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Summary Extraction of salt by leaching process is used intensively nowadays. In this analysis about cavity dissolution modeling, we consider the case of a binary system characterized by a chemical solute corresponding to the solid that is dissolved by a "solvent". Salt dissolution is controlled by thermodynamic equilibrium at the interface, i.e., equality of the chemical potentials. In this paper, a local non-equilibrium Diffuse Interface Model and an explicit treatment of the brine-salt interface are introduced in order to solve such dissolution problems. Equations are obtained by upscaling micro-scale equations for a solid-liquid dissolution problem using a volume averaging theory. Based on this mathematical formulation, dissolution test cases are presented. We introduce and discuss the main features of the method. Illustrations of the interaction between natural convection and forced convection in dissolution problems are presented and the time and space evolution of the rock salt-fluid interface is shown through several examples.

INTRODUCTION

Dissolution of porous media or solids is widely concerned in many industrial fields, e.g., acid injection into petroleum reservoirs, dissolution of rocks caused by underground water, etc. In the latter, rock dissolution creates underground cavities of different shapes and sizes, which induce a potential risk of collapse as shown in Fig.1. In most applications, modeling such liquid/solid dissolution problems is of paramount importance.
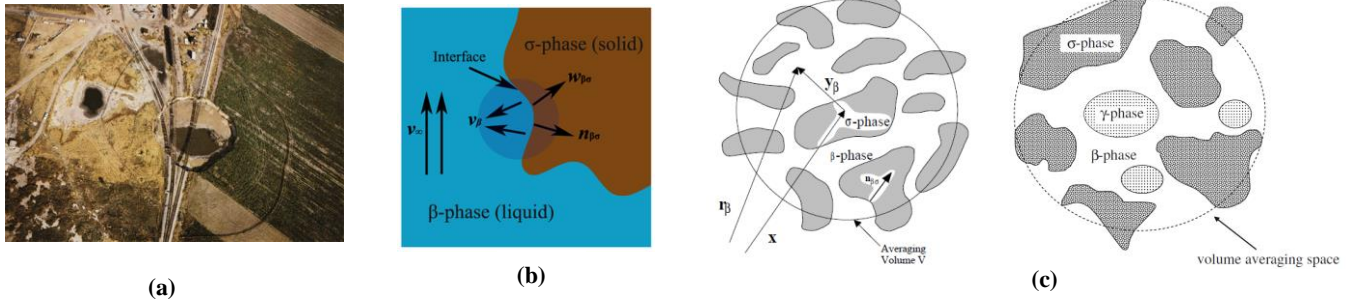

Fig. 1: Land Subsidence in Central Kansas Related to Salt dissolution (a), explanation of the variables at the local level to the interface (b) and averaging volume at pore scale level with material point position vector and 3-phases model (the third phase may be insoluble species for instance) (c).[1]

Among all methods used for modeling dissolution process, we present two generic ways for simulating such problems. The first one is a direct treatment of the evolution of the fluid-solid interface, for instance using an ALE (Arbitrary Lagrangian-Eulerian) method. The second uses a Diffuse Interface Model (DIM) to smooth the interface with continuous quantities [1, 3, 6], like the liquid phase volume fraction, species mass fractions, etc.

MATHEMATICAL MODEL

According to [1], the Darcy-scale diffuse interface model for Solid/Liquid dissolution problems in a binary system includes the 3 following balance equations: the mass balance for the β-phase, the mass balance for the σ-phase, the mass balance for species A.

$$\varepsilon_\beta \rho_\beta^* \frac{\partial \Omega_{A\beta}}{\partial t} + \rho_\beta^* \boldsymbol{V}_\beta \cdot \nabla \Omega_{A\beta} = \nabla \cdot \left(\varepsilon_\beta \rho_\beta^* \boldsymbol{D}_{A\beta}^* . \nabla \Omega_{A\beta} \right) + \rho_\beta^* \alpha \left(1 - \Omega_{A\beta} \right) \left(\omega_{eq} - \Omega_{A\beta} \right)$$

$$\frac{\partial \varepsilon_\beta \rho_\beta^*}{\partial t} + \nabla \cdot \left(\rho_\beta^* \boldsymbol{V}_\beta \right) = \rho_\beta^* \alpha \left(\omega_{eq} - \Omega_{A\beta} \right)$$

$$-\rho_\sigma \frac{\partial \varepsilon_\sigma}{\partial t} = \rho_\sigma \frac{\partial \varepsilon_\beta}{\partial t} = \rho_\beta^* \alpha \left(\omega_{eq} - \Omega_{A\beta} \right)$$

