Adsorption Processes in MEDUSA

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Availability: by appointment

Thematics: climate, environment and oceanography

Description:

Solute transport in porous media such as seafloor surface sediments is mostly by moecular or ionic diffusion in porewater. However, for some nutrients, such as ammonium or phospahte ions, transport by adsorption onto solids particles is another important pathways of transport.

Adsorption processes are currently not represented in the Models of Early Diagenesis in the Surface Sediment with Adaptable complexity, MEDUSA (Munhoven, 2021). While a reasonably realistic steady-state representation of adsorption processes (by diffusion coefficient enhancement) can be realised by code patching, it is unclear if this approach allows for selective adsorption on special types of solid particle (e. g., clay particles only). As a result, it would be more consistent to extend the code generator to allow for the explicit inclusion of adsorption processes.

Here, I propose to implement both approaches in MEDUSA and to perform a comprehensive sensitivity analysis of the two methods, and of the relative importance of transport by adsorption in general.

Requirements and prerequisites This thesis project requires advanced programming skills. The code generator for MEDUSA is written in Fortran 95 and needs to be adapted. Introductory training in Fortran 90/95 can be provided if required.

Basic knowledge of biogeochemical cycles (carbon, phosphorus, nitrogen) would be useful, but is not indispensable, as this can be easily acquired from textbooks and scientific literature (rich collection available in the lab).

Infrastructure Usual developments and test simulations can normally be done on the student's own computing devices (laptop, desktop PCs), but a calculation server is available in the lab if required.

Stays abroad This work can be completely done in Liège.