MEDIA: a modelling environment for surface sediment biogeochemistry

Meysman F.J.R.[1], C. Heip[2], P.M.J. Herman[2], and J.J. Middelburg[2]

[1] Ghent University, Marine Biology Section
K.L. Ledeganckstraat 35, B-9000 Gent, Belgium
E-mail: filip.meysman@rug.ac.be

[2] Centre for Estuarine and Marine Ecology
Korringaweg 7, NL-4401 NT Yerseke, The Netherlands

Surface sediments of oceans, estuaries and rivers are highly active geochemical environments. In recent years, there is a remarkable interest for a thorough quantitative understanding of the physical, chemical and biological processes governing sediment biogeochemistry. This new emphasis is being driven by both fundamental and applied objectives. Pressing environmental problems, such as predicting the fate and transfer rates of contaminants in aquatic sediments, now demand numerical answers. Moreover, mathematical models can assess the complex role of the sediment in the global biogeochemical cycles of carbon, nitrogen and other elements. Important topics include benthic-pelagic coupling (i.e. the quantification of fluxes across the sediment-water interface) and the interpretation of the historical sediment record in the light of ocean paleochemistry and climate studies.

Quantitative predictions and explanations of sediment biogeochemistry are possible through the application of so-called diagenetic models, which incorporate mass and momentum conservation equations for the different species in the surface sediment. Within the field of diagenetic modelling, a significant amount of problem-solving knowledge has been acquired from past modelling projects. Over the past four decades the field has shifted from simple analytic models, which need many simplifying assumptions and can only provide a limited qualitative understanding, to large and complex numerical models, which need extensive coding as a computer application, but give realistic and mechanistic description of sediment biogeochemistry. In recent years, a number of example applications have illustrated the capacities of such sophisticated numerical model codes for the integrated modelling of biogeochemical cycles (Soetaert et al., 1996; Wang and Van Cappellen, 1996; Boudreau et al., 1998). Although intrinsically powerful applications, the current numerical model codes still show a number of weaknesses: (1) models are site-specific, as they incorporate a fixed set of species and reactions, which limits the type of diagenetic problems and environments to be investigated (2) models lack flexibility and extendibility, and the associated need for low-level reprogramming and recompilation constitutes a major barrier for potential model users. A grand challenge is to encapsulate the present know-how into an easily used and flexible environment, and to bring this problem-solving power within reach of geochemists that are not familiar with computational issues.

Meeting this challenge constitutes the central philosophy behind the MEDIA project (Modelling Environment for DIAgenesis). The MEDIA environment comprises a flexible and extensible software system that provides problem-solving assistance for simulating the biogeochemistry of surface sediments. The MEDIA modelling environment is built on two fundamental strongholds:

(1) Problem solving environments, a modern concept from the field Computation Science and Engineering (CSE). Rather than focusing at a single model, a Problem Solving Environment (PSE) comprises a computer application that provides all the computational facilities necessary to solve a *target class* of related problems. These features include model construction possibilities, advanced solution methods and ways to easily incorporate novel solution methods. Moreover, a PSE uses the 'natural language' of the target class of problems, so users can run them without specialized knowledge of the underlying computer hardware or software.

(2) Object-oriented technology, the ground breaking new paradigm from the field of Industrial Software Engineering. Within MEDIA generic model construction was introduced i.e. the application user is allowed to assemble a diagenetic model from a toolbox of available model components (species, processes). Due to the introduction of an object-oriented database new

components (e.g. new species and reactions) can be added without the need for writing a single line of new code.

Succinctly stated, the MEDIA environment transfers the control on diagenetic model formulation from the application author to the application user, enables the design of customer-tailored diagenetic models built from a set of basic building blocks and provides an efficient numerical solution procedure for these models.