject partners fulfil their legal and contractual obligations towards the Commission and the other project partners. The reports and audits must be submitted to the Project Co-ordinator at least 3 weeks before the deadline. After the Co-ordinator and, where necessary, the PCC have checked their scientific content and legal implications, all these materials and documents are forwarded to the Commission. The PCC can refuse to accept documents if they do not meet the desired scientific quality or the legal requirements of the Commission or if they do not correspond to decisions previously made by the GA.

High scientific quality will be guaranteed by the fact that all collaborators in this consortium are highly motivated individuals and leading European scientists who have successfully devoted their careers to understanding fundamental problems in environmental science. In addition, the future careers of all depend greatly on maintaining a high output of innovative fundamental and applied environmental research that is published in the leading peer reviewed journals. This in itself provides additional "automatic" control of quality, guaranteed by the international review system. Quality control of methodological approaches and data is part of the work plan. Technical meetings will organised for standardising sampling methods and controlling quality of data.

To guarantee (1) an optimised communication between science and end-users (2) targeted dissemination of MODELKEY results and innovative tools, (3) high value training activities for end-users and (4) a rapid conversion of new scientific knowledge in current and future monitoring programs, risk assessment and prioritisation as well as management activities by environmental agencies a **end-user communication board** is established within the first months of MODELKEY (see Fig. B.6-1). It will assemble the Project Co-ordinator (UFZ), the heads of the subprojects DECIS (CVR) and DIS/TRAIN (RIKZ), the end-users that are full members of the MODELKEY consortium (EWQMA, ACA, CEFAS and RIKZ) as well as a group of external end-users such as listed in B3. RIKZ is the most important end-user in the Scheldt river basin and at the same time head of the subproject DIS/TRAIN on result dissemination and training ensuring an optimal flow of knowledge and demands between scientists and end-users.

Table B.6.1: Members of the MODELKEY PCC

Co-ordination	**PCC members**	**Deputies**
General management	Werner Brack (UFZ, D)	Mechthild Schmitt-Jansen (UFZ, D)
Scientific Co-ordinator	NN (UFZ, D)	-
Subproject heads		
KEYTOX	Kevin Thomas (CEFAS, UK)	Maria Lamoree (VUA, NL)
BASIN	Eric de Deckere (UA, B)	Barbara Frank (EWQMA, D)
EXPO	Arthur Baart (Delft, NL)	Bernhard Westrich (UoS, D)
EFFECT	Sovan Lek (CNRS, F)	Bas Kooijman (VUA, NL)
SITE	Mechthild Schmitt-Jansen (UFZ, D)	Helmut Segner (UB, CH)
DECIS	Claudio Carlon (I, CVR)	Dick de Zwart (RIVM, NL)
DISS/TRAIN	Joop Bakker (RIKZ, NL)	Barbara Frank (EWQMA, D)
Case study team leaders		
Elbe basin	Pavel Jurajda (IVB, CZ)	Miroslav Machala (VRI, CZ)
Scheldt basin	Erwin Winter (RIVO, NL)	Eric de Deckere (UA, B)
Llobregat basin	Isabel Muñoz (UdG, E)	Maria Jose Lopez de Alda (CSIS, E)

Communication flow, partnership meetings, workshops and reporting

Communication flow

A full position (twice 50% part-time) for the MODELKEY management in the PO (Project Office) will be responsible for **maintaining regular contact** with the PCC members - by phone, letter, and email, ensuring all partners keep to work schedules as listed in the proposal and also to be agreed at partnership meetings, and ensuring that all reporting deadlines are understood and adhered to by all partners. In addition, she/he will be responsible for the **communication flow** by setting up a system for exchange of data, results, co-ordination decisions, and information material, and for reporting among partners primarily using email and the Internet:

- all partners have a well functioning email,
- an internal webpage (only accessible for project members) will be installed and regularly updated by the manager as well as a generally accessible webpage for the interested public to be designed together with partners of the subproject DISS/TRAIN.

Part of the consortium co-ordination will be the establishment of an open electronic communication platform to enhance data access and broad discussion possibilities whenever needed – in a consortium as voluminous as this the need might arise.

Meetings, workshops, conferences and staff exchange

Within the first two months of **MODELKEY** a **start-up meeting** for the whole consortium will be organised, where the first scientific activities will again be discussed and agreeded on in all details.

Each year, there will be one **main workshop** for the whole consortium (GA) and an additional meeting of the PCC. These meetings will review progress and control quality of results. Further **technical meetings** on the subproject level and across subprojects and work packages will take place to standardise sampling methods, to control quality of data, and to exchange results. They are called by the respective head of the respective subproject. Additional **status review meetings** every 6 months may be demanded by the PCC.

For standardisation of methodology and approach and data integration, there will be an **exchange of scientists** among partners for extended periods (activities within DIS/TRAIN 2). National teams will further consult regularly with local managers. Two main **conferences** will be organised to discuss results within the whole consortium and with the scientific community and a broad group of users. Meetings will take place in as many different participating member states as possible.

Reporting

There will be three **levels of regular reporting** within MODELKEY. An annual report will be prepared for internal reporting and reviewing and for the EU. After 18 months and after year 3 there will be larger mid-term reports and at the project's end a final report to the EU. We will implement an additional e-mail based 6-monthly brief reporting system to ensure that time and work schedules are maintained. A mailbox for continuous information exchange will be established.

Consortium agreement and plan for the management of knowledge, of intellectual property and of other innovation-related activities arising in the project.

Consortium Agreement

The entire work plan of MODELKEY has been established in close collaboration of all participants. Hence, the details description of the implementation plan is the well elaborated basis for the scientific co-operation. The management structure has been established in a way that it directly represents the management structure used in the consortium agreement.

The consortium agreement used for MODELKEY is strongly based on the consortium agreement elaborated by a consortium of German research organisations, universities and industry which is one of the most frequently used model consortium agreements in Europe at the moment. This consortium has been headed by the Hermann-von-Helmholtz Association of National Research Centres consisting of fifteen large research centres. As UFZ is member of the Helmholtz Association, UFZ will receive strong support from the Brussels Helmholtz Office and all members of the consortium who scheduled this model consortium agreement. The model consortium agreement can be found at
http://www.helmholtz.de/de/Publikationen/Aktualisierte_Muster-Konsortialvertraege.html .

UFZ has already negotiated several consortium agreements under FP6, including the one as co-ordinator of ALARM, an IP with 53 partners.

The model consortium agreement has already been modified according to specific needs of MODELKEY.

Intellectual Property

The procedures to be used to disseminate, protect and exploit the intellectual property will be clearly covered in this consortium agreement. Aim of this agreement is to balance the requirements necessary to protect such intellectual property and the foreseen dissemination objectives. Participating Small and Medium sized Enterprises (SMEs) are preferred partners for commercial exploitation of project results and materials. The Project Co-ordination Committee will ensure that the consortium agreement is strictly adhered to.

Research results will belong to the institutions where the research was carried out and the intellectual property rights will be applied individually according to the rules of the employer under the applicable European and national laws. In addition, ownership of intellectual property will depend on whether it results from one partner or joint contribution.

The consortium will provide all necessary endeavor for optimum valorisation of patentable inventions involving several institutions. In general, it is intended that the institutions responsible for a collective invention will be jointly in charge for filing an application for a patent, with shared intellectual ownership right negotiated between the relevant partners on a case-by-case basis. Any party not intending to seek adequate and effective protection of certain of its knowledge from the project shall notify the co-ordinator.

Principles of good scientific practice

Furthermore, the principles of good scientific practice are to be obeyed within MODELKEY, which follow the following rules:

Rule 1 - Responsibility: The UFZ as co-ordinator as well as all partners entrusted with personnel management tasks in the scientific field are responsible for withholding the principles of good scientific practice as laid out in different national memoranda. In particular this includes securing specialised counselling for newly employed scientists and bringing these scientists closer to such fundamental principles.

Rule 2 - Organisation: The heads of subprojects hold particular responsibility for a high level of organisation and are irrelevant of the size of the subproject particularly responsible for ensuring that management tasks, supervision, conflict management and quality control are guaranteed and clearly fulfilled.

Rule 3 - Good Scientific Practice: Good scientific practice is based on the principles of scientific eloquence, conscientiousness, and communication. This includes the encouraging constructive criticism backed by scientific evidence and freedom to voice one's opinions independent of the hierarchical position of those involved, the responsibility, to acknowledge, respect and quote the priorities of others in terms of ideas and results in the past and present as well as being able to accept constructive criticism and admit to one's own errors and mistakes. Dealing with such issues constructively without discrediting other scientists –is an integral part of scientific communication and belongs to the most meaningful achievements of our scientific culture.

To enable the verifiability as well as the objective criticism of scientific results, scientific primary data are indispensable. As long as such data are the basis of publications, patents or running R&D work, they should be kept on a secure medium, accessible to the partner organisation for at least ten years.

Originality and quality are given preference over quantity as performance and evaluation criteria for job appointments within MODELKEY.

Rule 4 - Incorrect Conduct: Incorrect conduct in the scientific field is considered to take place when in a scientifically considered context consciously or negligently false statements are made, the intellectual ideas of others are violated or research activities of others restricted, as well as the rules of good scientific practise ignored. In particular the following are considered as incorrect conduct in the scientific field.

Manipulation of scientific facts for example by:

- Making up data
- Manipulation of data through elimination of "undesirable" results, as well as the manipulation of charts and diagrams
- Ignorance of contradictory relevant results of others
- Intentional distorted interpretation of results
- Intentional distorted inclusion of the research results from others

A deliberate attempt to mislead through scientifically false statements in the form of:

- Applications
- Grant proposals and reports on the use of grant funds
- Publications, i.e multiple publications without reference to quoted sections

Violation of intellectual ideas for example:

- Unauthorized use under the presumption of authorship
- Presumption or unfounded assumption of scientific authorship or co-authorship
- Refusal of co-authorship for others in spite of adequate contributions
- Exploitation, publication or making accessible fixed ideas, methods, research results or research steps of others without the authorization of the original author (theft of ideas)
- Concealing essential and relevant preliminary work undertaken by others
- Falsification of the content of a document

Attempted sabotage through damaging, destruction of or manipulation of materials i.e.:

- Appliances and experiment order
- Data, documents, software
- Consumables (e.g. chemicals)

Responsibility for the incorrect conduct of others can for example occur through:

- Active involvement in the incorrect conduct of others
- Knowledge of and toleration of misconduct of others
- Co-authorship of publications containing false information
- Negligence of obligation to exercise supervision

Rule 5 - Punishment: It is part of the ethics of science, not to tolerate the scientific misconduct of others. The common way of dealing with suspicion of misconduct should be to approach the initiator about the misdemeanour and to seek clarification and correction of the problem.

Rule 6 - MODELKEY conduct on suspicion of scientific misconduct: MODELKEY institutionalises a procedure which is to be followed when a suspicion or reproach of scientific misconduct occurs against a member of MODELKEY which cannot be resolved at the subproject or project level. The procedure adapted will be oriented at similar procedures of the particular partner institutions.

B7: Project resources:

B8 – Detailed implementation plan – first 18th months

MODELKEY focuses on a better diagnosis, prediction and forecasting of the impact of environmental pollution on freshwater and marine ecosystems. This goal will be met by a close integration of deterministic and probabilistic approaches of hazard assessment interlinking highly innovative modelling tools with state-of-the-art experimental approaches. To achieve its objectives MODELKEY is composed of 6 subprojects on specific scientific subjects including KEYTOX (key toxicant identification), BASIN (basin-specific database), EXPO (exposure modelling of contaminants), EFFECT (effect modelling), SITE (site assessment), DECIS (decision making), and 2 integrating subprojects on dissemination and training (DIS/TRAIN) and scientific co-ordination (COOR).

The close integration and the respective synergies can be only achieved if all subprojects run over the whole duration of the project. Thus, the components of MODELKEY are basically the same for the first 18 months and the entire duration of the project (see Fig. B4.1). However the weight and the tasks of the subprojects change significantly during the term of MODELKEY.

In the first 18 months BASIN plays a key role by delivering a meta database that collects existing monitoring data on hydrological conditions, physico-chemical parameters, concentrations of chemicals, toxicity data, and data on aquatic communities in the three river basins selected as case studies by MODELKEY. In addition links to other databases are established (e.g. that of the EU project REBECCA). Most projects rely on this databases as the basis for exposure (EXPO) and effect (EFFECT) modelling, for hot spot selection for key toxicant identification (KEYTOX) and in depth site assessment (SITE). Also the decision support system is based on TRIAD-like data from BASIN.

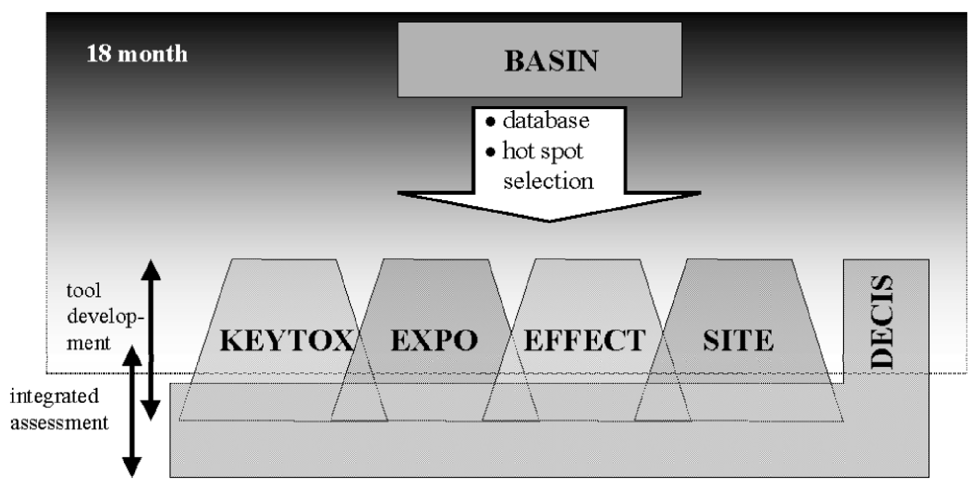


Fig. B8.1: Pert diagram on MODELKEY subprojects within the first 18 months.

All of the subprojects KEYTOX, EFFECT, EXPO, SITE, and DECIS have two basic focuses: (1) the development of innovative tools enhancing the state-of-the-art of impact assessment of toxic pollution on biodiversity and (2) application of these tools for integrated assessment in selected case studies (Fig. B8.1). In the first 18 months the clear focus is on the development of innovative tools that will be applied in the second part of the project for key toxicant identification and integrated risk assessment based on the BASIN data base. DECIS focuses in the first 18 months on the development of the conceptual framework and of the decision support system.

Risks and contingency plans

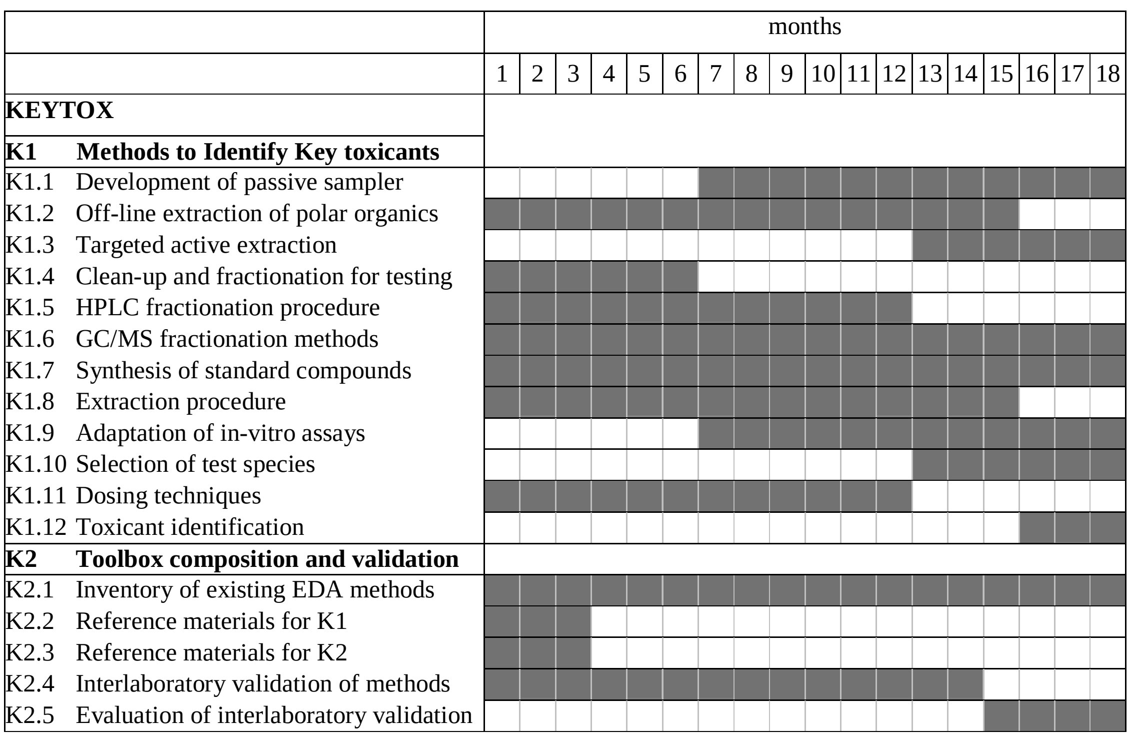
For all components, the risk for the research as such is limited as it will be done by highly experienced scientists. MODELKEY is a highly integrated project. It will use state-of-the-art methods for an integrated impact assessment on freshwater and marine ecosystem. This research is based on existing material and the staff capacity to do the in depth research with established methodologies is already available.

MODELKEY will enhance the state-of-the-art in three ways:
1) Integration of state-of-the-art methods
2) Development of several truely novel and innovative tools
3) Integration of these innovative tools into the impact assessment approch.

It is always possible that the development of novel tools fails. However, that is no risk for integrated impact assessment approach in MODELKEY. In the case of failure the approach will use the respective existing state-of-the-art tool, which is already available in the consortium.

Temporal sequence

The prospective time schedule for the first 18 months is given in the gantt chart (Fig. B8.2)



K3 Site-specific toxicant identification																		
K3.1 Review EDA studies/ EDA at hot spots	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
K4 Key Toxicant Identification Database																		
K4.1 Inventory of existing databases	■	■	■	■	■	■												
K4.2 Development of the KEYTOX-database							■	■	■	■	■	■	■	■	■	■	■	■
BASIN																		
B1 Establishment of river basis database																		
B1.1 Collecting information on monitoring and research programs	■	■	■	■	■	■	■											
B1.2 Overview / Collection of additional data	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■		
B1.3 Distinguish potentially hazardous sites																	■	■
B2 Quality assessment / guideline deduction																		
B2.1 Overview on methodologies													■	■	■			
B2.2 Triad development													■	■	■	■	■	■
B2.3 Distinguish potentially hazardous sites													■	■	■	■	■	■
B2.4 Effect / pollution in Elbe (CZ)													■	■	■	■	■	■
EXPO																		
EX1 Erosion and sedimentation processes																		
EX1.1 Literature review	■	■	■	■	■	■												
EX1.2 Analysis and evaluation of data	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
EX1.3 Evaluation of physical data of hotspots													■	■	■	■	■	■
EX1.4 Description of organism/property relation													■	■	■	■	■	■
EX1.5 Parameterisation of erosion processes	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
EX1.6 Parameterisation of transport conditions	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
EX1.7 Improvement of formulations															■	■	■	■
EX1.8 Evaluation of the Elbe flood 2002	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
EX2 Transport and fate of contaminants																		
EX2.1 Data analysis	■	■	■	■	■	■	■	■	■	■	■	■						
EX2.2 Literature review	■	■	■	■	■	■												
EX2.3 2D/3D modelling of Scheldt estuary	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■			
EX2.4 2D modelling of river Elbe	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
EX2.5 Calibration of models													■	■	■	■	■	■
EX2.6 Parameterisation of transport processes	■	■	■	■	■	■	■	■	■	■	■	■						
EX2.7 Sensitivity analysis													■	■	■			
EX2.8 Sediment origin analysis											■	■	■	■	■	■	■	■
EX2.9 Classification of river/estuary types													■	■	■	■	■	■
EX2.10 Development of model set													■	■	■	■	■	■
EX2.11 Detailed modelling of Elbe portion	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
EX2.12 Sensitivity analysis							■	■	■	■	■	■	■	■	■	■	■	■
EX2.13 Hydrological discharge scenarios										■	■	■	■	■	■	■	■	■
EX3 Bio-availability and food web																		
EX3.1 Review of exposure assessment models	■	■	■	■	■	■	■	■										
EX3.2 Evaluation of in-situ assessment methods	■	■	■	■	■	■	■	■										
EX3.3 Model formulation	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
EX3.4 Review of models in RA approaches	■	■	■	■	■	■	■	■										
EX3.5 Setup of database	■	■	■	■	■	■												
EX3.6 Classification of food webs					■	■	■	■	■	■								
EX3.7 Parameterisation of food web module									■	■	■	■	■	■				
EX3.8 Application of the model													■	■	■	■	■	■
EX3.9 Sensitivity analysis											■	■	■	■	■	■	■	■
EX4 Integrated modelling																		
EX4.1 Specification of user requirements		■	■	■	■	■	■	■										
EX4.2 Input data requirements		■	■	■	■	■	■	■										
EX4.3 Output data requirements		■	■	■	■	■	■	■										

EX4.4 Organising meeting										X								X
EX4.5 Designing user interface									X	X	X	X	X	X	X	X	X	X
EX4.6 Overview of environmental conditions		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
EX4.7 Generation of Default sets										X	X	X	X	X	X	X	X	X
EX4.8 River schematisation method		X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
EX4.9 Incorporation of parameters of EX1-3																X	X	X
EFFECT																		
EF1 Integrated diagnosis of effects on community patterns																		
EF1.1 Data analysis	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
EF2 Development of component model, predicting effects on species success																		
EF2.1 Database building	X	X	X	X	X	X	X	X	X	X	X	X						
EF2.2 Pattern analysis	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
EF2.3 Overview of modelling methods	X	X	X	X	X	X	X	X	X	X	X	X						
EF3 Mechanistic modelling of effects in canonical communities																		
EF3.1 Literature study	X	X	X	X	X	X	X	X										
EF3.2 Establishment of GAM	X	X	X	X	X	X	X	X	X	X								
EF3.3 Establishment of fish test	X	X	X	X	X	X	X	X	X	X								
EF3.4 Data collection	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
EF3.5 Classification of food webs	X	X	X	X	X	X	X	X										
EF3.6 Modelling of closed communities	X	X	X	X	X	X	X	X										
EF3.7 Effect simulation in model ecosystems							X	X	X	X	X	X						
EF3.8 Evaluation of stressed food chain behaviour							X	X	X	X	X	X						
SITE																		
S1 Sediment properties, erosion and sedimentation																		
S1.1 Sediments sampling				X	X	X	X	X	X	X								
S1.2 Measurement of sediment stability							X	X	X	X	X	X	X	X	X			
S1.3 Sedimentation rates				X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
S2 Bioavailability, bioaccumulation in food webs																		
S2.1 Tenax desorption	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
S2.2 Field study on desorption							X	X	X	X	X	X	X	X	X	X	X	X
S2.3 Bioaccumulation in invertebrates				X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
S2.4 Bioaccumulation in microorganisms				X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
S2.5 Biomimetic methods	X	X	X	X	X	X	X	X	X	X	X	X						
S2.6 Food web accumulation										X	X	X	X	X	X	X	X	X
S3 Pollution induced effects on biofilm communities																		
S3.1 Diagnostic toolbox development	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X		
S3.2 PICT-approach					X	X	X	X	X	X	X	X	X	X	X	X		
S3.3 Site assessment and toolbox application					X	X	X	X	X	X	X	X	X	X	X	X	X	X
S4 Effect on invertebrate communities																		
S4.1 Toolbox development	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
S4.2 Selection of sampling sites	X	X	X	X	X	X	X											
S4.3 Data analysis of BASIN data	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
S4.4 Assessment of selected sites								X	X	X	X	X	X	X	X	X	X	X
S5 Effects on fish communities																		
S5.1 Selection of study sites / screening							X	X	X	X	X	X	X	X	X			
S5.2 Selection of target fish species							X	X	X	X	X	X	X	X	X			
S5.3 Diagnostic toolbox development										X	X	X	X	X	X	X	X	X
DECIS																		
D1 Conceptual framework																		
D1.1 Decision support system	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
D1.2 Site prioritisation module	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X	X
D2 Integrated Risk Index																		
D2.1 Risk Index for basin scale							X	X	X	X	X	X	X	X	X	X	X	X

D2.2 Risk Index for site-specific assessment							■	■	■	■	■	■	■	■	■	■	■	■
DIS/TRAIN																		
DT1 Dissemination																		
DT1.1 Personal unions	■	■	■															
DT1.2 Workshops, conferences											■							
DT1.3 Internet sites	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■
CO1 Co-ordination																		
CO1.1 Co-ordination	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■	■

Fig. B8.2: Gantt chart for the first 18 months

Version of the A3 form for the first 18 months

Work package list (18 months)

WP No	Work package title	Leader No	PM	Start month	End month	Deliver-able No
K1	Methods to identify the key toxicants present in freshwater and marine ecosystems: EDA toolbox development	VUA	88	1	18	KD1.1-KD1.8
K2	Toolbox composition and inter-laboratory comparison and validation of existing and developed techniques and preparation of reference materials	RIVO	64	1	18	KD2.1-KD2.3
K3	Site-specific key toxicant identification on the Scheldt, Elbe and Llobregat basins	VRI	31	1	18	KD3.1 KD3.2
K4	Development of a key toxicant identification internet database	RIKZ	19	1	18	KD4.1 KD4.2
B1	Establishment of river basin specific (meta) data bases	EWQMA	60	1	18	BD1.1-BD1.4
B2	Data collection, quality assessment and guideline deduction	UA	20.5	13	18	BD2.1-BD2.4
EX1	Sedimentation and erosion processes	UoS	17	1	18	EXD1.1-EXD1.8
EX2	Transport and fate of contaminants	DELFT	16	1	18	EXD2.1-EXD2.11
EX3	Bio-availiability and foodweb	VUA	21	1	18	EXD3.1-EXD3.5
EX4	Generic exposure assessment model	DELFT	17	1	18	EXD4.1-EXD4.9
EF1	Integrated diagnosis of observed effects on community patterns in a multiple stressed environment	RIVM	7	1	18	EFD1.1-EFD1.5
EF2	Development of a component model, predicting effects of exposure to single and combined toxicants on species success and community composition	CNRS	30	1	18	EFD2.1-EFD2.5
EF3	Mechanistic modelling of toxic effects in canonical communities and in simple food chains	VUA	56	1	18	EFD3.1-EFD3.8
S1	Sediment properties, erosion and sedimentation	UoS	12.5	4	18	SD1.1-SD1.4
S2	Bioavailability, bioaccumulation, biomagnification in food webs	VUA	77.2	1	18	SD2.1-SD2.10
S3	Pollution induced effects on biofilm communities	UFZ	53	1	18	SD3.1-SD3.4
S4	Effects on invertebrate communities	UA	66	1	18	SD4.1-SD4.6
S5	Effects on fish communities	UB	36	6	18	SD5.1-SD5.4
D1	Development/Refinement of the conceptual framework and hot spots prioritization module	CVR	28.5	1	18	DD1.1-DD1.6
D2	Integrated Risk Index	RIVM	17	6	18	DD2.1-DD2.3
DT1	Dissemination	UFZ	7.5	1	18	DT1.1-DT1.5
DT2	Training	RIKZ	0	25	18	-

Deliverables list (18 month plan)

Deliver-able No	Deliverable title	Delivery date	Nature	Dissemination level
KD1.1	Pre-mutagenicity testing clean up method for crude sediment extracts.	6	R	PU
KD1.2	Selection, development and evaluation of individual fractionation steps for subsequent development of automated multi-step fractionation method for sediment-associated PACs.	12	R	PU
KD1.3	Tailored protocols for high-efficiency accelerated solvent extraction (ASE) of toxicants with selected physico-chemical properties from biota tissues.	15	R	PU
KD1.4	Off-line extraction method for polar organic compounds.	15	R	PU
KD1.5	Identification and optimisation of injection, separation and trapping parameters for the development of preparative GC/MS fractionation.	18	R	PU
KD1.6	Synthesis of alkylated and heterocyclic PAC standards with MW>250	18	O	PP
KD1.7	Passive integrated sampling method for polar organic compounds.	18	R	PU
KD1.8	Initial database for the development of computer tools for toxicant identification.	18	O	PP
KD2.1	Reference materials of key toxicants in water, sediment, mussel and fish for KEYTOX 1 and 2.	3	O	PP
KD2.2	Validation report on sample pre-treatment and bioassay response of EDA method, including performance characteristics.	18	R	PU
KD2.3	Evaluation of relative performance of applied EDA techniques at different laboratories.	18	R	PU
KD3.1	Literature review on previous EDA studies in the basins of interest. Key toxicant suggestion on this basis.	6	R	PU
KD3.2	Toxicity characterisation at selected hotspots in the basins of Elbe, Scheldt and Llobregat.	18	R	PU
KD4.1	Inventory of existing databases and their specifics.	6	R	PU
KD4.2	Specification of the final MODELKEY database (platform, parameter list, features), including SITE data, based on existing databases.	18	R	PU
BD1.1	Status report on monitoring programmes	6	R	PU
BD1.2	First meta database on available data with links to data originating databases	6	O	PU
BD1.3	TRIAD database and identification of missing data for each case study river basin as input to the research items of BASIN 2	16	O	PU
BD1.4	First selection (on limited data set) of potentially hazardous sites and respective key effects as a crucial input to SP SITE and KEYTOX	18	O	PP
BD2.1	Report on the use of integrated biological-	18	R	PU

	effect based assessment methods			
BD2.2	A triad assessment methodology that will be used after month 18 for evaluation of the sediment quality based on the available data	18	O	PP
BD2.3	Revision and Identification of potentially hazardous sites and respective key effects as a crucial follow up to SP SITE and KEYTOX	18	O	PP
BD2.4	Survey data of in vitro and chemical analysis in the Czech part of the riverElbe basin	18	R	PU
EXD1.1	Overview of processes: sedimentation, erosion, mixing and consolidation	18	R	PU
EXD1.2	Analysis and evaluation of data on river morphology, flow velocity field and transport characteristics to identify sedimentation and erosion areas for Elbe, Scheldt and Llobregat	18	R	PU
EXD1.3	Compilation, evaluation and synopsis of physical and chemical data of hotspots deposits	18	R	PU
EXD1.4	Description of relations between benthic organism and the physical and chemical properties of the sediment	18	R	PU
EXD1.5	Parameterised formulations and rules for the beginning and intensity of sediment erosion to be used in EXPO 2 and 4 based on master variables	18	R	PU
EXD1.6	Parameterised formulations and rules of local transport conditions for the beginning of suspended contaminated particle edimentation and their sedimentation rates for the EXPO 2 and 4 models	18	R	PU
EXD1.7	Description and specification of additional necessary and actual data on sediments which must be provided by targeted field measurements in SITE 1 for the respective rivers: Elbe, Scheldt and Llobregat	18	R	PU
EXD1.8	Report overview Elbe flood 2002	18	R	PU
EXD2.1	Data analysis (of data collected in BASIN)	12	R	PU
EXD2.2	Preliminary results of detailed 2D/3D modelling of Scheldt estuary including the marine coastal zone	15	R	PU
EXD2.3	Preliminary results of detailed 2D modelling of river Elbe	18	R	PU
EXD2.4	Results of calibration of models on collected data (from BASIN)	18	R	PU
EXD2.5	Sediment origin analysis (determining the origin and retention time of sediment)	18	R	PU
EXD2.6	Review and description of the state-of-the art transport and bio-chemical processes that determines the behaviour of contaminants in riverine and estuarine systems	6	R	PU
EXD2.7	Initial simplified parameterisation/generalisation of transport and sedimentation processes	12	O	PP
EXD2.8	Sensitivity analysis parameters and processes	15	O	PP
EXD2.9	Classification of river/estuary types and environmental conditions	18	O	PP
EXD2.10	Model parameter sensitivity analysis by	18	O	PP

	application of principle component method and/or Monte Carlo simulation			
EXD2.11	Specification of characteristic hydrological discharge scenarios (low, medium, high discharge and flood) with significant impact of sediment bound toxicants on the ecosystem	18	R	PU
EXD3.1	Review report on factors affecting bioavailability in aquatic systems and the current status of inclusion of bioavailability in exposure assessment and risk assessment models	8	R	PU
EXD3.2	Report with proposed parameterization and model formulations for sediment bioavailability, parameter estimates and uncertainties, to be used in the prototype model EXPO4	18	R	PU
EXD3.3	Report on current status of food chain transfer / biomagnification modelling and inclusion in regulatory risk assessment practices and potential for inclusion in the generic model	8	R	PU
EXD3.4	Report on selection of food chain accumulation models, parameterization, and literature-based inventory of parameter estimates and uncertainties, to be used in the prototype model EXPO WP 3.4 and compatible with EFFECT and DECIS	18	R	PU
EXD3.5	Joint database with EFFECT3	8	O	PP
EXD4.1	Specifications user requirements	8	R	PP
EXD4.2	Input data requirements	8	R	PP
EXD4.3	Output data requirements	8	R	PP
EXD4.4	Conceptual design of generic exposure model, including the procedures to obtain “candelabrum” and “trumpet” shaped river/estuary network from GIS maps	18	R	PP
EXD4.5	Classifications riverbasins/estuaries	18	R	PU
EXD4.6	Incorporation of transport and fate parameters from Expo 1,2,3 into design	18	O	PU
EXD4.7	Proposed default set for parameters	18	R	PP
EXD4.8	Prototype of user interface of the generic exposure model	18	P	PU
EXD4.9	Modellers meetings	10, 18	O	PP
EFD1.1	Overview and interpretation of required data available and identification of data gaps in close collaboration with BASIN 1	6	R	PU
EFD1.2	Conversion of concentration data of individual toxicants to overall combined toxic risk also for the benefit of WP EFFECT 2	12	O	PP
EFD1.3	Construction of a site oriented MS Access database for model input data in collaboration with EFFECT 2 on the basis of the meta database from BASIN 1	12	O	PU
EFD1.4	Overview of existing modelling techniques and decision on modelling techniques to apply in the next stage of the WP	14	R	PU
EFD1.5	Preprogramming of required models	18	P	PU
EFD2.1	MS Access database for the river basins Elbe,	12	O	PU

