Ecological modelling - formulation of the pelagic model.

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Summary

We have developed various ecological modules that can be incorporated in the ultimate OMEX ecological model, which must be operational in the third year of OMEX.
The choice whether or not to include a module will depend on the requirements imposed by the data set as well as on computational restrictions; 1-D model runs allow more complex modules than 3-D model runs. The various modules will be described in short.

Water column processes

Nutrients, dissolved substances.

Ammonium and nitrate are modeled. This allows assessment of the importance of new versus regenerated production and the quantification of water column nitrification compared to benthic nitrification.
Oxygen dynamics is included as an additional constraint on phytoplankton production and heterotrophic respiration estimates.
These are essentially modules that were already implemented during OMEX I (Soetaert et al., subm.).

Phytoplankton.

The phytoplankton is able to adapt its physiological condition to the environment. For instance, the amount of chlorophyll per cell as well as the cellular nitrogen to carbon ratio are adjusted as a function of light, nutrient availability and temperature. In stratified water masses, the light and nutrient gradients are in an opposite direction and consequently, the nitrogen to carbon ratio and the chlorophyll to carbon ratio of algae may change substantially as a function of water depth. In addition, it may be expected that algae experience physiological changes when they are 'upwelled'. In that case they will need to adapt from low-light, nutrient-rich waters to high-light, nutrient-rich waters, and after depletion of nutrients to high-light, low-nutrient waters.
Not all phytoplankton models are able to describe these physiological adaptations of algae to varying environmental conditions. As yet there does not exist a single model that describes the adaptation on the level of the nitrogen to carbon ratio as well as the chlorophyll to carbon ratio.
We have implemented several existing phytoplankton routines with varying abilities to represent these physiological adaptations (See Figure 1). In addition we have developed a new model that encompasses the adaptation on both the level of the Chl/C and N/C ratio.

- (1) Balanced growth model:

Nitrogen and carbon assimilation occurs with fixed stoichiometry. Both the chlorophyll to carbon ratio and the nitrogen to carbon ratio is fixed.

This model describes only one state variable (Phytoplankton carbon or phytoplankton nitrogen). It is the model most often used in dynamic simulations.

- (2) Droop kinetics model (Tett & Droop, 1988)

Nitrogen and carbon assimilation are decoupled and depend on the N/C quotum of the phytoplankton. The variable N/C ratio is assumed to reflect luxury consumption of DIN. The chlorophyll to nitrogen ratio depends on the N/C quotum. This is the original OMEX I module. There are two state variables: phytoplankton carbon and phytoplankton nitrogen.

- (3) Photoadaptation model (Geider et al., 1997)

This is a balanced growth model (fixed N/C ratio) but including the adapation of cellular chlorophyll concentration as a response to light, temperature and external nitrogen concentration. There are two state variables, phytoplankton chlorophyll and phytoplankton carbon.

- (4) Energy budget model (Lancelot et al., 1991), model AQUAPHY.

Nitrogen and carbon assimilation are decoupled; nitrogen uptake depends a.o. on the availability of cellular carbohydrates (used as a carbon source for protein synthesis and as a substrate for respiration providing energy for protein synthesis). The N/C ratio is variable and reflects the protein/total carbon ratio. The chlorophyll to nitrogen ratio is constant. The original model has been slightly modified (i.e. to prevent unrealistic NC ratios under high-light, low-nutrient conditions).

There are three state variables: small metabolites, reserve molecules and functional macromolecules (proteins). The first two are carbohydrates and contain carbon only; the last state variable consists mainly of proteins and contains C and N.

- (5) Energy budget model with photoadaptation.

This is essentially the model of Lancelot et al. (1991), but the functional macromolecules have been subdivided in 'photosynthetic' and 'biosynthetic' molecules as described in Geider et al. (1996). In addition to a variable N/C ratio, this model also describes the adaptation of the algal chlorophyll content.

This is a new model that is now being calibrated based on literature data of culture conditions (for an example of model calibration, see Fig. 2).

There are four state variables: small metabolites, reserve molecules, biosynthetic and photosynthetic macromolecules. Only the biosynthetic and photosynthetic molecules contain N, only the photosynthetic macromolecules contain chlorophyll.

Zooplankton

This is the module implemented during the OMEX I project; it consists of the model of Henderson & Steele (1995).

