1 Research proposal, NWO-program Computational Life Sciences (CLS)

1.1 Project Title

Understanding the 'organic carbon pump' in meso-scale ocean flows

1.2 Project Acronym

DEBpump

1.3 Principle Investigator

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2 Project summaries

2.1 Summary

The 'organic carbon pump' is the rate at which algae bind atmospheric carbon dioxide, and transport it to deep waters in the form of organic carbon. In this project, a systematic 'first principle' multidisciplinary approach is followed to determine the effect of transport properties of oceanic meso-scale flows to the efficiency of the organic carbon pump. We do so by combining a realistic algal physiology model, based on the Dynamic Energy Budget theory, with simulations in a very high-resolution ocean model. The simulation results will be tested against in-situ data obtained during the Dutch MARE (Mixing of Agulhas Rings Experiment) project and the SeaWiFS (Sea-viewing Wide Field-of-View Sensor) satellite data. Our approach is unique in the combination of (i) the biological model which contains explicit energy and nutrient balances, while biomass composition is variable, (ii) the high-resolution ocean model to simulate flows details of the meso-scale flows and (iii) the advanced numerical methods used for determining the transport properties of nutrients and biomass.

2.2 Samenvatting

De organische koolstof pomp is de snelheid waarmee algen atmosferisch koolstof dioxide binden en transporteren naar diep water in de vorm van organische koolstof. In dit project wordt een systematische, multidisciplinaire studie voorgesteld om de effecten van het transport door meso-schaal stromingen in de oceaan op de efficientie van de organische koolstof pomp te bepalen. Hiertoe combineren wij een realistisch algenfysiologisch model dat gebaseerd is op de Dynamische Energie Budget theorie, met simulaties in een hoog-resolutie oceaan circulatie model. De resultaten van de simulaties zullen op hun realisme getoetst worden tegen waarnemingen gedurende het MARE (Mixing of Agulhas Rings Experiment) project en SeaWiFS (Sea-viewing Wide Field-of-View Sensor) satelliet waarnemingen. Onze aanpak is uniek in de koppeling van (i) het biologisch model dat expliciete

energie- en nutrient-balansen representeert, terwijl de samenstelling van biomassa variable is, (ii) het hoogresolutie oceaanmodel dat grote details van de meso-schaal structuren kan weergeven en (iii) de geavanceerde numerieke methoden voor transport die gebruikt worden om het transport van nutrienten en biomassa te kunnen bepalen.

3 Classification

Van model naar simulatie

4 Composition of the Research Team

Name	Discipline	Affiliation
Prof. Dr. Ir. H.A. Dijkstra	Physical Oceanography	IMAU, UU Utrecht
OIO	Physical Oceanography	NWO-CLS, (based at IMAU)
Prof. Dr. J.G. Verwer	Mathematics	CWI Amsterdam
Dr. B.P. Sommeijer	Mathematics	CWI Amsterdam
Drs. Pham Thi, N.N.	Mathematics	CWI Amsterdam
OIO	Mathematics	NWO-CLS, (based at CWI)
Prof.Dr. S.A.L.M. Kooijman	Theoretical Biology	VU Amsterdam
Dr. B.W. Kooi	Mathematics	VU Amsterdam
Drs. T. Troost	Biology	VU Amsterdam
Drs. L. Kuijper	Biology	VU Amsterdam
OIO	Physics/Biol	NWO-CLS, (based at VU)

Promotores: Kooijman, Dijkstra and Verwer.

5 Research School

SENSE, BBOS, Stieltjes

6 Description of the Proposed Research

6.1 Motivation

This project is strongly motivated by a desire to understand the physical-chemical processes which control the level of atmospheric carbon dioxide. Apart from fundamental reasons, there is also an urgent need for this knowledge: there are strong indications that the level of CO2 in the atmosphere is affecting the global temperature. The increase of CO2 due to anthropogenic activities, may lead to substantial climate change (Houghton et al., 2001).

Although there is still much discussion on closing the planetary carbon budget, it is well-established that processes in the marine biosphere can act as an important sink of carbon from the atmosphere (Jacobson et al. 2000, Falkowski et al. 2000, Falkowski 2002). Carbon is, for example, taken up by organisms to build biomass structure and is eventually transported to the deep ocean as Particulate Organic Matter (POM) where it is partly buried into sediments. Carbon uptake also occurs within the terrestial biosphere, but organic matter on land is oxidized prior to incorporation into soils. Hence, this leaves the burial of POM and biogenic calcium carbonate as a main pathway by which carbon is removed from the biosphere (Kooijman, 2003).

There is a central role for plankton in this organic carbon pump. Most of the carbon is used by autotrophic organisms during photosynthesis in the surface waters of the ocean (the euphotic zone). Through the food chain, this carbon is transported to higher trophic levels and hard parts of these organisms eventually form the main contribution to POM. Hence, the distribution of phytoplankton is central to the efficiency of the organic carbon pump (Mann and Lazier, 1996).