	Scheldt & Llobrogat and corresponding dataset			
EFD2.2	Integrative datamatrix within GIS interface	12	O	PU
EFD2.3	Overview of modelling methods for component patterns of community	12	R	PU
EFD2.4	Patterns of community (ordination and clustering)	18	R	PU
EFD2.5	Preliminary results on patterns of toxins and environmental factors vs community	18	R	PU
EFD3.1	Literature study on theory for and experiments with simple closed communities (8 months)	8	R	PU
EFD3.2	Standard Operational Procedure for the gnotobiotic aquatic microcosm	10	R	PU
EFD3.3	Standard Operational Procedure for specific effects testing with a benthic fish species under laboratory conditions	10	R	PU
EFD3.4	Toxicity data for two or three key toxicants (selected by KEYTOX) derived from single species tests with organisms representing three trophic levels related to the theoretical concept of canonical communities.	18	R	PU
EFD3.5	Collection of data for ecophysiology of relevant species and toxico-kinetics and effects of target toxicants; both from literature and from experiments at ECT	18	R	PU
EFD3.6	Joint database on relevant food chains with EFFECT3	8	O	PP
EFD3.7	Computer simulation of effects of toxicants with various modes of action in canonical communities	8	O	PP
EFD3.8	Computer simulation of toxico-kinetics and effects in food chains, using parameter values of selected target organisms and toxicants in the SITE studies	12	O	PP
SD1.1	Completion of the BASIN 1 and EXPO 1 data set and providing actual data for input in the EXPO 2 model	10	R	PU
SD1.2	Supply of undisturbed sediment cores from hotspots for key toxicant identification in KEYTOX	12	O	PP
SD1.3	Intercomparison of field and laboratory techniques for contaminated sediment sampling and erosion stability measurements (CSM, SETEG, EROMOB) using data from Elbe, Scheldt, Llobregat)	15	R	PU
SD1.4	Mapping of the SITE 1 results for a comprehensive assessment in EXPO and DECIS	18	R	PU
SD2.1	Detailed characteristics of sediment samples form the three catchments	10	R	PU
SD2.2	Desorption rate constants of model contaminants for different organic fractions	18	R	PU
SD2.3	Data on the structural parameters governing desorption rates of model contaminants	18	R	PU
SD2.4	Report on rapidly and slowly desorbing fractions of contaminants in field sediments in the Scheldt estuary	18	R	PU
SD2.5	Data on uptake of contaminants sorbed to	18	R	PU

	organic matter by benthic invertebrates			
SD2.6	Progress report on development of methods to study bioavailability and bioacumulation in micro-organsisms	18	R	PU
SD2.7	Biologically available concentrations in the Scheldt determined with biomimetic methods	12	R	PU
SD2.8	Internal concentrations of key toxicants in laboratory test organism in connection with canonical community modelling	18	R	PU
SD2.9	Workshop report describing the organisation, planning, and protocols for the freshwater food web studies	14	R	PU
SD2.10	Report on the results of marine food web study in the Scheldt	18	R	PU
SD3.1	Overview over approaches for the verification of cause-effect relationships between exposure to key pollutants (selected by KEYTOX) and effects on biofilm communities including their biodiversity	6	R	PU
SD3.2	Effect assessment of key-toxicants on the structure, biodiversity and functioning of the biofilm communities	16	R	PU
SD3.3	Establishment of standardised testsystems to measure pollution induced community tolerance of biofilms	16	O	PP
SD3.4	*In-situ* application of the toolbox, developed within the project to derive a causal analysis of community disturbance at selected hotspots	18	O	PP
SD4.1	overview of existing tools for biological effects-based sediment quality assessment	7	R	PU
SD4.2	identification of suitable bio-indices to toxicity assessment	18	R	PU
SD4.3	intercalibrated sampling strategy and design	7	O	PP
SD4.4	evaluation of the role of invaders as indicators	12	R	PU
SD4.5	overview of site – specific base line data, community structure and species diversity extracted from data collection in BASIN 1	18	R	PU
SD4.6	preliminary application of the toolbox at hotspots	18	O	PP
SD5.1	toxicological and ecological screening of selected sites	15	R	PU
SD5.2	selection of target species	15	O	PP
SD5.3	method-oriented diagnostic toolbox for toxicological site assessment	18	O	PP
SD5.4	Toxicological and ecological data to feed into EFFECT models	18	O	PP
DD1.1	Review of models/tools/decision frameworks and conceptual framework	10	R	PU
DD1.2	Preliminary list of recommendations for the design of monitoring programs of biodiversity impacts at basin scale	10	R	PU
DD1.3	Socio-economic characterisation of three case studies	16	R	PU
DD1.4	DSS Structure Interim Report	18	R	PU
DD1.5	Review and preliminary proposal for prioritization of hot spots based on risk and economic assessment of biodiversity and	18	R	PU

	ecological impairment			
DD1.6	Design of investigation on biodiversity value	18	R	PU
DD2.1	Critical review of Weight of Evidence approaches and tools	10	R	PU
DD2.2	Proposed preliminary Weight of Evidence procedures for Basin scale IRI	18	R	PU
DD2.3	Proposed preliminary Weight of Evidence procedures for Site Specific IRI	18	R	PU
DT1.1	Scientific brochure and flyer on the existence of MODELKEY	3	R	PU
DT1.2	MODELKEY Website launch	12	O	PU
DT1.3	MODELKEY Newsletter 1	6	O	PU
DT1.4	1st yearly update Workshop on the MODEL-KEY progress, all subprojects reporting	12	O	PU
DT1.5	Establishment of an end-user communication board	12	O	PU

WP KEYTOX 1- Methods to Identify the Key Toxicants Present in Freshwater and Marine Ecosystems

Work Package No.	K1	Starting date:					Month 1		
Participant	CEFAS	CSIC	RIKZ	RIVO	SPbU	VRI	VUA	UFZ	XEN
Person Months	10	0	16	6	19	4	10	18	5

Objectives

The overall objective of this work package is to develop a series of methods that fill the current gaps in key toxicant identification (Effect Directed Analysis [EDA]). This will be realised by meeting the following objectives:

- To develop, validate and standardise a series of procedures for the effective extraction of key toxicants as unknowns from water, sediment and biota.
- To develop, validate and standardise a series of key toxicant isolation techniques.
- To develop, validate and standardise techniques for the identification of key toxicants
- To provide a battery of bioassays suitable for EDA.

Description of work

The first 18 months of work in KEYTOX1 will see a start to the development of techniques for the identification of key toxicants in freshwater and marine ecosystems:

Task K1.1. Development of a passive integrated sampler for organic compounds (CEFAS). The suitability of POCIS for the extraction of polar key toxicants from marine and freshwaters will be evaluated through the deployment of POCIS samplers in flow through tanks that will be quantitatively dosed with a number of known polar organic compounds (log K_{OW} 0.5 to 4) that are known to affect a number of the bioassay systems being evaluated in KEYTOX. The extracts from these will be tested on relevant bioassays to quantitatively determine whether POCIS can extract the relevant material. If POCIS are effective in the extraction of these model toxicants then they will be tested in the field. If they are not effective then different extraction configurations will be tested and evaluated. For field evaluation POCIS will be deployed at fixed points in an effluent gradient from a sewage treatment works (STW) on the Tees estuary (UK) and the river Thames (UK). Following 30 days exposure the samples will be eluted and the extracts tested using relevant bioassays (YES, YAS). The results of the field-testing will also be evaluated and an assessment made as to whether they are suitable for use with EDA.

Task K1.2 Off-line extraction of polar organic compounds (log K_{OW} < 3) (CEFAS). CEFAS has already published a solid phase extraction (SPE) technique suitable for the extraction of a broad range of polar (log K_{OW} < 3) organic compounds using a polymeric resin marketed as Isolute ENV+ (IST, Hengoed, UK) (Thomas et al., 1999). Since the development of this technique a wider range of resins (e.g. StrataX by Phenomenex) have been developed and have successfully been applied to extract polar compounds such as pharmaceuticals and their metabolites from STW effluents (Hilton and Thomas, 2003). The purpose of this work is to evaluate the existing method against stricter criteria using a greater range and number of authentic reference compounds, whilst also comparing a range of new SPE packings with ENV+. Both freshwater and marine samples will be spiked with the same range of reference compounds used to test the POCIS system and extracted in triplicate using a number of modern SPE packings suitable for the extraction of polar compounds. The packing material giving the best performance in terms of the recovery of analytes and reproducibility will be evaluated further by extracting ten-replicates of spiked water to establish performance data for the method.

Task K1.3 Targeted active extraction (CEFAS, VUA, RIKZ). Preparatory work will be done on the development of immunoaffinity extraction methods for the highly selective extraction of androgenic and estrogenic compounds.

Task K1.4 Rapid pre-mutagenicity testing clean up and fractionation method (UFZ, XEN). KEYTOX will develop simple and rapid initial clean up and fractionation procedures including size exclusion and normal-phase chromatography that will be evaluated for their potency to provide a realistic picture of the mutagenic potency of complex mixtures.

Task K1.5 Development of robust automated multi-step and multi-column HPLC fractionation procedures. (UFZ) The development will be based on existing experience with available automated two-step and off-line multi step fractionation procedures. The major focus is on combined size-exclusion, normal-phase and electron-donor-acceptor separation procedures on different stationary phases.

Task K1.6 Development of preparative GC/MS fractionation methods and optimisation of injection, separation and trapping parameters. (UFZ, XEN, SPbU). Preparative GC/MS will be developed at the example of the separation of PAC isomers with a molecular weight of above 250 with specific focus on alkylated and heterocyclic compounds. Previous studies indicated that this highly complex group of compounds includes potent mutagenic and Ah-receptor mediated toxicants.

Task K1.7: Synthesis of authentic standards of alkylated and heterocyclic PACs of a molecular weight above 250 for GC/MS fractionation and mutagenicity testing (SPbU).

Task K1.8. Novel EDA design for biota. Development of high-efficiency ASE based extraction methods for biota (UFZ, CEFAS and RIVO). As shown for plant material extraction efficiency and thus the recovery of bioaccumulated toxicants can be significantly enhanced by applying ASE. However, particularly for complex biological matrixes optimised conditions such as solvent selection, pressure and temperature are crucial. KEYTOX will aim at the development of tailored extraction procedures for biofilms, invertebrates and fish tissues.

Task K1.9 Development and adaptation of in vitro assays for application to environmental matrices *(VUA, RIKZ, VRI)*
Initial work on the development of in vitro assays determining genotoxicity, tumour promotion, hormonal disruption (androgenicity, thyroid hormone inhibition), neurotoxicity and antibiotic resistance for use in EDA will be done.

Task K1.10 Initial selection of test species for high-throughput in vivo bioassays (CEFAS, RIKZ, RIVO). The existing battery of *in vivo* bioassays will be assessed and those deemed suitable for development as high-throughput bioassays in EDA selected. The selection procedure will evaluate bioassays currently considered recommended for environmental monitoring whilst also evaluating emerging techniques that may also be of considerable value to the EDA field.

Task K1.11 Novel dosing techniques for in vitro and in vivo assays (CEFAS, VUA, RIKZ). Work will be started to develop dosing techniques that create well-defined and constant exposure levels of test compounds - and eventually environmental extracts - in in vitro and in vivo assays.

Task K1.12. Toxicant identification
Initial work on the evaluation of identification techniques (GCxGC-ToF-MS) for unknown compounds (RIVO) will be developed.

Deliverables

KD1.1 Pre-mutagenicity testing clean up method for crude sediment extracts (month 6). (Task K1.4)
KD1.2 Selection, development and evaluation of individual fractionation steps for subsequent development of automated multi-step fractionation method for sediment-associated PACs (month 12). (Task K1.5)
KD1.3 Tailored protocols for high-efficiency accelerated solvent extraction (ASE) of toxicants with selected physico-chemical properties from biota tissues (month 15). (Task 1.6)
KD1.4 Off-line extraction method for polar organic compounds (month 15). (Task K1.2)
KD1.5 Identification and optimisation of injection, separation and trapping parameters for the development of preparative GC/MS fractionation (month 18). (Task K1.6)
KD1.6 Synthesis of alkylated and heterocyclic PAC standards with MW>250 (month 18) (Task K1.7)
KD1.7 Passive integrated sampling method for polar organic compounds (month18). (Task K1.1)
KD1.8 Initial selection of test species for high-throughput *in vivo* bioassays (month 18). (Task K1.10)

Milestones[1] and Expected Results

- Pre-mutagenicity testing clean up method for crude sediment extracts (month 6).
- Selection, development and evaluation of individual fractionation steps for development of automated multi-step fractionation method for sediment-associated PACs (month 12).
- Tailored protocols for high-efficiency accelerated solvent extraction (ASE) of toxicants with selected physico-chemical properties from biota tissues (month 15).
- Off-line extraction method for polar organic compounds (month 15).
- Identification and optimisation of injection, separation and trapping parameters for the development of preparative GC/MS fractionation (month 18).
- Passive integrated sampling method for polar organic compounds (month18).
- Initial selection of test species for high-through *in vivo* bioassays (month 18).

WP KEYTOX 2 Toolbox composition and inter-laboratory comparison and validation of existing and developed techniques and preparation of reference materials

Work Package No.	**K2**	**Starting date:**				**Month 1**			
Participant	CEFAS	CSIC	RIKZ	RIVO	SPbU	VRI	VUA	UFZ	XEN
Person Months	7	13	8	17	2	3	12	1	1

Objectives

The overall objective of this work package is to validate the various EDA steps: sample pre-treatment, bioassays and identification. This will be realised by meeting the following objectives:

- To prepare suitable marine and freshwater reference materials (water, biota, sediment) for the validation of different EDA preparative analytical methods and bioassay responses.
- To prepare suitable marine and freshwater reference materials (biota and sediment) for the inter-laboratory comparison study of existing EDA techniques.
- To organise an inter-laboratory comparison study of existing EDA techniques for water, biota and sediment.

Description of work

The work will be performed in the following steps:
Task K2.1: Inventory of existing EDA methods (sample preparation and bioassays) to be applied for inter-laboratory comparison. (CEFAS, RIKZ, RIVO, VUA, UFZ).

Task K2.2: Preparation of suitable reference materials for water, mussel, fish and sediment for KEYTOX 1 (RIVO, RIZK). For all compartments a marine and freshwater material will be prepared. Materials will be spiked with deuterated, 13C-labelled, or native compounds. All candidate materials will be tested for homogeneity. Reference materials will be used for chemical validation of the sample pre-treatment step in KEYTOX 1 (recoveries of the key toxicants, repeatability, and ruggedness of the sample pre-treatment techniques). Methods that are validated are SPMDs, silicon rubber, POCIS, SPE, normal-phase HPLC, reverse phase HPLC, gel permeation chromatography (UFZ, CEFAS, RIVO, RIKZ, VUA). In addition, the reference materials will also be used for the validation of the bioassay (suitability of the sample pre-treatment techniques, ruggedness, and the link with the chemical data). Existing *in vivo and in vitro* assays will be validated (see table 2 in B4 KEYTOX 2) by VRI, VUA, XEN, CEFAS, and RIKZ. The innovative pre-treatment methods and bioassays will be validated in the next inter-laboratory study.

Task K2.3: Preparation of reference materials (water, mussel, fish and sediment) with unknown solutions of a number of selected key toxicants for the first inter-laboratory study for KEYTOX 2 (RIKZ, RIVO). Materials will be spiked with key toxicants based on bioassay responses and analytical detection limits.

Task K2.4: Organisation of the first inter-laboratory study for validation of the sample pre-treatment methods and bioassays (RIVO, RIKZ). In this step standardised extraction, clean-up and general fractionation methods will be validated, and all KEYTOX laboratories (UFZ, CEFAS, RIVO, RIKZ, VUA, CSIC) will chemically determine the key toxicants, and fractions will be tested with validated bioassays (*in vivo* and *in vitro* assays) (VRI, VUA, XEN, CEFAS, and RIKZ). Validation of the specific fractionation techniques will take place by the laboratories that developed these methods only; fractions will be sent to the laboratories that perform the validated bioassays.

Task K2.5: The interlaboratory step is immediately followed by an evaluation including statistical treatment of the results at a workshop for the KEYTOX partners (CEFAS, RIVO, RIKZ, VUA, CSIC , VRI, VUA, XEN). A preliminary assessment of relevance of applied sample pre-treatment methods and bioassays. The performance characteristics of the pre-treatment methods and bioassays will be reported (RIVO, RIKZ).

Deliverables

KD2.1 Reference materials of key toxicants in water, sediment, mussel and fish for KEYTOX 1 and 2 (month 3). (Tasks K2.2, K2.3)
KD2.2 Validation report on sample pre-treatment and bioassay response of EDA method, including performance characteristics (month 18). (Tasks K2.1, K2.4, K2.5)
KD2.3 Evaluation of relative performance of applied EDA techniques at different laboratories. (18 Months) (Task K2.5)

Milestones[1] and Expected Result

KM2.1 Production and delivery of reference materials for KEYTOX 1 and 2 (water, sediment, mussel and fish) (month 3).
KM2.2 Assessment of relevance of bioassays for use in EDA (month 18)
KM2.3 Organisation of intercomparison exercise for sample pre-treatment and bioassay response, followed by a workshop to evaluate the data (month 12).
KM2.4 Intercomparison exercise for sample pre-treatment and bioassay response (Month 13).
KM2.5 Report on performance characteristics of pre-treatment and bioassay EDA methods (month 18).

WP KEYTOX 3 Site-specific key toxicant identification on the Scheldt, Elbe and Llobregat basins

Work Package No.	**K3**	**Starting date:**				**Month 1**			
Participant	CEFAS	CSIC	RIKZ	RIVO	SPbU	VRI	VUA	UFZ	XEN
Person Months	2	9	0	0	0	6	0	2	1

Objectives

KEYTOX 3 has the following three objectives in the first 18 months:

- Review previous EDA studies in the basins of interest.
- Begin toxicity characterisation at selected hotspots.
- Establish techniques for the synthesis of authentic reference materials.

Description of work

Task K3.1 (UFZ, CEFAS, CSIC, VRI, XEN): A desk review of all EDA studies conducted in the basins will be conducted in order to establish which key toxicants have been previously identified. The output of this review will be also be used to inform BASIN, SITE and KEYTOX 4 as to the previous data available for the three basins being studied. Following hotspot selection in BASIN, water, sediment and biota samples will be screened using various bioassays in order to establish which types of compounds are occurring at the hotspots. The data will be reported as toxic equivalents. The data will then be fed into BASIN 1 and cross-referenced with available monitoring data. The bioassay results will also determine which tests will direct the EDA process later in KEYTOX 3.

Deliverables month 1- 18

KD3.1 Literature review on previous EDA studies in the basins of interest. Key toxicant suggestion on this basis (month 6). (Task K3.1)

KD3.2 Toxicity characterisation at selected hotspots in the basins of Elbe, Scheldt and Llobregat (month 18). (Task K3.1)

Milestones[1] and expected result month 1-18

KM3.1 Review on previous EDA studies on the basins of the Elbe, Scheldt and Llobregat (month 6)

KM3.2 Toxicity equivalent data for a range of bioassay end-points for samples collected from the Elbe, Scheldt and Llobregat (month 18)

WP KEYTOX 4 Development of a Key Toxicant Identification Internet database

Work Package No.	**K4**	**Starting date:**				**Month 12**			
Participant	CEFAS	CSIC	RIKZ	RIVO	SPbU	VRI	VUA	UFZ	XEN
Person Months	1	1	7	1	6	0	1	1	1

Objectives

To develop an Internet accessible database providing environmental data on key toxicants identified during the project as input to the MODELKEY models and the consequent DSS.

Description of work

Task K4.1 (RIKZ, CEFAS, CSIC, RIVO, SPbU, VUA, UFZ, XEN): The basic concept of **KEYTOX DATABASE** is to build further on already existing databases. The starting point, therefore, is an inventory of these (Internet) databases that offer site specific information (water, sediment, biota, key toxicants), data on toxicity, physico-chemical properties, production, and application data of individual compounds, including those present in synergistic/antagonistic mixtures.

Using the QPID database system (developed and supported by RIKZ-NL) and the results of the database inventory, the specifications of the 'zero-version' of the ModelKey database are specified in the second phase of this sub-project.

Task K4.2 (RIKZ): Information requisites of KeyTox partners (in particular EXPO and EFFECT), together with available data, are used for further development and harmonisation of this 'zero version', and will be the extending work within KEYTOX.

The database will provide access to the following data:

- Sample specific data (locations, GIS coordinates., chemical- and bio-analytical worksheets, analytes, responses, etc.)
- names, synonyms, CAS, other key data (using internet sites *e.g.* http://chemfinder.cambridgesoft.com/)
- Analytical-chemical data (system specific, *e.g.* Kovats retention index for GC-MS, GLP)
- Physico-chemical data (several internet databases)
- Toxicity data (KEYTOX data and several internet databases)
- Bioassay specific response data (KEYTOX, internet, literature search, research data of KEEYTOX-partners)
- Integrated software (like AMDIS, toxicity calculation and key toxicant prioritising modules)
- Site, toxicant, source etc. searching facilities
- Generation of DSS essential parameters (DECIS)

Deliverables

KD4.1 Inventory of existing databases and their specifics (Month 6) (Task K4.1)
KD4.2 Specification of the final **MODELKEY** database (platform, parameter list, features), including **SITE** data, based on existing databases (Month 18) (Task K4.2)

Milestones[1] and expected result

KM4.1 Information gaps, determining KEYTOX development program by comparing MODELKEY specifics and INTERNET databases functionality. (Month 18)

WP BASIN1 – Establishment of river basin specific (meta) databases

Work Package No.	B1	Starting date:					Month 1		
Participant	UA	CSIC	UdG	VRI	IVB	EWQMA	RIKZ	RIVO	ACA
Person Months	16	13.5	3	2	3	17	1.9	2	1.3

Objectives

- to compile a meta database including monitoring data and site specific data
- to link modelling and assessment tools to a database
- to provide data for the other sub projects

Description of work

Basin 1 will provide a data distribution platform for the other subprojects. The first step will be to develop a meta database. Subsequently the required data for the other subprojects will be collected and made available by the website of the project. BASIN 1 is divided into 6 tasks.

Task B1.1 Collecting all information regarding relevant monitoring and research programs in the three river basins. This information will be put in a meta-database. (Month 1-6)

Task B1.2 Getting an overview of the data required in the other subprojects. The coordinators of the other work packages will be asked to give a list of the information they need. This information must be as detailed as possible. Based on this information additional data are collected and added to existing databases or a link will be made to databases containing the information. (Month 1-16)

Task B1.3 Distinguish potentially hazardous sites based on the collected information of water managers. (Month 17-18)

Deliverables

BD 1.1 Status report on monitoring programmes (month 6) (task B1.1).

BD 1.2 First meta database on available data with links to data originating databases (month 6) (task B1.1).

BD 1.3 TRIAD database and identification of missing data for each case study river basin as input to the research items of BASIN 2 (month 16) (task B1.2)

BD 1.4 First selection (on limited data set) of potentially hazardous sites and respective key effects as a crucial input to SP **SITE** and **KEYTOX**. (month 18) (task B1.3)

Milestones[1] and Expected Results

BM1.1 Questionnaire send to all water managers of the three river basins (month 2)

BM1.2 Overview of all available monitoring data, evaluation of the results of the questionnaire (month 6)

BM1.3 Overview of the data required by the other work packages (month 16)

BM1.4 River basin-specific databases will be available on the MODELKEY website (month 16)

BM1.5 Workshop to discuss the results collected for the database (month 18)

WP BASIN 2 - Data collection, quality assessment and guideline deduction

Work Package No.	**B2**	**Starting date:**					**Month 13**			
Participant	UA	CVR	CSIC	UdG	VRI	IVB	SZU	RIKZ	RIVO	ACA
Person Months	2	1	1.5	1	2	2	2	7.7	1	0.3

Objectives

- to reveal hot spots and lacking information on the case study river basins and their marine coastal areas.
- to apply and improve TRIAD-like environmental quality assessment tools, as input into the decision support system of DECIS

Description of work

Basin 2 will provide additional data to fill the data gaps within BASIN 1 and will make a scientific evaluation of the data to distinguish hot spots, to improve integrated asssement methods and to deduct sediment guidelines.

Task B2.1 An overview will be made of the methodologies used for the evaluation of monitoring data. (Month 13-15)

Task B2.2 Development of a Triad like assessment methodology, based on the Flemish Triad, to evaluate the collected monitoring data (Month 13-18).

Task B2.3 Expert judgement of the data with a TRIAD like approach to distinguish potentially hazardous sites. The Flemish triad system will be used for this (Month 13-18)

Task B2.4 Survey on in vitro effects and chemical pollution in the Czech part of the Elbe river basin to fill gaps in monitoring data (Month 13-18)

Deliverables

BD 2.1 Report on the use of integrated biological-effect based assessment methods (month 15) (task B2.1)
BD 2.2 A triad assessment methodology that will be used after month 18 for evaluation of the sediment quality based on the available data (month 18) (task B2.2)
BD 2.3 Revision and Identification of potentially hazardous sites and respective key effects as a crucial follow up to SP SITE and KEYTOX (month 18) (task B2.3)
BD 2.4 Survey data of in vitro and chemical analysis in the Czech part of the river elbe basin (month 18) (task B2.4)

Milestones[1] and Expected Result

1. Overview of the monitoring programs will be extracted from BASIN 1 (month 13)
2. Evaluation of the existing assessment methods (month 15)
3. Workshop to discuss the triad assessment methodology and possible changes (month 17)
4. Adapted triad assessment method (month 18)
5. Results of the quality assessment with the Flemish methodology to distinguish potential hot spots (month 18)

WP EXPO1: Erosion and sedimentation processes (18 month plan)

Work Package No.	EX1	Starting date:				Month 1		
Participant	UoS	UA	DELFT					
Person Months	13	2	2					

Objectives

The overall objective of this work package is to analyse and evaluate all the existing data from river Elbe, Scheldt and Llobregat on hydrology, morphology, sediment properties and contaminated hot spots provided by BASIN 1 and SITE 1 subprojects. Special emphasis will be given to the consistency, compatibility, representation, uncertainty and variability of the data with regard to their applicability for numerical modelling of erosion and sedimentation processes. The data collection and analysis comprises:

(a) Discharge and water level records including flood hydrographs,

(b) Concentration and total load of suspended sediments, physical properties of deposited and suspended sediments,

(c) Identification of location and estimation of mass of hot spots and contamination level,

(d) Estimation of polluted sediment erosion stability and contaminated grain size fraction. The overall goal is: classification of sediments in terms of erosion risk, mobility, and potential impact of sediment associated pollutants on aquatic ecosystem.

(e) Assessment of sediment residence time related to erosion /sedimentation dynamics

Description of work

- **Task EX1.1 Literature review on sedimentation, erosion, mixing and consolidation** (UoS, Delft)
- **Task EX1.2 Analysis and evaluation of data** on river morphology, flow velocity field and transport characteristics to identify sedimentation and erosion areas such as near bank zones, Groyne fields (especially Elbe), harbours (Elbe, Scheldt , Llobregat) from BASIN 1 (UoS, UoA, Delft)
- **Task EX1.3 Compilation, evaluation and synopsis of physical and chemical data of hotspot deposits**: grain size distribution, sediment layers, water and gas content, total organic carbon, bulk density; contamination profile, contaminated sediment age (e.g. Cs 137 label for Elbe) (UoS)
- **Task EX1.4 Description, evaluation and parameterisation of relations between benthic organism and the physical and chemical properties of the sediment** (Delft)
- **Task EX1.5 Parameterisation and simplification** of the erosion and sedimentation process formulations for numerical modelling in EXPO 2 and 4 (UoS, Delft)
- **Task EX1.6 Parameterisation and simplification of local transport conditions** for the beginning of suspended contaminated particle sedimentation and their sedimentation rates for the EXPO 2 models (UoS, Delft)
- **Task EX1.7 Improvement of formulations** by using recent results from SITE 1 investigation (UoS)
- **Task EX1.8 Evaluation of the Elbe flood 2002: erosion of hot spots and sedimentation on flooded areas, estimation of contaminant mass balance; findings, lessons and conclusions. (UoS)**

Deliverables

EXD 1.1: Overview of processes: sedimentation, erosion, mixing and consolidation (task EX1.1) (month 18)

EXD 1.2: Analysis and evaluation of data on river morphology, flow velocity field and transport characteristics to identify sedimentation and erosion areas for Elbe, Scheldt and Llobregat (Task EX1.2) (month 18)

EXD 1.3 Compilation, evaluation and synopsis of physical and chemical data of hotspot deposits (Task EX1.3) (month 18)

EXD 1.4: Description of relations between benthic organism and the physical and chemical properties of the sediment (month 18) (Task EX1.4)

EXD 1.5: Parameterised formulations and rules for the beginning and intensity of sediment erosion to be used in EXPO 2 and 4 based on master variables (month 18) (Tasks EX1.5, EX1.7)

EXD 1.6 Parameterised formulations and rules of local transport conditions for the beginning of suspended contaminated particle sedimentation and their sedimentation rates for the EXPO 2 and 4 models (month 18). (Tasks EX1.6, EX1.7)

EXD 1.7: Description and specification of additional necessary and actual data on sediments which must be provided by targeted field measurements in SITE 1 for the respective rivers: Elbe, Scheldt and Llobregat (months 6, 12 and 28) (Task EX1.2)

EXD 1.8: Report overview Elbe flood 2002 (month 18) (Task EX1.8)

Milestones and Expected Results

EXM1.1 Overview of processes: sedimentation, erosion, mixing and consolidation (month 18)

EXM1.2 Analysis and evaluation of data on river morphology, flow velocity field and transport characteristics to identify sedimentation and erosion areas for Elbe, Scheldt and Llobregat (month 18)

EXM1.3 Compilation, evaluation and synopsis of physical and chemical data of hotspot deposits (month 18)

EXM1.4 Initial description of relations between benthic organism and the physical and chemical properties of the sediment (month 18)

EXM1.5 Initial parameterised formulations and rules for the beginning and intensity of sediment erosion to be used in EXPO 2 and 4 based on master variables (month 18)

EXM1.6 Initial parameterised formulations and rules of local transport conditions for the beginning of suspended contaminated particle sedimentation and their sedimentation rates for the EXPO 2 and 4 models (month 18)

EXM1.7 Description and specification of additional necessary and actual data on sediments which must be provided by targeted field measurements in SITE 1 for the respective rivers: Elbe, Scheldt and Llobregat (months 6, 12 and 28)

EXM1.8 Evaluation of Elbe flood 2002, erosion of hot spots, sedimentation on flooded areas: findings, lessons and conclusions (month 18)

WP EXPO2: Transport and fate processes of contaminants (18 month plan)

Work Package No.	EX2	Starting date:				Month 1		
Participant	UoS	DELFT						
Person Months	8	8						

Objectives

The overall objective of this work package is to improve understanding and forecasting of the governing processes in river basins that determine the behaviour of transport and fate of contaminants in fresh and saline waters. For this, the river Elbe and the Scheldt estuary have been selected as appropriate test cases. Based on detailed 2D and 3D numerical modelling of transport and bio-chemical processes, simplified formulations will be generated. These formulations/knowledge rules will be generically applicable and as much as possible based on readily available (GIS-based) data. The rules and parameterisations describing the behaviour of contaminated sediments will be incorporated in the generic exposure assessment model of WP4. The work package covers the implementation of specific erosion and sedimentation processes formulated in WP1 to model the interaction between the sediment and flow field which then allows to predict the spatial and temporal distribution of concentrations of dissolved and particulate key toxicants in selected river portions with hot spots. A hierarchical model concept consisting of a 2 –dimensional (TELEMAC/ EXSUBIEF) and a 1- dimensional model (COSMOS) will allow the exposure prediction at a local or optionally regional scale for the following up project EFFECT for the Elbe river. The Delft3D model suite will be used for developing a detailed transport and fate model of contaminant sediments in the Scheldt estuary, including the adjacent marine coastal zone. This includes formulations for detailed sediment-water exchange for prediction of both sediment quality and the return fluxes of sediment-bound contaminants to the overlying water.

