Reactive transport in complex biogeochemical systems

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This contribution reviews recent progress and trends in reactive transport modeling (RTM) of biogeochemical systems, and discusses remaining challenges. Our premise is that a combination of process-oriented laboratory experiments, RTM and field validation is the most appropriate strategy to improve our understanding of the chemical dynamics of biogeochemical systems. Focus is on the use of RTM as intellectual support to interpret field-based data, design experimental studies and test implications of hypotheses. In this context, model development occurs iteratively, as new knowledge is continuously incorporated, and sensitivity analyses, rather than prediction, take central stage. Sensitivity analyses help identify the dynamical variables that dominate the behaviour of the system, but they also allow to compare and rank alternative model structures and process formulations. Powerful new approaches in RTM consist in combining traditional forward simulations with inverse, stochastic and adjoint modeling. Illustrative examples of RTM, applied to rivers, estuaries, sediments and aquifers, are discussed, with an emphasis on issues related to parameter identification, calibration, uncertainty and heterogeneity.

Present and past export of Southern Ocean deep water to the Pacific

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We present new Pb, Nd and Hf isotope time-series for two ferromanganese crusts, which have grown from central Pacific bottom water (D137-01, north of Samoa Passage, 7219 m water depth) and southern Pacific deep water (63KD, Tasman Basin, 1700 m water depth) over the past 38 and 23 Ma, respectively. Age models for both crusts were obtained by combining $^{10}Be/^{9}Be$ profiles and Co-flux modelling. Continuous time-series for Pb, Nd and Hf isotopes were measured at high precision using a Nu Plasma MC-ICPMS.

D137-01 is the deepest ferromanganese crust so far investigated for isotope time-series. Lead isotopes show a very different pattern from previously reported central Pacific records. Prior to ~ 17 Ma $^{206}Pb/^{204}Pb$ ratios are radiogenic (>18.80) and similar to "Atlantic" values whereas the present day $^{206}Pb/^{204}Pb$ ratio of 18.75 is intermediate between Southern Component Waters (≤18.85) and Pacific deep water (≤18.70). Two possible explanations for the observed trend are (i) a change in the isotopic composition of deep water exported from the Southern Ocean to the Pacific with time or (ii) a decrease in the flux of water masses from the Circum Antarctic Current to the Pacific Ocean. The likelihood of these interpretations can be tested by comparison with the second new record from the Tasman Basin. Overall there is a striking similarity of the two profiles and a remarkable agreement with general Pb isotope patterns in Southern Ocean crusts (Frank et al., 2002) and records from the Western Boundary Current in the South Pacific (Baker et al., 2001) over the past 14 Ma. Consequently, we suggest that the observed changes have been related to the export/composition of Southern Ocean water masses.

Final interpretations have to take into account the Nd and Hf isotope time-series from the same crusts as well. D137-01 shows relatively invariable ε_{Nd} and ε_{Hf} values over the past 38 Ma which are consistent with a two component mixture of Southern Ocean waters and Central Pacific bottom water. The picture for the Tasman Basin looks more complicated. Here we observe drastic changes (3 ε units) in Nd isotopes over the past 10 Ma which are accompanied by substantial changes in ε_{Hf} (2.5 ε units).

Frank M., Whiteley N., Kasten S., Hein J.R. and O'Nions K. (2002), *Paleoceanography*, in press

Baker J.A., Waight T.E., Graham I.J. and Wright I.C. (2001), *Eos Trans. AGU*, **82**(47), Fall Meet. Suppl., Abstract OS31C-0438