FASTREACT – Efficient reactive transport modelling for long-term repository safety assessments

P. TRINCHERO[1]*, J. MOLINERO[1], G. ROMÁN-ROSS[1], STEN BERGLUND[2] AND JAN-OLOF SELROOS[3]

[1] Amphos 21 Consulting S.L., Passeig Garcia Faria, 49-51, E-08019, Barcelona, Spain
[2] HydroResearch AB Stora Marknadsvägen 15S SE-18334 Täby Sweden
[3] Swedish Nuclear Fuel and Waste Management Company, Box 250 101 24 Stockholm, Sweden

Reactive transport modelling is commonly used to provide support for repository engineering activities and safety assessment studies [1]. Yet, the very large temporal and spatial scales involved in these types of studies along with the non-linearity of the underlying processes pose formidable computational challenges that usually force modellers to simplify the problem.

In this work, we present a numerical tool, denoted as FASTREACT, for the efficient solution of large-scale reactive transport simulations. The tool, which relies on the theory of Stochastic-Convective models [2], decomposes complex three-dimensional geometries into a set of independent streamlines. Reactive transport processes are then solved over the whole set of streamlines using one single reference simulation that incorporates explicitly all the relevant geochemical processes. FASTREACT has been developed for safety assessment calculations of radionuclide transport in fractured rock and thus provides efficient handling of the coupling between advection, reactions and matrix diffusion processes for large amounts of input and output data.

The methodology is tested against a synthetic case study where a radionuclide transport problem is solved over a set of heterogeneous conductivity fields. The results compare favourably with those obtained using an Eulerian approach whereas the computational performance of FASTREACT is proved to be much more efficient when compared with the "traditional" Eulerian 3D simulations.

[1]. Selroos, J.-O. (2008) Site-descriptive modeling of geological repository sites in Sweden International Geological Congress, Oslo (Norway). [2]. Cvetkovic V, Dagan G, 1994. Transport of kinetically sorbing solute by steady random velocity in heterogeneous porous formations. J. Fluid Mech., 265, pp 189-215.

High-precision Neodynium isotope analyses by MC-TI-MS

ANNE TRINQUIER[1], CLAUDIA BOUMAN[1] AND JOHANNES SCHWIETERS [1]

[1] Thermo Fisher Scientific, Bremen, Germany, anne.trinquier@thermofisher.com

Resolving Nd isotope anomalies at the ppm level for materials with a wide range of compositions and Nd concentrations is key to unraveling fundamental relations in geochronology, geochemistry, cosmochemistry and environmental sciences. Nd isotope Thermal-Ionization Mass Spectrometry (TIMS) has proven successful in running Nd both as Nd^+ on multiple filament assembly (300-500ng) [1] and NdO^+ on single filament assembly (1-10ng) [2].

The present study on a Thermo Scientific TRITON *Plus* instrument assesses precision and accuracy of Nd analyses adapting the above mentioned protocols on two Nd standards (Merck # 170335 and JNdi [3]) for sample loads ranging from 0.5 µg to the ng range, using 10^{11} Ω amplifiers, automatized mode and shortened analysis time compared to literature. Nd^+ analyses of 500ng and 100ng loads on double Re filament assemblies in static mode with rotation of the amplifier-cup association ("virtual amplifier") yield indistinguishable isotopic ratios. The 1-yr 2RSD reproducibility R_i for $^{i}Nd/^{144}Nd$ ratios expressed in ppm: R_{143} = 5 and $R_{142\text{-}150}$ = 4 to 21 (n=70, 3.6-10V $^{142}Nd^+$, 100 or 500 ng). Notably, analyses with 10V $^{142}Nd^+$ ion beams could be limited to 1hr. NdO^+ analysis of 10ng loads on single Re filament assembly, a different ion-beam setting, in static mode, yields Nd isotopic ratios indistinguishable from those obtained in Nd^+ analyses. This validates the stability of the instrument ion optics, the Faraday cups, and the current amplifier system, as well as accurate oxide interference correction. The 2RSD reproducibility expressed in ppm: R_{143} = 16 (n=13, 1.5V $^{142}Nd^{16}O^+$). Notably, one analysis was limited to 25min.

With acquisition times ≤90min and a reproducibilty on $^{143}Nd/^{144}Nd$ of 5ppm (Nd^+) and 16ppm (NdO^+), this study holds promise for achieving highly reproducible results with ever smaller sample amounts. A TRITON *Plus* Nd^+ study on 100 pg loads using 10^{12} Ω amplifiers reported 2RSD reproducibility of 176 ppm on $^{143}Nd/^{144}Nd$ [4]. Detection limit, precision and accuracy of Nd isotope TIMS analysis are thus expected to be further improved by the combined use of 10^{12} Ω amplifiers and NdO^+ analysis.

[1] Caro et al. (2003) Nature 423, 428-432. [2] Harvey and Baxter (2009) Chem. Geol. 258, 251-257. [3] Tanaka et al. (2000) Chem. Geol. 168, 279-281.[4] Koornneef et al. (2013) J.Anal.At. Spectrom. , in press.

www.minersoc.org
DOI:10.1180/minmag.2013.077.5.20