Description of work

- **Task EX2.1** Data analysis (of data collected in BASIN) (UoS, Delft)
- **Task EX2.2** Literature review and description of the state-of-the art transport and bio-chemical processes that determines the behaviour of contaminants in riverine and estuarine systems (Delft)
- **Task EX2.3** Detailed 2D/3D modelling of Scheldt estuary including the marine coastal zone (Delft)
- **Task EX2.4** Detailed 2D modelling of river Elbe(UoS)
- **Task EX2.5** Calibration of models on collected data (from BASIN) (UoS, Delft)
- **Task EX2.6** Initial parameterisation/generalisation of transport and sedimentation processes, e.g. derive empirical formulations describing the retention of sediments and contaminants based on typical and easy to derive characteristic features of river basins (UoS, Delft)
- **Task EX2.7** Sensitivity analysis parameters and processes (UoS, Delft)
- **Task EX2.8** Sediment origin analysis (determining the origin and retention time of sediment) (UoS, Delft)
- **Task EX2.9** Classification of river/estuary types and environmental conditions (Delft)
- **Task EX2.10** Development of a hierarchical model set: 2-d model coupled with or optionally embedded in a 1-d contaminant transport model for large scale and long time simulation (UoS)
- **Task EX2.11** Detailed 2-d modelling of the most important portion of the river Elbe (60 km) that include the two major contaminant contributors: Mulde and Saale (UoS)
- **Task EX2.12** Model parameter sensitivity analysis by application of principle component method and/or Monte Carlo simulation (UoS, Delft)
- **Task EX2.13** Specification of characteristic hydrological discharge scenarios (low, medium, high discharge and flood) with significant impact of sediment bound toxicants on the ecosystem (UoS, Delft)

Deliverables

EXD2.1: Data analysis (of data collected in BASIN) (Task EX2.1) (month 12)

EXD2.2: Preliminary results of detailed 2D/3D modelling of Scheldt estuary including the marine coastal zone (Task EX2.3) (month 15)

EXD 2.3: Preliminary results of detailed 2D modelling of river Elbe (Tasks EX2.4, 2.10, 2.11), including erosion risk and impact assessment for identified hot spots in the rivers (Elbe etc.) and quantification of mobilized hotspots and contaminant mass balance caused by the Elbe flood 2002 (Task EX2.4) (18 month)

EXD 2.4: Results of calibration of models on collected data (from BASIN) (Task 2.5) (18 month)

EXD 2.5: Sediment origin analysis (determining the origin and retention time of sediment) (Task EX2.8) (18 month)

Description of proposed parameterisation of transport and fate processes including:

EXD 2.6: Review and description of the state-of-the art transport and bio-chemical processes that determines the behaviour of contaminants in riverine and estuarine systems (Task EX2.2) (month 6)

EXD 2.7: Initial simplified parameterisation/generalisation of transport and sedimentation processes (Task EX2.6) (month 12)

EXD 2.8: Sensitivity analysis parameters and processes (Task EX2.7) (month 15)

EXD 2.9: Classification of river/estuary types and environmental conditions (Task EX2.9) (month 18)

EXD 2.10: Model parameter sensitivity analysis by application of principle component method and/or Monte Carlo simulation (Task EX2.12) (month 18)

EXD 2.11: Specification of characteristic hydrological discharge scenarios (low, medium, high discharge and flood) with significant impact of sediment bound toxicants on the ecosystem (Task EX2.13) (month 18)

Milestones and Expected Results

EXM 2.1: Working 2D/3D model Scheldt (month 15)

EXM 2.2: Working preliminary 1D/2D model Elbe (month 18)

EXM 2.3: Results detailed model calculations (month 18), giving insight in

- erosion risk and impact assessment for identified hot spots in the rivers (Elbe etc.)
- quantification of mobilized hotspots and contaminant mass balance caused by the Elbe flood 2002
- Results of calibration of models on collected data (from BASIN)
- Sediment origin analysis (determining the origin and retention time of sediment)

EXM 2.4: Initial proposed parameterisation of transport and fate processes (month 18)

EXM 2.5: Classification of river/estuary types and environmental conditions (month 18)

EXM 2.6: Specification of characteristic hydrological discharge scenarios (low, medium, high discharge and flood) with significant impact of sediment bound toxicants on the ecosystem (month 18)

WP EXPO3: Bio-availability and foodweb (18 month plan)

Work Package No.	**EX3**	**Starting date:**				**Month 1**	
Participant	VUA	DELFT	RIKZ	UJOE	IVB	UdG	UoA
Person Months	5	1	11	1	1	1	1

Objectives

The overall objective of this work package is to review and summarize current knowledge on bioavailability and food chain transfer of contaminants and to develop suitable parameterisation and formulations for the generic exposure assessment model of WP4

More detailed objectives:

- Comprehensive review of existing and innovative approaches for inclusion of bioavailability and food chain models in exposure assessment modelling
- Development of conceptual framework to derive components of a generic food web
- Development and testing of a tiered approach for parameterisation and model formulations for food chain transfer and biomagnification
- Development and testing of parameters and formulations to predict bioavailability of waterborne and sediment-bound key contaminants from innovative in-situ assessment methods (desorption studies, biomimetic methods)
- Evaluate the impact of uncertainty in parameters and data on model outcome
- Validate the food chain modules in the different case studies.

Description of work

- **Task EX3.1** Comprehensive review of current exposure assessment models and to what extent factors determining bioavailability of contaminants are included in those models. Factors to be included: organic matter composition and concentration (POM, DOM), pH, redox potential, sediment grain-size and specific area related parameters, and different classes of compounds (VUA, DELFT, RIKZ, UJOE)
- **Task EX3.2** Evaluation of currently available rapid in-situ assessment methods (tenax desorption studies, biometic techniques) used in SITE-2, and their suitability to incorporate in exposure assessment models (VUA, RIKZ, UJOE)
- **Task EX3.3** Based on this evaluation, parameters and model-formulations will be derived for inclusion in the prototype model (VUA, RIKZ, UJOE)
- **Task EX3.4** Critical review of food web accumulation models in current risk assessment approaches, ranging form including simple models based on experimental or predicted concentration factors (BCF, BAF, and biota/sediment accumulation factors (BSAF) to more complex toxicokinetic approaches, which may include feeding behaviour, lipid metabolism, biotransformation, and food web dynamics (VUA, RIKZ, UJOE)
- **Task EX3.5** Setup of joint database with EFFECT-3 containing relevant toxicokinetic parameters (BCF, BAF, BSAF, rate constants for uptake, elimination, biotransformation) for different species and compound classes (VUA, RIKZ)
- **Task EX3.6** Based on input from BASIN-1, SITE 3-5 a classification of food webs will made. In cooperation with EFFECT3 potentially suitable generic and prototype food webs will be designed, that may be applied in all catchments (VUA, RIKZ, IVB, UdG, UoA)
- **Task EX3.7** Development of parameterisation and formulations for prototype food web module (VUA, RIKZ, DELFT)
- **Task EX3.8** Application of the model will be applied to a small selection of hydrophobic neutral compounds, for which biodegradation and biotransformation is expected to be low and for which monitoring data have been identified in BASIN (VUA, DELFT, RIKZ)
- **Task EX3.9** Preliminary sensitivity analysis of propagation of uncertainty of input-parameters (VUA, DELFT, RIKZ)

Deliverables

EXD 3.1 Review report on factors affecting bioavailability in aquatic systems and the current status of inclusion of bioavailability in exposure assessment and risk assessment models. Report will include evaluation of currently available rapid in-situ assessment methods (month 8) (Task EX3.1, EX3.2)

EXD 3.2 Report with proposed parameterization and model formulations for sediment bioavailability, parameter estimates and uncertainties, to be used in the prototype model EXPO4 (month 18) (Task EX3.3)

EXD 3.3 Report on current status of food chain transfer / biomagnification modelling and inclusion in regulatory risk assessment practices and potential for inclusion in the generic model (month 8) (Task EX3.4)

EXD 3.4 Report on selection of food chain accumulation models, parameterization, and literature-based inventory of parameter estimates and uncertainties, to be used in the prototype model EXPO WP 3.4 and compatible with EFFECT and DECIS (month 18) (Task EX3.6, EX3.7, EX3.8, EX3.9)

EXD 3.5 Joint database with EFFECT3 (month 8) (Task EX3.5)

Milestones and expected results

EXM3.1: Overview of handling of bioavailability and food chain accumulation in exposure assessment models currently used in science and regulatory practices (month 6)

EXM3.2: Database of factors affecting bioavailability in relation to compounds and environmental conditions (in cooperation with SITE-2; month 8)

EXM3.3: Evaluation and selection of food web accumulation models suitable for Expo WP 3.4, Effect WP 5.1 and DECIS, SITE (month 12)

EXM3.4 Database of parameter estimates derived from literature and BASIN, uncertainty ranges (month 14)

EXM3.5: Development and model formulations for inclusion in prototype model (month 18)

WP EXPO4: Integrated modelling (18 month plan)

Work Package No.	**EX4**	**Starting date:**				**Month 2**		
Participant	DELFT	VUA						
Person Months	16	1						

Objectives

The overall objective is to integrate and transfer the knowledge and information from EXPO 1,2 and 3 into a generic exposure assessment model. This model will be able to assess and compare the exposure risks to the environment for each individual source of contaminated site in every European river basin/estuary with minimal requirements for model steering and use. The model can be used :

4. to assist local and regional authorities with an easy-to-use generic tool to provide insight in the behaviour of contaminated sites and to aid in prioritisation of clean-up strategies;
5. to assist in the development and optimisation of future monitoring strategies for ungauged catchments in European river basins including the estuaries;
6. to provide information and guidelines to set-up and apply a detailed model of contaminants for s specific river basin.

The model tool will be able to visualise the risk of remobilisation of contaminant sediments and to predict the abiotic and biotic exposure concentrations and contributions throughout the river basin originated from various polluted sources (e.g. hot-spots and point sources). As such, the generic exposure model contains a river/estuarine and coastal compartment to model transport and exposure from contaminated sediments and point sources. Schematisation and dimensioning of individual European river networks will be automated, based on GIS digital maps. Environmental conditions of each individual basin can be selected from defaults or can be provided by the user. The model can be applied with minimal data requirement. Default conditions will be available when no actual data is available. The model will be a stand-alone model that can be run on any Windows-based platform. The output of the model can be used in EFFECT to assess the impact on a population scale and in DECIS for further risk and economic assessment.

Description of work

- **Task EX4.1** Provide specification of user requirements (Delft)
- **Task EX4.2** Providing technical specifications to the level of spatial and temporal resolution for the parameterisations in WP 1-3 (Delft)
- **Task EX4.3** Providing technical specifications for the output of the model, which will be used in EFFECT and DECIS (Delft)
- **Task EX4.4** Organising meetings of all exposure modellers (DELFT, UoS, VUA) together with developers of the decision support system (CVR) (month 6, 12 and 18) to coordinate and gear activities to each other (Delft)
- **Task EX4.5** Designing and prototyping the user interface (Delft)
- **Task EX4.6** Overview and classification of typical environmental conditions in European riverbasins/estuaries (Delft, VUA)
- **Task EX4.7** Generating default sets of environmental conditions (Delft, VUA)
- **Task EX4.8** Developing a uniform and widely applicable method for automatically schematise a river network from a GIS map into various stream orders (Delft)
- **Task EX4.9** Incorporating transport and fate parameterisations from EXPO 1/2/3 (Delft)

Deliverables

EXD4.1: Specifications user requirements (Task EX4.1) (month 8)
EXD4.2: Input data requirements (Task EX4.2) (month 8)
EXD4.3: Output data requirements (Task 3.4.3) (month 8)
EXD4.4. Conceptual design of generic exposure model, including the procedures to obtain “candelabrum” and “trumpet” shaped river/estuary network from GIS maps (Task EX4.8) (month 18)
EXD4.5: Classifications riverbasins/estuaries (Task EX4.6) (month 18)
EXD4.6: Incorporation of transport and fate parameters from Expo 1,2,3 into design (Task EX4.9) (month 18)
EXD4.7: Proposed default set for parameters. (Task EX4.8) (month 18)
EXD4.8 Prototype of user interface of the generic exposure model (month 18) (Task EX4.5)
EXD 4.9 Modellers meetings (month 10, 18) (Task EX4.4)

Milestones and Expected Results

EXM4.1: Working prototype generic model (10 month)
EXM4.2: Conceptual design final model (18 month)
EXM 4.3: Modellers meetings (10 month, 18 month)

WP EFFECT1 - Integrated diagnosis of observed effects on community patterns in a multiple stressed environment (18 months plan)

Work Package No.	**EF1**	**Starting date:**				**Month 1**		
Participant	RIVM	CNRS	VUA					
Person Months	5	1	1					

Objectives

The primary objective of WP EFFECT 1 for the first 18 months is to collect, unify and store the data required for the sequence of models to be applied in this WP. Additionally, depending on the data available, the model structure will be defined and preprogrammed.

Description of work

Task EF1.1: The first 18 month of work in this work package will be devoted to gathering, sorting, interpreting and storing the required data. This work requires considerable interaction with the parties providing the data. This interaction may serve to fill gaps in the data and unify data coding. Especially the biological sensus data may require a lot of attention in order to cope with taxonomical imbalance and to ascertain a comparable effort in capturing biota across monitoring sites. Together with the sub-projects BASIN, KEYTOX and EXPO and mainly WP EFFECT 2, a versatile relational database structure will be constructed to store, combine and retrieve the required data of different nature and origin (topology, habitat, chemical, availability, toxicological and biotic). Additionally, model type selection and model preprogramming will be accomplished to enable a flying start of the modelling work that is planned for the next 2 years of the project.

Deliverables

EFD1.1 Overview and interpretation of required data available and identification of data gaps in close collaboration with BASIN 1 (Task EF1.1) (month 6)
EFD 1.2 Conversion of concentration data of individual toxicants to overall combined toxic risk also for the benefit of WP EFFECT 2 (Task EF1.1) (month 12)
EFD 1.3 Construction of a site oriented MS Access database for model input data in collaboration with EFFECT 2 on the basis of the meta database from BASIN 1 (Task EF1.1) (month 12)
EFD 1.4 Overview of existing modelling techniques and decision on modelling techniques to apply in the next stage of the WP (Task EF1.1) (month 14)
EFD 1.5 Preprogramming of required models (Task EF1.1) (months 18)

Milestones[1] and Expected Result

EFM 1.1 It is nearly certain that the existing data will suffer from short-comings. However, the most important data will be available. It is expected that the remaining data requirements (mainly habitat suitability data) can easily be met by a limited amount of expert judgement from the organisations monitoring the basins Elbe, Scheldt and Llobregat. (month 8).

EFM 1.2 By the end of month 14 a decision should be taken on the exact structure of the models and model links to apply. Limited freedom of choices ensures that this will not produce a problem in the progress of the WP. (month 14)

WP EFFECT2 – Development of a component model, predicting effects of exposure to single and combined toxicants on species success and community composition

Work Package No.	**EF2**	**Starting date:**				**Month 1**		
Participant	CNRS	VUA	RIVM					
Person Months	28	1	1					

Objectives

- to analyse the spatial and temporal patterns in toxins and ecological data from key sites to provide an integrated analysis and basis for the modelling work
- to begin an evaluation of toxin-ecological process interactions by starting with single action and combination of actions

Description of work

Task EF2.1: To build a MS access database for the case study river basins (Elbe, Scheldt & Llobrogat) and adjacent coastal area within the spatial and temporal variabilities in collaboration with EFFECT 1 and on the basis of the meta-database provided by BASIN 1. Data set will be built using ArcView GIS interface.

Task EF2.2: Analyses for spatial and temporal patterns in data from the case studies to identify those areas most sensitive to toxins and likely impacts to ecological population and community

Task EF2.3: Overview of modelling methods and begin of predictive effect modeling using the techniques of generalized sensitivity analysis and Monté Carlo based analysis using and the data set from task EF2.1

Deliverables

EFD 2.1: MS Access database for the river basins Elbe, Scheldt & Llobrogat and corresponding dataset; (months 12) (task EF2.1)

EFD 2.2: Integrative datamatrix within GIS interface; (months 12) (task EF2.1)

EFD 2.3: Overview of modelling methods for component patterns of community; (months 12) (task EF2.3)

EFD 2.4: Patterns of community (ordination and clustering); (months 18) (task EF2.2)

EFD 2.5: Preliminary results on patterns of toxins and environmental factors vs community (with intercomparison to EFFECT 1 for diagnose); (months 18) (task EF2.2)

Milestones and Expected Result

EFM 2.1: Integrative dataset for MODELKEY studied sites including rivers and estuarine areas; (month 10)

EFM 2.2: First calibrated modeling approaches to dataset (month 18)

WP EFFECT3: Mechanistic modelling of toxic effects in canonical communities and in simple food chains

Work Package No.	**EF3**	**Starting date:**				**Month 1**		
Participant	VUA	CNRS	RIVM	UFZ	ECT			
Person Months	20	3	3	2	28			

Objectives

Development of appropriate concepts to quantify effects in very simple theoretical communities; this knowledge will be helpful to recognize effects in the field, where feedbacks and species interactions complicate the recognition of small effects on integrated systems.

Modelling of the flux of compounds through a realistic food chain, and the effects of these compounds; this knowledge will be helpful to interpret the field data that are colleted in the SITE WP's

Study how feedback loops in closed ecosystems deal with toxic effects on individuals that belong to the different trophic categories (consumer, producer, decomposer)

Evaluate how effects propagate through a food chain, in which the body size of organisms and the lipid content depend on the place in the food chain

Establishment of experimental approaches for delivering the required input data for the models as well as for model verification

Description of work

Task EF3.1: Literature study on theory for and experiments with simple closed communities

Task EF3.2: To establish a simplified gnotobiotic aquatic microcosm (GAM) under laboratory conditions containing organisms representing different trophic categories (consumer, producer, decomposer) which later on in the project (after 18 months) will be exposed to “keytoxicants”. The design of the GAM and the selected measurement endpoints will allow assessing the theoretical concept of canonical communities.

Task EF3.3: To establish a fish test under controlled laboratory conditions which will allow evaluating model considerations on how chemical effects propagate from sediment through sediment dwelling organisms to benthic fish.

Task EF3.4: Collect ecophysiological, toxico-kinetic and effect data on relevant species

Task EF3.5: Based on input from BASIN-1, SITE 3-5 a classification of food webs will made. In cooperation with EXPO3 potentially suitable generic and prototype food webs will be designed, that may be applied in all catchments

Task EF3.6: Model closed communities under toxic stress and determine parameter values that are appropriate for small effects of selected compounds in selected species (using data from literature and experiments)

Task EF3.7: Simulate how effects show up in model ecosystems, depending on the mode of action of the compound

Task EF3.8: Derive properties of stressed ecosystems and evaluate the behaviour of stressed food chains in specified dynamic environments

Deliverables

EFD 3.1: Literature study on theory for and experiments with simple closed communities (8 months) (task EF3.1)

EFD 3.2: Standard Operational Procedure for the gnotobiotic aquatic microcosm (10 months) (task EF3.2)

EFD 3.3: Standard Operational Procedure for specific effects testing with a benthic fish species under laboratory conditions (10 months) (task EF3.3)

EFD 3.4: Toxicity data for two or three key toxicants (selected by KEYTOX) derived from single species tests with organisms representing three trophic levels related to the theoretical concept of canonical communities. (18 months) tasks EF 3.2 and 3.3)

EFD 3.5: Collection of data for ecophysiology of relevant species and toxico-kinetics and effects of target toxicants; both from literature and from experiments at ECT (month 18).(task EF3.4)

EFD 3.6: Joint database on relevant food chains with EFFECT3 (month 8)

EFD 3.7: Computer simulation of effects of toxicants with various modes of action in canonical communities (month 8) (task EF3.6)

EFD 3.8: Computer simulation of toxico-kinetics and effects in food chains, using parameter values of selected target organisms and toxicants in the SITE studies (month 12) (task EF3.7 and 3.8)

Milestones and Expected Result

EFM 3.1: Selection of the appropriate organisms representative for the theoretical concept of canonical communities (6 months)

EFM 3.2: Selection of the appropriate benthic fish species (6 months)

EFM 3.3: Establishment of single species cultures (12 months)

EFM 3.4: The analysis of results from experiments at ETC will show to what extend closed communities are stable enough for the evaluation of toxic effects; if they are too unstable, we turn to fed batch cultures (18 month)

EFM 3.5: We will be able to judge the link between closed spatially homogeneous communities and biofilms as ecosystem models for the study of effects; we will adjust the experimental program on the basis of these findings and select the most cost-effective exposure time and measurement frequency. (18 month)

WP SITE1 –. Sediment properties, erosion and sedimentation (18 month plan)

Work Package No.	S1	Starting date:				Month 4		
Participant	UoS	ACA						
Person Months	12	0.5						

Objectives

The overall objectives of this work package are

- to provide actual data on sediment key parameters for accomplishing the existing data set and to fill the gap in the EXPO 1 and BASIN 1 data base
- to make sediment profiling by applying innovative sediment investigation methods for sediment sampling and analyzing, sediment erosion stability measuring
- to provide reliable field data on erosion and sedimentation for calibration and validation of the numerical models in EXPO 2
- to provide undisturbed sediment samples for chemical and biological analysis in KEYTOX
- to facilitate intercomparison and transfer of different sediment erosion stability testing methods applied at selected sites in the basins of the rivers Elbe, Scheldt and Llobregat

Description of work

Task S1.1 Sediment sampling

Undisturbed sediment samples will be taken in representative hotspot identified in BASIN 1 areas along the river course. Those hotspots can be found in the groyne fields of the river Elbe where sampling activities are focussed on. The sediment core sampler will be applied to allow depth profiling in terms of physical sediment properties (grain size, bulk density, pore water content, gas content) and optionally other chemical and biological properties in KEYTOX. In addition, by applying the so called PEEPER system for some days it is also possible to measure the dissolved toxicants profile in the pore water via diffusion.

Task S1.2 Laboratory and in situ measurements of sediment stability

Measuring of the depth profile of local critical erosion shear stress and erosion rate through laboratory experiments with SETEG. Transfer of sediment profile test results from the lab to the field. (groyne field) sediment top layer erosion stability tests will be performed with EROMOB at the same hotspot to compare both methods. Sediment erosion stability will be also measured with the Cohesive Strength Meter (CSM) at the same site to allow the convertibility of the results. According to the test results the more simple CSM probe is planned to be applied for the Scheldt, the Llobregat and also for the Bilina river (Elbe).

Task S1.3 Sedimentation rates

To determine the sedimentation rates recently developed and calibrated sediment traps will be established in suitable areas. During low water season campaigns local flow velocities and suspended sediment concentration in the groyne fields (Elbe) will be measured. The experimental results on sedimentation are evaluated and applied to the above mentioned rivers addressed in EXPO. Special emphasis is put on a measuring activity to capture an erosive flood event for sediment and pollutant mass balance. Hereto, samples can be taken from bridges to cover the whole cross section which is necessary in case of overbank flow with flooded areas. For quantitative sediment mass balance echo sounding measurements for sediment surface and sediment layer thickness detection are planned.

Deliverables

SD 1.1 Completion of the BASIN 1 and EXPO 1 data set and providing actual data for input in the EXPO 2 model. (10 months) (task S1.1)

SD 1.2 Supply of undisturbed sediment cores from hotspots for key toxicant identification in KEYTOX (12 month) (task S1.1)

SD 1.3 Intercomparison of field and laboratory techniques for contaminated sediment sampling and erosion stability measurements (CSM, SETEG, EROMOB) using data from Elbe, Scheldt, Llobregat) (15 months) (task S1.1, S1.2)

SD 1.4 Mapping of the SITE 1 results for a comprehensive assessment in EXPO and DECIS (18 months) (task S1.3)

Milestones and expected results

MS 1.1 (month 12) Workshop on sediment sampling methods and sediment erosion stability measurements

MS 1.2 (month 18) Workshop on particle size and sedimentation rate measurement techniques

WP Site 2 Bioavailability, bioaccumulation, biomagnification in food webs (18 month plan)

Work Package No.	**S2**	**Starting date:**				**Month 1**		
Participant	VUA	UJOE	RIKZ	RIVO	UFZ	SZU	CSIC	
Person Months	3	36	13	5	4	10	3	
Participant	ACA	UdG	VRI					
Person Months	0.2	1	2					

Objectives

The main objective of this workpackage is to deliver improved exposure estimates to be used for input to and parameterisation of the exposure and effect models to be developed in EXPO and EFFECT, and for input to the community-based assessments (SITE 3-5) and integrated assessments in DECIS and BASIN. This will be realised in the first 18 month period by meeting the following specific objectives:

- To asses and quantify the main factors determining the bioavailability of sediment-bound contaminants in laboratory desorption and bioaccumulation studies (UJOE) and field desorption studies (RIKZ, VUA)
- To develop methods for the determination of exposure and bioavailability in micro-organisms (RIKZ, UFZ)
- To apply novel biomimetic techniques for the measurement of bioavailable exposure concentrations in sediments and the water column of the Scheldt (RIVO, RIKZ)
- To analyse the accumulation of contaminants in a marine food web in the Scheldt estuary (RIVO, RIKZ, VUA)
- To prepare the freshwater food web studies in all basins in the 2nd phase of the project by harmonising methods, protocols, design, and organisation (all, in co-operation with SITE 3-5)
- To provide internal concentrations in test organisms (UFZ) for canonical community and food chain modelling (EFFECT3)

Description of work

Bioavailability, desorption studies and bioaccumulation in invertebrates

Task 5.2.1 Sediments from selected hot spots of the different basins will be selected and characterised (content and type of organic carbon, other elemental content, hardness/resistance to oxidation, and particle size distribution. For pore water DOM by organic carbon, macromolecular size distribution, aromaticity and functional groups (determined spectroscopically. Suitable model compounds will be selected in cooperation with other project members. Selected sediments samples will be spiked with relevant carbon-14 or tritium labelled contaminants and after 6-8 weeks contact time sorption (koc) and desorption of the model compounds will be measured. Relationships between desorption rate constants and contaminant and organic matter parameters and influence of aging and organic matter decomposition will be investigated in particulate and dissolved organic matter, in laboratory studies using the Tenax extraction method. Parameters to be included: kinetics of desorption, size of the different kinetic fractions, desorption rate constants, polarity of the pollutants, the mineral characteristics and the polarity of organic matter. The result will be used for the model formulations to be used in EXPO-3. (UJOE)

Task 5.2.2. The Tenax desorption method will be applied to field sediments in a salinity gradient in the freshwater and estuarine part of the Scheldt. For a range of compounds (to be selected in the first quarter of the project) the slowly and rapidly desorbing fractions will be determined. The results will be used in EXPO-3 (RIKZ, VUA).

Task 5.2.3 The bioavailability of sorbed contaminants to infaunal invertebrates in sediments will be determined in bioaccumulation experiments. The same sediments as in Task 5.2.1 will be spiked with the models compounds and after 6-8 weeks contact time bioaccumulation of the model compounds to *Lumbriculus variegatus* will be measured. This will provide information on, kinetics, BSAF, and the of role sediment characteristics and degradation and the relation between the tenax desorption results and the bioaccumulation. The results will be used in EXPO-3, SITE-4, EFFECT 1-3. (UJOE)

Bioavailability and bioaccumulation in microorganisms

Task 5.2.4. The role of microorganisms and food chain transfer to macro-zoobenthos will be investigated. Bacteria may be a major vehicle in mass transfer of hydrophobic compounds between sediment and macro-zoobenthos even more important than transfer from water, to be used in the EXPO models (Gunarsson et al, 1999). Methods will be developed and optimised for exposure and analysis. Deuterated modelcompounds (covering a broad range of Kow) will be applied. The role of bacterial contaminant transfer in relation to compound specific parameters (like Kow) and feeding behaviour of (test) organisms will be investigated. The outcome will be used in EXPO-3, EFFECT-3, SITE 3-4. (RIKZ)

In-situ assement with biomimetic methods

Task 5.2.5 An array of biomimetic methods (SPME, SPMD, SPE, Silicon rubber) tested and validated in KEYTOX will be applied in the Scheldt basin. With these methods an estimate will be obtained of the freely dissolved water concentration, which is assumed to be available for uptake by organisms. The output in the form of the bioavailable water concentrations will be used in EXPO 3-4, EFFECT 1-2, SITE 3-5. (RIVO, RIKZ)

Food web accumulation and biomagnification

Task 5.2.6 The bioaccumulation and food web transfer of contaminants will be studied in order to provide information on internal dosage levels in the effect and community-based workpackages (EFFECT 1-3; SITE 3-5, DECIS) and for parameter estimation and validation of the exposure and effect models (EXPO-3; EFFECT-3). As members of the SITE-2 team also participate in the workpackages where the results will be applied, the design and output of the food web studies will be tailored to the information needs.

The work in this task will be coordinated by VUA. With the prospect of freshwater food web studies in the 2nd phase of MODELKEY species, sites and target compounds will be selected, protocols harmonised and analysed for feasibility. Based on the information obtained from BASIN and SITE 3-5 on the presence and abundance of species, key pollutants of concern, concentrations in organism, and gaps in the data available, a preliminary selection will be made of relevant sites and species to select (in cooperation with EXPO-3, EFFECT-3). Classes of organisms to be considered are: algae, biofim-communities, zooplankton, benthic invertebrates, predatory fish, and possibly a piscivoreous bird species. For each basin proposals for organisms and contaminants to address will be made (basin coordinators IVB-VRI, CSIC-UdG, RIVO-UA), and to be discussed on a technical workshop on the preparation of the freshwater food web studies (organiser: VUA). Protocols for sampling (methods, season of preference, size/age classes, minimal required amount, taxa descriptions,), sample treatment (purging, dissection of tissues), transport, and storage (freezing conditions) will be provided to the partners that participate in SITE 3-5. The selection of validated chemical methods and quality assurance measures to be applied will be made by the laboratories that also participate in KEYTOX (RIVO, RIKZ, CSIC, UFZ, SZU, VRI, VUA). A joint report describing the outcome of the workshop, the protocols, and the organisation and planning of the freshwater sampling campaigns studies will be prepared (month 14; all, coordin. VUA).