There are still substantial problems to simulate patterns of primary production in the ocean using combined eddy-permitting ocean models and models of plankton dynamics (Oschlies and Garcon 1998, Malchow and Petrovskii 2002). One of the reasons is that much of the supply of nutrients to the eutrophic zone occurs at smaller scales than a typical eddy scale (Levy et al., 2001). However, also the model of plankton dynamics, such as the classical nitrate, phytoplankton, zooplankton, detritus (N-P-Z-D) model, is still oversimplified.

6.2 Scientific problem and expected results

The growth of phytoplankton in the ocean is dependent on the availability of light and nutrients, the latter depending on both the local flow conditions and on the local ecological scenery. For example, nitrogen is often a limiting factor for growth because it is quickly depleted in upper layers, but cannot easily be transported from depth because of a strong stratification which inhibits vertical mixing. The (species-specific) composition of POM and the heterotrophic activity strongly determine the depth at which the biomass is still present.

The problem is complicated because of the multitude of spatial and temporal scales involved. Processes in the surface (turbulent) mixed layer are central to the air-sea exchange of components such as carbon and nitrogen and hence for the background concentrations of these quantities even in case the biology is absent. These processes take place on time scales from days to weeks and spatial scales of several kilometers in the horizontal and the upper 500 m of the ocean. On larger horizontal scales, in particular on the internal Rossby deformation radius (10 - 100 km), meso-scale structures in the ocean such as eddies and ocean rings, are dominant in the mixing process. These processes, which occur on time scales of weeks have a substantial effect on the large-scale flow in an ocean basin such as the North Atlantic Ocean. They also have a strong impact on the spatial structures of primary production as has been well demonstrated by Oschlies and Garcon (1998). To assess the conversion of carbon from the atmospheric reservoir to the deep-sea reservoir on a basin scale, one has to address systematically the processes in the mixed layer and typical meso-scale structures.

Mixing processes in the upper 200 m of the ocean and on time scales of days to weeks are complex due to the high level of turbulence. The turbulent mixed layer is classically viewed as being generated by a spatially homogeneous flow structure, where the vertical profiles of tracers are determined from the kinetic energy budget and the background stratification. However, even in this turbulent flow region plankton patchiness can be found in the upper layers of the ocean (Abraham, 1998).

On the larger space and time scales, organized flow structures tend to contribute significantly to the mixing rate of nutrients and hence to the primary production. At mid-latitudes, instabilities of the main western boundary currents such as the Gulf Stream, generate eddies and rings, which may have diameters of about 100 km. These eddies may have vertical signatures of about 1000 m or even deeper and create a local physical environment which may be much different from the surroundings. A typical example are rings which are shed from the Agulhas Current near the tip of South Africa (Dijkstra and De Ruijter, 2001). Recently, the properties of these rings (including many plankton species) have been measured during three cruises of the Mixing of Agulhas Rings Experiment (MARE). Preliminary results indicate that different species are preferentially located at different locations in the ring.

It is not very well known how the mesoscale features, such as oceanic rings, affect production rates of phytoplankton and hence their role in the large-scale organic carbon pump is practically unknown (Oschlies and Garcon, 1998). In this project, a systematic approach is suggested to study the coupling of biological and hydrodynamical processes in ocean meso-scale flows. This is accomplished through a combination of a 'first principle' biological model based on Dynamic Energy Budget theory (Kooijman, 2000) with simulations in a very high resolution ocean model (Molemaker and Dijkstra, 2000) using advanced numerical methods (Van der Houwen and Sommeijer, 2002, Verwer et al. 2002, Hundsdorfer and Verwer, 2003). With the results, it will be possible to obtain quantitative estimates of the efficiency of the organic carbon pump and the contributions of each of the specific oceanic and biological processes to this efficiency.

6.3 Methods

The evolution of biomass in the flows is studied by using Dynamic Energy Budget (DEB) theory (Kooijman 2001, Kooijman and Nisbet 2000, Nisbet et al. 2000). This is the central innovative element in the project since it is one of few 'first principle' theories around that can describe the relevant biology for the carbon pump.

In a recent paper, a relatively simple model of mixotrophic organisms was described (Kooijman et al. 2002); these organisms have both autotrophic an heterotrophic capabilities. This model satisfies closed balances for mass within a system which is open with respect to energy. As such, it has much more realistic properties than many ecological models used in studies of the biology of the ocean. The DEB model allows for the intracellular accumulation of nutrients and carbohydrates, which is essential to model growth in the water column that has gradients in nutrients and light such that steady state growth is hardly possible at any given depth. The DEB model will be linked to models for sinking of detritus developed by Huisman and Sommeijer (2002a,b).

