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## Reactive Transport Modeling For CO<sub>2</sub> Sequestration With A Dual Mesh Method

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### Summary

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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 consists 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 modelling 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 of CO<sub>2</sub> injection in carbonate reservoirs illustrate this algorithm.

## Introduction

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This paper recalls the Compositional Dual Mesh Method, an original algorithm for a compositional flow modelling 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 of CO<sub>2</sub> injection in carbonate reservoirs illustrate this algorithm. The results were obtained in the project H-CUBE (Audigane *et al.*, 2014).

## Compositional Single-phase Flow Model with Chemical Reactions

Applying the multi-phase model of Marle (1982) to a single-phase flow with  $n$  components, the transport of components with chemical reactions is given by the convection-diffusion equation including the contribution of the chemical reactions becomes:

where  $\varphi$  is the porosity,  $\rho$  is the density,  $c_\alpha$  is the mass fraction of the specie  $\alpha$ ,  $\overline{\overline{D}}_\alpha$  is the diffusion tensor of the specie  $\alpha$ ,  $q_\alpha$  is the source term of the specie  $\alpha$ ,  $v$  is the Darcy flow,  $\overline{\overline{k}}$  is the absolute permeability tensor,  $\mu$  is the phase viscosity,  $p$  is the pressure,  $g$  is the acceleration due to gravity,  $M_\alpha$  is the molar mass of the specie  $\alpha$ ,  $\nu_{\alpha r}$  are the stoichiometric coefficients of the reaction  $r$  and  $\xi_r$  is the rate of chemical reaction  $r$ .

## Equilibrium and Kinetic Chemical Equations

The reaction system to solve, including both equilibrium and kinetics equations for a given timestep is:

$$\left\{ \prod \left( \gamma_\alpha \left( b_\alpha \right. \right. \right.$$

where  $\xi_\beta$  is the reaction rate of the reaction  $\beta$ ,  $n_r$  is the total number of reaction (both equilibrium and kinetics reactions). Note that  $\gamma_\alpha$  depends on the ionic strength of the solution which depends on the charge and concentration of the species.

### Compositional dual mesh formulation

The Compositional Dual Mesh Method (CDMM) (Guérillot and Bruyelle, 2017) 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 first application is done on a two-dimensional synthetic case (Guérillot and Bruyelle, 2017). The grid mesh geometry corresponds to the “SPE-10 2nd comparative solution” project (Christie and Blunt 2001). The HRM is composed of 13200 cells. The upscaled model (LRM) is generated by grouping three cells in each direction to obtain a model composed of 528 cells. Figure 1 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 CO<sub>2</sub> plume induced by the injection is similar between HR scale simulation and CDMM.

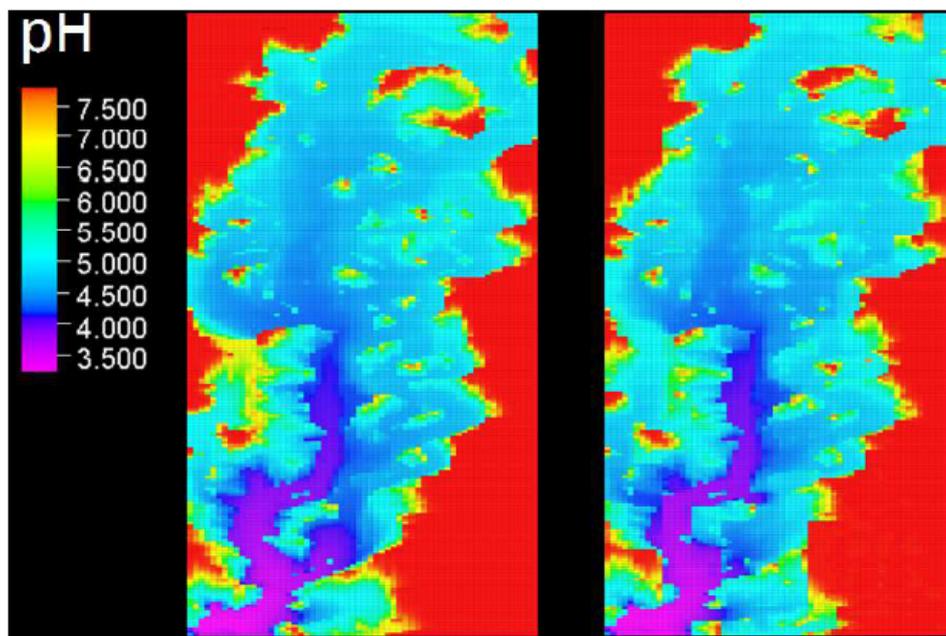
The second application is done on a fluvial sedimentary heterogeneous model (Bruyelle *et al.* 2017). The geometry of the heterogeneous geological model is similar based on to the Minjur Sandstone (Saudi Arabia) and was built by Issautier *et al.* (2013; 2014) to evaluate the role of compartmentalization of heterogeneous reservoir on CO<sub>2</sub> storage capacity estimate. This model represents a fluvial deposit with a complex realistic architecture and a high resolution of the heterogeneities. The HRM is composed of 217080 cells. The upscaled model (LRM) is generated by grouping three cells in each direction to obtain a model composed of 8040 cells. Figures 2 and 3 show respectively the evolution of the pH and the total concentration of dissolved inorganic carbon ( $C_T$ ) at the producer well of the homogeneous case. The results provided by the CDMM match with the results of the HR scale simulation.

