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Studying the cycling of trace elements and isotopes at the sediment-water interface using a diagenetic model with automated code generation for user defined problems

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The sediment-water interface (SWI) is identified by GEOTRACES as one of the four main interfaces across which material fluxes regulate sources and sinks of trace elements and isotopes (TEIs) in the ocean [1]. Given the significant logistical and analytical challenges of measuring TEI fluxes across SWI, and the complexity of biogeochemical reaction networks in marine sediments, modelling tools become critical in quantifying the mechanisms and processes regulating the cycling of TEIs across the SWI [2]. Diagenetic models, typically one-dimensional reaction-transport models, are the standard tools for modelling transfers of carbon, oxygen and nutrients across the SWI, but their applications in TEI studies are very limited. We design a diagenetic model specific for TEI studies. The model is written in Julia, an increasingly popular computer language for high performance scientific computing. The model includes a dynamic pH model [3] which enables TEI speciation calculations. The model can generate computer codes automatically, only requiring the user to provide an Excel file with tables of model species, chemical reactions and kinetic rate expressions. The model is thus highly flexible, and the generated codes are specific to the user defined problem, yet it has minimal requirement of the users' programming skills. The model is also designed with high performance in mind. The ultimate goal is to couple it to ocean circulation models, for example using the transport matrix method [4], which would eliminate the need for empirical parameterizations of TEI fluxes across the SWI, allowing more accurate biogeochemical modelling of TEIs in the ocean. We demonstrate the applicability of the model by simulating pore water profiles of TEIs from various depositional environments.

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