The project is logically divided into three interacting subprojects:

6.3.1 Subproject A: Mixed layer processes and the carbon pump (Biological Part)

The interaction of production and sinking will be studied first in one spatial dimension using the General Ocean Turbulence Model (Large et al, 1994; http://www.gotm.net).

We expect to find answers to the following problems

1 How does atmospheric carbon fixation relate to nutrient supply quantitatively and what are realistic estimates for the fixation rate, based on verified mechanism?

2 How does nutrient profiles build up as a result of growth, sinking, mineralization and mixing, including its diurnal and yearly dynamics?

3 What is the minimum level of ecophysiological detail algal growth models must have to capture the measured vertical profiles realistically? E.g. increasing the number of internal reserves increases the variability of biomass composition; to what extend is this essential to capture the basic patterns in primary production?

The verification material that will be used consists of eco-physiological data in laboratory study and field-data on vertical profiles of nutrients and biomass

6.3.2 Subproject B: Meso-scale mixing processes and phytoplankton growth (Oceanographical Part)

To model the typical upper-layer oceanographic flows, the three-dimensional non-hydrostatic ocean model developed at IMAU will be used. This model simulates full momentum and tracer equations at high resolution. It was used to study the development of meso-scale eddies under the presence of convection (Molemaker and Dijkstra, 2000). Recently, this code was made parallel and the national supercomputer (a 1024 processor SGI-Origin3000 machine) will create opportunities for very high-resolution simulations.

Using this flow model, simulations will be performed for the upper 1000 m of the ocean in an ocean basin for the case of a typical propagating Agulhas Ring (Van Aken, 2003). Different forcing conditions (day/night, seasonal, etc.) will be used over a typical time scale of Order(1-10) years. For each flow simulated, the biology will be calculated using the DEB model for the mixotrophs (Kooijman et al. 2002). Focus of the studies will be on the mechanisms of how flow structures and plankton properties affect the downward transport of carbon.

We expect to find answers to the following problems

1 Can we find first-principle explanations for chlorophyll distributions as observed by satellites?

2 Can we understand the plankton patterns as observed during the MARE experiments?

3 How do meso-scale flow phenomena modify the large-scale surface chlorophyll patterns?

6.3.3 Subproject C: Numerical simulation of complex flows with DEB (Numerical Part)

To be able to obtain reliable answers to the problems addressed in projects A and B, sophisticated numerical techniques are necessary. Several difficulties have to be faced, for which we expect to find an answer:

1 The first step will be the coupling of the flow solver (which is available from Project B) with a transport solver. In fact, the output of the flow solver (i.e., the velocity field) serves as input for the transport solver. A simultaneous solution of flow and transport requires an integrated approach. Therefore, the algorithms, the spatial grids, the size of the time steps, etc. need to be tuned (see e.g. Van der Houwen and Sommeijer, 2002). Next, in solving the transport problem it is highly important to preserve special properties. To achieve this, the numerical method should be chosen with great care. We will pay special attention to positivity in the solution. This requirement usually imposes a severe restriction on the time step. In this context, the use of so-called limiters is an often-used technique. We will investigate the most efficient approach in the current application.

2 A next computational complication is that we have to deal with complex source terms. Moreover, these terms cause a coupling between the DEB and flow/transport model and certainly influence the choice of an appropriate numerical algorithm.

3 The different spatial scales require special treatment. To keep the number of grid points at a manageable level, the use of embedded models with different resolution might be an option. The difficulty in this approach is that we need to impose boundary conditions at the artificially introduced boundaries between the various embedded models. Another possibility is to use local grid refinement on part(s) of the grid where we observe large spatial variation. Furthermore, in our 3D simulations on irregular domains we have to make a choice on the type of grids that we use. A uniform Cartesian grid may be inefficient. Transformed grids, or even fully unstructured grids can provide a remedy.

4 An interesting question related to the preceding research item is the use of small timesteps in spatially refined regions and large timesteps elsewhere. This idea of advancing some part of the system faster in time than other parts is called multirating and originates from the ODE-field. There it has successfully been used, e.g. in the simulation of electrical circuits. Applying the same idea in a PDE context is much more difficult. In our application this approach will have an impact on both the flow solver and the transport solver. Some first applications of multirating to PDEs have been made (see Flaherty et al. 1997 and Logg, 2003). However, for sophisticated numerical techniques it is not yet clear how to arrange this efficiently and to maintain classical numerical properties like stability and accuracy.

6.4 Scientific significance

The project will be highly innovative in several respects

1 It will contribute essential information for understanding the global carbon balance, and it does so in a mechanistic, rather than descriptive way. This allows, among others, estimation of primary production in the geological past, which is of importance for climate reconstructions.

2 It will join physics, chemistry, biology and advanced computational techniques using first principles, rather than descriptions.

