Open Archive TOULOUSE Archive Ouverte (OATAO)

OATAO is an open access repository that collects the work of Toulouse researchers and makes it freely available over the web where possible.

This is an author-deposited version published in: http://oatao.univ-toulouse.fr/
Eprints ID : 12104

To cite this version : Guo, Jianwei and Quintard, Michel and Laouafa, Farid *Upscaling and large-scale modeling of the dissolution of gypsum cavities.* In: 12èmes Journées d'Études des Milieux Poreux 2014, 9 October 2014 - 10 October 2014 (Toulouse, France).

Any correspondance concerning this service should be sent to the repository administrator: staff-oatao@listes-diff.inp-toulouse.fr

Upscaling and large-scale modeling of the dissolution of gypsum cavities

Jianwei Guo*[1], Michel Quintard[1, 2] & Farid Laouafa[3]

[1] Université de Toulouse; INPT, UPS; IMFT (Institut de Mécanique des Fluides de Toulouse), 31400 Toulouse, France

[2] CNRS; IMFT; 31400 Toulouse, France

[3] Institut National de l'Environnement Industriel et des Risques, 60550 Verneuil-en-Halatte, France

*jguo@imft.fr

1.   INTRODUCTION

The dissolution of geological formations containing gypsum can rapidly create various karstic features, and may potentially generate great risks such as subsidence and collapse [1]. To understand the gypsum dissolution mechanism is very important to develop safety measures. It is not feasible to take into account all the pore-scale details at a large-scale by direct numerical modeling, and some sort of macro-scale models are essential. Such a macro-scale porous medium model can also serve as a diffuse interface model to describe the dissolution at a fluid/solid interface, as done in [2].

The objective of this study is to develop a macro-scale model, starting from the pore-scale transport problem with boundary condition corresponding to non-linear reaction or thermodynamic equilibrium, making use of the method of volume averaging [3], and then implement it for a large-scale cavity dissolution modeling.

2.   UPSCALING

The porous medium under consideration consists of three phases at the pore-scale: two solid phases, one being soluble (gypsum), the other insoluble, and a liquid phase (water + dissolved species). To implement upscaling for the pore-scale mass transport problem, we follow the traditional decomposition of the mass fraction ω_l, into an intrinsic average, Ω_l, and a deviation term $\tilde{\omega}_l$. Approximate solutions in terms of closure variables are then proposed for the deviation. Closure problems for the closure variables are subsequently obtained and used to calculate the effective properties involved in the macro-scale model. The originality here lies into the treatment of the non-linear reaction and couplings.

The generalized macro-scale expression for the mass balance of Ca^{2+} can be written as

$$\frac{\partial \varepsilon_l \rho_l \Omega_l}{\partial t} + \nabla \cdot \left(\varepsilon_l \rho_l \Omega_l \mathbf{U}_l + \varepsilon_l \rho_l \left(\Omega_l - \omega_{eq} \right) \mathbf{U}_l^* \right) = \nabla \cdot \left(\varepsilon_l \rho_l \mathbf{D}_l^* \cdot \nabla \Omega_l \right) - \dot{m}_l \tag{1}$$

with the mass exchange term for Ca^{2+}, $\dot{m}_l$, given under different forms depending on the pore-scale boundary condition at the liquid/solid interface. We have

$$\dot{m}_l = -a_{vl} M_{Ca} \left(1 - \frac{\Omega_l}{\omega_{eq}}\right)^n k_{s,eff} + a_{vl} M_{Ca} \left(1 - \frac{\Omega_l}{\omega_{eq}}\right)^{n-1} \mathbf{h}_l^*.\nabla\Omega_l \qquad (2)$$

for a non-linear reactive boundary condition at the pore-scale, or, more classically

$$\dot{m}_l = \omega_{eq}\dot{m} + \rho_l\alpha_l\left(\Omega_l - \omega_{eq}\right) + \rho_l\mathbf{h}_l.\nabla\Omega_l \qquad (3)$$

for a thermodynamic equilibrium boundary condition at the pore-scale, where, $\dot{m}$ is the mass exchange term of gypsum, $\mathbf{U}_l$ the intrinsic average velocity, $\mathbf{U}_l^*$, $\mathbf{D}_l^*$, $k_{s,eff}$, α_l, $\mathbf{h}_l^*$ and $\mathbf{h}_l$ are effective parameters which can be obtained by solving the related closure problems.

For the macro-scale momentum balance, we can have, for instance, Darcy's law, or penalized versions of Navier-Stokes equations, i.e., Darcy-Brinkman or Darcy-Navier-Stokes equations.

3.   LARGE-SCALE MODELING

A numerical implementation of the above obtained macro-scale model in COMSOL® is used to solve for large-scale cavity dissolution examples, typical of situations leading to sink-hole formations with a thermodynamic equilibrium boundary condition at the pore-scale. Given the uncertainties about the rock formation, a simplified form of Eq.(3) is used to estimate the mass exchange of Ca^{2+}:

$$\dot{m}_l = \rho_l\alpha_l\left(\Omega_l - \omega_{eq}\right) \qquad (4)$$

A work-flow is proposed to choose properly the parameters in the model that would reproduce as accurately as possible the concentration field and fluxes and, consequently, the interface recession. Additional tests are performed to check which type of momentum balance equation should be used. The results show that a proper choice for the mass exchange coefficient α_l leads to satisfactory results with the macro-scale model, and that Darcy-Darcy and Darcy-Navier-Stokes formulation give almost the same cavity formation for the studied cases.

4.   REFERENCES

1. A.H. Cooper, "*Subsidence hazards caused by the dissolution of Permian gypsum in England: geology, investigation and remediation*", in: Geohazards in Engineering Geology, (eds J.G. Maund and M. Eddleston). Geological Society of London, Special Publications in Engineering Geology, 15, pp. 265-275 (1998)

2. H. Luo, F. Laouafa, J. Guo and M. Quintard, *Numerical modeling of three-phase dissolution of underground cavities using a diffuse interface model*. International Journal for Numerical and Analytical Methods in Geomechanics. DOI:10.1002/nag.2274 (2014)

3. S. Whitaker, *The Method of Volume Averaging, Theory and Applications of Transport in Porous Media*, Vol.13. Kluwer Academic Publishers (1999)