Bacterial dynamics, dissolved organic matter

The model of Billen and Servais (1989) has been implemented. There are 3 state variables (or 5, if variable N/C stoichiometry is allowed): dissolved organic polymers, dissolved organic monomers and bacteria.
Dissolved organic matter is produced in the form of dissolved organic polymers which are first hydrolysed by bacterial exoenzymes. The ensuing dissolved organic monomers can be taken up by the bacteria, inducing growth.

Particulate organic matter

Up till now only the OMEX I module is available. It considers 4 fractions, particulate nitrogen and carbon that is either fast or slow sinking. The decay rate of carbon and nitrogen depends on the N/C quotum and is higher for nitrogen than for carbon compounds. This induces a decreasing N/C ratio and degradability with ageing of the organic matter.
The distinction between two sinking classes and the variable degradability is important for the sediment model, whose behaviour to a large extent depends on the reactivity of the organic matter falling on the sediment surface.

Design of a detrital model will be the main focus during the second year of OMEX II-II.

Sediment-water exchange processes

There are several options implemented to describe exchange across the sediment-water interface, and the main features of each have been tested. Models (1) and (2) were developed during OMEX I; models (4)-(7) are often used in shelf sea models.

- (1) Fully coupled dynamic diagenetic model

This is the module developed during OMEX I (Soetaert et al., 1996). It is the most complete module, but computationally too demanding for coupling to a detailed water column model.

- (2) Semi-dynamic diagenetic model

Only the profiles of two detritus fractions are described dynamically, the dissolved substances are assumed to be at steady state with the profiles of organic detritus and their fluxes are computed based on the gradients at the sediment-water interface.

The behaviour of this module is comparable to the full diagenetic model (Soetaert et al., 1996), while imposing less computational demands.

- (3) Integrated sediment detritus model

The total amount of sediment detritus is described dynamically and the fluxes of dissolved constituents are derived based on mass budget considerations or using a metamodel approach. This module is less flexible than (2) but very fast.

- (4) Reflective boundary

The settling detritus is translated into a flux of dissolved inorganic nitrogen compounds and oxygen, assuming immediate mineralization of all the settling organic matter. This model is unable to reproduce characteristic seasonality in sediment response, lacks denitrification but there are no computational constraints.

- (5) Imposed bottom water concentration boundary

Detritus settles on the sediment and is lost to the water column. The bottom water concentrations of nitrate, ammonium and oxygen are imposed. This parameterization violates mass budget; no computational constraints.

- (6) Imposed flux condition

Detritus settles on the sediment and is lost to the water column. The fluxes of nitrate, ammonium and oxygen to or from the sediment are imposed. This parameterization violates mass budget; no computational constraints.

- (7) No solute flux

Detritus settles on the sediment and is lost to the water column. There is no flux of dissolved substances associated. This is clearly incorrect for the oxygen components, but is equivalent to a reasonable degree of denitrification for the nitrogen compounds. No computational constraints.

- (8) No sediment

It is assumed that all mineralization occurs in the water column. This conserves mass, but denitrification cannot be reproduced; this parameterisation of sediment-water exchange imposes no computational constraints.