During the first 18 months the estuarine food web in the Scheldt will be studied (RIVO, RIKZ, VUA). The selection of compounds will include reference compounds (PCBs, chlorinated pesticides, PAHs, Hg, Cd) for validation of the proto-type food web model in EXPO-3, model compounds from the bioaccumulation studies in this workpackage, in order to allow field-laboratory comparisons, and a first selection of contaminants of concern from KEYTOX-3 in month 6, and BASIN, such as e.g. brominated flame retardants (PBDEs, PBBs). Validated methods for sampling, sample treatment and chemical analysis are available from the joint monitoring programme (JMP) in which RIKZ and RIVO participate. Planning, organisation and design of the sampling programme will be addressed at an early stage (month 1-3, RIVO), sampling (RIVO) and chemical analysis (RIVO, RIKZ, VUA) will be executed between month 4-12. The results will be described in a report (RIVO, RIKZ, VUA, month 18) that will be used by EXPO-3 for validation of the prototype marine food web model.

Deliverables

SD2.1 Detailed characteristics of sediment samples form the three catchments (Task S2.1) (month 10) (UJOE)
SD2.2 Desorption rate constants of model contaminants for different organic fractions (Task S2.1) (month 18) (UJOE)
SD2.3 Data on the structural parameters governing desorption rates of model contaminants. (Task S2.1) (month 18)(UJOE)
SD2.4 Report on rapidly and slowly desorbing fractions of contaminants in field sediments in the Scheldt estuary (Task S2.2) (month18) (RIKZ, VUA)
SD2.5 Data on uptake of contaminants sorbed to organic matter by benthic invertebrates. (Task S2.3) (month 18) (UJOE)
SD2.6 Progress report on development of methods to study bioavailability and bioacumulation in micro-organsisms (Tasks S2.4) (month 18) (RIKZ, UFZ)
SD2.7 Biologically available concentrations in the Scheldt determined with biomimetic methods (Task S2.5) (month 12) (RIKZ, RIVO)
SD2.8 Internal concentrations of key toxicants in laboratory test organism in connection with canonical community modelling (EFFECT 3) (month 18) (UFZ)
SD2.8 Workshop report describing the organisation, planning, and protocols for the freshwater food web studies. (Task S2.6) (month 14) (all, coordin. VUA)
SD2.9 Report on the results of marine food web study in the Scheldt (Task S2.6) (month 18) (RIVO, RIKZ, VUA)

Milestones and Expected Results

M S 2.1 Technical workshop on preparation of sampling campaign of food web study (month 14)
M S 2.2 Results of biomimetic exposure concentrations in the Scheldt estuary (month 12)
M S 2.3 Results of sediment desorption and invertebrate bioaccumulation studies (month 18)
M s 2.4 Results of concentrations of contaminants in the marine food web in the Scheldt basin (month18)

WP SITE3 –Pollution induced effects on biofilm communities

Work Package No.	**S3**	**Starting date:**				**Month 1**		
Participant	UFZ	UdG	DW					
Person Months	20	30	3					

Objectives
The overall objectives of this work package are

- to develop a diagnostic toolbox for assessing adverse effects of site specific key toxicants on microbenthic communities including structural and functional parameters of biofilms, taxonomic based bioindices and metabolic profiling (all wp- partners)
- to establish metabolic toxicity test systems considering sensitive endpoints in dependence of mode of action of key toxicants (UdG, UFZ)
- to derive a causal analysis of effects of site specific key toxicants on community level by applying the concept of pollution induced community tolerance (PICT) (UdG, UFZ)
- to identify disturbances of microbenthic communities and ecosystem function at hotspots (UdG (Llobregat), DW (Elbe)
- to derive a causal analysis of community disturbance by applying the toolbox developed within the project (regional scale) (all wp-partners)

Description of work

Task S3.1 diagnostic toolbox development

Aim of the first 18 month of this work package will be, to develop an advanced toolbox for community based toxicity assessment of site-specific toxicants by integrating structural, physiological and functional parameters of microbenthic communities and community-based ecotoxicological assessment approaches. This will include (I) a literature-based collection of available methods, which are suitable to detect and quantify toxic effects in biofilm communities considering the specific mode of action of a contaminant (II) the development of methods to quantify toxic effects on biofilms in microcosm approaches.

Changes of community structure (biomass, taxonomy (all wp-partners) and metabolic profiling (e.g. HPLC-based pigment profiles, elemental composition, (C, N and P)) will be studied under non-toxic and toxic exposure as well as pollution induced changes of the microenvironment in biofilms (microgradients of pH and redox, measured by microelectrodes, (UdG); content of extracellular polymeric substances (EPS) (UFZ)), which could affect the bioavailability of toxicants. Effects on functional parameters of biofilms will be assessed through a variety of methods. The algal functioning front of toxicants will be assessed by non destructive pulse-amplitude modulated fluorescence-based methods (PAM). PAM – investigations will cover different scales by using whole community approaches (phyto - PAM) as well as single cell assessment within intact consortia (microscopy - PAM) (UFZ). Bacterial and fungal functioning will be assessed by analysis of extracellular enzyme activities in intact biofilms by applying fluorescence-labelled substrates (4-methyl-umbelliferyl – labelled compounds). Changes in maximal velocity and affinity for the substrate will be assessed under different toxic conditions (UdG).

Task 3.2 Pollution induced community tolerance - approach

Pollution induced community tolerance will be measured by short-term toxicity tests and quantified by shifts in EC_{50}. The backbone of the PICT - method is an acute metabolic test system, which addresses the specific mode of action of a toxicant and which is able to detect tolerance development. One aim of the first phase of this project is, to enlarge the applicability of PICT for a broad variety of toxicants. Considering the results of the method collection within the first part of this work package, metabolic test systems will be developed, addressing sensitive endpoints of a selection of site specific key toxicants. This will include effects on photosynthesis (algal component), extracellular enzyme activities (bacterial and fungal component), and percent of active bacteria (CTC and DAPI stain) or bacterial secondary production (bacterial component) (UdG, UFZ).

Task S3.3 Site assessment and toolbox application

During this phase of the project, key toxicants will be addressed, derived from already well characterised contaminated sites in the Elbe and Llobregat River Basin, covering a variety of mode of actions (according to the results of BASIN). This will include pesticides, the herbicide s-Triazin prometryn, n-Phenylnaphtylamin and heavy metals (all wp-partners).

Deliverables

SD 3.1 Overview over approaches for the verification of cause-effect relationships between exposure to key pollutants (selected by KEYTOX) and effects on biofilm communities including their biodiversity (6 months) (task S3.1)

SD 3.2 Effect assessment of key-toxicants on the structure, biodiversity and functioning of the biofilm communities (16 months) (task S3.1) .

SD 3.3 Establishment of standardised testsystems to measure pollution induced community tolerance of biofilms (16 months) (task S3.2)

SD 3.4 *In-situ* application of the toolbox, developed within the project to derive a causal analysis of community disturbance at selected hotspots (regional scale) (18 months) (task S3.3)

Milestones and Expected Results

M S 3.1 (month 6) 1st workshop: summary of approaches, assessing effects of key toxicants on microbenthic communities.

M S 3.2 (month 16) PICT-testsystems available

M S 3.3 (month 18) toolbox applied in case studies of Elbe (UFZ, DW) and Llobregat (UdG)

WP SITE 4 – Effects on invertebrate communities

Work Package No.	**S4**	**Starting date:**				**Month 1**		
Participant	UA	UJOE	IVB	UdB	DW			
Person Months	12	2	2	23	27			

Objectives

The overall objectives of this work package are

- To develop a diagnostic tool box of current and promising new tools for biological effects-based sediment quality assessment based on sediment contact testing (UJOE), macroinvertebrate community structure and metrics, including bio-indices (all wp-partners)
- To link bio-indices to contamination (UA, UdB, DW)
- To identify information gaps in the available datasets for the application of earlier identified tools (Schelt (UA), Elbe (DW, IVB) and Llobregat (UdB)
- To compile an overview of community structure and biodiversity of the macro-invertebrates in the studied river basins (Schelt (UA), Elbe (DW, IVB) and Llobregat (UBA)

Description of work

SITE 4 will make an overview of the state-of-the-art biological effects-based sediment quality assessment tools and the data required to apply the selected tools. Therefore SITE 4 will be divided into three tasks:

Task S4.1 Toolbox development

Collecting and scientific evaluation of currently used and new promising tools for quality and impact assessment related to contamination. Intercalibrations and adaptations, that have to be made for optimisation of the methods regarding a general usage for toxicity assessment, will be made for available tools. Available and used evaluation methods and bio-indices will be viewed and optimised for toxicity effect assessment of macroinvertebrates.

Task S4.2 selection of sampling sites and development of sampling strategy for the three basins

An overview will be made of what kind of information is needed to apply and develop the methods selected in task 1. This information will be asked to the work package BASIN 1. A plan will be made for the collection of missing information and for the sampling of the hot spots that will be studied. In a workshop, the methods theoretically and experimentally developed in task 1 will be discussed and a base of a comparable strategy will be decided by the partners, preferably applied in the field.

Task S4.3 data analysis of available data from BASIN

Based on available data in BASIN 1, analyses will be made of the biodiversity in the three river basins compared to other river basins. It will be clarified which role invaders, masking the indication of toxic effects play in the ecosystem of the rivers studied and whether they will be regarded or neglected. Information for other river basins will be collected from the literature to ensure the general practicability of the tools.

Task S4.4 site assessment of selected contaminated sites

First sampling campaigns will be performed in order to collect experiences for possible adaptations of the design, to validate the toolbox and to provide site-specific baseline data.

Deliverables

SD 4.1 overview of existing tools for biological effects-based sediment quality assessment (7 months) (task S4.1)

SD 4.2 identification of suitable bio-indices to toxicity assessment (18 months) (task S4.1)

SD 4.3 intercalibrated sampling strategy and design (7 months) (task S4.2)

SD 4.4 evaluation of the role of invaders as indicators (12 months) (task S4.3)

SD 4.5 overview of site – specific base line data, community structure and species diversity extracted from data collection in BASIN 1 (18 months) (task S4.3, S4.4)

SD 4.6 preliminary application of the toolbox at hotspots (18 months) (task S4.4)

Milestones[1] and Expected Result

M S 4.1 (month 7) Literature search and information compilation completed

M S 4.2 (month 7) Workshop discussing the collected tools and bio-indices for sediment quality assessment based on the macroinvertebrate community and further experimental needs

M S 4.3 (month 7) List of the data needed for the application of the selected tools which will be delivered to BASIN 1

M S 4.2 (month 12) Scientific evaluation and intercalibration of suitable methods and experiences of the pilot field work

M S 4.4 (month 18) Report of the biodiversity on the three selected river basins in comparison with other European river basins

WP SITE 5 – Effects on fish communities (18 month plan)

Work Package No.	**S5**	**Starting date:**				**Month 6**		
Participant	UB	VRI	IVB	RIVO				
Person Months	10	10	10	6				

Objectives

The overall objectives of this work package are

- to select field sites and fish species for toxicological and ecological analysis (RIVO, VRI, IVB)
- to perform experimental studies to develop a diagnostic toolbox for site-specific toxicity assessment (all wp-partners)
- to generate data for the ecological EFFECT models (all wp-partners)
- to provide site-specific baseline data on toxic hazards and fish communities (all wp-partners)

Description of work

Task S5.1 selection of study sites and toxicological/ecological screening

In a first phase (months 6-15), study sites will be selected in the two river systems, Elbe (limnic) and Westerscheldt (brackish to marine). The selection will be based upon a) information and data collected by BASIN 1 during the initial months of MODELKEY, and b) preliminary toxicological and ecological screening within SITE 5 at candidate field sites in Elbe and Westerscheldt, measuring sediment-borne toxic potentials (by means of *in vitro* bioassays) and fish community parameters.

Task S5.2 selection of target fish species

At each field site, one fish species will be selected for *in vivo* biomarker measurements and for incorporation in the EFFECT models. The target species used in those experiments will be identified on the basis of its abundance at the study sites and its toxicological (biomarker response etc.) as well as ecological characteristics (benthic species, position in the food chain, etc.). The latter point is important in order to feed experimental and field data into the models developed in EFFECT. Candidate species are flounder for the Westerscheldt and stickleback or chub for the Elbe; the final decision on these candidate species will be made upon the results of the initial field surveys..

Task S5.3 diagnostic toolbox development

The second phase during the initial 18 months of SITE 5 (months 9-18) has two aims: Firstly, to develop methods for the diagnostic toolbox for *in situ* toxic effects assessment; this part will be finished at month 18. Secondly, to generate initial experimental data sets to be used as a “conceptual toolbox” in subsequent site assessment and verification of the EFFECT models. To this end, laboratory experiments with the selected target fish species will be performed to generate basic toxicological and ecological data. For exposure, major contaminants of the river basins as identified by BASIN will be used. This part will extend beyond month 18. In vitro and in vivo toxicological endpoints to be part of the diagnostic toolbox will include ER- and AhR mediated effects (CALUX assays), cytotoxicity, histomorphology and ATP contents, and, finally, genotoxicity (comet assay). Using these endpoints, in vitro bioassays will determine the toxic potential being present in river sediments. In vivo biomarker measurements as well as in vitro bioassays on fish tissue extracts will determine will verify to what extent the toxic potencies being present in the sediment are transferred into the fish. The ecological measurements will include population-relevant parameters of individuals (growth, survival, fecundity/fertility).

Deliverables

SD 5.1 toxicological and ecological screening of selected sites (15 months) (task S5.1)

SD 5.2 selection of target species (15 months) (task S5.2)

SD 5.3 method-oriented diagnostic toolbox for toxicological site assessment (18 months) (task S5.3)

SD 5.4 Toxicological and ecological data to feed into EFFECT models (18 months) (task S5.2, S5.3)

Milestones[1] and Expected Result

M S 5.1 (month 9) Selection of candidate study sites (in collaboration with BASIN, DECIS)

M S 5.2 (month 15) Final identification of the study sites and target fish species in Westerscheldt and Elbe

M S 5.3 (month 18) finalisation of a first series of experimental studies on toxicological and population-level responses of target fish species to basin-relevant contaminants

WP DECIS1 - Development/Refinement of the conceptual framework and hot spots prioritization module

Work Package No.	**D1**	**Starting date:**					**Month 1**	
Participant	CVR	UFZ	UA	CEFAS	DELFT	CNRS	CSIC	
Person Months	22	1	1	1	1	1	1.5	

Objectives

Development of decisional framework and Decision Support System (DSS) structure
The primary objectives of this task for the first 18 months are:

- to develop a common decisional framework to integrate project deliverables for management purposes
- to ensure a coherent development of projects deliverables to be integrated within the DSS
- to formulate a preliminary structure for the DSS

Site prioritisation module
Primary objectives for the first 18 months are:

- socio-economic characterisation of the three case studies
- design of the investigation on biodiversity valuing

Description of work

Task D1.1 Development of decisional framework and Decision Support System (DSS) structure

In order to define a conceptual framework, a review of existing models, decision frameworks, legislations and policy-driven actions will be performed. The review will be focused on the identification of potentialities and gaps which may be elaborated and fulfilled within the DSS. Links with legislations and management tools will be highlighted. The review will end with a report summarizing main findings.

For the first definition of a monitoring program, an initial overview of existing programs at the light of data required by Modelkey models and tools will be performed. A preliminary list of recommendation for monitoring biodiversity impacts at basin scale will be derived, which will be revised and completed based on the three case studies.

The DSS structure will be preliminarily defined. Demands of selected groups of end-users will be collected and evaluated. The main functionalities of the systems will be identified. During this phase, better solutions for the DSS structure and organization in terms of general contents, diagrams, step procedures and links will be studied and then proposed for the definitive version, to be confirmed for the 30th month.

Task D1.2 Site prioritisation module

Socio-economic data of the three case studies will be collected and analysed. The zoning of the three river basins based on socio-economic variables will be accomplished. The investigation activities on biodiversity valuing will be designed and preliminary proposal for prioritization of hot spots will be defined.

Deliverables

DD1.1: Review of models/tools/decision frameworks and conceptual framework, Report (month 10) Task D1.1
DD1.2: Preliminary list of recommendations for the design of monitoring programs of biodiversity impacts at basin scale (month 10) Task D1.1
DD1.3: Socio-economic characterisation of three case studies (month 16) Task D1.2
DD1.4: DSS Structure Interim Report (month 18) Task D1.1
DD1.5: Review and preliminary proposal for prioritization of hot spots based on risk and economic assessment of biodiversity and ecological impairment (month 18) Task D1.2
DD1.6: Design of investigation on biodiversity value (month 18) Task D1.2

Milestones and Expected Result

1. By the month 8th, the general conceptual framework should be agreed by all project partners
2. By the month 16th, definition of one or two methods and preliminary set of criteria for the hot spots prioritization procedure should be available.

WP DECIS2 – Integrated Risk Index

Work Package No.	**D2**	**Starting date:**				**Month 6**		
Participant	RIVM	CVR	CNRS	UA	CEFAS	DELFT		
Person Months	1	12	1	1	1	1		

Objectives

Integrated Risk Index for basin scale hot spot prioritization

1. To review Weight of Evidence approaches and tools
2. To develop a preliminary Weight of Evidence procedure

Integrated Risk Index for site-specific assessment

1. to develop a first proposal for the WoE procedure to be applied in the site-specific assessment

Description of work

Task D2.1 - Integrated Risk Index for basin scale hot spot prioritization

A review of open literature will be accomplished in order to assess and to compare developed and proposed step-wised Weight of Evidence methodologies, as well as procedures to formulate risk indexes. The evaluation of criteria for weighting, selecting, and integrating the ecological, chemical and toxicological data (i.e., lines of evidence), will provide a series of recommendations for the implementation of BASIN 1 database. A Final Report concerning the review results will be produced.

In the second period different tiered WoE methodologies will be developed. Criteria for assessing, weighting and integrating the exposure and effects data (i.e., experimental and model results) by means of Multi Criteria methodologies will be formulated.
At least two preliminary Weight of Evidence procedures, for example one qualitative and one quantitative, will be proposed.

Task D2.2 - Integrated Risk Index for site-specific assessment
As for the first task, at least two Weight of Evidence procedures will be compared and selected in order to propose a preliminary approach for the site-specific assessment.

Deliverables

DD2.1 Critical review of Weight of Evidence approaches and tools (report) (month 10) (Task D2.1 9)
DD2.2 Proposed preliminary Weight of Evidence procedures for Basin scale IRI, Interim Report (month 18) (Task D2.1)
DD2.3 Proposed preliminary Weight of Evidence procedures for Site Specific IRI, Interim Report (month 18) (Task D2.2)

Milestones and Expected Result

1. In the first 18 months, DECIS 2 will provide a methodological development of a preliminary Weight of Evidence approach, proposing two or more adaptable procedures characterized by different (or increasing) site-specificity (i.e. basin vs. site-specific scale) and complexity (i.e., qualitative vs. quantitative).
2. The development of preliminary WoE procedures will require the coordination with BASIN 1, in order to interpret and assess the chemical, ecological and eco-toxicological data in terms of exposure and effects.

WP DECIS3 – Development and application of DECIS DSS

Work Package No.	**DECIS 3**	**Starting date:**				**Month 30**			
Participant	CVR	EWQMA	RIKZ	CSIC	UFZ	ACA	IVB	RIVO	UdB
Person Months									

Objectives

- No activities in DECIS 3 are planned during the first eighteen months.

WP DIS/TRAIN 1- Dissemination (18 month plan)

Work Package No.	**DT1**	**Starting date:**				**Month 1**		
Participant	CEFAS	CSIC	RIKZ	RIVO	SPbU	VRI	VUA	UFZ
Person Months	1	1.5	0.5	1				2
Participant	CVR	RIVM	UdG					
Person Months	1		0.5					

Objectives

- To disseminate relevant information with European and world-wide communities (policy makers, end-users, stakeholders, and scientists) in the field of assessing and forecasting the impact of environmental pollutants on marine and fresh water ecosystems and biodiversity
- To make these communities aware of the existence of MODELKEY, its partners and its ambition.
- To optimise communication by establishing an end-user communication board.

Description of work

The MODELKEY work and its partners are strongly linked to European Research Networks and Integrated Projects. Dissemination and exchange of knowledge are of mutual interest to all European scientific, policy, and stakeholder communities. This exchange process is stimulated by three types of tasks:

Task DT1

The public communication strategy of MODELKEY consists of (1) Web-site, (2) newsletter, (3) brochures, flyers and press releases. A newsletter every half year, flyers when considered necessary (e.g. yearly workshop, courses), describing the activities and progress of MODELKEY. The written dissemination strategy consists of submission of scientific and informative on several issues of the MODELKEY project to international and management journals respectively. Presentations / Posters at national and international symposia constitute the verbal dissemination.

Task DT2

The first of yearly workshops, addressing both the scientific and executive community on the progress of the project, will be organized in M12. A workshop newsletter will be prepared, and distributed by the MODELKEY Web-site and E-mail. The proceedings will be published in a scientific and management journal.

Task DT3

The networking strategy consistst of (1) actively approaching other European networks and integrated projects (e.g. SEDNET, REBECCA, AQUATERRA, ALARM), (2) an end-user communication board to facilitate direct transfer of knowledge and demands between end-users and science. The board consists of project coordinator, subprojects leaders, selected key end-users. An inventory of end-users will serve the selection. The boards main tasks are (1) to optimise the communication (DIS/TRAIN1), (2) advice workpackages how to optimise scientific approach and end-user benefit (3) guarantee knowledge flow directly into decision making by environmental agencies and authorities (DECIS), (4) organise the mid-term review of MODELKEY (Month 30).

Deliverables

DT 1.1 Scientific brochure and flyer on the existence of MODELKEY, its anticipated program and the central MODELKEY contact point. To be distributed amongst the European / world wide scientific Networks and Projects (Month 3)

DT 1.2 MODELKEY Website launch (Month 4)

DT 1.3 MODELKEY Newsletter 1 (Month 6)

DT 1.4 1st yearly update Workshop on the MODELKEY progress, all subprojects reporting (Month 12)

DT 1.5 Establishment of an end-user communication board (Month 12)

Milestones and Expected Result

- Course evaluation during the 1st workshop (M12)
- Progressive tuning with other European Networks and Projects (*a.o.* SedNet, REBECCA, AQUATERRA, ALARM)
- Establishment of end-user communication board selection list (M3)

WP DIS/TRAIN 2- Training and Education

Work Package No.	7.2	Starting date:				Month 20		
Participant	CEFAS	CSIC	RIKZ	RIVO	SPbU	VRI	VUA	UFZ
Person Months	0	0	0	0	0	0	0	0
Participant	CVR	RIVM	UdG					
Person Months	0	0	0					

Objectives

- Training activities for PhD students and other young researchers in the sense of a hands-on training process start already within the first 18 months. For these activities no additional person months are reserved since these activities are included in the scientific WPs.

Description of work

Hands-on training for young researchers

Deliverables

no specific deliverables

Milestones and Expected Result

- no specific milestones

WP CO1: Scientific coordination and Project Management

Work package number	CO1	Start date or starting event:				Month 1	
Participant id	UFZ						
Person-months per participant	9						

Objectives (months 1-18)

- The project success is dependent on successful communication between all participating research groups (e.g. in the selection of scenario assumptions, in dealing with the pilot sites, etc.), and an electronic tool permitting a systematised information exchange plus open debates is helpful in structuring discourses, filing data to make them easily accessible, and for mutual information about the state of research. As this information has different characteristics regarding the public access to it (see the deliverables list), different access levels will be established.
- The knowledge to be generated by the project needs broad dissemination, beyond the scientific community to make it available to decision makers and to make sure it is taken into due account in the decision making process.
- Scientific co-ordination supports all other subprojects and workpackages. However, a specific focus is on the support of dissemination activities. These are already mentioned in WP DIS/TRAIN 1. However, they are also tasks of Scientific co-ordination.

Deliverables

COD 1.1: Start-up meeting for the whole consortium (Month 2)

COD 1.2: MODELKEY Website launch (Month 4)

COD 1.3: 1st yearly update Workshop on the MODELKEY progress (Month 12)

COD 1.5: Establishment of an end-user communication board (Month 12)

Milestones and expected result

COM 1.1: Start-up meeting for the whole consortium (Month 2)

COM 1.2: MODELKEY Website launch (Month 4)

COM 1.3: 1st yearly update Workshop on the MODELKEY progress (Month 12)

COM 1.5: End-user communication board established (Month 12)

B.9 Other issues

Ethical issues

This proposal does not include research on modifications of the human genome or research involving cloning. It does not interfere with principles expressed in widely recognised texts such as the conventions of the Council of Europe on human rights and biomedicine, the Helsinki declaration and the UNESCO Declaration on the human genome. The research fulfils all legal and ethical requirements of the member states where it is carried out.
The project can be specified as to ethical aspects as follows:

- Human embryos or foetus	No
- Use of human embryonic or foetus tissue	No
- Use of other human tissue	No
- Research on persons	No
- Children	No
- Persons unable to consent	No
- Pregnant women	No
- Healthy volunteers	No
- Use of non-human primates	No
- Use of transgenic animals	No
- Use of other animals	Yes
- Genetic modification of animals	Yes
- Genetic modification of plants	No

Animal experiments:
There is also a small number of studies planned in the project (KEYTOX 1 and 2, SITE5), which involve experimental animals (fish). The reason for using animal experiments is because this project is focussing mainly on improving the understanding between *in vitro*, *in vivo* responses and possible changes in biodiversity in relation to exposure of toxicants. These data are necessary for the integrated effect and exposure models to be performed in EXPO and EFFECT. There are no alternatives for addressing these questions.
All animal experiments performed within MODELKEY will strictly follow the rules of the respective national ethical committees on animal experimentation. There is an ongoing EU-wide discussion on establishing standards for maintenance of fish. Some of the MODELKEY partners (e.g., H. Segner) are involved in these discussions and will ensure that the rearing of fish in the MODELKEY partner laboratories will follow those standards. This will be further ensured by the fact that the experimental facilities of the partner laboratories are especially equipped for maintenance of fish, and the involved scientists have long-standing experience and know-how in the culture of fish. The animal treatments foreseen in MODELEY include exposure of fish to chemicals at concentrations that correspond to concentrations in the environment, i.e. very low concentrations which most likely will not induce pain or severe distress, and the fish will not suffer more than in its natural environment.
Wherever possible, we will rely on *in vitro* methods instead of animal experimentation. Several MODELKEY partners have outstanding experience in the use of *in vitro* systems for environmental hazard assessment (e.g, W. Brack, M.

Machala, H. Segner), as it is evident for instance from the participation of one partner (H. Segner) in the ECVAM Task Force on Alternatives in Ecotoxicology.

Studies involving genetically modified cell lines

In KEYTOX 1 and 2 of this project, genetically modified cell lines (the so-called CALUX™ assays) will be used as reporter gene assays for use as bioassays for toxicants by partner 3, 6, and 11. All necessary authorisations on storage, handling and use of these cell lines have been obtained from the National Committee on Genetically Modified Organisms (Dutch COGEM committee). All cells and materials thereof will be held in the proper containments and be treated/handled according to “good laboratory practice” as specified by the COGEM and by the “Hinderwet vergunning”, to exclude release of GMOs, or materials thereof in the environment.

EC Policy issues

Issues relating to environmental and sustainable development policies are addressed in section B3.1.

B.10 Gender issues

B.10.1 Gender Action plan

MODELKEY will follow employment policies laid down by the individual participant institutes and will consequently reflect specific national gender action plans. All universities and research institutions of the Consortium support the implementation of international resolutions and programmes aiming at the full and equal participation of women in all spheres of society, and most of them possess their own equal opportunity programmes (usually addressing ”equality” in all spheres, not just ”gender”.
The implementation of these equal opportunity programmes aim for the full participation of women and comprise different measures such as an *Action Plans for the Promotion of Women, Working Groups for Gender Equality, or Committees for Equal Opportunities*. A specific example found in many of these plans is that in the case of equal qualifications, female applicants are preferred to male candidates to attain a balanced proportion of women at all levels. The promotion of gender mainstreaming is a difficult task and needs continuous promotion, since the results achieved so far are generally considered unsatisfactory. Women are still significantly under represented at more senior grades in research . Only a low percentage of professors are women or hold leading positions in RTD projects

In **MODELKEY** about 30% of PCC members and deputies will be women including the deputy of the project co-ordinator, subproject leaders, case study leaders and deputies (see Table B.6.1). The role of female scientists in the project covers a wide range of scientific activities untertaken at all levels from professor to post-doctoral scientist and technicians.

Although the subject matter of MODELKEY is in no way gender-discriminatory, specific activities to ensure and promote gender equality within the Project will include:

Affirmative action Procedures for the hiring of staff will follow the specific conditions of the individual institutes (see above), which usually include a preference for female applicants where they have equal qualifications to male applicants. Application of female researchers will be specifically encouraged, aiming to bring more women into the project. Our aim is to increase the proportion of female researchers during the project.

Gender advisory group One representative of the network will be chosen as the responsible person for gender issues within the Project, and charged with establishing a small gender advisory group. This group will review procedures (e.g.. invitations to training courses/workshops), identify women scientists in the community that may have been overlooked, develop, review and refine the *gender action plan* and organise internal audits on gender issues. A key task will be to set up an inclusion policy that will not only ensure the project follows an equal opportunities agenda but will also identify barriers to female involvement and progression and develop strategies to remove them. An example will be the provision of travel assistance bursaries to encourage participation at project conferences and workshops of external female scientists.

Internal audits We will untertake an audit on gender issues in Year 2 and Year 4 of the Project. These will be supplemented with an external review untertaken as part of the Project interim review during Month 18.

B.10.2. Gender issues

As fare as we are aware there are no specific gender issues associated with **MODELKEY** beyond those addressed in the Gender Action Plan. However, the *gender advisory group* will regularly review and assess the situation.

ANNEX B.5: Detailed description of MODELKEY partners

1. UFZ Centre for Environmental Research (UFZ)

The UFZ (Centre for Environmental Research) was established in 1991 as the first and only establishment in the Helmholtz Community of German Research Centres (HGF) to be exclusively devoted to environmental research. It currently employs around 650 staff in total. The UFZ is 90 percent funded by the Federal Ministry of Education and Research, with the regional governments of Saxony and Saxony-Anhalt sharing the remaining 10 percent equally. Since its foundation in 1991 UFZ has participated in 44 EU projects, coordinating 14 of them. 22 of these projects have started in the 5^{th} EU Framework Programme.

The Department of Chemical Ecotoxicology (http://www.ufz.de/spb/tox/index.html) currently consisting of 14 scientists, 15 technicants, and 6 PhD students is headed by **Prof. Dr. Gerrit Schüürmann**. It aims at unravelling mechanisms of deleterious effects of chemical substances, and at deriving assessment criteria for their ecotoxicological potential in the field. The experimental and theoretical studies focus on two complementary approaches: In the substance-oriented approach, single compounds, mixtures and environmental samples are analyzed with respect to their biological activities and underlying modes of toxic action. Responsible toxicants are identified and cause-effect relationships are established. The effect propagation on higher levels of biological organization is considered in the system-oriented approach, where the stress response of communities in the field is studied in terms of reaction patterns and interactions. The link between effect parameters and exposure parameters as well as underlying compound properties enables the development of strategies for a process-oriented risk assessment of contaminations in the field.

