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Coupling Diagenetic Effects in a Basin Model for Mass Transfer Predictions at the Regional Scale

Background

Most petrographic studies in sedimentary reservoirs show common diagenetic transformations of prevalent rock-forming minerals, such as feldspar dissolution and kaolinite precipitation at low temperature or illitization associated with silicification in sandstones under higher temperature conditions. Lenses of carbonate cementations are reported under very variable conditions. Over geologic relevant time periods, these effects might give rise to significant porosity changes, to more or less irreversible sealings and therefore control the permeability pattern and the migration of fluid and solutes.

The present contribution show how a geochemical module was integrated in a preexisting 3D basin simulator. This code, refered to as NEWBAS (see table), is already able to account for heterogeneous sediment deposition/uplift/erosion sequences and reproduces vertical compaction phenomena, according to a classic elasto-plastic rheology for the sediments. Mass conservation principles for both fluid and solids are used. A single equation is assembled and solved for fluid pressure using a finite volume approach and iterative numerical schemes. Results of the simulator are mainly the evolution of the flow pattern at the global scale, which may exhibit compaction disequilibrium accompanied by the generation of over-pressure regimes. A visco-plastic rheology for the sediments has been considered to analyse over-compaction phenomena. Taking advantage of the knowledge of fluid velocities through the heterogeneous porous sediments, thermal history can be reconstructed. The aim of the present version of the code is to reflect the main geochemical interactions between moving solutes and solids, in an attempt to describe the diagenetic processes that are affecting basins during their life.

Principles of the geochemical sub-model

This recent part of the numerical model is based on the local thermodynamic equilibrium principle. Redox processes are disregarded at this stage. Bulk composition is expressed in terms of components known as basis species (Bethke, 1996). Briefly, the total aqueous concentration of these components are found when solving a system of non-linear algebraic equations (1) which is built by substituing mass action equations (2) into mass conservation equations (3).

$$tot(C_\ell) = \sum_{j=1}^{NES} \alpha_{j,\ell} K_j \prod_{i=1}^{NCB} (C_i)^{\alpha_{j,i}} \quad (1)$$

$$E_j = K_j \prod_{i=1}^{NCB} (C_i)^{\alpha_{j,i}} \qquad (2)$$

$$tot(C_\ell) = \sum_{j=1}^{NES} \alpha_{j,\ell}(E_j) \qquad (3)$$

where NCB is the number of basis components, NES is the total number of considered species, K_j is the thermodynamic coefficient for the formation of the j^{th} species, (C_i) the activity of the i^{th} basis component, (E_j) the activity of the species number j $\alpha_{j,i}$ the stoichiometric coefficient of the j^{th} species in the i^{th} basis component.
The thermodynamic constants K are temperature dependant. These parameters are extracted from the CHEMVAL database.
Ionic strengh corrections are introduced using Davies formalism. Coefficients γ_i relating activities to concentrations are given by $log(\gamma_i) = -Az_i^2(\frac{\sqrt{I}}{1+\sqrt{I}} - bI)$ where the I is the ionic strength of the solution.
For basin modeling purposes, a range of minerals are selected that are numerous enough to capture the spatial variability of the present day lithologies. Aqueous species that are necessary to produce these minerals are then selected. A local set of basis species (*i.e.* building blocks) is then attached to each cell of the 3D mesh, but for transfer modeling, the speciations are also expressed in a common set, with minimum size, of basis elements refered to as the global basis. All the basis have the same dimension. At each time step, the algorithm seeks for a stable mineral assemblage, namely look at undersaturated minerals or at new supersaturated minerals. Therefore minerals are allowed to precipitate or disolve as the basin geometry evolves.