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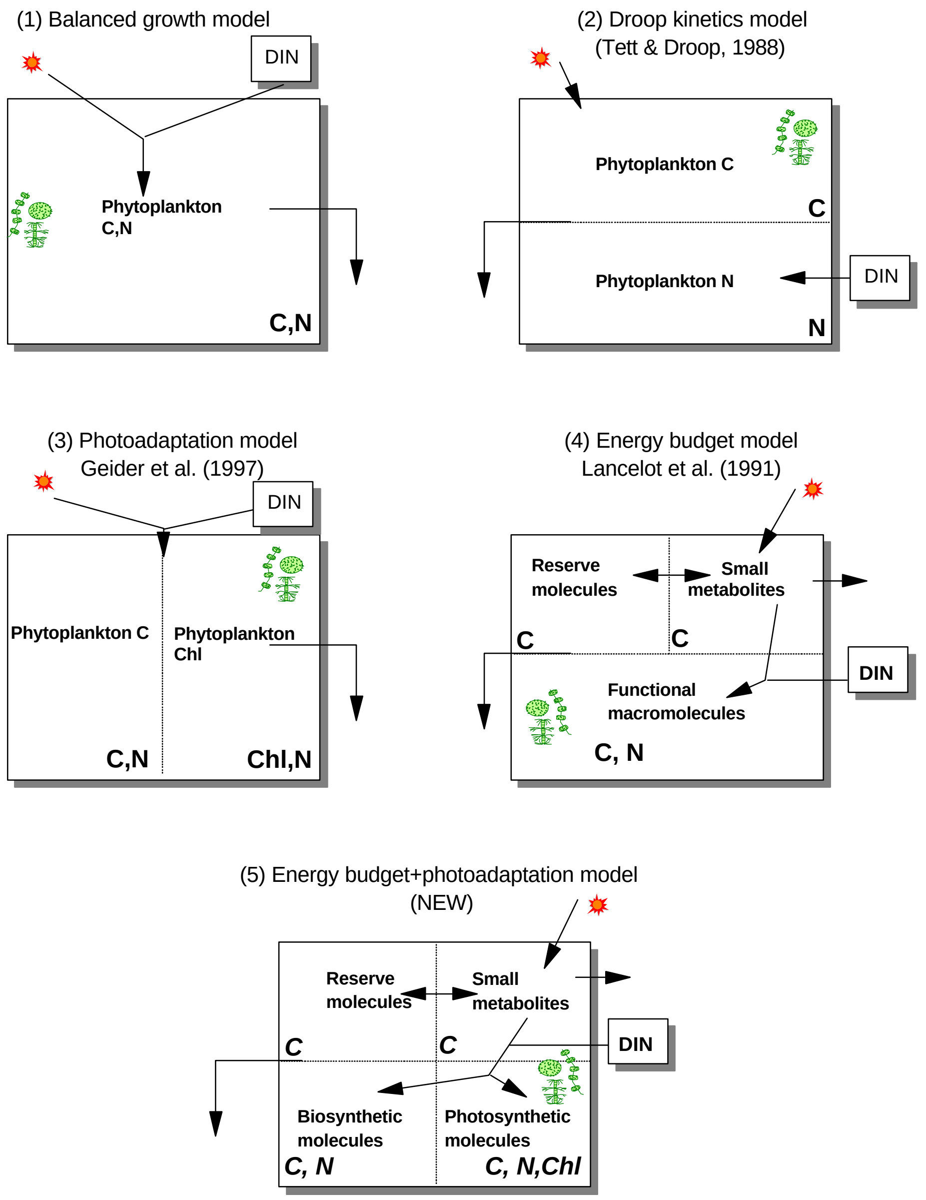

Fig. 1. A schematic representation of the various phytoplankton models implemented.

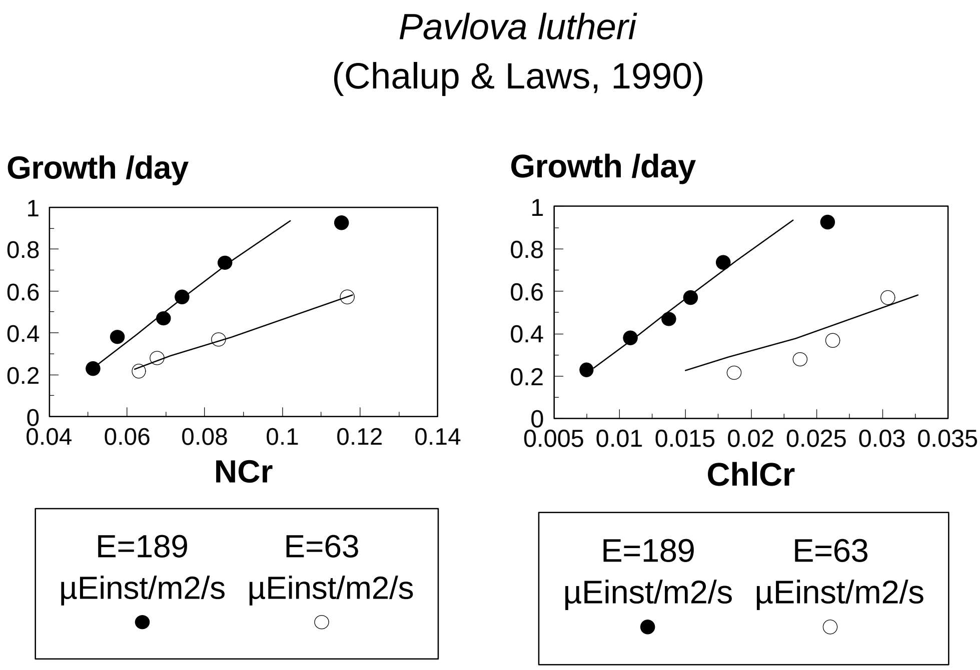

Fig. 2. An example of goodness of fit of the newly developed phytoplankton model with laboratory data (Chalup & Laws, 1990) of the species Pavlova lutheri.

