Reactive Transport Modeling in Porous Media with an Innovative Dual Mesh Method

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Introduction

Acidic fluid injection in rock formations may generate geochemical reactions that can modify the mineral assemblage of the rock and disturb thermodynamic equilibria. Numerical difficulties of reactive transport simulation are that geochemical reactions are at the pore scale, may appear in short time period and are very sensitive to the mesh size and/or time step. The classical approach for reservoir engineers consist in upscaling the high resolution petrophysical values to assign to a low-resolution model. For reactive transport modelling, the upscaling step will impact not only the mass fraction of each species but also the mineral dissolution and/or precipitation processes that highly depend on mass fractions.

This paper recalls the Compositional Dual Mesh Method, an original algorithm for a compositional flow modeling in porous media with rock-fluid interactions using two different space and time discretization: one mesh, as usual for the pressure equation and a much finer one for the chemical reactions. The interest of this scheme is that the calculation of the flow on the high-resolution grid is done solving a local problem on each coarse cell. Two examples will illustrate this algorithm: one for an injection of CO2 in a carbonate reservoir and the second one will address reactions during the injection of an acidic water for improving well injectivity again in a carbonate reservoir.

Compositional single-phase flow model with chemical reactions

From the equation derived by Marle [1], the partial differential equation that we are considering and which has been implemented in an innovative software are given below. It allows considering n species and consider gravity. Chemical reactions are considered with both equilibrium reactions, precipitation and dissolution reactions:

$$\begin{cases} \partial_t(\varphi\rho\, c_\alpha) + div\left(\rho\, c_\alpha v - \varphi\rho\bar{\bar{D}}_\alpha \nabla c_\alpha\right) + M_\alpha \sum_{r\in R} \nu_{\alpha r}\Psi_r = q_\alpha,\ \alpha = 1,n \\ v = -\dfrac{\bar{\bar{k}}}{\mu}(\nabla p + \rho g \nabla z) \\ \sum_\alpha c_\alpha = 1 \\ \prod_{\alpha=1}^{n_{aq}} (\gamma_\alpha b_\alpha)^{\nu_{\alpha r}} - K_{eq,r} = 0\,, \quad r = 1..n_{re} \\ \Psi_r = A_r^0 \dfrac{N_r}{N_r^0} k_r \left(1 - \dfrac{\prod_{\alpha=1}^{n_{aq}} (\gamma_\alpha b_\alpha)^{\nu_{\alpha r}}}{K_{eq,r}}\right) 0\,, \quad r = 1..n_{rm} \end{cases} \tag{1}$$

where φ is the porosity, ρ is the density, c_α is the mass fraction of the specie α, $\bar{\bar{D}}_\alpha$ is the diffusion tensor of the specie α, q_α is the source term of the specie α, n is the number of species, v is the Darcy flow, $\bar{\bar{k}}$ is the absolute permeability tensor, μ is the phase viscosity, p is the pressure, g is the acceleration due to gravity, M_α is the molar mass of the specie α, γ_α is the activity coefficient, b_α is the molality of α (mole per kg of H_2O), $\nu_{\alpha r}$ are the stoichiometric coefficients of the reaction r, $K_{eq,r}$ is the chemical equilibrium constant for the reaction r, Ψ_r is the rate of chemical reaction r, k_r is the reaction rate constant ($mol.m^{-2}.s$), A_r^0 is the reactive surface area at initial time, N_r is the mole number of the mineral r per unit block grid volume. Note that, $c_\alpha = b_\alpha M_\alpha$ and $b_\alpha = n_\alpha / m_{H2O}$, where n_α is the amount of specie α (in moles) and m_{H2O} is the mass of H_2O (in kg).

Compositional dual mesh formulation

The Compositional Dual Mesh Method (CDMM) [2,3,4] is based on an approach that consider two meshes interacting with each other. A specific spatial and temporal discretization for each unknown (Pressure and mass fractions for each

species) allow to perform an adaptive homogenization. The HRM can be view as a set of local systems. Each local system is defined by the fine cells composing a coarse cell. The LRM is used to solved the pressure equation while the HRM is used to solved the transport equation and chemical equilibrium. The following steps are performed at each iteration on the LRM.

- Step 1- Properties upscaling. This modelling with two meshes implies an upscaling step of the pressure equation parameters (porosity, permeability and transmissibility) from the HRM to the LRM.
- Step 2 - Resolution of pressures on LRM. The resolution of the matrix system coming from the implicit finite volume discretization of the pressure equation give the pressure field. The LR velocity field is computed from the pressures field.
- Step 3 - Resolution of the Velocity Field on HRM. For each local system, the coarse fluxes deduced at the step 3 are used as boundary conditions. The coarse flux is weighted by the fine scale transmissibility in order to maintain the HR scale heterogeneities. For each local system, a steady state flow problem is considered that leads to solve a matrix system with Dirichlet and Neumann boundary conditions. The HR velocity field is computed from the pressures field.
- Step 4 - Resolution of mass fractions of the species on the HRM. An explicit scheme is used to solve the transport equations on the HRM.
- Step 5 - Flash and reaction solver on the HRM. Geochemical equilibrium and the mineral precipitation and dissolution kinetics are solved block-by-block to update the mass fractions.

Applications

The application on a CO2 injection in a carbonate reservoir [2] shows that the results are close to the results obtain with the HR scale simulation, more accurate than simulations performed on LRM and faster than simulations done on HRM. The CO2 plume induced by the injection is similar between HR scale simulation and CDMM.

The application on acidic water injection in a carbonate reservoir [4] show a gradual decrease in the amount of calcite under the effect of the acid. On the HRM, all the calcite contained in the meshes directly connected to the well is consumed in less than 500 seconds. This decrease in calcite results in an increase in the porosity and permeability of these meshes.

Conclusions

The simulation of reactive transport requires fine meshes with the most detailed geological description representing complex heterogeneities at very fine scales in order to accurately represent the phenomena generated by geochemical reactions such as changes in porosity, pH, etc. The competitive advantage of the CDMM approach is that the global computation time is reduced while maintaining the chemical equilibrium and transport of species on the HRM. The methodology is easily parallelized by distributing each local problem data amongst computing nodes.

The applications on different synthetic case studies demonstrate the practicability of this approach to perform accurate reactive transport simulations on cases that cannot be treated by conventional approaches which do not allow to maintain all the detailed information needed to capture the fluid rock interactions.

References

[1] Marle, C.M. [1982]. On macroscopic equations governing multiphase flow with diffusion and chemical reactions in porous media. International Journal of Engineering Science, 20(5), 643-662.

[2] Guérillot, D. and Bruyelle, J. 2017. Compositional dual mesh method for single phase flow in heterogeneous porous media - Application to CO2 storage. J. Comput Geosci. https://doi.org/10.1007/s10596-017-9645-0

[3] Bruyelle, J., Audigane, P., & Guérillot, D. (2017, June 12). Accurate Reactive Transport Modeling in Heterogeneous Reservoirs with the Dual Mesh Method. Society of Petroleum Engineers. doi:10.2118/185842-MS

[4] Guérillot, D. and Bruyelle, J. [2017]. Coupling Fluid Flow around Wells with Rock-Fluid Interactions Equations for Simulating Acid Stimulations with a Dual Mesh Approach. In Second EAGE Workshop on Well Injectivity and Productivity in Carbonates.