Effective kinetic laws for cement in contact with a CO_2-rich solution

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The management of the processes triggered by CO_2 injection in deep geological formations is still a challenge owing to the associated risk of CO_2 leakage and its negative impact on the environment and also on human health. CO_2 leakage from the reservoir to other permeable layers due to a deficient sealing in the well cement plugs and annulus is a probable situation that needs a specific evaluation.

As a consequence of the interaction between a CO_2-rich solution and the cement different reaction fronts appear. In this study we aim at determining the effective kinetic laws and diffusion of cement alteration by combining an experimental and a numerical study.

To this end we first performed diffusion experiments of CO_2-rich solutions using Class G Portland cement samples at P = 12 MPa and T = 60 °C. Measurement of aqueous chemistry by ICP-MS enabled the determination of net reaction rates. SEM images of the reacted cement samples were taken to identify the occurring reactions and measure the position and the thickness of the different reaction fronts.

The experimental results are then used in an automatic calibration process whose objective is to infer the optimal set of effective reaction rate coefficients and effective surface area of the solid phases and the parameter linking diffusion to porosity changes. For this purpose we coupled a diffusion-reaction modeling tool, a geochemical library, Cheproo++ [1] and a finite-difference approximation of the multicomponent diffusion problems, to PEST [2]. The statistics provided in the estimation procedure allow to quantify the effect of each parameter on the numerical results, and therefore to identify those with a consistent impact on the processes identified in the experiments.

[1] Gaspari, F. D. (2015). *Doctoral thesis*. [2] Doherty, J. (1994). In *Water Down Under 94*, 551-554.