### Conclusions

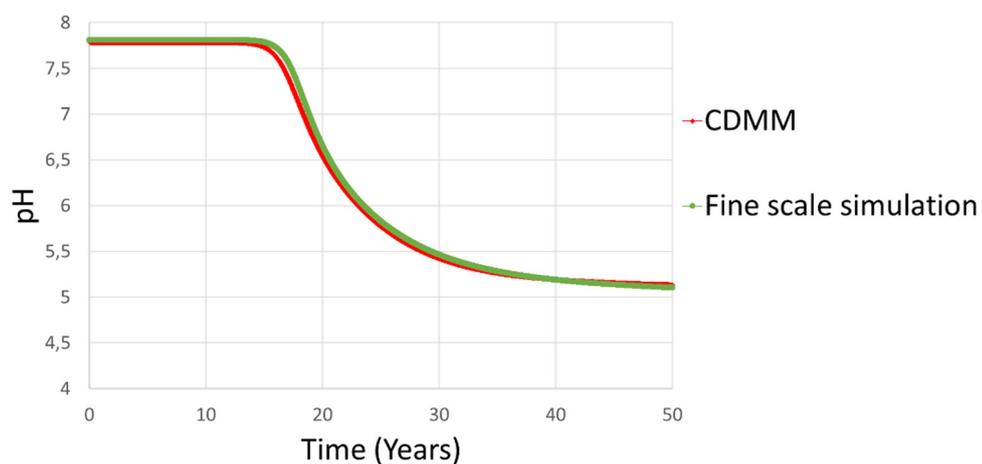
The simulation of reactive transport requires fine meshes with the most detailed geological description representing complex heterogeneities at very fine scales in order to accurately represent the phenomena generated by geochemical reactions such as changes in porosity, pH, etc. The competitive advantage 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.

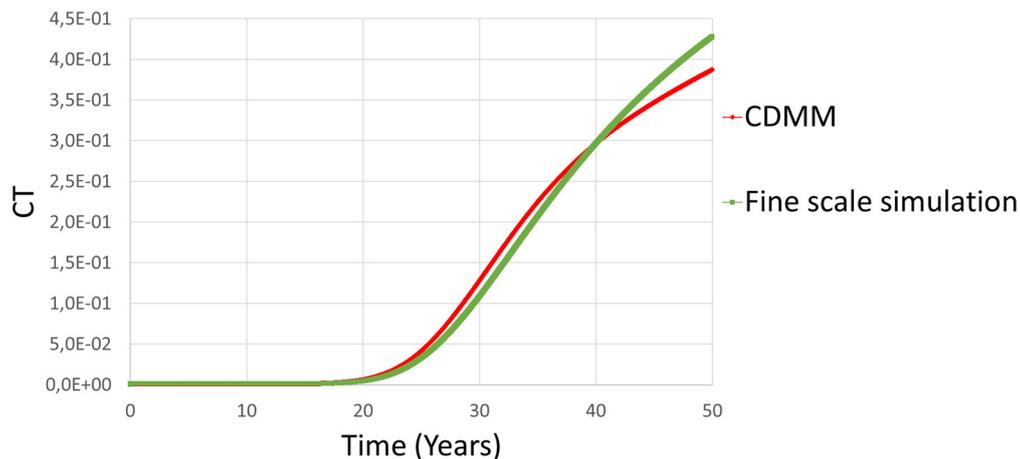
The applications on different synthetic case studies demonstrate the practicability of this approach to perform accurate reactive transport simulations on cases that cannot be treated by conventional approaches which do not allow to maintain all the detailed information needed to capture the fluid rock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



**Figure 1** Spatial development of pH induced by 5 years of injection. Left: fine scale simulation. Right: Compositional Dual Mesh Method (Guérillot and Bruyelle, 2017).



**Figure 2** Comparison of pH evolution for production well (Bruyelle et al. 2017).



**Figure 3** Comparison of CT breakthrough curves for production well (Bruyelle et al. 2017).

### Acknowledgements

This work is part of the project Hydrodynamics, Heterogeneity, and Homogenization in CO<sub>2</sub> Storage (H-CUBE). This project is partially sponsored by the French National Research Agency <http://www.agence-nationale-recherche.fr/en> (Under the reference ANR-12-SEED-0006) and by Terra 3E SAS <http://www.terra3E.com>. The authors acknowledge these financial supports.

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