Research Team

Werner Brack Ph.D. in Environmental Chemistry. Leader of a research group on effect-directed analysis. Teaching at the Universities of Leipzig and Ouro Preto (Brazil). Member of the editorial board of Chemosphere. He is coordinator of the national project CHEMSTRESS on “Chemical key stressors and their distribution and transformation in river ecosystems” and a German-Canadian project titled “Influence of sunlight on the toxicity of complex environmental mixtures of PAHs – Identification of toxic photomodification products”. As a member of the core group of the European Sediment Research Network (SedNet) he is involved in the development and standardisation of methods of sediment quality assessment on an European scale. His scientific focus is on method development for effect-directed analysis of complex environmental samples including sediments, groundwaters and leachates. His role in MODELKEY is that of the overall coordinator. His group will play a major role in subproject KeyTox (key toxicant identification).

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W. Brack, K. Schirmer (2003) Effect-directed identification of oxygen and sulphur heterocycles as major polycyclic aromatic cytochrome P4501A-inducers in a contaminated sediment. Environ. Sci. Technol. 37:3062-3070
W. Brack (2003) Effect-directed analysis – A promising tool for the identification of organic toxicants in complex mixtures?. Anal. Bioanal. Chem. 377:397-407

Mechthild Schmitt-Jansen (Ph.D.) as a limnologist is involved in national and international actions concerning the evaluation of potential ecological risks of stressors on algal communities. The research focuses on approaches to ascertain causal links between toxic exposure and effects on higher levels of biological organisation by using multispecies approaches (pollution induced community tolerance). She has long-standing experience in the assessment of regulation mechanisms of aquatic primary production including process measurements and structural analysis of microalgae - communities, using taxonomy approaches as well as biomarkers.

Selected relevant references

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Schmitt-Jansen, M. & Nixdorf, B. (submitted): Longitudinal dynamics of lake phytoplankton in a lowland outlet stream. Journal of Plankton Research.
Altenburger R, Schmitt-Jansen M. (2003). Predicting toxic effects of contaminants in ecosystems using single species investigations. in: Breure AM, Markert BA, Zechmeister HG. (Eds) Bioindicators, Biomonitors: Principles, Assessments, Concepts. Elsevier. pp. 153-198.
Schmitt, M. (2000): A comparison of methods to investigate the species composition and population structure of aquatic Heteroptera. Mitt. dtsch. Ges. allg. angew. Entomologie 12, 245-248.
Schmitt, M. & Nixdorf, B. (1999): Spring phytoplankton dynamics in a shallow eutrophic lake. Hydrobiologia 408/409, 269-276.

Gerrit Schüürmann is the head of the Department of Chemical Ecotoxicology and serves as editor for *Environmental Toxicology and Chemistry* and on the editorial board of three other journals, and has published over 170 articles. He participates in several international and national projects. Examples are the EU projects IMAGETOX and TUBERCULOSIS, which was co-ordinated by him. He focuses on structure-activity relationships and on modelling compound properties and exposure, with a longstanding knowledge in computational chemistry and advanced statistics. His work is devoted to developing and applying mechanistically sound molecular descriptors for predicting phase partitioning, degradation and toxicity of compounds from chemical structure.

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Albrecht Paschke (Ph.D. in Physical Chemistry) is the head of the research group “exposure analysis”. Major research interests are the experimental determination of physicochemical properties of xenobiotics, waste, soil and sediment leaching tests for characterisation of the pollutant mobilisation and bioavailability, and the development/calibration and field validation of passive samplers for organic micropollutants in water and air. He is running national and international projects on “time-integrated determination of dissolved organic micropollutants in surface waters using semipermeable membrane devices and novel passive samplers” and “particle-size specific pollutant content of sediments and waste materials”.

Selected relevant references

Paschke A, Popp P, (2003): Solid-phase microextraction fibre-water distribution constants of more hydrophobic organic compounds and their corrrelations with the octanol-water partition coefficients. *J. Chromatogr. A*, 999 (2003) 35-42.

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Klaus-Dieter Wenzel (Ph.D. in Chemistry) is a senior scientist in the research group “exposure research” and responsible for the coordination of the German-Israeli-Palestinian project “Groundwater availability and the fate of pesticide input – fundamentals of human health in the Middle East”. His research focuses on fate assessment of pesticides, persistent organic pollutants (POPs) and PAHs in terrestrial and aquatic environments and the development of extraction, clean-up and analytical procedures for these compounds in soils, sediments and complex biological matrixes.

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Wenzel K-D, Hubert A, Manz M, Weißflog L, Engewald W, Schüürmann G 1998. Accelerated Solvent Extraction of Semivolatile Organic Compounds from Needles and Mosses. *Anal. Chem.* 70:4827-4835.

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Rolf Altenburger Ph.D. in Natural Sciences, venia legendi in Ecology and Ecotoxicology, University lecturer at University of Bremen (Germany). He was participant in the EU-projects BEAM (5. FP) and PREDICT (4.FP). His main expertise as relevant for MODELKEY are techniques for identification, assessment and quantification of biological effects in response to chemical exposure including estimation of dose-response and time-response functions, and his expertise on the assessment and prediction of combined effects of chemical mixtures. He has published more than 40 peer-reviewed papers and a similar amount of book contributions. Rolf Altenburger is co-ordinator of the proposed project EUFP6 RAMSES and thus not directly involved in MODELKEY. However, he will act as an advisor in questions relevant to his expertise, which may rise in MODELKEY.

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2. University of Antwerp (UA)

The research group Ecosystem Management (http://www.ua.ac/ecobe) is one of the research units of the department of Biology at the University of Antwerp. The main objective of the research group is to provide a sound scientific basis for nature- and ecosystem management in general and integrated water management in particular. Therefore the research is focussed on ecology of stagnant and running inland waters and estuaries and the associated wetlands. The processes in the land water interaction along the whole river continuum from source to sea are studied at different scales:

from individual organism over populations and communities towards ecosystems and the landscape. These studies, both descriptive field and experimental studies, will be integrated to make predictions on the impact of different management options on the functioning and biodiversity of the system.

Next to studies on the effect of water quality on fish, macroinvertebrates and macrophytes, studies on developing ecosystem management programs for several rivers systems, including the Schelde estuary and on integrated water management are undertaken. Further several studies on characterisation of the ecological quality of river sediments and the impact of sediment quality on biota are running. The group is involved in the coordination of the working group “Quality and impact assessment” of the EU network SedNet, and coordinates the research project OMES which object is the development of an ecosystem model for the Schelde estuary with special emphasis on the nutrient cycle and the role of the intertidal area in the ecosystem functioning. Nine different universities and scientific research institutes are involved in this OMES project.

The research group has a certified laboratory for water quality analyses and for determination of macroinvertebrates in function of the application of the Belgian Biotic Index.

Research Team

Patrick Meire studied biology at the University of Ghent. I started my PhD work at the Laboratory of Animal Ecology, Nature Conservation and Biogeography of the University of Gent first with a research grant from the Belgium National Fund for Scientific Research, later as a research assistant. In 1990 I became senior researcher at the Institute of Nature Conservation, a research Institute of the Flemish Government. Since 1995 I hold the chair of Integrated Water Management at the Institute of Environmental Studies of the University of Antwerp (part time visiting professor) and since 1999 I am full time professor at the University of Antwerp, Department of Biology and head of the ecosystem research group.
My research dealt mainly with studying the impact of human activities (pollution, reclamation, dredging etc.) on the estuarine ecosystem and with translating this knowledge in management plans.

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Eric de Deckere studied environmental science at the Agricultural University of Wageningen. He specialised in integral water management. He prepared a manual for the treatment of eutrophication in freshwater lakes at the Dutch Institute for Inland Water Management and Waste Water Treatment. Worked as a PhD student at the Centre for Estuariene and Mariene Research in Yerseke, looking at the effect of benthos on the behaviour of sediments. For this, he was involved in the Dutch research project BOA and the European Mast-III project INTRMUD (Morphology and processes of intertidal mudflats). Currently he is working at the University of Antwerp, coordinating the development of Flemish monitoring method for sediment quality assessment. He is also involved in the European LIFE-SED project on contaminated sediments. He recently passed his doctoral degree and is appointed doctor assistant in the European project Sednet.

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Stefan Van Damme studied agricultural sciences, followed by a specialised study in environmental technologies, at the University of Ghent. He performed a three year study on denitrification in tidal areas of the Scheldt estuary at the University of Ghent. At the Free University of Brussels he participated in a study on nitrogen cycling in the same estuary. At the Université Libre de Bruxelles he performed the validation of a one year dataset of an automated measurement station. Currently he is preparing a PhD at the University of Antwerp, looking at the evolution of the water quality of the Scheldt estuary with focus on nitrogen. He is also involved in the practical organisation and scientific integration of the integrated scientific programme OMES, which focuses ecological research on the Scheldt estuary.

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Chris Van Liefferinge studied Biology, option organisms and populations, at the University of Antwerp, where he also graduated in the supplementary study of environmental sciences. After his studies he followed a course fish stock management. Since 1998, he works at the University 'Campus Drie Eiken' as scientific assistant in the ecosystem management research group, where he is responsible for the research of fish communities and the relation between the water quality and the aquatic life communities (macro-invertebrates : Belgian Biotic Index and fishes : Index of Biotic Integrity). He has experience on the field of fresh water fish ecology, Flemish protection programmes of rare and endangered fish species, evaluation of the methodology and use of the Flemish index of Biotic Integrity for fresh waters, the determination of the possibilities and the monitoring of river restoration and rehabilitation projects, including the amelioration of fish migration. In addition he is responsible for the certified laboratory of biological water quality assessment using macro-invertebrate indexation.

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Van Liefferinge C., Seeuws P., Meire P. & Verheyen R.F. (in prep.) Microhabitat use and preferences of the endangered species *Cobitis taenia* L. (spined loach) in the Flanders, Belgium - A tool for ecosystem management

Van Liefferinge, C. Simoens, I. Breine, J., Ercken, D., Goethals, P., Verhaegen, G., Ollevier, F., De Pauw, N., Belpaire, C. & Meire, P. (in prep.) Is a standardised electric fishing sample of a 100m section enough for an accurate estimation of species diversity and IBI evaluation as mentioned in the water framework directive?

3. Centre for Environment, Fisheries and Aquaculature Science (CEFAS)

CEFAS (www.cefas.co.uk) is an internationally renowned scientific research and advisory centre working in fisheries management, environmental protection and aquaculture. CEFAS undertakes a wide range of research, advisory, consultancy, monitoring and training activities. Our customer base includes Government departments (UK and foreign, central and local), international agencies, commercial companies and aid organisations. Much of our work is conducted for the UK Government and the European Union where our research and advice is utilised by policy makers, but in the past six years we have developed an increasingly worldwide client base. CEFAS has a staff compliment of approximately 550 who are based at three specialist laboratories within the UK. We have two ocean going research vessels and our facilities are equipped with the latest laboratory, tank and aquatic field based equipment. CEFAS has a long track record in EU framework programme particpation, being involved in over 30 projects under FP 3 and 4, over 20 in the 5th Framework Programme. We are currently particpating in 13 newly awarded FP6 projects, of which we are coordinating two.

The Hazardous Substances Research area is currently comprised of approximately 30 scientists from the Analytical Chemistry, Contaminant, Fate and Effects, and Pollution Effects teams and is led by **Dr. Kevin V. Thomas**. Work in this area is primarily concerned with research into the effects of hazardous substances on aquatic organisms. The present portfolio of work is carried out within 3 main themes; Causality, Emerging Contaminants and Risk Assessment.

Research Team

Kevin V Thomas PhD in Environmental Science. Topic leader for hazardous substances research. Invited lecturer at Dublin City University (Eire). He brings to the project extensive experience in environmental research. Dr Thomas specialises in the characterisation and effects of contaminants and leads a very active research group that are at the forefront in this area. Dr Thomas has extensive experience of successfully managing complex research projects for the UK Department for the Environment, Northumbrian Water Plc, Solutia Plc, Corus Plc, the UK Oil Operators Association (UKOOA), the UK Environment Agency, the UK Department of Trade and Industry, the Norwegian Research Council, Daiwa Foundation, Ecosea Ltd., WRc-NSF, the UK Health and Safety Executive. Shell, Posford Haskoning Ltd, and multi-national industry consortia. He currently manages programmes investigating the characterisation of toxicants in produced water, environmental occurrence of pharmaceutical compounds, environmental fate and effects of antifouling compounds and the bioavailability of copper. He advises the UK and Foreign Governments, Industry, EU, ICES and OSPAR on marine environmental matters concerning hazardous substances. His role in MODELKEY will be as sub-project leader for KEYTOX, whilst his research group will play a major role in this subproject.

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Hilton, M. and Thomas, K.V. (2003) Determination of selected pharmaceutical contaminants in water samples by liquid chromatography-electrospray tandem mass spectrometry. *Journal of Chromatography A*. 1015, 129-141.

Thomas, K.V., Barnard, N., Collins, K. (2003) Toxicity characterisation of sediment pore waters collected from UK estuaries using a *Tisbe battagliai* bioassay. *Chemosphere* 53, 1105-1111.

Thomas, K.V., Hurst, M.R., Reynolds, W., Klungsøyr, J., Meier, S and J.E.Thain (2002) *In vitro* ecotoxicological assessment of pelagic ecosystems. ICES ASC CM 2002/X:07.

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Thomas, K.V., Hurst, M.R., Matthiessen, P., and Waldock, M.J. (2001) Identification of oestrogenic compounds in surface and sediment pore water samples collected from industrialised UK estuaries. *Environmental Toxicology and Chemistry*. 20(10) 2165-2170.

John Thain is CEFAS's senior ecotoxicologist and has who has over twenty-six years experience in marine and freshwater ecotoxicology, and is responsible for the planning, guiding and conducting of biological effects studies in the aquatic environment. His research experience includes the development of new biological effects techniques, biomarkers, chronic and acute sediment bioassays, equilibrium partitioning and biodegradation. Current project management includes the development of a National Marine Ecotoxicological Analytical Control Scheme for Defra. He provides advice to Defra and other bodies such as EA, industry and working groups of PARCOM and ICES on the use and application of biological effects techniques and the interpretation of data.

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Thain J E (1992). Use of the oyster *Crassostrea gigas* embryo bioassay on water and sediment elutriate samples from the German Bight. Mar Ecol. Prog. Ser Vol 91: 211-213.

Thain J E, Matthiessen P, Bifield S and McMinn W (1994). Assessing sediment quality by bioassay in UK coastal waters and estuaries. Proc. Scientific Symp. On the North Sea Quality Status Report of the North Sea Task Force, Ebeltoft, Denmark, 18-21 April 1994

Thain J E, Allen Y and Matthiessen P. (1996). Monitoring sediment toxicity in UK estuaries and off shore waters from 1990-1993. In Development and Progress in sediment quality Assessment: Rationale, Challenges, Techniques & Strategies, p 127-142. Edit by M. Munawar & G Dave. Ecovision World Monograph Series, SPB Academic Publishing, Amsterdam.

Matthiessen P & Thain J E et al (1997). An Assessment of Sediment Toxicity in the River Tyne Estuary, UK by Means of Bioassays. Mar Environ. Res. Vol 45:1 p 1-15.

Thain J E, Davies I M, Rae G H and Allen Y. (1997). Acute toxicity of ivermectin to the lugworm *Arenicola marina*. Aquaculture 159: 47-52.

Jan Balaam MSc in Chemistry. Team Co-ordinator for Contaminant Fate and Effects team. She brings to the project substantial experience in marine environmetnal science. She specialises in the characterisation of toxicants in complex matrices. She has worked on a number of research contracts for the UK Oil Operators Association (UKOOA), the UK Environment Agency, the UK Department of Trade and Industry and the Norwegian Research Council, using specialist skills to identify unknown compounds in matrices such as sediment, pore water, surface water, produced water from oil installations and biota. Her role in MODELKEY will be to work on many aspects of the sub-project KEYTOX.

Selected relevant references

Thomas, K.V., Balaam, J., Hurst, M.R. Thain, J.E. (In press) Identification of *in vitro* oestrogen and androgen receptor agonists in offshore produced water discharges. *Environmental Toxicology and Chemistry*

Thomas, K.V., Balaam J., Hurst M.R., Matthiessen P. and Waldock M. (2004) The *in vitro* potency and characterisation of oestrogen receptor (ER) agonists in UK marine sediments. *Environmental Toxicology and Chemistry 23* 471–479.

Thomas, K.V., Balaam, J., Lavender, J., Jones, C. (2002). Characterisation of genotoxic compounds in sediments collected from United Kingdom estuaries. *Chemosphere*. 362, Vol 49 Iss 3, 247-258.

Mark Hurst BSc in Chemistry and with over eight years experience in environmental science research. He has a wide experience in conducting research into the biological effects and impact of hazardous substances in the aquatic environment. His specialises in the development and application of *in vitro* and *in vivo* bioassays for the assessment of environmental contamination.

Selected relevant references

Mark R. Hurst, Jan Balaam, Yin L. Chan-Man, John E. Thain and Kevin V. Thomas. (In Press). Determination of Dioxin and Dioxin-Like Compounds in Sediments from UK Estuaries Using a Bio-analytical Approach: Chemical-Activated Luciferase Expression (CALUX) Assay. Marine Pollution Bulletin

Mark R. Hurst and David A. Sheahan. The Potential For Oestrogenic Effects Of Pesticides In Headwater Streams In The United Kingdom. The Science of the Total Environment 2003; 301: 87-96.

Ioanna Katsiadaki, Alexander P. Scott, Mark R. Hurst, Peter Matthiessen and Ian Mayer. Detection of Environmental Androgens: A Novel Method Based On Enzyme-Linked Immunosorbent Assay of Spiggin, The Stickleback (Gasterosteus aculeatus) Glue ProteinEnvironmental Toxicology and Chemistry 2002; 21: 1946-1954.

Peter Matthiessen, Yvonne Allen, Shaw Bamber, John Craft, Mark Hurst, Tom Hutchinson, Steve Feist, Ioanna Katsiadaki, Mark Kirby, Craig Robinson, Sandy Scott, John Thain and Kevin Thomas. The Impact Of Oestrogenic And Androgenic Contamination On Marine Organisms In The United Kingdom – Summary Of The Edmar Programme. Marine Environmental Research 2002; 54:645-649.

J.K. Fawell, D. Sheahan, H.A. James, M. Hurst, S. Scott. Oestrogens and Oestrogenic Activity in Raw and Treated Water in Severn Trent Water. Water Research 2001; 35: 1240-1244.

4. WL| Delft Hydraulics (Delft)

WL| Delft Hydraulics is an independent research institute and specialist consultancy based in the Netherlands, with a staff of over 350 people, performing innovative research on water-related issues in both freshwater and salt water systems for over 70 years. WL| Delft Hydraulics conducts a host of research and development projects, both national and international and its expertise, facilities and collaboration with universities support both applied and fundamental research. Delft Hydraulics will provide expertise in detailed dynamical numerical, deterministic and expert modelling approaches used for linking water quality and hydrological parameters to biological groups and habitat requirements. Delft Hydraulics is currently involved in several EU-projects dealing with both chemical-ecological issues (e.g. HABES, DANUBS, REBECCA) and implementation of the WFD (e.g. BMW, Harmoni-QUA and Harmon-IT).

The team from Delft Hydraulics consists of experts in various field of research relevant to MODELKEY.

MSc **Johan Boon** has a broad experience in projects related to water quality and its management. As a senior project advisor he is involved in a wide variety of projects and studies related to the analysis of water quality and ecology and the development and applications of assessment tools in estuarine and marine systems. He is an expert in the field of modelling suspended matter and toxic substances and the risk assessment of calamitous oil spills. Mr Boon has lectured various courses on water quality and sediment modelling. Some recent publications concerning his tasks are:

Boon, J.G., Dardengo, L.V., Mulder H.P.J. and J.C. Winterwerp, (2004): Impact assessment of alternative dumping sites in the Ems-Dollard estuary (in preparation). Journal of environmental management.

Boon, J.G., de Goede, E.D., van Ormondt, M. and J.A. Roelvink,(2003): Impact of the Venice Lagoon storm surge barriers on the morphology and circulation of waters. Proceedings of the sixth Medcoast conference . pp. 1257-1269

Villars, M., Nauta, T., Husken, M.O., J.G. Boon and F. Kleissen, (2002): Framework for coastal discharge assessment. Proceedings of second conference on Marine Waste Water Discharges

Gerritsen, H., Boon, J.G., Kaaij, van der T, and R.J. Vos., (2001): Integrated modelling of suspended matter in the North Sea. Estuarine, Coastal and Shelf Science, 53, 581- 594

Gerritsen, H, Vos, R.J., Kaaij, van der Th, Lane, A and J.G. Boon. (2000): Suspended sediment modelling in a shelf Sea (North Sea). Coastal engineering 41 (2000), 317-352

MSc **Arthur Baart** is a senior water quality expert, specialised in water quality related risk assessment and model design. He has a broad experience in the application of water quality models and has been responsible for the design and implementation of industry funded exposure models as GEMCO: generic estuary model for contaminants and MAMPEC estuary and harbour model for anti-foulants.

Baart A.C, J.G. Boon, M.T. Villars (2003). Generic estuary model for contaminants (GEMCO), Z2725, Delft Hydraulics , Delft.

Baart A.C, J.G. Boon, M.T. Villars (2001). Generic model for contaminants concentrations in estuaries (GEMCO), in From Basic science to decision making, Setac , Brussel.

Van Hattum, B. A.C. Baart, J.G. Boon (2002). Computer model to generate predicted environmental concentrations (PECs) for antifouling products in the marine environment - 2nd edition accompanying the release of Mam-Pec version 1.4. Report. nr. E-02/04. Institute for Environmental Studies, Vrije Universiteit, Amsterdam.

Dr. **Tony Minns** is head of the section Ecological Modelling and has extensive experience in numerical methods, database management, mathematical modelling and environmental modelling. His expertise covers not only the mathematical and technical aspects of constructing mathematical models but also the practical applications of modelling systems and their schematisation, calibration and validation. He has considerable practical experience in the development and application of integrated modelling systems involving hydrodynamics, water quality and ecology. With his work in hydroinformatics, he has gained experience in the application of new, emergent technologies like artificial neural networks, evolutionary algorithms and cellular automata in hydraulic engineering, hydrology and water management. Consequently, he used various data mining techniques for the purposes of classification, model extraction and knowledge discovery.

Minns, A.W., 2000, Subsymbolic methods for data mining in hydraulic engineering, Journal of Hydroinformatics, IWA, 2(1), 3-13

Hall, M.J., Minns, A.W. & Ashrafuzzaman, A.K.M., 2002, The application of data mining techniques for the regionalisation of hydrological variables, J. of Hydrology and Earth Science Systems, AGU

Abbott M.B. and Minns A.W., 1998, Computational Hydraulics, 2nd Edition, Ashgate Publishing, Aldershot, U.K

CUR, 1993, Hydrology and Water Management of Deltaic Areas, Minns A.W. (ed.), Centre for Civil Engineering Research and Codes (CUR), 93-5, Gouda

Minns, A.W., 1998, Artificial Neural Networks as Sub-symbolic Process Descriptors, PhD thesis, Balkema, Rotterdam

Msc. **Jos van Gils** has over 16 years experience in projects related to water quality and its management. He has considerable experience in both inland and coastal water studies, and he is an expert in water quality modelling. Furthermore, he has often played an integrating and co-ordinating role between specialists of different disciplines. Since 1988, he has been active as a project leader, in the Netherlands but also in many projects abroad, especially in Southern Europe (Greece) and Eastern Europe (Poland, Danube countries). In 1993-1994, he has been working in Greece full-time and he has specialised in water quality problems and their management under Mediterranean circumstances. In 1995-1997, he has been the product manager of the one-dimensional modelling system SOBEK, for WL| Delft Hydraulics' and the Ministry of transport and Public Works of the Netherlands. He has considerable experience as a teacher and trainer.

Gils, J.A.G. van and Argiropoulos, D., "Axios river basin water quality management", Water Resources Management 5: 271-280.

Gils, J.A.G. van, Ouboter, M.R.L., and Rooij, N.M. de, "Modelling of water and sediment quality in the Scheldt Estuary", Netherlands journal of Aquatic Ecology, 27(2-4) 257-265.

Gils, J. van, and Bendow, J., (2002): "The Danube Water Quality Model and its role in the Danube River Basin Pollution Reduction Programme", Poceedings of the XX-th Conference of the Danubian Countries on Hydrological Forecasting and the Hydrological Basis of Water Management, Bratislava, Slovakia, September 2000.

M. Zessner and J. van Gils (2001): "Nutrient fluxes from the Danube basin to the Black sea", Proceedings of the Second International Black Sea Conference in Varna, Bulgaria, June 2001.

Jos van Gils, Horst Behrendt, Adrian Constantinescou, Ferenc Laszlo and Liviu Popescu, (2004): "Changes of the nutrient loads of the Danube since the late eitghties: an analysis based on long term changes along the whole Danube river and its main tributaries." Submitted to the Fourth International Black Sea Conference in Varna, Bulgaria, June 2004.

MSc **Harm Duel** is a senior ecologist and head of the section Water Quality and Ecology within the Inland Water Systems Division. He is a specialist in the assessments of ecological responses to changes in abiotic conditions. Mr. Duel is one of the key figures in international networks on habitat modelling: IAHR-ecohydraulics committee (secretary), European Aquatic Modelling Network and the International Aquatic Modelling Group. In those capacities, he is initiating new developments and technologies with respect to habitat modelling of instream habitats and floodplain habitats.

Duel, H., M.J. Baptist, G.J. Geerling, A.J.M. Smits, J.S.L. van Alphen.(2003) Cyclic floodplain rejuvenation as a strategy for both flood proection and enhancement of the biodiversity of the river Rhine. In: King et al. (eds). Environmental flows and ecohydraulics. Proceedings of International Conference. Cape Town.

Baptist, M.J., H. Duel, W.E. Penning, A.J.M. Smits, G.W. Geerling & J.S.L. van Alphen (2001). Assesment of cyclic floodplain rejuvenation on flood levels in the Rhine river. River Research and Application, special issue.

Van der Lee, G., H. Duel, D. van der Molen & R. Pouwels (2000). Uncertainty analysis of habitat evaluation methods applied at different levels of scale. International Symposium: Ecology of Scale, Wageningen, the Netherlands. Paper.

5. Consorzio Venezia Richerche (CVR)

The Consorzio Venezia Ricerche (CVR, i.e. Venice Research Consortium) is a non profit research organization including the two Universities of Venice (University Ca' Foscari of Venice and Architecture University Institute of Venice), public and private institutions. The research activity of CVR is mainly focused on integrated water management, risk assessment/management and development of GIS-based decision support systems for the rehabilitation of contaminated sites (sediments, industrial megasites and regional sites). CVR environmental unit currently consists of ca. 12 Ph.D. or postgraduated researchers and includes environmental scientists, chemists and economists and Geographical Information System (GIS) specialists, thus enhancing the capability of interdisciplinary studies. The extensive use of geographical information systems and the development of decision support systems, provide effective tools for integrated management and spatial planning.
CVR shares valuable expertise with the consortium partners, and in particular with the Dept. of Environmental Sciences and the Interdepartmental Centre for Sustainable Development at the University Ca' Foscari in Venice. CVR has an advanced GIS (geographical information system) laboratory and consortium partners provide a large number of other facilities (e.g. analytical laboratories).
Relevant research projects carried out over the last three years includes: "Desyre: Gis-based decision support system for the rehabilitation of large contaminated sites" and "Sertech: development of an integrated system for the treatment of contaminated sediments" (funded by the Italian Ministry of Research and Technological Development); "Environmental Database Integration for the Lagoon of Venice Drainage Basin to support eco-management"; "ERA-MANIA: ecological risk assessment Italian national procedure for the rehabilitation of regional contaminated sites", in collaboration with the Dutch National Research Institute for Health and Environment (RIVM).

Research Team

Key persons in the Modelkey project will be:

Claudio Carlon, PhD in Environmental Chemistry. Specialized in the integration of environmental risk assessment within GIS-based decision support systems, coordinator of the CVR Environmental Unit. Teaching "Environmental Risk Assessment" at the International PhD Programme on Analysis and Governance of Sustainable Development, University of Venice. Coordinator of the project Desyre, funded by the Italian Ministry of Research and Technological Development (concluded in November 2003). Desyre combines environmental risk, socio-economic and technological assessment within a Geographical Information System to derive alternative rehabilitation scenarios for regional contaminated sites. Coordinator of the project "Environmental Database Integration for the Drainage Basin of the Lagoon of Venice to support eco-management", funded by the Veneto Region. Member and/or participant in several International Networks and Scientific Committees, such as CLARINET (EU concerted action), SEDNET (EU Demand Driven Sediment

Network), NICOLE (Network for Industrially Contaminated Land in Europe), NATO-CCMS (North Atlantic Treaty Organisation-Challenges of Modern Society), he is involved in the definition of risk assessment and management best practices and guidelines. His role in Modelkey is that of coordinator of the DECIS subproject.

Antonio Marcomini, full Professor of Environmental Impact Assessment and of Pollution Chemistry at the University Ca' Foscari of Venice (UNIVE), president of CVR, chairman of the Venice Gateway for Science and Technology. Past academic international experiences include a postdoctoral fellow at the University of Toronto (Canada) and research at the EAWAG-ETH (Polytechnic of Zürich, Switzerland). Member of the national steering committee of the Environmental Chemistry Division of the Italian Chemical Society. As environmental consultant for the Italian Ministry of the Environment and the Ministry of the Public Works, he works for water quality management in the Venice lagoon. He is member of the EU network CLARINET on contaminated sites. Prof. Marcomini has also been coordinator or principal investigator for research projects of the European Commission (over the last years: EUMAC, Eutrophication and Macrophytes, 1995; ANACAD, Analysis of Concrete Admixtures,1997; SUITE, Sulphonated in the Terrestrial Environment, 1998; ACE, Analysing Combination Effects of Mixtures of Estrogenic chemicals in Marine organisms, 2001), of public institutions (CNR-PRISMA 1 and PRISMA 2, MURST, MUIR, etc.) and private companies (Federchimica, EniChem Augusta, Condea, AIS-CEFIC, etc.). Author of more than 150 articles on peer reviewed international journals, he has a long-standing experience in the assessment of contaminated water and sediment, encompassing chemical analysis, risk modeling and management aspects. His role will be mainly focused on the integration of Modelkey deliverables within a common conceptual framework, which is addressed in DECIS sub-project.

Silvio Giove, associate professor of Applied Mathematics at UNIVE, member of the Scientific Referee Panel of CVR, coordinator of the CVR team on Multi-Criteria Analysis, Associate Professor of Applied Mathematics in the University of Venice. His main scientific interest covers Artificial Intelligence methodology and applications, like neural nets and fuzzy sets, multi-criteria and multi-objective decision analysis, dynamic system, time series and signal analysis. The most significant applications regards ecological topics, together with economic and finance, bio-engineering. He is a collaborator member for National and International Research Projects and of Scientific Societies, and referee for some International Journals in the field of fuzzy logic and bio-engineering. The didactical activity regards Applied Mathematics, Computer Sciences, Financial Mathematics, Control and System Theory, Decision Theory. He will contribute to the development of the DECIS decision support system with special regards for the general structure and the application of multi-criteria and fuzzy methodologies.

Andrea Critto, Ph.D. in Environmental Science, has a long-standing experience in environmental risk assessment of contaminated sediments and land. Teaching Environmental Risk Assessment at the University of Venice. He is member of SETAC Europe. He has solid experience in the coordination of multidisciplinary research projects concerning the definition of environmental monitoring plan based on Ecological Risk Assessment (e.g., MAP project: Ecological risk analysis and chemical pollution characterization in the Venice Lagoon, funded by Venice Water Authority;

LAGOON METABOLISM project: Metabolic processes in the Venice Lagoon. Productivity, cycles of nutrients and effects of contaminants on biota. Integration between experimental approaches and environmental risk modelling, funded by Consortium for Venice Lagoon Research). He is currently coordinator of ERA-MANIA project concerning the application of Ecological Risk Assessment to develop remedial scenarios and monitoring plan for contaminated megasite in Italy, funded by Italian Ministry of Environment and in collaboration with RIVM (The Netherlands). He has published in a variety of international journals including Environmental Pollution, Environmental Toxicology and Chemistry, Environmental International and Chimia. His scientific focus is on method development for screening and site specific ecological risk assessment. His role will be mainly focused on the development of an integrated risk indicator in DECIS sub-project.