The transport equation and the coupling strategy

Among the variety of solutions available in the reactive transport literature, we adapt a two-step method, with a sequential iterative approach (SIA), starting at each time step with an explicit source term in the transport equations, derived from the solution of the thermodynamic problem in each cell. The set of partial differential equations (PDEs) is solved for the total concentration of each non conservative component.
This reaction source terms R_k expresses the mass transfer in each cell for a given basis component in between the solution and the minerals, which is required to insure the thermodynamic equilibrium within the time step.
Denoting by L the diffusive-convective transfer operator, we successively solve for each component C_ℓ, the transport equation

$$\frac{(C_\ell^{*n+1} - C_\ell^n)}{\delta t} = L(C_\ell^n) + R_k^n \qquad (4)$$

starting from C_ℓ^n and from the source terms R^n known at time step n. An intermediate concentration C^{*n+1} is derived at time step $n+1$ which is used as a starting value for looking at the thermodynamic equilibrium at the time step $n+1$. In the present stage of development, the iterative algorithm has not been fully implemented.

The back effect on the model

The redistribution of minerals has an influence on the porosity distribution, but we may expect much more important impacts on permeability. The classic K formulation is therefore modified to account for the fractional contributiof mineral classes (*i.e.* typicaly sand, silt, clay, carbonate) in the estimation o f the porosity. As in Revil and Cathles (1999), Gouze et al. (2001), we suggest an interaction in between the gradually evolving sediment composition and the exponent of in the KC law. However more research is needed in this area.

Application and discussion

The new capabilities of this integrated quantitative diagenesis simulator are here below illustrated using simplified 1D vertical sections extracted from the central part of the intracratonic Paris basin (France). In this situation, transformation are controlled by the temperature, because an hydrostatic regime is very rapidly established.
As an academic sample, jurassic clays are initialy defined as a mixture o f microcline and gibbsite. Ca-Montmorillonite precipitates very rapidly and is replaced later on by Kaolinite. As soon as temperature is about 25C, after 20My of burial, Muscovite is over saturated. The final composition is described at the final depth of 2500m as an assemblage of muscovite-gibbsite-kaolinite, with a PH of about 6 at a temperatutre of 95C. The figure 1 shows the total aqueous Si content in triasic sandstone layers, and also in thin jurassic strata. Quartz tends to dissolve as temperature increases.
Results will serve as a basis for a comparison with open systems. The next step of the study will be made on a cross section through a small structural gas trap where ground water flow is lately controlled by the topography. Partly sealed aquifers above this trap may indicate fluid circulations through the faults segments that delineate the trap. This may give indications on the timing for fluid motion around this system.

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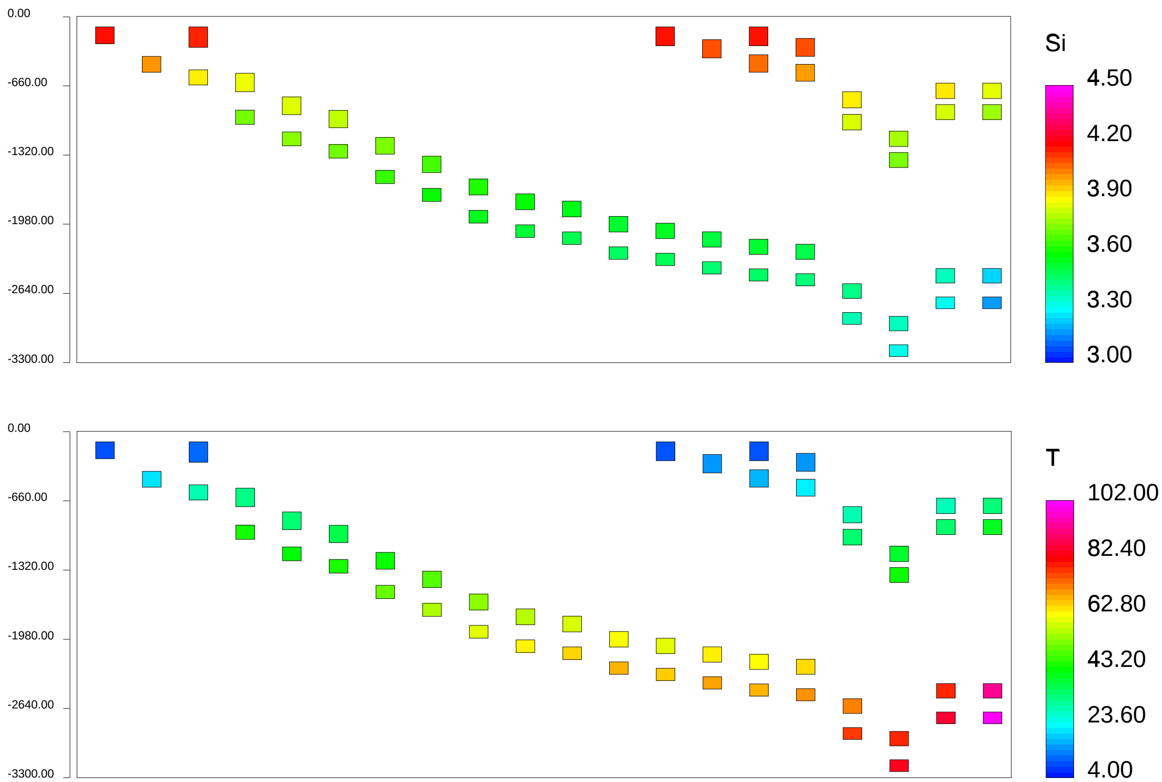