3 It will link scales in time and space in relation to production that are far apart, from minutes to years, from cubic centimeters to ocean basins.

6.5 Relation with other research of related interest

Simulations of primary production that we know of are hardly realistic from a biological and/or from an ocean circulation point of view. This project will be unique in dealing with a variable algal biomass composition, while still observing stoichiometric constraints on production and a full mass and energy balance, as well as state of the art implementation of ocean circulation modelling.

6.6 Project in context of current research by team members

The group at the VU developed the DEB theory for the metabolic organisation of life; quantification of primary production has been among the applications of this theory in the context of European programs (MAST II), and National Programs (NOP II). This research focused on algal ecophysiology; an implementation in ocean circulation models has not been attempted before.

The development of models for mixotrophs has been a preparation for this project to reduce the complexity of producer-consumer-decomposer models for ecosystems (Kooijman and Nisbet, 2000). The necessity of such a simplification for implementation in circulation models revealed during the interaction between Dijkstra and Kooijman in the NOP II program.

This project will interact with parallel projects that have been started by the team members, which aim to find answers to the following problems of related interest such as

1 To what extend mimic mixotrophic communities that of producers, consumers and decomposers in its functional aspects? (research by Kuijper)

2 What is the effect of grazing in the transport of organic carbon, and how can this effect be summarized most efficiently in a model that deals with algae only. (research by Kuijper)

3 Under what environmental conditions will mixotroph populations evolve into auto- and heterotrophic populations on an evolutionary time scale and how does this effect nutrient turnover? (research by Troost)

4 How does biodiversity, i.e. ecosystem structure, affect nutrient recycling, i.e. ecosystem function? (research by Troost) Information about these projects can be found at http://www.bio.vu.nl/thb/

The group at IMAU is involved in high-resolution ocean modelling, in particular of meso-scale structures such as ocean rings. The group is involved in the MARE cruises that investigated the properties of Agulhas rings. Moreover, there is a large expertise in the use and interpretation of satellite data.

The group at CWI has a long lasting experience in numerical methods for partial differential equations, including applications in algal growth and sinking. This experience is the result of joint work with the UvA-group Aquatic Microbiology, headed by Huisman (see Huisman & Sommeijer, 2002a and 2002b, and Huisman et al., 2002). Another topic intensively studied at CWI concerns the construction and analysis of flow and transport solvers (see Sommeijer 1999 and Van der Houwen and Sommeijer, 2001 and 2002).

7 Working programme and time schedule

7.1 Project A: Mixed layer processes and the carbon pump

Year 1 Numerical implementation of the mixotroph model with 0, 1 and 3 reserves in the (one dimensional) General Ocean Turbulance model. Calibration of parameter values using data from eco-physiological literature.

Year 2 Understanding the formation of POM and the rate it is transported to deeper levels and compare these with measurements using sediment traps.

Year 3 Determining which physical/biological processes are dominant in the POM transport.

Year 4 Finishing papers and writing of Ph. D. thesis.

7.2 Project B: Meso-scale mixing processes and phytoplankton growth

Year 1 Implementation of the DEB model into a three-dimensional non-hydrostatic model and numerical improvements in cooperation with project C. Mixed layer simulations and comparison with the GOTM results in project A.

Year 2 Complete simulation studies of the meso-scale flows. Verification of results with measurements in Agulhas rings and satellite data on chlorophyll distributions (SeaWiFS). Understanding the surface patterns of the phytoplankton.

Year 3 Assessment of the efficiency of the carbon pump due to the meso-scale ocean flows. Coupling of the results with those of project A.

Year 4 Finishing papers and writing of Ph. D. thesis.

7.3 Project C: Numerical simulation of complex flows with DEB

Year 1 In close co-operation with project B the flow and and transport solver will be coupled with special emphasis on research item 1, as formulated in Section 6.2. Next, the biology component will be added to arrive at the combined DEB-transport model for which an efficient numerical method will be constructed (research item 2).

Year 2-3 Upscaling of the problem. Here the research items 3 and 4 (regarding non-uniformity in space and time, respectively) will be studied. Furthermore, a parallel implementation on the SGI Origin 3000 will be carried out.

Year 4 Finishing papers and writing of Ph. D. thesis.

We aim at 4 till 5 papers per sub-project (so 15 papers in total, excluding the thesis), three co-authored by sister sub-project members.

8 Toegang tot nationale computerfaciliteiten

We will use the SGI-Origin3000 machine for the circulation simulations.

9 Literature

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9.1 Five most important references from team members

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Most papers from the team members can be downloaded from their websites, which also give additional information about their scientific activities:
http://www.bio.vu.nl/thb/
http://www.phys.uu.nl/ dijkstra/
http://db.cwi.nl/personen/publiek/zoek_show.php4?persnr=87
www.cwi.nl/ janv

10 Requested Budget

3 OIO's, standard benchfees.