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where ε_β is the volume fraction of β-phase, $\Omega_{A\beta}$ is the mass fraction of species A in the β-phase, ω_{eq} is the equilibrium mass fraction at the σ–β interface, α is the mass exchange term, ρ_β^* and ρ_σ are respectively the β-phase and σ-phase densities, and $\boldsymbol{D}_{A\beta}^*$ is the effective diffusion tensor for species A. $\boldsymbol{D}_{A\beta}^*$ is the macroscopic diffusion/dispersion coefficient, ρ_β^*: such that $\langle \rho_\beta \omega_{A\beta} \rangle = \varepsilon_\beta \rho_\beta^* \Omega_{A\beta}$ and α is the mass exchange coefficient between the two phases. The macroscopic diffusion/dispersion coefficient and the mass exchange coefficient are obtained by solving "closure problems" over representative unit cells of the pore-scale geometry, characterized by two boundary value problems for two "mapping variables" (closure variables In the DIM model, there is no "pure liquid phase" since ε_β is used continuously to represent the fluid as well as the solid regions. Therefore, the Navier-Stokes equations are no longer suitable for this situation. Instead, we can adopt a Darcy-Brinkman model to take the place of Navier-Stokes equations for the momentum equations,

$$\frac{\mu_\beta\left(\Omega_{A\beta}\right)}{\varepsilon_\beta}\Delta V_\beta - \left(\nabla P_\beta - \rho_\beta^* \boldsymbol{g}\right) - \mu_\beta\left(\Omega_{A\beta}\right)\boldsymbol{K}^{-1}\cdot V_\beta = 0$$

where $\boldsymbol{K}$ is a permeability function of ε_β. The Darcy-Brinkman equation will approach Stokes equation when $\boldsymbol{K}$ is very large and will simplifies to Darcy's law when $\boldsymbol{K}$ is very small. If inertia terms are not negligible, a similar penalization of Navier-Stokes equations may be used by adding Darcy-Forchheimer contributions.

NUMERICAL MODELLING

Whenever density variation is present in the fluid phases, gravity (buoyancy force) plays an important role in mass and heat transports, through natural convection mechanisms. This natural convection phenomenon, often called salt fingering, is well illustrated by our model Figures 2 [2].
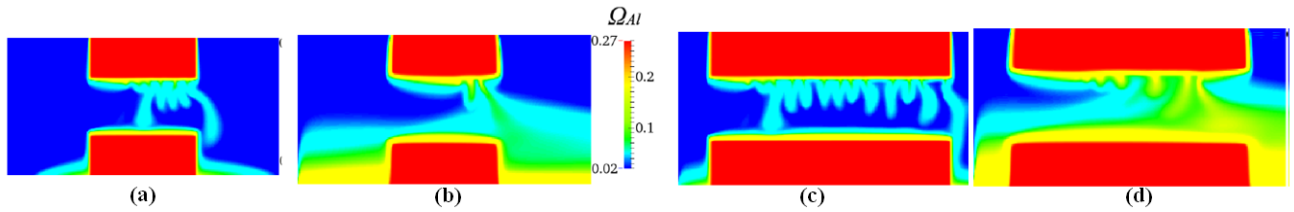

Fig 2: Examples of concentration plumes for a 2D simulation with gravity at time 100 s (a) and 1000 s (b) and salt block size 8 mm, and for a salt (c) and (d) block size 16 mm (from [2]).

The second illustration deals with the modeling of an experimental leaching test performed in a salt layer (Fig. 3). The numerical model was extended to gypsum material and one can observe the significant difference in terms of rate of dissolution (at the beginning of the test there was no cavity).
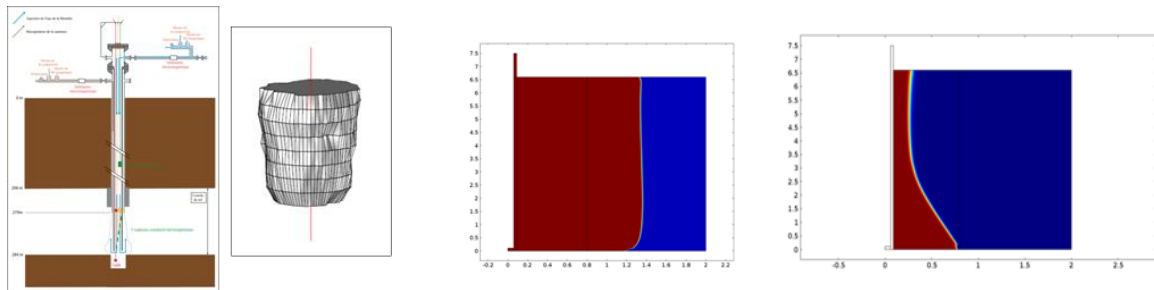

Fig 3: From left to right: experimental dissolution-leaching test (and final cavity shape) in a salt layer, cavity after in salt after 12 day and then cavity shape in case of gypsum material after 3years. (The cavity is in red and the solid material in blue).

References
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