Figure 1: Evolution in time (MY, left to right, one column per new deposited strata, starting 215 MY ago) and space (vertical scale) of temperature (bottom) and aqueous total Si (top) for sandstone cells solely in a vertical sedimentary column. The quantity -log10[total] is reported by colours. The top of the column follows the paleobathymetry.

ANNEX : Main characteristics of the hydraulic module

code	NEWBAS
principle	3D Finite Volumes
geometry	Evolutive, infered from backstripping
meshing	multi-layered - nested square cells
hydraulics	○ Mass conservation principle for fluids - single phase ○ Darcy's law ○ Kozeny-Carman relationship $K(\varphi) = \frac{0.2\varphi^3}{S_0^2(1-\varphi)^2}$ ○ $\bar{\bar{K}} = K(\varphi)\begin{bmatrix}\lambda_x & 0 \\ 0 & \lambda_y\end{bmatrix}$ ○ $\mu(\theta), \rho(\theta)$ ○ Main unknown fluid pressure ψ
mecanics	○ Vertical deformation ○ Mass conservation for solids during burial ○ Effective stress principle $\sigma = S - \psi$ ○ Plastic deformation, $\varphi(\sigma) = \varphi_0 + \varphi_1 e^{-\sigma/\sigma_1} + \varphi_2 e^{-\sigma/\sigma_2}$ ○ Visco-plasticity, $\frac{\partial \varphi}{\partial t} = a(\sigma)\frac{\partial \sigma}{\partial t} + b(\sigma)$ ○ Elasticity for over-consolidated materials $\frac{\partial \varphi}{\partial \sigma} = 1/E_e$
boundaries	○ Paleobathymetry - eustatic level - topography ○ Hydrostatic head profiles or no flow at vertical lateral boundaries, ○ Lower limit - free for mechanics, impervious for flow
Heat transfers	○ Conduction $\gamma = \gamma_w^{\varphi}\gamma_s^{(1-\varphi)}$ ○ Convection ○ Volumic source term q_r - radiogenic ○ Heat flux $\Phi(x, t)$ at the basement

Table 1: φ porosity, $K(\varphi)$ intrinsec permeability, S_0: specific surface for a given lithology, λ_{xx}, λ_{yy}: anisotropy factor for K in strata and orthogonal to strata, ρ fluid density, μ fluid dynamic viscosity, θ temperature, γ thermal conductivity for the porous rock, $S = \int \rho(z) g\, dz$ total vertical stress, σ effective stress, ψ pore pressure.