Stefano Foramiti, Ms. equivalent on Environmental Science, specialized in Geographical Information Systems (GIS). His work is devoted to the development of GIS based Multiple Objectives Decision Support Systems for environmental applications.

Christian Micheletti, Ph.D. Student in Environmental Science. His research interests are in Ecological Risk Assessment, applied to transitional environments (i.e. the Venice lagoon), focusing on methods to estimate site-specific ecological risk for the benthic organisms and for the whole aquatic food web. He is also interested in the integration of Ecological Risk Assessment with Human Health Risk Assessment, GIS and spatial stochastic processes.

Paola Agostini, Ph.D. student. Her scientific focus is on the integration of risk assessment and social risk within decision support systems for environmental management.

Petra Scanferla, Ms. Equivalent on Environmental Science. Her scientific interest is focused on the bioaccumulation of contaminants in benthic organisms.

Selected relevant references on environmental chemistry and spatial data analysis

M. Dalla Valle, A. Marcomini, A. Sfriso, A. J. Sweetman, K.C. Jones, (2003) Estimation of PCDD/F distribution and fluxes in the Venice lagoon, Italy: combining measurement and modelling approaches. *Chemosphere*, 51: 603-612

Di Corcia A, Cassassa F, Crescenzi C, Marcomini A, and Sampieri R (1999). Fate of linear alkylbenzenesulfonates and co-products in sewage treatments plants and in receiving river waters. *Environmental Science Technology*, 33:4119-4125

Marcomini A, Pojana G, Sfriso A, and Quiroga JM (2000). Behavior of anionic and nonionic surfactants and their persistent metabolites in the Venice lagoon (Italy). *Environmental and Toxicological Chemistry*, 19:2000-2007

Carlon C., Critto A., A. Marcomini A., (2000) Risk based characterisation of a contaminated site using multivariate and geostatistical tools. *Environmental Pollution* 111**,** 3, 417-427.

Carlon, C., Marcomini, A., Della Valle, M. (2003) Regression models to predict water-soil heavy metals partition coefficients in risk assessment studies. *Environmental Pollution J.* **127**, 109-115

Carlon, C., Nathanail, C.P., Critto, C., Marcomini, A. (2003) Comparison of different procedures to define sampling strategies for contaminated sites. *Soil and Sediment Contamination. An International Journal.* In press

Selected relevant references on risk assessment and management

Pojana, G., Critto, C., Micheletti, C., Carlon, C., Busetti, F., Marcomini, A. (2003) Analytical and Environmental Chemistry in the Framework of Risk Assessment and Management: the lagoon of Venice as a case study. *Chimia* 57, 242-249

Critto, A., Carlon, C., Marcomini, A., Quercia, F. (2002) Ecological Risk analysis for contaminated sites rehabilitation. International framework and development of Italian national guidelines. Manual 11/2002 ANPA (Italian Environmental Protection Agency) Rome, Italy, pagg. 1-104 (In Italian)

Carlon C., Norbiato C., Critto A., Marcomini A., (2000) Risk analysis applied to a contaminated site. Determination of risk based remedial targets. *Ann Chim.* 90, 5-6, 349-358

Critto, A., Carlon, C., Marcomini, A.. (2004) Screening ecological risk assessment for the benthic community: the Venice lagoon as case study. *Environment International*, in press

Micheletti C., A. Critto, C. Carlon, A. Marcomini (2004). Ecological Risk Assessment of Persistent Toxic Substances for the Clam *Tapes philipinarum* in the Lagoon of Venice. *Environmental Toxicology and Chemistry*, In press

Selected relevant references multi-criteria and fuzzy analysis

Canestrelli E., Giove S., "Optimizing a quadratic function with fuzzy linear coefficients", *Control and Cybernetics*, **20**, 1991, 25-36

Canestrelli E., Fuller R., Giove S., "Sensitivity analysis in possibilistic quadratic programming", *Fuzzy Sets and Systems*, **82**, 1996, 51-56

Giove S., "Piecewise linear approximation of monotonic fuzzy operators among L-R type fuzzy numbers", *Central European Journal of Operations Research*, vol. 7, (4), 2000, 305-320

Giove S., “Interval TOPSIS for multicriteria decision making”, *Neural Nets*, Springer, 2002, 56-63

Giove S., “Fuzzy measures and the Choquet Integral for Group Multicriteria Decision Making”, *Neural Nets*, Springer, 2001, 77-84

Selected relevant references on GIS and decision support systems

Carlon, C, Critto A, Nadal N, Samiolo M. Marcomini A., Petruzzelli, G.A. (2003) Desyre – decision support system for rehabilitation of contaminated sites. Consoil 2003 8th International Conference on Contaminated Soil, 12-16 May 2003 Extended proceedings

Critto, A., Bertazzon, S., Carlon, C., Marcomini, A., Zanetto, G., (2000). Integration of spatial analysis and ecological risk assessment in a GIS environment: the case study of the venetian lagoon contaminated sediments. Proceedings of the 4th International Conference on Integrating Geographic Information Systems and Environmental Modeling: problems, prospects, and needs for research; 2000 Sep 2-8; Boulder, CO. Boulder: University of Colorado, Cooperative Institute for Research in Environmental Science. (www and CD)

Facchinetti, G., Mannino, I., Mastroleo, G., Soriani, S., Zanetto, G., Carlon, C., Marcomini, A. (2003) A decision support system for the requalification of contaminated sites: a fuzzy expert approach for comparing alternative end uses 8th International Conference on Contaminated Soil, 12-16 May 2003 Extended proceedings

Critto, A., Carlon, C., Giove, S., Nadal, N., Samiolo, M., Silvoni, S., Foramiti, S., Marcomini, A., (2002) DESYRE – DEcision Support sYstem for REhabilitation of contaminated sites: objectives and structure. Peer reviewed extended proceedings of the *International Conference on Integrated Assessment and Decision Support*, pagg. 211-216. International Environmental Modelling and Software Society, Canberra, ACT, Australia

Bertazzon S., Micheletti C., Critto A., Marcomini A., (2004). Spatial Analysis of the Bioaccumulation of Distributed Pollutants in Clams *Tapes philipinarum*: the Venetian (Italy) lagoon case study. *Ecological and Environmental Statistic*. resubmitted with revision

University Ca’ Foscari of Venice (IDEAS) (Subcontractor of CVR)

IDEAS (www.unive.it/ideas) is the Interdepartmental Centre for Sustainable Development at the University Ca’ Foscari of Venice and hosts the Centre of Excellence for Sustainable Development in the Mediterranean Coastal Areas (CESD, www.unive.it/cesd). IDEAS undertakes research and education activities for the evaluation and promotion of sustainable development. Research activities address the environmental, economic and cultural dimensions of sustainable development. Main topics are integrated water management, integrated coastal zone management, soil and sediment rehabilitation. IDEAS works in close cooperation with Consorzio Venezia Ricerche (CVR), a non-profit research consortium which mission is to transfer technological innovation and scientific know-how to public and private companies in order to support sustainable development. Main research topics of this collaboration are risk assessment and GIS-based decision support systems. The close collaboration of research teams of environmental experts, engineers and socio-economists allows a comprehensive understanding of the problem.

IDEAS has a proved experience in the economic valuation of environmental goods (contingent evaluation, cost-benefit analysis, travel costs methods) and in the socio-economic analysis of how environmental problems affect economic uses and the planning framework

Research team

Paulo Augusto Lourencio Dias Nunes

PPhD in Economic Science. He is Senior Researcher and Lecturer for the Interdepartmental Centre for Dynamic Interactions between economy, environment and society (IDEAS) of University Ca' Foscari of Venice. He is also Professor of Environmental and Resource Economics at The Johns Hopkins University (Bologna Center, Italy) and Senior Economist for the Foundation Eni Enrico Mattei, Venice, Italy. He has been involved during his research period at the Department of Spatial and Environmental Economics, Vrije Universiteit, Amsterdam, in projects related to biodiversity valuation and analysis of regional sustainable development, in particular for the use and conservation of biodiversity in marine ecosystems. He has collaborated with the Portuguese Ministry of Science and the Portuguese National Institute for the Conservation of nature in relation to the economic analysis and valuation of non-market goods.

Selected relevant references

Nunes, P.A.L.D. (2002) Measuring the Economic Benefits from Protecting the Parque Natural do Sudoeste Alentejano e Costa Vicentina of Commercial Tourism Development: Results from a Contingent Valuation Survey, Portuguese Economics Journal, vol. 1., 71-87.

Nunes, P.A.L.D. (2002) The Contingent Valuation of Natural Parks: Assessing the Warmglow Propensity Factor, Edward Elgar Publishing (UK), New Horizons in Environmental Economics Series.

Nunes, P.A.L.D., J.C.J.M. van den Bergh and P. Nijkamp (2001) Integration of Economic and Ecological Indicators of Biodiversity, in Valuation of Biodiversity Studies: Selected Studies, 153-182, OECD, Environment Directorate, Paris, France.

Nunes, P.A.L.D. and J.C.J.M. van den Bergh (2001) "Economic Valuation of Biodiversity: Sense or Nonsense", Ecological Economics, vol. 39, 203-222.

Nunes, P.A.L.D. (2000) The nonuse benefits of forest ecosystems, in Economische Waardering van Bossen – een case study van Heverleebos-Meerdaalwoud, Moons et al. (eds), 177-226.

Soriani Stefano

Stefano Soriani is Senior Lecturer of economic and political geography at the Department of Environmental Sciences and at the Interdepartmental Centre for Dynamic Interactions between

Economy, Environment and Society (IDEAS) (Università Ca' Foscari of Venice), also member of the Steering Committee of AGEI (Association of Italian Geographers). He currently teaches economic geography, coastal systems and conflicts for the use of natural resources, cost-benefit analysis and economic valuation of the environment. He studied economy and geography in Venice (Università Ca' Foscari, Dipartimento di Economia) and Rotterdam, The Netherlands (Erasmus Universiteit Rotterdam, Department of port, transport and regional economics). His main fields of research include port development and transportation, urban waterfront redevelopment, integrated coastal zone management, the role of culture in the modern and postmodern debate about nature conservation. He collaborates with COSES (Consorzio per la Ricerca e la Formazione, Venezia), International Centre Cities on Water (Venezia), Fondazione Eni Enrico Mattei, EURICUR (European Institute for Comparative Urban Research, Erasmus Universiteit Rotterdam), CVR (Consorzio Venezia Ricerche).

Selected publications

"Tourism and Environmental Degradation: the Northern Adriatic Sea", in **Sustainable Tourism? European Experiences**, H. Coccossis, J. A. Edwards and G. K. Priestley eds., Wallingford, CAB International, 1996, pp. 137-152 (con G. Zanetto).

"The Venice Port and Industrial Area in a Context of Regional Change", in **Cityports, Coastal Zones and Regional Change: International Perspectives on Planning and Management**, B. S. Hoyle ed., Chichester, John Wiley and Sons, 1996, pp. 235-248.

"Crafting the new public spaces of postmodern urbanism: the emergence of "historic waterfronts" as new social and functional places ", in **Geographies of Diversity. Italian Perspectives**, a cura di S. Conti, Roma, Società Geografica Italiana, 2000, pp. 225-242, con C. Minca.

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Paola Minoia

PhD in human geography with specialisation in water management and spatial issues. Interest in water demand management, policy issues in middle eastern countries, social analysis, public participation and decision-making processes. Programme coordinator of the Sustainability project CESD (Centre of Excellence for Sustainable Development) at the interdepartmental centre IDEAS of the University of Venice. Experience in EC-funded projects (coordination of a LIFE programme for eco-tourism in the Venice Lagoon), working experience in African and Middle-Eastern countries within the UN system (programme officer at UNDP environmental program in South Africa and Egypt, expert of the Italian Ministry of Foreign Affairs for cooperation agencies' Report on Social Development in Egypt), participation in research programmes on environment and water management with African Universities (Niamey, Khartoum, Cairo).

6. Faculty of Earth and Life Sciences, Vrije Universiteit, Amsterdam, The Netherlands (VUA)

The Faculty of Earth and Life Sciences of the Vrije Universiteit, Amsterdam, The Netherlands, is the result of the merger in 2002 between the former Faculty of Earth Sciences, Faculty Biology and the Institute for Environmental Studies (IVM). The faculty offers education and does research in the fields of earth sciences, biology, biomedical sciences, geoarcheology, public health and environmental sciences. Research is organized around research institutes and centers, with the goal of promoting multidisciplinary research, combining the knowledge of several institutes.

Institute for Environmental Studies (IVM)

IVM is a multidisciplinary research institute focussing on environmental chemistry, (eco)toxicology, environmental economics and international and legal aspects of environmental management and was founded at the Vrije Universiteit (VU) Amsterdam in 1971. IVM employs about 80 people of which 60 are directly involved in research. IVM researchers co-operate with partners from other national and international research institutes. About three quarters of IVM's resources are obtained from contract research. IVM's clients include national and international research funding organisations, business, governmental and non-governmental organisations, and international (UN) organisations. The main areas of research include environmental chemistry, (eco)toxicology, environmental economics and international and legal aspects of environmental management.
The *Department of Chemistry & Biology* is headed by professor **Abraham Brouwer**, who leads a research group that currently consists of 8 scientists, 8 technicians and 4 PhD students. He has over 15 years of experience in the field of environmental and nutritional toxicology, with special emphasis on mechanisms of action, endocrine toxicology, design and validation of molecular biomarkers and developmental and reproductive toxicology.
The IVM scientists and researchers have a vast experience in the fields of chemical analyses of environmental contaminants, development of *in vitro* and *in vivo* bioassays, and combined effects of chemicals *in vivo*. There are two well-equipped laboratories. Technicians of both the chemical laboratory and the biological laboratory are highly qualified. IVM chemistry technicians are experienced in the fields of chemical analyses of environmental contaminants at trace levels, bioassay directed fractionation and analytical method development. The technicians at the biological laboratory are specialized in *in-vitro* bioassays such as the DR- and ER-CALUX and have extensive experience with cell lines and primary cell culture.

Research Team

Marja Lamoree (PhD) is an analytical chemist trained in the coupling of various separation techniques to mass spectrometry. She has been employed at the IVM from 2000 as a researcher in environmental chemistry. Her expertise lies in the combination of up-to-date analytical-chemical and biological-based techniques and their application in an iterative mode in order to identify novel and "unknown" substances, to contribute to the evaluation of their biological relevance and estimation of the total potency of complex mixtures of new and well known contaminants.
In the framework of several projects, for instance EU funded research like the ACE project, attention is paid to analytical method development for determination of environmental contaminants at trace levels such as endocrine disrupters and novel antifouling compounds, including sample pretreatment and bioassay directed fractionation.

Selected relevant references

M.H. Lamoree, C.P. Swart, A. van der Horst, B. van Hattum (2002). Determination of diuron and the antifouling paint biocide irgarol 1051 in Dutch marinas and coastal waters. J. Chromatogr. A. 970, 183-90.

C.J. Houtman, P.H. Cenijn, T. Hamers, M.H. Lamoree, J. Legler, A.J. Murk and A. Brouwer (2004). Toxicological profiling of sediments with in vitro bioassays with emphasis on endocrine disruption. Environ. Toxicol. Chem., 23, 32-40.

C.J. Houtman, A.M. van Oostveen, A. Brouwer, M.H. Lamoree, J. Legler (2004). Identification of estrogenic compounds in fish bile using bioassay directed fractionation. Submitted to Environ. Sci. Technol.

Timo Hamers, PhD in Environmental Toxicology, has been employed by IVM since 2003. Recent research activities mainly included *in vitro* pre-screening of the endocrine disrupting potency of brominated flame-retardants (BFRs) within the framework of EU project FIRE. Through this research and his PhD research on the toxic potency of diffuse air pollution, he gained much experience on the application of small scale *in vitro* and *ex vivo* test systems to screen the toxic potency of complex mixtures and on the relevance of such systems for the actual field situation.

Selected relevant references

T. Hamers, M.D. van Schaardenburg, E.C. Felzel, A.J. Murk, J.H. Koeman (2000). The application of reporter gene assays for the determination of the toxic potency of diffuse air pollution. Sci. Total Environ. 262, 159-74.

T. Hamers, K.R.J. Molin, J.H. Koeman, A.J. Murk (2000). A small-volume bioassay for quantification of the esterase inhibiting potency of organophosphate and carbamate insecticides in rainwater: development and optimisation. Toxicol. Sci. 58, 60-67.

T. Hamers, P.J. van den Brink, L. Mos, S.C. van der Linden, J. Legler, J.H. Koeman, A.J. Murk (2003). Estrogenic and esterase-inhibiting potency in rainwater in relation to pesticide concentrations, sampling season and location. Environmental Pollution 123, 47-65.

B. van Hattum (PhD) is a senior scientist in environmental chemistry and ecotoxicology with more than 15 years of experience, and has been involved in many field, experimental and modelling studies on chemical fate, bioaccumulation and food chain transfer, within the scope of PhD projects, contract research for government and industry, and various EU Framework projects. Through memberships of professional and network organizations (IAWR, SETAC, SEDNET) and the editorial board of the journal Environmental Pollution (1993-1999) he has an extensive network. Recent and current studies include the development of models for the exposure assessment of antifoulants (Mam-Pec), models for bioaccumulation in estuarine food webs, whole effluent testing of industrial effluents with biological and chemical methods, evaluation frameworks for sediment quality assessment, bioavailability of sediment-bound contaminants, and organotins in marine invertebrates and mammals.

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Van Hattum, B. and J.F. Cid Montañés (1999). Toxicokinetics and bioconcentration of polycyclic aromatic hydrocarbons in freshwater isopods. Environ. Sci. Technol. 33, 2409-2417.

Den Besten, P.J. , D. ten Hulscher and B. van Hattum. (2003). Bioavailability, uptake and effects of PAHs in aquatic invertebrates. In: P. Douben (ed.). PAHs: an ecological perspective. John Wiley & Sons Ltd, London. (in press)

Leonards, P.E.G., Broekhuizen, S., de Voogt, P., Van Straalen, N.M., Brinkman, U.A.T., Cofino, W.P. & Van Hattum, B. (1998) Studies of bioaccumulation and biotransformation of PCBs in mustelids based on concentration and congener patterns in predators and preys. Archives Of Environmental Contamination And Toxicology 35, 654-665.

R.J.C.A. Steen, E.H.G. Evers, B. van Hattum, W.P. Cofino, U.A.T. Brinkman (2002). Net fluxes of pesticides from the Scheldt Estuary into the North Sea: a model approach. Environmental Pollution 116, 75-84.

J.F. Stronkhorst, F. Ariese, B. van Hattum, P.J. den Besten, M. Bergman, R. Daan, M. de Kluijver, J.F. Postma, T. Murk, D. Vethaak (2003). Environmental monitoring and recovery at two dumping sites for dredged material in the North Sea. Marine Pollution Bulletin 124, 17-31.

Department of Theoretical Biology

The *Department of Theoretical Biology*, headed by professor **S.A.L.M. (Bas) Kooijman**, is part of the Institute of Health Sciences of the Faculty of Earth and Life Sciences of the Vrije Universiteit. The main object of the research programme of the Department can be labelled as quantitative bio-energetics. This topic has been chosen because of its relevance for a wide variety of biological specialisms: the availability of nutrients and energy is frequently the most important limiting factor in the development and functioning of living systems. The aim of the research programme is to develop a quantitative and coherent theory for energy and mass transduction that links theories concerning all levels of organization, from membrane physiology to ecosystem dynamics. The Dynamic Energy Budget theory, that is developed by Bas Kooijman, offers good opportunities for use in ecotoxicology, e.g. to describe toxicity of chemicals in relation to toxicokinetics and in combination with other stressors. This application resulted in the development of the DEBtox method for the analysis of toxicity data, which was recently accepted by the ISO and OECD as one of the valid methods to analyse such data (Kooijman et al, 2004).

Research team

Professor Dr. **S.A.L.M. (Bas) Kooijman** graduated in biology (1974), and obtained his PhD degree (1974) on the statistical analysis of point patterns at Leiden University. During this period he teached in and advised on applications of mathematics in biology. During 1977-1985 he was affiliated at the TNO laboratories in Delft as study director, and supervised research in ecotoxicology. Since 1985 he was appointed as professor and head of the Department of Theoretical Biology of the Vrije Universiteit, and was advisor at the TNO laboratories till 1995. He (co)authored about 200 articles, book chapters, including 3 books. Since 1979 most work relates to the Dynamic Energy Budget theory that he created; this theory is about quantitative aspects of metabolic organisation. Extensive information about his professional activities can be found at http://www.bio.vu.nl/thb/.

Selected relevant references

Kooijman, S.A.L.M. and Bedaux, J.J.M. (1996). The analysis of aquatic toxicity data. VU University Press, Amsterdam.

Kooijman, S.A.L.M. (2000). Dynamic Energy and Mass Budgets in Biological Systems. Cambridge University Press.

Kooijman, S. A. L. M. (2001) Quantitative aspects of metabolic organization; a discussion of concepts. *Phil. Trans. R. Soc. B,* **356**: 331--349.

Kooijman, S.A.L.M., Bedaux, J.J.M., Péry, A.R.R. and Jager, T. (2004) Biology-based methods. In: H. Magaud (ed) Draft guidance document on the statistical interpretation of ecotoxicity tests. ISO and OECD, TC 147/ SC 5/ WG 10/ N0390, Paris.

Péry, A.R.R., P. Flammarion, B. Vollat, J.J.M. Bedaux, S.A.L.M. Kooijman and J. Garric (2002). Using a biology-based model (debtox) to analyse bioassays in ecotoxicology: Opportunities & recommendations. Environ. Toxicol. Chem., 21:459-465.

7. Centre Nationale de Recherche Scientifique – Midi-Pyrénées (CNRS)

In the past 5 years, CNRS and University Paul Sabatier (UPS) have combined their efforts to promote excellence in research on biodiversity and ecosystem functioning. The ecological research centre (Fédération de Recherche) has been created, confirming the dynamism of Toulouse in this research area. Research units now support 80 research fellows, plus post-doctoral researchers, PhD and MSc students and visiting international scientists. Members are participating as partners or coordinators in the previous EU-FP projects.
The present proposal is an investigation from a group of internationally known researchers belonging to the "Laboratoire Dynamique de la Biodiversité" (LADYBIO, http://www.ladybio.ups-tlse.fr, UMR 5172, the joined research unit) headed by **Dr. Eric Chauvet**. This lab includes 36 permanent scientists (23 researchers and 13 engeniers and technicians) and 32 PhD students and 4 post-docs. It aims studying spatial and temporal biodiversity dynamics according to natural or/and anthropogenic disturbances. The involved team namely "Aquatic Community Ecology" focus research on macroinvertebrates and fish community in freshwater systems and has high expertise on ecological modelling. It was coordinator of the PAEQANN project in the 5th FP (EVK1-CT1999-00026). This team included 6 researchers, 2 technicians, 6 PhD students. The major research topic concerns the understanding of the factors that govern the structure of biodiversity and ecological communities at global, regional and local scales of fish and macroinvertebrate in freshwater systems. As modelling techniques, machine learning methodology, especially artificial neural networks (ANN) are used to pattern and predict aquatic diversity and structure.

Research Team in Modelkey:

Prof. Sovan Lek (http://aquaeco.ups-tlse.fr/slek) is leader of the group. He has published more than 100 papers, in peer-reviewed journals, and 2 books. He is editorial board member of *Ecological Modelling* and *Ecosystems & Community*. He is founding member of "International Society for Ecological Informatics" (ISEI). He will contribute to the coordination of subproject (Effect Modelling). **Dr Sébastien Brosse** (associate professor, University Paul Sabatier) is junior scientist of LADYBIO. He will contribute to subproject SP5 (Decision making and management) in model selection and quality of exposure data. **Dr James Gagneur** (associate professor) will contribute to WP EFFECT2. **Dr Muriel Gevrey** and **Géraldine Loot** (assistant professor, LADYBIO) are junior scientists involving in subproject SP4 (Effect Modelling) for species sensitivity distribution. All members are familiar to the ANN modelling techniques and .

Selected, relevant publications

LEK S., GUEGAN J.F.2000 (eds). Artificial Neuronal Networks: application to ecology and evolution. *Springer-Verlag* 262p
BROSSE S., GIRAUDEL J.L. & LEK S., 2001. The temporal dynamic of fish populations assemblage and community structure. *Ecological Modelling* 146(1-3): 159-166.
GEVREY M., DIMOPOULOS I., LEK S. 2003. Variables contributions in Artificial Neural Network to model Ecological Data: review and comparison of methods. *Ecological Modelling* (in press)
GIRAUDEL J.L. & LEK S., 2001. A comparison of self-organizing map algorithm and some conventional statistical methods for ecological community ordination. *Ecological Modelling* 146(1-3): 329-339
PARK Y.-S., VERDONSCHOT P.F.M., CHON T.-S. & LEK S. 2002. Patterning and predicting aquatic macroinvertebrate diversities using artificial neural network. *Water Resarch* (in press)

8. IIQAB Chemical and Environmental Research Institute of Barcelona – CSIC Spanish Council for Scientific Research (CSIC)

The IIQAB (Chemical and Environmental Research Institute of Barcelona), former CID (Centre for Research and Development), was established in 1999 as a research institute devoted mainly to environmental sciences (http://www.iiqab.csic.es). It is part of the CSIC (Spanish Council for Sientific Research), the main scientific organism in Spain. The **IIQAB** is divided in five departments and their human resources include around 340 staff in total. The founding comes from the European Union (~ 40%), the Spanish and Catalan governments (~ 50%) and the industry (~10%).

The Department of Environmental Chemistry currently consisting of 14 scientists, 7 technicants, and 35 PhD students is headed by **Prof. Dr. Damià Barceló**. It aims at the study of the source, transport, and fate of environmental pollutants, and their effecs on organisms (fish, molluscs, and man). The Department is organized in 5 different research groups or units. During the last years, the *Water Quality and Soil-Related Aspects Unit* headed by Prof. Dr. Damià Barceló has been involved in various EU scientific ativities. Its main activity within the EU 4FP was the coordination of the Waste Water Cluster, which was integrated by five research projects: PRISTINE, PRENDISENSOR, SANDRINE, OWWA and INEXsPORT. Within the 5FP, the group is or has been involved in 10 research projects/nets, including EXPRESS-IMMUNOTECH, FATEALLCHEM, SEDNET, P-THREE, STAMPS, and PHYTOHEALTH. The group is also currently participating in the following recently funded 6FP projects: AQUATERRA, SWIFT-WFD, EMCO (coordinator) and HORIZONTAL-ORG. The main research activities and expertise of the group are in the fields of (a) advanced analytical chemistry based on mass spectrometric analysis and biosensors, (b) transport, fate and bioavailability of priority and emerging organic pollutants and endocrine disruptors in water-soil systems and biota and (c) evaluation of the sources and distribution of pollutants by chemometric analysis and modelling.

Research Team

Damià Barceló Ph.D. in Analytical Chemistry (1984). Since 1999 full Research Professor at IIQAB-CSIC and Head of the Environmental Chemistry Department. He has published more than 350 scientific papers in SCI journals. He is editor of 5 books on Environmental Analysis and co-author of a pesticide book. Other relevant activities are: networking experience at the EU (1997-2002); coordinator of the Waste Water Cluster (2002-2004); working group leader of the EU network and/or CA SEDNET, HARMONI-CA, SOWA and JOINT, and partner of the RTD EU projects (2001-2005, 5FP, under the Water Key action) WATCH, CLOSEDCYCLE, AWACSS, STAMPS, P-THREE and ARTDEMO (2003-2007); subproject leader of the integrated project AQUATERRA (6FP); supervisor of 16 Ph D thesis on environmental analysis (1992-2003). His scientific focus is on method development for environmental analysis of priority and emerging pollutants. His role in MODELKEY is the overall coordination (project manager) of the CSIC participation in the IP. His group will play a major role in the subprojects BASIN and SITE (for the Llobregat river basin) and KeyTox (key toxicant identification).

Selected relevant references

M. Castillo, M.C. Alonso, J. Riu, D. Barceló (1999) Identification of Polar, Ionic, and Highly Water Soluble Organic Pollutants in Untreated Industrial Wastewaters. Environ. Sci. Technol. 33: 1300-1306.

M. Castillo, D. Barceló (1999) Identification of Polar Toxicants in Industrial Wastewaters using Toxicity-Based Fractionation with Liquid Chromatography/mass Spectrometry. Anal. Chem. 71: 3769-3776.

M. Petrovic and D. Barceló (2000) Determination of anionic and nonionic surfactants, their degradation products and endocrine disrupting compounds in sewage sludge by liquid chromatography/mass spectrometry. Anal. Chem. 72: 4560-4567.

M. Farré, I. Ferrer, A. Ginebreda, M. Figueras, L. Olivella, Ll. Tirapu, M. Vilanova, D. Barceló (2001) Determination of drugs in surface water and wastewater samples by liquid chromatography-mass spectrometry: methods and preliminary results including toxicity studies with Vibrio fischeri. J. Chromatogr. A, 938: 187-197.

M. Petrovic, A.R. Fernandez-Alba, F. Borrull, R.M. Marce, E. Gonzalez-Mazo, D. Barceló (2002) Occurrence and distribution of nonionic surfactants, their degradation products and linear alkylbenzene sulfonates in coastal waters and sediments in Spain. Environ. Toxicol. Chem., 21: 37-46.

S. Lacorte, M. Guillamón, E. Martínez, P. Viana, D. Barceló (2003) Occurrence and Specific Congener Profile of 40 Polybrominated Diphenyl Ethers in River and Coastal Sediments from Portugal. Environ. Sci. Technol. 37: 892-898.

Maria José López de Alda Ph.D. in Pharmacy (1994). Since 1999, Research Scientist at the Department of Environmental Chemistry, IIQAB-CSIC and head of the laboratory for chemical analysis. She is involved in several national and international projects. Examples of them are the EU projects AWACSS and ARTDEMO where she acts as assistant of the project manager. She has more than 40 papers published in international refereed journals. She focuses on the development of advanced LC-MS^n analytical methods for determination of endocrine disrupting compounds, and priority and emerging pollutants in environmental samples. Main tasks within MODELKEY project: assistant of the project manager, supervision of PhD work, and coordination of sampling activities and data compilation for the Llobregat river.

Selected relevant references

S.A. Wise, M.M. Schantz, D.L. Poster, M.J. Lopez de Alda, L.C. Sander (1999) Standard reference materials for the determination of trace organic constituents in environmental samples. In: Barceló D (Ed) Sample Handling and Trace Analysis of Pollutants: Techniques, Applications and Quality Assurance. Elsevier, pp. 649-687.

N. García-Reyero, E. Grau, M. Castillo, M.J. López de Alda, D. Barcelò, B. Piña (2001) Monitoring of endocrine disruptors in surface waters by the yeast recombinant assay. Environ. Toxicol. Chem. 20: 1152-1158.

M. Petrovic, E. Eljarrat, M.J. López de Alda, D. Barceló (2001) Recent advances in the mass spectrometric analysis related to endocrine disrupting compounds in aquatic environmental samples. J. Chromatogr. A 974: 23-51.

M. Petrovic, M. Solé, M.J. López de Alda, D. Barceló (2002) Endocrine Disrupters in Sewage Treatment Plants, Receiving River Waters and Sediments. Integration of Chemical Analysis and Biological Effect on Feral Carp. Environ. Toxicol. Chem. 21: 2146-2156.

P. López-Roldán P., M.J. López de Alda, D. Barceló D. (2004) Simultaneous determination of selected endocrine disrupters (pesticides, phenols and phthalates) in water by in-field solid-phase extraction (SPE) using the prototype PROFEXS followed by on-line SPE (PROSPEKT) and analysis by liquid chromatography-atmospheric pressure chemical ionization-mass spectrometry.Anal. Bioanal. Chem. 378: 599-609.

S. Rodríguez-Mozaz, S. Reder, M.J. López de Alda, G. Gauglitz, D. Barceló (2004) Simultaneous multi-analyte determination of estrone, isoproturon, and atrazine in natural waters by an optical immunosensor river analyser (RIANA). Biosens. Bioelectron. 19: 633-640.