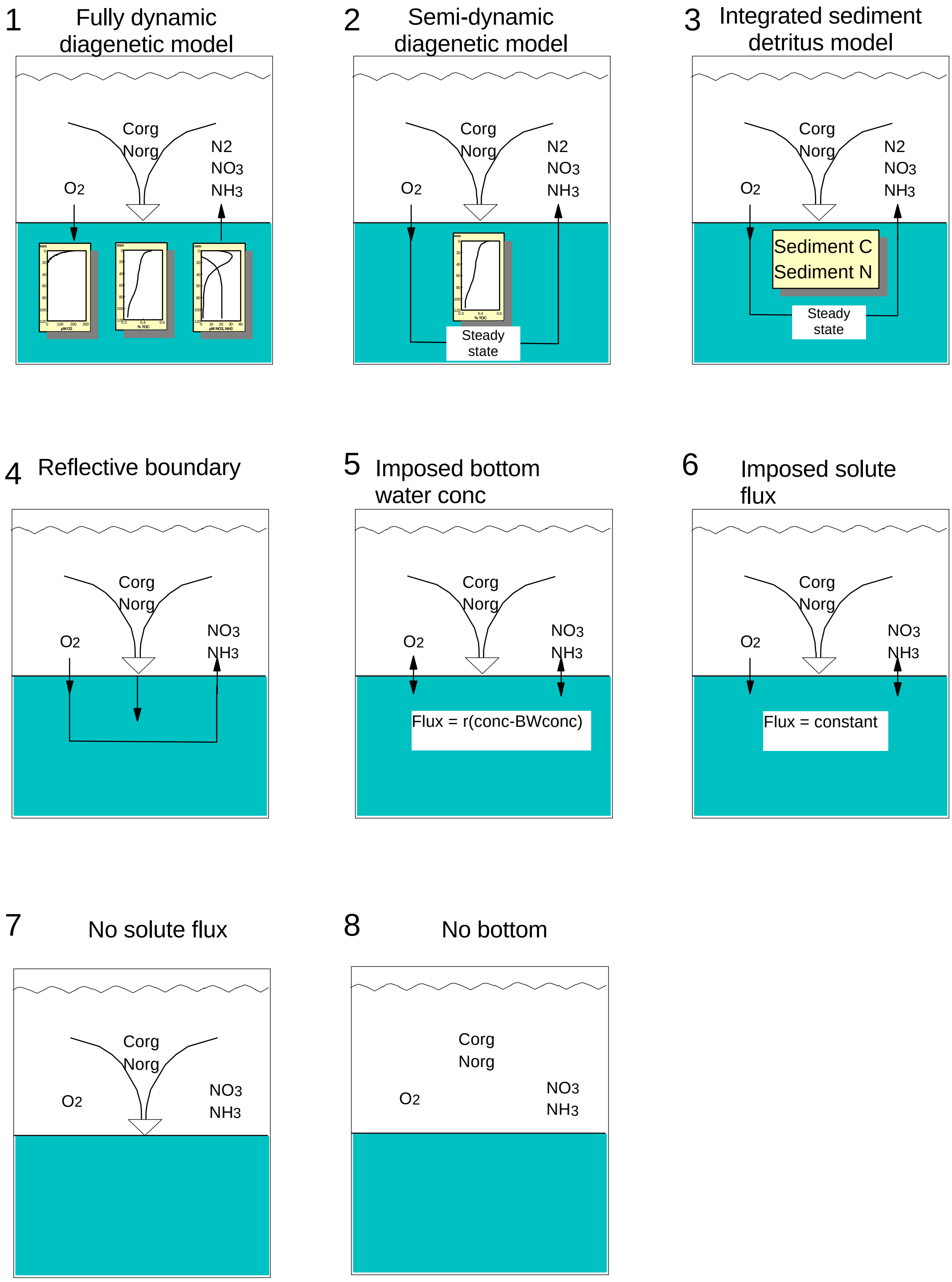

Figure 3. A schematic representation of the various sediment-water exchange models implemented.