Silvia Díaz-Cruz Ph.D. in Chemistry (2001). Assistant Professor in the Department of Analytical Chemistry, Faculty of Chemistry, University of Barcelona from 2000 to 2003. Since 2002 Research Scientist at the Department of Environmental Chemistry, IIQAB-CSIC, Barcelona, Spain. She is involved in the EU project ARTDEMO dealing with the analysis of estrogens, progestogens and drugs in the aquatic environment. She has more than 20 papers published in international refereed journals. Her research activities focus on the determination of environmental emerging contaminants, such as antibiotics, by LC-MS^n techniques. Her work within Modelkey will be devoted to the identification of unknown pollutants by LC-ToF-MS^n.

Selected relevant references

S. Diaz-Cruz, M.J. López de Alda, D. Barceló (2003) Environmental behaviour and analysis of veterinary and human drugs in soils, sediments and sludge. TrAC-Trend. Anal. Chem. 22: 340-351.

M.J. López de Alda, S. Diaz-Cruz., M. Petrovic, D. Barceló (2003) Liquid chromatography (tandem) mass spectrometry of selected emerging pollutants (steroid sex hormones, drugs and alkylphenolic surfactants) in the aquatic environment. J. Chromatogr. A 1000: 503-526.

S. Díaz-Cruz, M.J. López de Alda, R. López., D. Barceló (2003) Determination of estrogens and progestogens by mass spectrometric techniques (GC-MS, LC-MS and LC-MS-MS). J. Mass Spectrom. 38: 917-923.

9. UdG Universitat de Girona

The UdG (Universitat de Girona) was established in 1992 as a new University in Spain. In its very young existence this University has excelled on several areas of Biology, Environmental Sciences and Chemistry. It currently employs around 1000 staff in total. The Ecology Unit at the Institute of Freshwater Ecology and at the Department of Environmental Sciences includes 22 researchers. It aims at the description of the biodiversity components of the aquatic ecosystems, as well as the unraveling of the mechanisms justifying their functioning. The Institute (http://ciencies.udg.es/iea) has developed research in several types of water bodies (lakes, lagoons and rivers) in NE Spain. It supports several lines of research developing aspects such as faunal and plant taxonomy, ecotoxicology, lake ecology, fish ecology and river ecology. The research covers basic and applied aspects, several of them being developed on the application of the WFD to the NE Spain waters.

Research Team

Sergi Sabater Ph.D. in Biology. Professor of Ecology and leader of the research group on stream and river ecology at the University of Girona. Teaching at the Universities of Barcelona and Girona (Spain). Member of the editorial board of Annales de Limnologie-International Journal of Limnology, and currently serving as the President of the Spanish Limnological Society . He is coordinator of a Spanish joint project on “Structure and function of fluvial biofilms: effect of the riparian forest and implications for water quality ” that involves the Universities of Girona and Barcelona. Has participated in 4 different EU programs within the 4th and 5th Framework as the National Leader of the respective consortia. His scientific interests are on general stream and river ecology, algal ecology, ecotoxicology and use of biological indicators. His role in MODELKEY is that of the developing the tools on biofilm detection for the effect of toxicants, and the implications this may have for the ecosystem functioning . His group will play a major role in subproject SITE (Biofilms).

Selected relevant references

Sergi Sabater, E.Vilalta, A.Gaudes, H.Guasch, I.Muñoz, A.Romaní. 2003. Ecological implications of mass growths of benthic cyanobacteria in rivers. Aquatic Microbial Ecology 32:175-184

Sabater, S., T. Buchaca, J. Cambra, J. Catalán, N. Ivorra, H. Guasch, I. Muñoz, E. Navarro, M. Real, A. Romaní. Structure and function of benthic algal communities in an extremely acid river. Journal of Phycology 39:481-489.

Real, M., I.Muñoz, H.Guasch, E.Navarro, S.Sabater. 2003. The effect of copper exposure on a simple aquatic food chain. Aquatic Toxicology 63: 283-291.

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Sabater, S., Navarro, N. & H. Guasch. (2002). Effects of copper on algal communities at different current velocities. Journal of Applied Phycology 14:391-398.

Sabater, S. , Helena Guasch, Anna Romaní, Isabel Muñoz. 2002. The effect of biological factors on the efficiency of river biofilms in improving water quality. In: “Ecological processes and ecosystems: functioning towards water purification”. Ostroumov, S., S.C. Mc Cutcheon, Ch. E. W. Steinberg (eds.). Hydrobiologia 469: 149-156.

Ivorra, N., J. Hetelaar, MHS Kraak, S. Sabater & W Admiraal. 2002. Responses of biofilms to combined nutrient and metal exposure. Environmental Toxicology and Chemistry 21, 3: 626-632.

Sabater, S., Armengol, J., Comas, E., Sabater, F., Urrizalqui, I. 2000. Algal biomass in a disturbed Atlantic river: water quality relationships and environmental implications. The Science of the Total Environment 263, 1-3: 185-195.

Helena Guasch. PhD (biology), aquatic ecology and ecotoxicology. University lecturer at the University of Girona (Spain). She has participated in the EU projects Biofilms (5 FP) and “Microbenthic communities used to assess effects of land-derived toxicants” (ENV4-CT96-0298) and several national research projects focused on the study of river periphyton structure and functioning. Her main expertise gaining during the past 12 years: Primary production. Nutrient dynamics. Ecophysiology of algal communities in fluvial systems. Use of algae for monitoring rivers. Ecotoxicology in fluvial systems focusing on atrazine, copper and zinc toxicity in periphyton. Developing techniques for phyto-toxicity assessment. She is now leader of a national research project titled "Dynamics of toxic substances in river ecosystems: effects on biofilms and consequences for water quality". She has published more than 30 peer reviewed papers or book chapters.

Selected relevant references

Guasch, H., E. Navarro, A. Serra, S.Sabater. Phosphate limitation influences the sensitivity to copper in periphytic algae. *Freshwater Biology*, in press.

Guasch, H., Guasch H, Admiraal W, Sabater S. 2003. Contrasting effects of organic and inorganic toxicants on freshwater periphyton. *Aquatic Toxicology*.64: 165-175.

Guasch H, Paulsson M, Sabater S. 2002. Effect of copper on algal communities from oligotrophic calcareous streams. *Journal of Phycology.* 38: 241-248.

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Guasch H, Sabater S. 1995. Seasonal variations in Photosynthesis-Irradiance responses by biofilms in Mediterranean streams. *Journal of Phycology* 31:727-735.

Anna M. Romaní Ph.D. in Biology. Researcher at the University of Girona. Her research focusses on biofilm structure and function in river ecosystems. She has long experience in extracellular enzyme activity measurements as a tool to assess the heterotrophic capacity to use specific molecules and, as a consequence, the relevance for the whole carbon cycling in the ecosystem. The relationship of such enzyme activities to both degradation processes and nutrient concentrations and balance are evaluated in natural and polluted rivers. She evaluates the biofilm metabolic and estructural responses to perturbations and the relationship with the environmental variables. Experiences have been done investigating sediment (surface and hyporheic) and epilithic biofilms, measuring the relevance of the heterotrophic organisms (bacteria, fungi, micro and meiofauna) as well as their trophic interactions.

Selected relevant references

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Emili Garcia-Berthou (Ph.D. in Biology) is Associate Professor at the Department of Environmental Sciences (Univ. of Girona) and leads several projects on the ecology of freshwater fish. His team has the necessary equipment and wide experience on the assessment of freshwater fish populations in rivers, lakes and reservoirs, including boat and wading electrofishing, seines, gillnets, and echosounding. His research focuses on the ecology of invasive species (such as common carp *Cyprinus carpio*) and the use of fish as indicators of water quality.

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Vila-Gispert A., García-Berthou E. & Moreno-Amich R. 2002. Fish zonation in a Mediterranean stream: Effects of human disturbances. *Aquat. sci.* 64: 163-170.

10. Centre for Fish and Wildlife Health (FIWI), University of Bern (UB)

The Centre for Fish and Wildlife Health (FIWI) at the University of Bern, Switzerland, executes research on the impact of environmental stressors, both infectious and non-infectious ones, on fish health. The Centre has long-lasting experience and is internationally recognized in studies on pathology and toxicology of fish. The FIWI is the Swiss National Reference Centre for fish diseases, being accredited according to ISO standards, and it participates in the network of the European Reference Laboratories. Currently, the FIWI consists of 6 senior scientists, 3 technicians and 7 PhD students. The research aims of the FIWI are a) interaction between pathogens and the fish host. This includes research both on the pathogenic factors of the infectious agent and research on the factors modulating the response of the host, for instance, immune parameters, temperature, age etc. b) the impact of toxicants on fish. Here, emphasis has been given on biomarker responses of fish as indicators of environmental pollution, particularly biomarkers of exposure and effects of organochlorines (e.g., CYP1A), endocrine disruptors (e.g., vitellogenin) or genotoxins (e.g., comet assay). Current field-oriented research activities of the FIWI on biomarker responses in contamination-exposed fish include, among others, a project on the impact of endocrine-disrupting chemicals on brown trout in Swiss rivers, a project on the impact of water quality on the health status and CYP1A expression of fish in Swiss rivers, and a project on biomarker expression in fish from the Danube river.

The methods required for the contribution of the FIWI to MODELKEY are established (some of them were established within the EU-project “Diagnostic Ecotoxicology, coordinated by H. Segner: see special issue of Aquatic Toxicology, vol. 53, Nos. 3-4, 2001). Further, all the necessary equipment and infrastructure is available, including a biochemical lab with fluorescence/absorbance plate readers, ELISA equipment etc, a histopathology lab, and fish culture facilities.

Research Team

Helmut Segner, Doctor in Natural Sciences, venia legendi and habilitation in zoology, university lecturer in Biology and Veterinary Medicine at the University of Bern. To date, he participated in five EU projects, and coordinated two of them: "Diagnostic ecotoxicology: cell-based methodology to develop markers for early, sublethal effects assessment" (contract No ENV4-CT96-0223); "IDEA-Identification of Endocrine Disrupting Effects in Aquatic Organisms" (ENV4-CT97-0509). Furthermore, he was involved in EU-supported teaching and training activities, for instance, he hosted Marie Curie postdoctoral students, he participated in ERASMUS and LEONARDO teaching courses, and he received a Marie Curie training site on „Application of in vitro cellular approaches in Ecotoxicology" (HPMT-CT-200000118). Currently, he is involved in the EU project "EDEN". H. Segner serves on the editorial board of six international journals in the field of fish toxicology and fish diseases. His main research interest is in understanding the impact of environmental factors, including toxicants, on fish physiology and phenotypic plasticity. Segner has published more than 100 peer-reviewed publications.

Daniel Bernet, Doctor in Natural Sciences, postdoctoral fellow at the FIWI.. D. Bernet did his PhD thesis on the impact of water quality on fish health. In particularly, he aimed at developing a health index that integrates biochemical and histopathological marker responses. He was involved in more than 10 national projects (with 5 of them coordinated by him), mainly field studies on fish health assessment in contaminated environments. Currently, he is involved in a project on the occurrence of gonadal malformations in fish from Swiss Lakes and the search for the etiological agents – possibly endocrine-disrupting compounds – of those pathological effects. From his studies, D. Bernet has in-depth experience on a broad array of methods, from molecular to histological ones, and he is also well experienced in statistical and epidemiological approaches, as they are essential components of any field study on pollutant-induced responses in fish and fish communities. He has published about 20 peer-reviewed publications.

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11. VRI, Department of Chemistry and Toxicology

Veterinary Research Institute was established in 1956 as only institution in the Czech Republic which research is focused on veterinary virology, mictrobiology, immunology, reproduction diíseases, and food safety. It currently employs around 220 staff in total. The VRI is 80 percent funded by the Czech Minsitry of Agriculture and the Czech Ministry of Environment and grant agencies (Grant Agency of the Czech Republic, National Agency of Agricultural Sciences, Internal Grant Agency of the Czech Ministry of Health). VRI currently participates in 8 EU projects, mostly in the 5th EU Framework Programme.

The Department of Chemistry and Toxicology (http://www.vri.cz/labs/biochem/default.htm) currently consisting of 5 scientists, 2 technicants, and 3 PhD students is headed by **Dr. Miroslav Machala**. At present, research activities are focused on combined chemical and in vitro bioassay techniques and study of modes of action of polycyclic aromatic hydrocarbons (PAHs) and polychlorinated biphenyls and their derivatives. The research is focused on assessment of toxicity of xenobiotics using specific biochemical and cellular *in vivo* and *in vitro* biomarkers of toxicity mechanisms (dioxin-like toxicity, oxidative stress, estrogenicity, modulations of cell kinetics, mutagenicity etc.) using various biological models: chick embryo, freshwater fish - rainbow trout, chub (*Leuciscus cephalus*), carp, transgenic hepatoma H4IIE cell line (for CALUX assay), MVLN cell line (MCF-7 cells permanently transfected with the p-Vit-tk-Luc plasmid, for estrogenicity in vitro), rat epithelial WB-F344 cell line (for in vitro detection of adverse effects associated with tumor promotion of xenobiotics, namely inhibition of gap junctional intercellular communication and proliferative activity). Chemical analysis is complemenmtary to toxicologuical studies and involves determination of concentrations of large sets of PAHs and their derivatives and PCB congeners, in total more than one hundred individual compounds.

Research Team

Miroslav Machala, Ph.D. in Biochemistry. Leader of the Department. Teaching at the Masaryk University, Faculty of Science, Brno He is coordinator of several national projects in the field of in vitro and in vivo toxicology and chemical analysis of organic environmental pollutants. His role and contribution to the project: specific in vitro bioassays for assess of endocrine-disrupting effects, genotoxic and tumor-promoting activities of aquatic contaminants present in sediments, water samples and/or biota (modulations of AhR-, ER-dependent activities, p53 protein accumulation, post-confluent cell proliferation assay). His work is planned within the following workpackages: BASIN1-3, KeyTox1-4, Site2, Site5.

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Jan Vondracek, PhD in Cellular Biology, employed at VRI & Institute of Biophysics, Brno, Czech Republic, teaching at the Masaryk University, Faculty of Sciences, Brno. Research activities: development and implementation of in vitro bioassays, in vitro effects of toxicants. His role in the project, see M. Machala.

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12. Institute of Vertebrate Biology (IVB)

The IVB belongs to the Academy of Sciences of the Czech Republic. The staff includes 26 regular research scierntist, 18 scientist and PhD students contracted on the basis of research grant funding and 18 technicians. Goal of Institute is to develop knowledge and expertise in the basic and applied research of vertebrate biology. Institute was founded in 1953 and now has a 6 research departments. IVB has participated in 45 national and international projects,

The Department of Fish Ecology currently consisting of 2 scientists and 4 PhD students and 2 Master students. Department is oriented to investigating the biology and ecology of the early life stages of fishes. Research is conducted to evaluate and develop appropriate sampling and censusing techniques for fishes, conduct behavioural studies and identify the ecological requirements of fishes in a variety of aquatic habitats. Research aims are directed at using a combination of field studies, laboratory experiments and modelling to understand and predict the effects of the environment and biotic interactions, such as competition, predation and parasitism, on reproduction and recruitment in fishes. The results of many studies have wide implications for fisheries and wildlife management and conservation. The department is headed by Dipl. Ing **Pavel Jurajda**, PhD, with major research interest is natural reproduction of fish, fish behaviour and habitat improvements.

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JURAJDA , P., ONDRAČKOVÁ, M., REICHARD, M., (in press): Managed flooding as a tool for supporting natural fish reproduction in man-made lentic waterbodies. *Fisheries Management and Ecology*.

13. University of Joensuu, Department of Biology (UJOE)

The University of Joensuu (http://www.joensuu.fi/englishindex.html) is located in North Karelia and has six faculties: Education, Forestry Humanities, Science, Social Science and Theology. In 2002, the student enrolment for degree programmes was about 7200 and for non-degree programmes about 5700. International students constitute 3.5 percent of the student population. The University has a teaching staff of about 500 and, in addition, about 650 research scientist, assistant or technician. The task of the University is to provide research, educational and cultural facilities in broad and varied fields with a special view of satisfying the needs of Eastern Finland.

The aquatic ecology and ecotoxicology is one of main interest areas at the University. The Laboratory of Aquatic Ecology and Ecotoxicology (http://bio.joensuu.fi/ekotox/) at the Department of Biology (http://bio.joensuu.fi/e_index.html) is led by **Prof. Dr. Jussi Kukkonen** and it has modern facilities to conduct aquatic and sediment toxicity and bioaccumulation assays and other experiments, as well as chemical analyses, needed for the project. In sediment toxicology and aquatic bioavailability tests the laboratory has the leading role in Finland. The main focus being the fate and effects of xenobiotics in aquatic systems (water phase and sediment), and how different environmental factors (pH, temperature, humus, water hardness, UV-radiation) modify the effects. **Dr. Matti Leppänen** is involved the project and his current research interests are focused on bioavailability of sediment associated organic contaminants like polycyclic aromatic hydrocarbons, polychlorinated bifenyls and polybrominated difenylethers. **Dr. Tiina Ristola** has been working with sediment bioassays with *Chironomus riparius*. Her work has focussed on developing laboratory and *in situ* chronic bioassays which use larval development, adult emergence and reproduction as endpoints. **Dr. Jarkko Akkanen** is currently working on the DOM characterization and bioavailability issues in pore waters. **MSc. Merja Lyytikäinen** is currently working on the analysis of the organic pollutants in different matrixes and bioavailability related questions.

Selected, relevant publications.

Akkanen J. and Kukkonen J.V.K. 2003: Measuring the bioavailability of two hydrophobic organic compounds in the presence of dissolved organic matter. Environ. Toxicol. Chem. 22: 518-524.

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Ristola T., Parker D. and Kukkonen J.V.K. 2001: Life-cycle effects of sediment-associated 2,4,5-trichlorophenol on two groups of the midge Chironomus riparius with different exposure histories. Environ. Toxicol. Chem. 20: 1772-1777.

14. Elbe Water Quality Monitoring Agency (EWQMA)

The EWQMA (www.arge-elbe.de) is the national agency for the “Working Group for the Protection of the River Elbe (”Arbeitsgemeinschaft für die Reinhaltung der Elbe”, resert to as ARGE ELBE in the following text). The EWQMA currently has a staff of 10, of whom the Director is Prof. Dr. H. Reincke. The remaining members are a biologist, a chemist, three engineers, two technicans and two secretarial staff. The main aspects of our work are the monitoring and evaluation of data from biological, chemical and ecological (toxicological) investigations.

The EWQMA was reorganised and expanded to include the newly established Federal States in Eastern Germany in July 1993. The scope of investigations of the EWQMA covers water quality management measures involving the river Elbe and its main tributaries in cooperation with the seven Federal States of Saxony, Sachsen-Anhalt, Lower Saxony, Brandenburg, Mecklenburg-Vorpommern, Hamburg and Schleswig-Holstein. The type of data required is laid down in a nationally and internationally agreed sampling programme; the EWQMA is responsible for gathering, managing, analysing and publishing the data. The purpose of this cooperation between the Federal States is to take planning decisions and determine measures with the aim of documenting the pollutant load of the Elbe and its main tributaries, reducing toxin and nutrient emissions and improving the ecological situation. A further aim is to enable water quality requirements for drinking water and for irrigation purposes to be fulfilled and maintained.

EWQMA performs planning, coordination, execution and evaluation of sampling programmes in cooperation with the member States of the ARGE ELBE, with the IKSE, the Joint Federal/State Monitoring Programme for the North Sea, the Federal Environment Ministry and the Working Group of the Federal States on Water Problems (“LAWA”) as well as scientific institutions such as universities and research establishments (GKSS, UFZ Leipzig/Halle, in particular the ad-hoc research project 'Elbe Flood August 2002'). EWQMA tasks are carrying out monitoring programmes and special investigation programmes, sampling longitudinal profiles (by helicopter), establishing freight balances, public relations, providing support for tasks of individual States, systematic documentation of weirs and similar constructions in the German and Czech river sections in cooperation with our partners, publishing results in reports and in scientific journals and augmentation of standard quality control measures.

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Elsholz O., Frank C., Matyschok P., Steiner F., Wurl O., Stachel B., Reincke H., Schulze M., Ebinghaus R. and Hempel M.: On-line determination of mercury in river water at the German monitoring station Schnackenburg/Elbe. Fresenius J Anal Chem 366: 196-199 (2000)

Mrs **Barbara Frank** is a biologist (Dipl.-Biol.) with a wide range of experience in managing environmental data. Since 1994 she has worked in different projects dealing with water quality and data management. This included e.g. statistical evaluations for trend detection of water contaminants as well as the development of the Internet-based geographical information system ELBIS for use by ARGE ELBE. She is currently working within the research project MINOS at the Nationalpark Office of the Schleswig-Holstein Waddensea (Tönning, D) in the field of ecological impacts of offshore wind farms. Her tasks are project coordination, public relations including the project´s web site and moreover the construction of an overall project data base (ORACLE 8). She has the project coordination and data base construction within MINOS (Marine warm-blooded animals in the North and Baltic Seas: Foundations for assessment of offshore wind farms) at the National Park Office for the Schleswig-Holstein Waddensea, funded by German Federal Environment Ministry.

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Frank, B., Geschwandtner, D., Janson, K., Löffler, J. (2004) ELBIS, an Internet Information System on the Water Quality of the River Elbe. Acta hydrochimica et hydrobiologica. Sonderheft "10 Jahre gesamtdeutsche Magdeburger Gewässerforschung" (im Druck).

15. RIKZ / National Institute for Coastal & Marine Management

The *RIKZ* is the national knowledge and consultation centre in the proces of policy decision making and management of the marine and estaurine areas of the Netherlands. These include the North Sea and Wadden Sea and the estuaries of Scheldt, Meuse, Rhine, IJssel and Ems.

RIZA, the sister organisation does the same for the fresh water areas of Rhine, Meuse, Scheldt, Ems and inland waters.

Both *RIKZ* and *RIZA* are part of the Ministry of Public Transport and Water Management of The Netherlands, subdivision Rijkswaterstaat.

The *RIKZ* employs 350 to 390 people, organised into 3 general main departments and 3 research departments directly involved in knowledge and consultation: "Advisory and Management" (AB), "Development and Strategy" (OS) and "Monitoring and Information management" (MI). AB is specialised in consultancy, OS in applied scientific development, MI in monitoring information and analytical laboratories.

The *RIZA* employs some 500 people, organised in the research departments "Water systems", "Information and Measurements", "Emissions" and "Planning and Restoration"

RIKZ and *RIZA*, as part of Rijkswaterstaat, are primarily funded by the Ministry and work on behalf of the policy making Directorate General Water and the Rijkswaterstaat Head Quarters within national and international projects related to safety against flooding and environmental water quality. They do have Rijkswaterstaat (research) vessels to their disposal to dispatch into field surveys. *RIKZ* and *RIZA* do perform the task of environmental monitoring in the Dutch watersystems and manage the monitoring database DONAR and related databases *viz.* Dutch input into the OSPAR/ICES database.

The departments involved in MODELKEY do have several scientists and supporting staff in expertises of environmental chemistry, ecotoxicology, biology, physics and morphology. Dr. Dick Vethaak, Drs. Martine van den Heuvel-Greve and Dr. Hannie Maas are taking part in Work Packages BASIN and SITE as (eco)toxicologist. Dr. Joop F. Bakker, Drs. Hans Klamer and Foppe Smedes are taking part in Work Packages "KEYTOX", "SITE" and "EXPO" as biogeochemist, environmental chemist and analytical chemist respectively. Dr. Jan Hendriks is taking part as foos web modeller in "EXPO". They represent an extensive experience in research on ecology, bioassays, chemical-analytical and field and laboratory experience.

Dr. Joop F. Bakker is contactperson for both *RIKZ* and *RIZA* and coordinator of the Ems reference basin.

Selected, relevant publications

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16. Netherlands Institute for Fisheries Research (RIVO)

The Netherlands Institute for Fisheries Research (RIVO) is an institute that has developed a broad experience in biological, technical, technological and environmental aspects of fisheries research over many years. Its abilities and strengths in these fields are recognised by national and international fish related communities (governmental and commercial), by the scientific community and by nongovernmental organisations (NGOs). It is also recognised as a Dutch research institute for marine ecology and an excellent laboratory for chemical analysis. Three departments of RIVO will participate in MODELKEY. The department of Biology and Ecology investigates the anthropogenic and naturally induced changes in annual fish stock size. The ecological research of the department is oriented towards understanding anthropogenic impacts on the coastal zone. The department investigates how changes in an ecosystem due to e.g. large infrastructure projects, such as offshore airports and wind farms, can impact on fish. The department of Environment and Food Safety is responsible for strategic and applied research in the area of the aquatic environment and safety of fishery products. The research concentrates on three key areas: environmental research (e.g. monitoring, occurrence, fate of contaminants in the aquatic environment, identification of unknown contaminants), food safety research (e.g. monitoring of contaminants in food), and natural compounds (e.g. monitoring of trace metals and shellfish toxins). The department has gained international recognition for its development of techniques for the analysis of flame retardants, PCBs, and related organic substances, and involvement in the organisation of interlaboratory studies for organic contaminants, *e.g.* for QUASIMEME. The department Seafood and Aquaculture is responsible for the research related with topics from fish farming or catch until the product is on the plate of the consumer. The department has three different projectgroups: Evaluation of product and fresh chain, Aquaculture, and Well being and genomics. The Aquaculture group has a large expertise in development of new fish species for farming, production of fish foods for fish larvae, modeling of streams of nutrient in fish farm systems, and hatching of fish.

Research Team

Pim EG. Leonards, PhD, is head of the Environment research section. The main focuses of the group are i) the development of analytical methods for new contaminants in the environment, ii) the monitoring of contaminants in the aquatic environment (e.g. flame retardants), iii) the chemical optimization/validation of bioassay methods, and iv) the identification of unknown contimants. He has worked at the Free University, Amsterdam (post-doc) on the detection, identification and quantification of new and unknown environmental contaminants using GC-AED/MS and time integrate samplers (SPMDs, SPME, empore disks). He obtained a Ph.D. degree at the Institute for Environmental Studies (IVM) of the Free University, Amsterdam. During the time at the IVM, dr. Leonards was a participant in several EU projects (Planar CBs (SMT), FAME and EQUATE). At RIVO he is a participant in the EU projects DIAC, STAMPS and is subcoordinator of the EU project FIRE. He has a broad experience in trace organic analysis (*e.g.* brominated flame retardants), ecotoxicology, risk assessment and the organisation of workshops on contaminants. His expertise and interest is also in the field of combining analytical chemistry with ecology and bioassays. His role in MODELKEY is the principle scientist, and his group will play a major role in subproject KeyTox (key toxicant identification).

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van Stee LL, Leonards PE, van Loon WM, Hendriks AJ, Maas JL, Struijs J, Brinkman UA. 2002. Use of semi-permeable membrane devices and solid-phase extraction for the wide-range screening of microcontaminants in surface water by GC-AED/MS. Water Res. 36(18):4455-70.

Heather Leslie, PhD, is currently working as project leader at the Department of Environment and Food Safety at the Netherlands Institute for Fisheries Research in IJmuiden, the Netherlands. This work is focused on the analysis of (persistent) organic chemicals, such as brominated flame retardants, in various environmental compartments, the analysis of complex contaminant mixtures in effluents using solid-phase microextraction (SPME), water quality monitoring and quality control of environmental analyses. Her past research at Utrecht University, the University of Amsterdam and RIZA focused on different ecotoxicological topics as internal effect concentrations in aquatic biota and the prediction of body residues and narcotic toxicity with SPME fibers, specific modes of toxic action and chronic toxicity of NPAHs, as well as the impact of point source pollution on the structure of benthic macroinvertebrate communities in rivers. She is involved in a number of research or scientific cooperation initiatives at both national and international level.

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Leslie, H.A., T.L. ter Laak, F.J.M. Busser, M.H.S. Kraak and J.L.M. Hermens. 2002. Bioconcentration of organic chemicals: is a solid-phase microextraction fiber a good surrogate for biota? Environ Sci Technol 36:5399̃5404.

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Ger-Jan Piet, PhD, has over 10 years experience in ecosystem-oriented research focussed on fish and benthic communities. He is member of several ICES working groups including WGECO (Ecosystem effects of fishing) and is chairman of the ICES WG on Beam Trawl Surveys. He has been involved in several national and international projects (e.g. EFEP "European Fisheries Ecosystem Plan" EU Q5RS-2001-1685, MAFCONS "Managing fisheries to conserve roundfish and benthic invertebrate species diversity" Q5RS-2002-00856) that involve biodiversity issues.

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Erwin (H.V.) Winter is a specialist on fish monitoring and fish migration in river basins. He is the project leader of the yearly performed fish monitoring surveys in the great rivers of the Netherlands. He is a scientific member in the EU-project FAME, involved with developing ecological assessment tools to qualify the integrity of fish communities in European rivers in relation to the EU-Water Frame Directive. He is the Dutch representative in the Diadromous Fish Committee (species using both riverine and marine environments) of ICES, International Councel for Exploration of the Sea.

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Winter, H.V. & W.L.T. van Densen, 2001. Assessing the opportunities for upstream migration by non-salmonid fishes in the weir-regulated River Vecht. Fisheries Management and Ecology 8: 513-532.

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Ingeborg J. de Boois. She participates in EU projects Monitoring Biodiversity (1999-2001) and MAFCONS (Managing fisheries to conserve groundfish and benthic invertebrate species diversity, 2003-2006). She is responsible for the identification of epibenthos and fish species. She has great experience with the taxonomy and determinantion of fish and epifauna species.

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Zühlke, R., J. Alsvåg, I. de Boois, J. Cotter, S. Ehrich, A. Ford, H. Hinz, A. Jarre-Teichmann, S. Jennings, I. Kröncke, J. Lancaster, G. Piet & P. Prince, 2001. Epibenthos diversity in the North Sea. Senckenbergia marit., 31(2): 269-281.

Edward Schram M.Sc. in Aquaculture. Projectleader in the aquaculture group of the department of Seafood and Aquaculture. He is involved in a number of CRAFT projects in the field of aquaculture: ‘Bio-economic feasibility of intensive pikeperch culture’, ‘Design and development of commercial scale farming technologies for sole’ and ‘Biological optimization and development of processing methods for turbot farming’. His scientific focus is on rearing of marine larvae and recirculating aquaculture systems. The project group Aquaculture has been involved in research on intensive fish farming in recirculation systems for 15 years and is the leading institute in this field in The Netherlands. Within RIVO the project group Aquaculture has extensive expertise in experimental research on fish in all its life stages.

Schram, E., 1995. The reliability of phosphorus balances in intensive recirculation systems of the African catfish, Clarias gariepinus. MSc- thesis no.1507 Wageningen University (Netherlands).

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Schram, E., Kamstra, A. and J.W. v.d. Heul. 2002 Density dependent growth in Dover sole (Solea solea). Seafarming Today and Tomorrow. Abstracts and extended communications of Aquaculture Europe 2002. EAS special publication No. 32.

17. Research Base of the Slovak Medical University – Institute of Preventive and Clinical Medicine (SZU)

The Institute of Preventive and Clinical Medicine (IPCM) with its 250 employees is focused on research in the field of environment related diseases, promotion of health and quality of life by means of prevention, control and therapy. The Institute was established in 1979 and since September 2003 it has become a component of the Slovak Medical University. IPCM belongs to the most active research institutions in Slovakia as regards its participation in international projects. Some of its departments including the National Reference Centre for Dioxins and Related Compounds (NRC-Diox) are incorporated in the EU Centre of Excellence in Environmental Health Research at IPCM since 2002.

The NRC-Diox, currently consisting 6 permanently employed researchers (4 are PhD’s) and 2 technicians, studies relations between environmental pollution, food contamination and human exposure to persistent organic pollutants (POPs). NRC-

Diox headed by **Anton Kocan** (PhD) is equipped with three HRGC/LRMS systems, one high resolution sector mass spectrometer coupled with two HRGC's, several HRGC's with EC detectors, and corresponding laboratory facilities for sample processing. It is accredited according to EN ISO/IEC 17025 for POPs analysis in environmental, feed/food and human matrices. NRC-Diox regularly participates in international intercalibration studies covering sediment, soil, flyash, food and blood samples.

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A. Kocan, J. Petrik, H. Uhrinova, B. Drobna, J. Chovancova (1999) The occurrence of semivolatile persistent organic pollutants in ambient air in selected areas of Slovakia. Toxicol. Environ. Chem. 68:481-493

18. RIVM: The Netherlands National Institute for Public Health and the Environment

RIVM is a large (≈1500 staff) national research centre, devoted to environmental and public health research with 35 research departments (http://www.rivm.nl/en/overrivm/). RIVM is founded in 1984, as a fusion product of several older national research institutions (RIV, RID and IVA).

The Laboratory for Ecological Risk Assessment is a part of the Environmental Risk and Safety Division (MEV) of RIVM. The mission of LER is to develop scientific knowledge about effects of anthropogenic and natural stress on ecosystem functioning and translate this knowledge into operational approaches for regulatory agencies. The research involves integration of different threats in a coherent way. Focus is on determining which stressors (disturbance, chemical substances, ...) deserve most regulatory attention. Activities of LER comprise laboratory- and field-based experiments, as well as application and development of mathematical models and decision-support systems. The work is primarily commissioned by the Netherlands Ministry of Spatial Planning, Housing and the Environment (VROM). In addition, projects are undertaken in charge of other ministries, municipalities, provinces, non-governmental institutions and the European Community. The Laboratory for Ecological Risk Assessment (LER) currently consists of 21 scientists, 15 technicants, 2 PhD students and administrative personnel. The ModelKey project will be an integral part of the strategic development project "Quantitative ecological risk assessment", headed by **Dr Leo Posthuma** with major research interests in probabilistic risk assessment. **Dick de Zwart (Drs)** is executing eco-epidemiological studies on "attributing field observed effects to the underlying causes". One of these studies is a joint project with Proctor and Gamble Corp., USA and the Utah State University. His role in ModelKey is that of the overall coordinator. His group will contribute to subproject SP4 (effects modeling) and the validation of the effects models with field data (SP1). Other contributers to the ModelKey project will be **Prof. Dr Dik van de Meent** (exposure modeling), **Dr Willie Peijnenburg** (bioavailability) and **Tom Aldenberg (Drs)** (theoretical biology and probabilistic risk assessment).

Selected, relevant publications

Aldenberg, T., Jaworska, J. S. (2000) Uncertainty of the Hazardous Concentration and Fraction Affected for Normal Species Sensitivity Distributions. Ecotox. Env. Safety, 46, 1-18.

De Zwart, D. 2002. Observed regularities in SSDs for aquatic species. In: Posthuma L., Traas T.P. Suter, G.W. (2002) The use of Species Sensitivity Distributions in Ecotoxicology. Lewis Publishers, Boca Raton, FL, USA.

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Van den Brink P.J., T.C.M. Brock and L. Posthuma. 2002. The value of the Species Sensitivity Distribution concept for predicting field effects: (non-)confirmation of the concept using semi-field experiments. In: Posthuma, L., Suter G.W. and Traas T.P. (2002) Species Sensitivity Distributions in Ecotoxicology. CRC Press, Boca Raton, FL, USA..

19. University of Stuttgart, Institute of Hydraulic Enginieering

Research Group:

Bernhard Westrich, Prof. Dr.-Ing. habil., is head of the Hydraulic Department at the Institute of Hydraulic Engineering, Faculty of Civil Engineering and Environmental Science, University of Stuttgart. His research activity is on the field of flow and transport processes in surface waters focussing on experimental investigation and numerical modelling of sediment and pollutant transport processes. He has broad experience in sediment physics, developed an innovative experimental method for direct erosion measurements of cohesive sediments and is supervisor of several interdisciplinary projects on contaminated sediment issues. Beside the academic commitment he is an active member of different professional organisations: chairman of the Task Force Committees of International (IAHR, ICOLD) and National Associations (ATV-DVWK) dealing with contaminated sediment issues and, a member of the SEDNET working core group 2.

Selected references:

Witt, O., Westrich,B.: Quantification of erosion rate for undisturbed contaminated cohesive sediment cores by image analysis, Hydrobiologia, Vol. 494(1-3), pp 271-276, 2003

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Westrich, B., Jancke,Th., Schmid,G. : Experimental investigation on comprehensive analysis of cohesive sediment erosion , Intern. Confer. Hydraulic Engineering , Thassaloniki ,2003

20. Saint-Petersburg State University, Institute of Chemistry (SPbU)

St.Petersburg University is the second largest university in Russia, and one of the oldest. The Institute of Chemistry is a large research centre integrated with the Department of Chemistry (a teaching unit). The two form PUSCC – Petrodvoretz University Scientific Centre for Chemistry. PUSCC currently employs more than 500 staff.

The Division of Physical Organic Chemistry currently consists of 5 Professors, 10 scientists, 9 technicians and engineers, and 2 Ph.D., 3 M.Sc. students and 2 Post-doctoral fellows.The division incorporates the University NMR laboratory. The head of the division is **Professor Vladimir S. Karavan**. The traditional research field is "Structure – Property" relationship for organic compounds. Following the acquisition of modern NMR the most developing research direction in the past decade became isolation, structure elucidation and prediction of environmental behavior of persistent organic pollutants. The group leader is Dr**. Vladimir A. Nikiforov.** The group will contribute mainly into SP2 (Key Toxicant Identification). It is supposed that in the second half of the project SPbU scientists will work also on other SPs in order to assure good dissemination of the approaches and results on the Russia national level. Key scientists working on the project will be **Dr. Serguei A. Miltsov** (synthesis), **Dr. Vadim. P. Boyarsky**(synthesis, databases) and **Dr. Stanislav I. Selivanov**(databases, structure elucidation). It is planned that Ph.D., M.Sc. and graduate students will be actively involved into the project. The group has experience in cooperation with EC countries through grants of INTAS, Nordic Council, Academy of Finland, The Research Council of Norway and via direct contracts.

Research team

Vladimir Nikiforov Ph.D. in Organic Chemistry. Leader of a research group on synthesis, isolation and structure elucidation of organic environmental pollutants. His main research interst in environmental chemistry is development of novel synthetic approaches to emerging classes of newly discovered contaminants.The group has experience in synthesis of all classes of organic compounds for preparation of standard solutions for environmental analysis and of specially purified substances for toxicological investigation. Standard solutions of Toxaphene congeners and of Polychloronaphthalenes are the best world-wide acknoledged achievements of the group. The group has experience in synthesis of ^{13}C and Deuterium labelled environmental contaminants and of enantiomeres of chiral toxicants.

Selected relevant references

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Vladimir A. Nikiforov, Vladimir S. Karavan, Sergei A. Miltsov, Stanislav I. Selivanov, Erkki Kolehmainen, Elina Wegelius, Maija Nissinen.(2003) Hypervalent iodine compounds derived from onitroiodobenzene and related compounds: syntheses and structures. ARKIVOC, Vol 2003, part(VI), pp 191-200. http://www.arkat-usa.org/ark/journal/2003/Varvoglis/AV-744A/744A.pdf

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J. Koivisto, E. Kolehmainen, V. Nikiforov, M. Nissinen, J. Linnanto, M. Lahtiперд, S.A. Miltsov and V.S. Karavan, (2001) A New Potential Toxaphene Congener: Synthesis, GC/EI-MS Study, Crystal Structure, NMR Analysis, and ab initio Calculations of 3-endo-,5-endo-Dichloro-7,7-bis-chloromethyl-4-dichloromethyl-tricyclo[2.2.1.02.6]heptane, Chemosphere, 44, 671-679.

Vadim Boyarsky Ph.D. in Organic Chemistry. He is one of the leading teachers and researchers in St.Petersburg university in the field of Physical Organic Chemistry and in homogemeous catalysis with transition metals complexes. The latter interest derives from his work in the Russian petrochemical Institute where he first prepared and studied Alkyl Cobalt Carbonyls, catalytic carbonylation of Aryl and Benzyl Halides. In recent years he developed a unique catalytic system for carbonylation of polychlorinated aromatic compounds (PCBs, PCDFs, PCNs, PBDEs etc.). In cooperation with University of Incheon, Korea, he is carrying out research project on chemistry of peroxynitrous acid. The most recent direction of his research is QSAR for PCB-carboxylic acids.

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on a modified cobaltcarbonyl catalyst. International Conference “Mechanisms of catalysis”, Moscow, p. 88.

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Dneprovskii A. S., Iz’’urov A. L., Boyarskii V. P.(1999) Polar Effect in the Substituted Benzyl Radicals Reaction with Tetrachlorocarbon, Zh. Org. Khimii. v.35., p.1477-1481 (Russ).

Zhesko T. E., Boyarsky V. P., Nikitina A. G. (1998) Aryl Halide Carbonylation via Catalysts Based on Modified Cobalt Carbonyl // Zh. Obshch. Khimii. v.68, p.85-89 (Russ).

Sergei Miltsov Ph.D. in Organic Chemistry. He has more than 20 years of experience in mechanisms and selectivity of free radical substitution reactions, which will be an important factor in development of synthetic methods for methylated PAHs. He also is a principial scientist in synthesis of polychlorinated ecotoxicants (dibenzodioxines, dibenzofuranes, biphenyls, naphtalenes and products of their metabolism as haptenes for immunoassay). In cooperation with Sensors and Biosensors Group, Chemistry Department of Autonomous University of Barcelona he is developing synthesis and investigation of properties of cyanine dyes. Another area of his research is MO calculation of physico-chemical properties of polyaromatic compounds.

Selected relevant references

M.Puyol, S.Miltsov, I.Salinas, J.Alonso (2002) Ketocyanine dyes: new H+-selective ionophores for use in Integrated waveguides absorbance optodes, Analytical Chemistry, vol.74, p.570-576.

S.Miltsov, C.Encinas, J.Alonso (2001)Novel synthesis of ketocyanine dyes, Tetrahedron Letters,vol 42, p.6129-6131.

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V.Nikiforov, A.Firsov, V.Karavan, S.Miltsov. (2001)Direct substitution of aromatic nitrogroup to chlorine by reaction with hexachlorocyclopentadiene. Reaction Mechanisms and Organic Intermediates, St.Petersburg, p. 11-14.

E.Kolehmainen, J.Koivisto, V.Nikiforov, K.Laihia, R.Kauppinen, K.Tuppurainen, M.Perakyla, S.Miltsov and V.Karavan (1999) NMR Spectroscopy in Environmental Chemistry: 1H and 13C NMR Parameters of Chlorinated Dibenzothiophenes Based on Two Dimensional NMR Techniques and ab initio MO and DFT/GIAO calculations. Magn. Reson. Chem. vol.37, p.743-747.

Stanislav Selivanov Ph.D. in Chemistry is a one of the leading experts in St.Petersburg in all aspects of modern NMR spectroscopy. His main research interest is exploration of NOE and other 2D technics for 3D structure elucidation and studying molecular dynamics of complex organic molecules, including biologically active compounds (synthetic steroid analogs, polypeptides, glycoside derivatives and others), transition metals clusters and flexible molecules of environmental contaminants (e.g. polychloroterpenes).

Selected relevant references

Selivanov S.I., Shavva A.G. (2002)NMR Spectroscopy for investigation of 3D-structure and molecular dynamics of modified steroid hormones. Bioorganicheskaya Khimia, V. 28, no. 3, p. 220-235.

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Tunik S.P., Pilyugina T.S., Koshevoy I.O., Selivanov S.I., Haukka M, Pakkanen T.A. (2004) Reaction of S-BINAP with $H_4Ru_4(CO)_{12}$. The first example of face-bridging BINAP coordination and 100% stereoselectivity in formation of chiral tetranuclear cluster framework. – Organometallics, V. 23, N 3, pp. 568-579.

21. ACA Centre for Environmental Research

The ACA (Agència Catalana de l'Aigua; in English Catalan Water Agency, CWA.), is a public enterprise belonging to the Ministry of Environment of the Autonomous Government of Catalonia, exerting the role and functions of Water Authority (basin agency) as it is referred in Water framework Directive. Within this context, it has all the competences related to management and administration of all aspects related to the water cycle at the catchment level, including hydrologic planning, execution and operation of hydraulic infrastructures, water quality control, preservation of aquatic ecosystems, administrative intervention, resource allocation and tax collection.

One of the main activities of the ACA (http://www.gencat.es/aca) is the survey of the quality of the continental waters (rivers and ground water), as well as, coastal and estuarine waters, in accordance with the local legislation and UE Directives. For that purpose, the C.W.A. carries out extensive quality monitorization programs aimed to obtain a knowledge of the pollution status of the water masses, and to prevent further deterioration of water quality and aquatic ecosystems through the implementation of diverse pollution abatement policies. ACA also maintains close cooperation with research centers, such as the IIQAB-CSIC and Universities.

Antoni Ginebreda PhD in Chemical Engineering 1980. Postdoctorates: Sloan Kettering Institute for Cancer Research (New York, USA), Instituto de Química Bio-orgánica, Consejo Superior de Investigaciones Científicas (CSIC, Barcelona) and Instituto Químico de Sarriá (Barcelona). Postgraduate degrees :DD - IESE, Universidad de Navarra, 1993. Since 1992 Head of the Laboratory of Water Quality Control of ACA. He is author of 34 research papers, 19 scientific communications and 10 patents. He is involved in several national and international projects. Examples of them are the EU projects/nets STREAM, JOINT, P-THREE, AND AQUATERRA, where he acts as project manager. His role in MODELKEY is that of providing the necessary sources of information for compilation of the environmental data available for the Llobregat river basin and participating in the validation of the Decision Support System through its application to the Llobregat case study.

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M. Farré, A. Oubiña, M.P. Marco, A. Ginebreda, L. Tirapu and D. Barceló (1999) 4-Nitrophenol ELISA equivalent for assessing the origin of organic pollution in waste water treatment works. Env. Sci. Technol. 33: 3898-3904.

T. Garrido, J. Fraile, J.M. Niñerola, M. Figueras, A. Ginebreda, L. Olivella (2000) Survey of Ground Water Pesticide Pollution in the Rural Areas of Catalonia (Spain). Int. J. Env. Chem. 78: 51-65.

E. Teixidó, L. Olivella, M. Figueras, A. Ginebreda, R. Tauler (2001) Multivariate exploratory data analysis of the organic micropollutants found in the Llobregat river (Catalonia, Spain). Int. J. Env. Chem. 81: 295-313.

J.Riu, E. Martínez, D. Barceló, A. Ginebreda (2001) LC-MS determination of linear alkylbenzene sulfonates and their carboxylic degradation products in influent and effluent water samples and sludges from sewage-treatment plants. Fresenius J. Anal. Chem. 371: 448-455.

E. Eljarrat, J. Caixach, J. Rivera, M. de Torres, A. Ginebreda (2001) Toxic Potency Assessment of Non-, Mono- and Di-ortho PCBs, PCDDs, PCDFs and PAHs in Northwest Mediterranean Sediments (Catalonia, Spain). Env. Sci. Technol 35: 3589-3594.

M. Farré, I. Ferrer, A. Ginebreda, M. Figueras, L. Olivella, L. Tirapu, M. Vilanova, D. Barceló (2001) Determination of drugs in surface water and wastewater samples by liquid-chromathography-mass spectrometry: methods and preliminary results including toxicity studies with *Vibrio fischeri*. J. Chromatogr. A. 938: 187-197.

22. Department of Ecology. University of Barcelona (UdB)

The University of Barcelona group, integrated at the Department of Ecology, has extended expertise on stream and river ecology. In this field, it has developed several aspects related with nutrient dynamics, riparian influences, ecotoxicology, river water quality, and dynamics of biological communities. Special focus has been given to the biology and ecology of invertebrates (micro, meio and macrofauna) and their interactions with natural biofilms (e.g. grazing, structure disturbances). A variety of aspects and techniques have been used for the study of invertebrates, ranging from density and biomass descriptions to determination of trophic interactions. Personnel

involved in the proposal are experts in the analysis of relationships between ecological dynamics of the communities and environmental variables, by using statistical tools. The research in the group has also focused in applied aspects, for example the ecotoxicological response of invertebrates to herbicides and heavy metals presence in the rivers. We have used mesocosms (artificial streams) to approach the relationships between physico-chemical factors in the ecotoxicological response of macroinvertebrate communities.
The group has been involved in different European projects (EVK1-CT-2000-3007, EV5V-CT94-0402, ENV4-CT96-0298, EVK1-CT1999-00005) with close collaboration with the group of the University of Girona.

Research group

Isabel Muñoz, Ph.D. in Biology. Full professor of Ecology at the Department of Ecology. She has been involved in national and international projects focused on structure and function of stream invertebrate community, ecotoxicology and water biological quality. She is coordinator of a national project on “the role of microfauna and meiofauna on stream natural biofilms”.

Ainhoa Gaudes, is a biologist. At present, she is postgraduate fellow of the University of Barcelona. Her research deals with the study of meiofauna community in streams.

Selected relevant references

Rosés, N.; Poquet, M.; Muñoz, I., 1999. Behavioural and histological effects of atrazine on freshwater molluscs (*Physa acuta* Drap. and *Ancylus fluviatilis* Müll. Gastropoda). Journal of Applied Toxicology, 19: 351-356.

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Muñoz, I.; Real, M.; Guasch, H.; Navarro, E.; Sabater, S. 2000. Resource limitation by freshwater snail (*Stagnicola vulnerata*) grazing pressure: an experimental study. Archiv für Hydrobiologie, 148: 517-532

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Real, M., Muñoz, I., Guasch, H., Navarro, E. and Sabater, S. 2003. The effect of copper exposure on a simple aquatic food Caín. Aquatic Toxicology, 63: 283-291.

Sabater, S., Vilalta, E., Gaudes, A., Guasch, H. Muñoz, I., and Romaní, A. 2003. Ecological implications of mass growths of benthic cianobacteria in rivers. Aquatic Microbial Ecology, 32: 175-184.

22. ECT Oekotoxikologie GmbH

ECT is a SME, which provides ecotoxicological services for industry and governmental authorities under the conditions of Good Laboratory Practise (GLP) that, qualify chemical products for registration and notification. These services include the performance of environmental risk assessments. ECT carries out research projects on behalf of or supported by the German Ministry of Education, Science, Research and Technology (BMFT), the German Federal Environmental Agency (UBA) and the European Commission (e.g. EVK1-CT-2000-00047). Objectives of these research activities have been inter alia the development of new ecotoxicological testing methods under laboratory and field conditions, e.g. bio-accumulation and toxicity in sediment dwelling organisms, biodegradation of chemicals in surface water and sediment, biodegradation of organic matter under field conditions, determination of endocrine effects in fish and determination of fate and effects of chemicals in terrestrial and aquatic mesocosms. Several of these methods have been ring-tested and have been or will be soon published as OECD and/or ISO Guidelines.

Research Team

Dr. Thomas Knacker graduated in Plant Physiology, Biochemistry and Microbiology. He is Managing Director of ECT and serves as editor-in-chief of the Journal of Soils and Sediments. His scientific work is focused on microcosm and mesocosm studies in the aquatic and terrestrial environment including fate and effects aspects of chemicals. He co-ordinated the EU-Project "The Use of Terrestrial Model Ecosystems (TMEs) to Assess Environmental Risks in Ecosystems" (ENV4-CT97-0470).

Selected relevant references:

Knacker T, Van Gestel CAM, Jones SE, Soares AMVM, Schallnaß H-J, Förster B, Edwards CA (2004) Ring-testing and field-validation of a terrestrial model ecosystem (TME) – an instrument for testing potentially harmful substances: conceptual approach and study design. *Ecotoxicology 13, 9-27*.

Weyers A, Sokull-klüttgen B, Knacker T, Martin S, Van Gstel CAM (2004) Use of terrestrial model ecosystem data in environmental risk assessment for industrial chemicals, biocides and plant protection products in the EU, *Ecotoxicology* 13, 163-176.

Knacker T, Förster B, Römbke J, Frampton GK (2003) Assessing the effects of plant protection products on organic matter breakdown in arable fields – litter decomposition test systems (Review). *Soil Biology Biochemistry* 35, 1269-1287.

Römbke J, Knacker T, Teichmann H (2001) Ecotoxicological evaluation of pharmaceuticals. In: Pharmaceuticals and personal care products in the environment: scientific and regulatory issues (Daughton CG & Jones-Lepp TL, eds.), 304-319. American Chemical Society, Washington D.C.

Dr. Philipp Egeler is Scientist at ECT. His Ph.D thesis was focused on bioaccumulation of organic contaminants in sediment dwelling organisms. Recently he studied the effects of plant protection products and other chemicals by applying aquatic and water-sediment test systems. Further he is coordinating two international ring-tests concerning effects and bioaccumulation of chemicals on sediment-dwelling organisms.

Selected relevant references:

Egeler P, Römbke J, Meller M, Knacker T, Franke C, Studinger G, Nagel R (1997) Bioaccumulation of Lindane and Hexachlorobenzene by Tubificid sludgeworms (Oligochaeta) under standardised laboratory conditions. Chemosphere, 35, 835-852.

Egeler P, Römbke J, Meller M, Spörlein P, Knacker T (2000) Assessment of biomagnification of hazardous substances from freshwater and marine sediments. Report for Research Project 296 28 3 on behalf of the Federal Environmental Agency (Umweltbundesamt), Berlin, Germany.

Egeler P, Meller M, Römbke J, Spörlein P, Streit B, Nagel R (2001) *Tubifex tubifex* as a link in food chain transfer of hexachlorobenzene from contaminated sediment to fish. *Hydrobiologia* 463, 171-184.

23. Xenometrix $_{\text{by Endotell}}$ GmbH (XEN)

Xenometrix by Endotell was established in by Nicole Weiland-Jäggi June 1997 in Allschwil, Switzerland. Xenometrix is a research and development company specialized in the production, distribution and services of test systems in Europe for molecular pharmacology, drug discovery and in vitro toxicity. Xenometrix strongly focuses on the development of new mutagenicity assays designed to help improve the effectiveness of drug discovery and development through lead compound optimization. With the increasing number of chemicals flowing through the drug development process, and the increasing demand for genotoxic analysis of environmental compounds, the number of screening assays required is growing year by year. The traditional full-format Ames *Salmonella* mutagenicity test cannot currently serve this market, since it requires too much time, labor and samplel to serve as a screening tool. The liquid format Ames II Mutagenicity assay, available exclusively through Xenometrix by Endotell, offers a higher speed format with new strains, colorimetry, automated plating and plate reading. The assay is fast and efficient, shows good correlation with the traditional Ames assay and was developed in the Ames lab at U.C. Berkeley.

Selected reference:

S. Flückiger-Isler, M. Baumeister, K. Braun, V. Gervais, N. Hasler-Nguyen, R. Reimann, J. van Gompel, H.-G. Wunderlich, G. Engelhardt. Assessment of the Performance of the Ames II™ Assay: a collaborative study with 19 coded compounds. Mutation ResearchGenetic Toxicology and Environmental Mutagenesis, In Press, Available online 26 Jan. 2004

24. Donabaum & Wolfram OEG (DW)

The managers and most of the employees of DONABAUM & WOLFRAM OEG are graduates of the University of Vienna (Biology, Zoology, Botany, Ecology or Chemistry). The well-founded and further education as well as the long-term experience form the basis for our activities in the field of applied limnology. We stand in close contact with other experts at home and abroad, cooperate with universities and civil engineers, and regularly participate in scientific conferences and seminars. As one of several partners of the Company for Ecological Planning, Environmental Analytics and Regional Development we are also involved in projects dealing with landscape ecological and socio-economic aspects. The most important fields of our work comprise hydrochemical and biological investigations, assessment of the pollution by industrial waste water, water quality monitoring of rivers, assessment of the ecological integrity, water rehabilitation techniques. Strong taxonomic expertises exist in aquatic macroinvertebrates, fish and freswater algae. Several international projects (covering pollution-related limnological issues in e.g. Germany, Vietnam, China, Tailand) provided for a high experience in transferring knowledge and expertise between regions.

Research team

As a biologist, **Georg Wolfram (PhD), scientist,** has wide experiences in taxonomy and community analysis of macrozoobenthos and fish ecology, ecology of standing and running waters, limnological management and rehabilitation of standing waters, hydrochemistry and water quality analysis. This expertise is founded on extensive activities as a lecturer at the University of Vienna and at a UNESCO Training Course of Limnology, on scientific work as a compagnion of Technical Bureau of Ecology, Vienna, and as a manager of the Donabaum & Wolfram OEG, Consulting Engineers of Ecology.

Five selected, relevant publications

Wolfram, G., M. Salbrechter, E. Weigand, U. Wychera & U.H. Humpesch, 2002. Variations in the epiphytic inverte-brate structure on Potamogeton perfoliatus L. in Traunsee (Austria): patchiness versus impacts by industrial tailings. In R. Schmidt & M. Dokulil (eds), Effects of industrial tailings on the ecological integrity of a deep oligotrophic lake (Traunsee, Austria). - Water, air and soil pollution 2: 117-136.

Wolfram, G., V. A. Kowarc, U. H. Humpesch & W. Siegl, 2002. Distrubution pattern of benthic inverte-brate communities in Traunsee (Austria) in relation to industrial tailings and trophy. In R. Schmidt & M. Dokulil (eds), Effects of industrial tailings on the ecological integrity of a deep oligotrophic lake (Traunsee, Austria). - Water, air and soil pollution 2: 63-91.

Wolfram, G., 1996a. Distribution and production of chironomids (Diptera: Chironomidae) in a shallow, alkaline lake (Neusiedler See, Austria). - Hydrobiologia 318: 103-115.

Wolfram, G., 1996b. A faunistic review of the chironomids of Neusiedler See (Austria) with the description of a new pupal exuviae (Insecta: Diptera: Chironomidae). - Ann. Naturhist. Mus. Wien 98B: 513-523.

Wolfram-Wais, A., G. Wolfram, B. Auer, E. Mikschi & A. Hain, 1999. Feeding habits of two introduced fish species (Lepomis gibbosus, Pseudorasbora parva) in Neusiedler See (Austria), with special reference to chironomid larvae (Diptera: Chironomidae). - Hydrobiologia 408/409: 123-129.

Claus Orendt (PhD), scientist, works mainly on several aspects of bioindiaction by macroinvertebrates. Most approaches of the environmental assessments performed focus on *in situ* bioindication based mainly on aquatic invertebrates including special groups (e.d. chironomids). Apart from extensive, over 15 years experiences in freshwater ecological analysis, faunistics and monitoring in many types of waters including the Elbe river, also studies on effects of toxicants (xenestrogenes, acid) on water organisms are performed. Activities as lecturer in courses at the University of Munich and the Technical Highschool of Anhalt, many presentations and publications of papers complete the working fields. Presently, several projects are concerned to the development of biological water assessment methods for the purpose of the EU-WFD. Also, Dr. Claus Orendt is the manager of Orendt-Hydrobiologie WaterBioAssessment Leipzig (www.orendt-hydro.de), which is founded in 1998 and co-operates with Donabaum & Wolfram. It is a small enterprise, in which several independent scientists and volunteers work on assessements and applied scientific studies of freshwater ecosystems embedded in a dense network of national and international specialists for ecological subjects and taxonomy. Partners and employers are universities, research institutes and regional and national agencies (see webpage) from home and abroad.

Five selected, relevant publications

ORENDT, C. (1999): Chironomids as bioindicators in acidified streams: a contribution to the acidity tolerance of chironomid species with a classification in sensitivity classes. - Int. Rev. Hydrobiol. 84 (5): 439-449.

ORENDT, C. (2000): The chironomid communities of woodland springs and spring brooks, severely endangered and impacted ecosystems in a lowland region of eastern Germany (Diptera: Chironomidae). – Journal of Insect Conservation 4:79-91.

ORENDT, C. (1998): Macroinvertebrates and diatoms as indicators of acidification in forest spring brooks in a region of eastern Germany (Leipzig-Halle-Bitterfeld) highly impacted by industrial activities. - Arch. Hydrobiol. 143 (4): 435-467.

ORENDT, C. & REINHART, U. (1997): The distribution of *Gammarus pulex* (L.), *Asellus aquaticus* L. and *Pisidium* sp. in an acidified forest brook and some tributary springs indicating problems in assessing the local state of acidity at a small scale level. - Limnologica 27(3-4): 271-280.

ORENDT, C. (2003): A classification of semi-natural northern prealpine river stretches based on chironomid communities. - Annls Limnol. 39 (3)

Gabriele Hofmann (Ph.D.) as a **limnologist** has a long-standing experience in the taxonomy and ecology of diatoms. She was involved in national and international projects concerning the development and standardization of methods of water quality assessment based on diatom community structure. Her scientific focus is on studying the stress response of diatom communities in the field, caused by different degress of acidification, salt-loading, eutrophication and organic pollution as well as the use of diatoms for monitoring ecological integrity.

Selected, relevant publications

Hofmann, G. & Schnelbögl, G. (1993): Biological indication of stream acidity by the use of diatoms. Proceedings of the 9th Task Force Meeting in Oisterwijk, the Netherlands: 14 p.

Hofmann, G. (1994): Aufwuchs-Diatomeen in Seen und ihre Eignung als Indikatoren der Trophie. Bibliotheca Diatomologica 30: 1-233.

Hofmann, G. (1996): Recent developments in the use of benthic diatoms for monitoring eutrophication and organic pollution in Germany and Austria. In: Whitton, B.A. & Rott, E. (eds.) Use of algae for monitoring rivers: 73-77.

Hofmann, G. (1997): Diatom communities in the Rivers Werra and Ulster (Germany) and their response to reduced salinity. Limnologica 27 (1): 77-84.

Lotter, A. & Hofmann, G. (2003): The development of the late-glacial and Holocene diatom flora in lake Sedmo Rilsko (Rila Mountains, Bulgaria). In: Tonkov, S. (ed.): Aspects of Palynology and Palaeoecology: 171-183.

Sebastian Höß (PhD), **biologist**, has wide experiences in the assessment of contaminated sediments and soils performed by ecological and ecotoxicological biomonitoring of meiofaunal in situ communities with special emphasis on nematodes and bioassays with whole sediment, soil, porewater, elutriates or extracts using the free living nematode Caenorhabditis elegans for the purpose of assessment of potentially contaminated natural sediments and testing of single substances in artificial sediments. A special expertise comprise the interpretation of the community analysis using metrics of major meiofaunal groups and the nematode community structure (species composition: indicator species, multivariate techniques, distribution of feeding types; maturity index: distribution of different life history strategists; biodiversity indices).

Selected, relevant publications

Höss S., Bergtold M., Haitzer M., Traunspurger W. & Steinberg C.E.W. (2001) Refractory dissolved organic matter can influence the reproduction of Caenorhabditis elegans (Nematoda). Freshwater Biology, 46, 1-10.

Höss S., Haitzer M., Traunspurger W. & Steinberg C.E.W. (1999) Growth and fertility of Caenorhabditis elegans (Nematoda) in unpolluted freshwater sediments - response to particle size distribution and organic content. Environmental Toxicology and Chemistry, 18, 2921-2925.

Höss S., Henschel T., Haitzer M., Traunspurger W. & Steinberg C. (submitted) Toxicity of cadmium to Caenorhabditis elegans (Nematoda) in whole sediment and porewater - the ambigous role of organic matter, Environmental Toxicology and Chemistry.

Haitzer M., Höss S., Traunspurger W. & Steinberg C. (1999) Relationship between concentration of dissolved organic matter (DOM) and the effect of DOM on the bioconcentration of benzo[a]pyrene. Aquatic Toxicology, 45, 147-158.

Haitzer M., Burnison B.K., Höss S., Traunspurger W. & Steinberg C.E.W. (1999) Effects of quantity, quality, and contact time of dissolved organic matter on bioconcentration of Benzo[a]pyrene in the nematode Caenorhabditis elegans. Environmental Toxicology and Chemistry, 18, 459-465.

[1] Milestones are control points at which decisions are needed; for example concerning which of several techniques will be adopted as the basis for the next phase of the project.

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