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A diffuse interface model for solid-liquid-air dissolution problems based on a porous medium theory

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► To cite this version:

Haishan Luo, Michel Quintard, Gérald Debenest, Farid Laouafa. A diffuse interface model for solid-liquid-air dissolution problems based on a porous medium theory. AGU Fall Meeting 2011, Dec 2011, San Francisco, United States. pp.0, 2012. hal-04023900

HAL Id: hal-04023900

<https://hal.science/hal-04023900>

Submitted on 10 Mar 2023

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Introduction

The underground rock may be dissolved by the flows of groundwater where the dissolution mainly happens at the liquid-solid interface. In many practical cases, the underground cavities are not occupied only by the water, but also the gas phase, e.g., air, CO₂. In this case, there are solid-liquid-gas three phases. Normally, the air does not participate the dissolution. However, it may influence the dissolution as the position of the solid-liquid interface may gradually change with the dissolution process. Simulating the dissolution problems with multi-moving interfaces is a difficult but rather interesting task. In this paper, we propose a diffuse interface model (DIM) to simulate the three-phase dissolution problem, based on a porous medium theory and a volume averaging theory. The interfaces are regarded as continuous layers where the phase indicator (mainly for the solid-liquid interface) and the phase saturation (mainly for the liquid-gas interface) vary rapidly but smoothly.

Diffuse Interface Model

Solid mass balance: $\frac{\partial \rho_s (1 - \varepsilon_f)}{\partial t} = -K_{sl}$

Liquid mass balance: $\frac{\partial \rho_l \varepsilon_f S_l}{\partial t} + \nabla \cdot (\rho_l \mathbf{V}_l) = K_{sl}$

Gas mass balance: $\frac{\partial \rho_g \varepsilon_f (1 - S_l)}{\partial t} + \nabla \cdot (\rho_g \mathbf{V}_g) = 0$

Species mass balance: $\rho_l \varepsilon_f S_l \frac{\partial \Omega_{Al}}{\partial t} + \rho_l \mathbf{V}_l \cdot \nabla \Omega_{Al}$

$= \nabla \cdot (\rho_l \mathbf{D}_{Al}^* \nabla \Omega_{Al}) + (1 - \Omega_{Al}) K_{sl}$

$\mathbf{V}_l = -\frac{\mathbf{K} \mathbf{k}_{rl}}{\mu_l} (\nabla P_l - \rho_l \mathbf{g})$

Darcy's Law :

$\mathbf{V}_g = -\frac{\mathbf{K} \mathbf{k}_{rg}}{\mu_g} (\nabla P_g - \rho_g \mathbf{g})$

Mass exchange between liquid and solid :

$K_{sl} = \rho_l \alpha (\Omega_{eq} - \Omega_{Al})$

$\alpha = f(D_{Al}, \varepsilon_f, S_l)$

Effective Diffusion coefficient :

$\mathbf{D}_{Al}^* = \mathbf{f}(D_{Al}, \varepsilon_f, S_l)$

Effective permeability :

$\mathbf{K} = K_\varepsilon \varepsilon_f^2 \mathbf{I}$

Relative permeability :

$k_{rl} = f(S_l)$

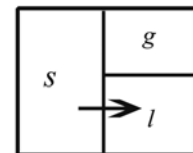
$k_{rg} = f(S_g)$

Capillary pressure :

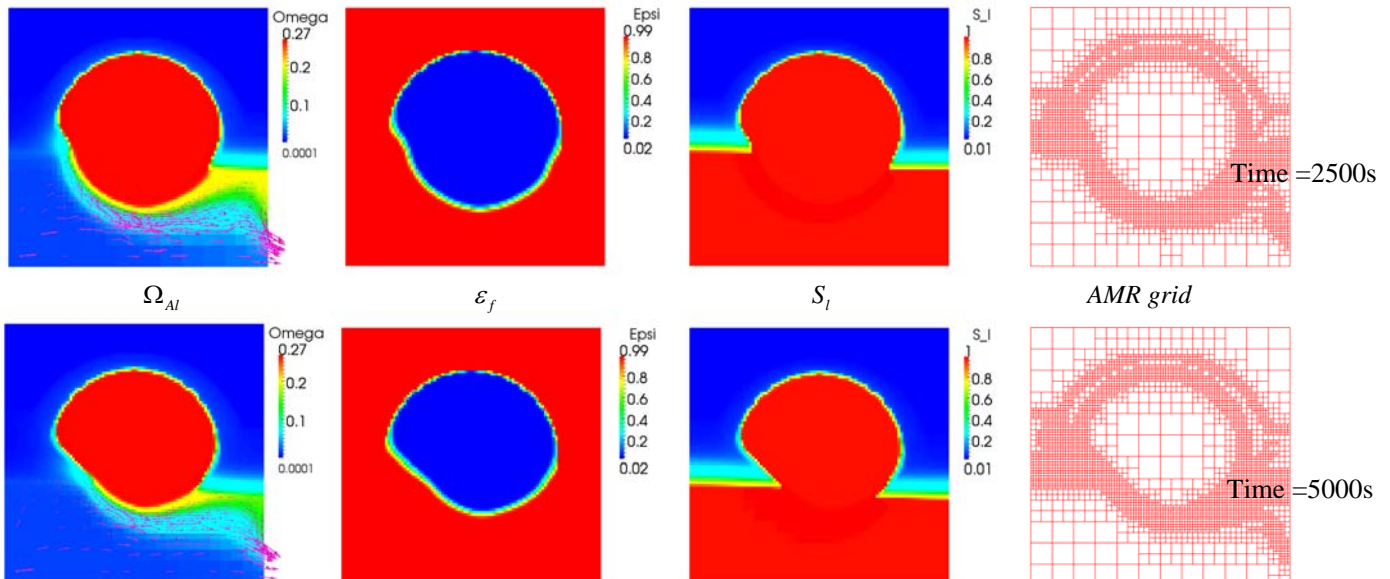
$P_c = P_g - P_l = f(S_l)$

Unit cell for the closure problem:

(s : solid; l : liquid; g : gas; f : fluid(liquid + gas))



Simulation Results with Adaptive Mesh Refinement



Conclusions

A diffuse interface model (DIM) is proposed to simulate the solid-liquid-gas three phase dissolution problems. The solid-liquid interface is diffused by the local non-equilibrium porous medium model, while the liquid-gas interface is diffused by the artificial capillary effects. The simulation results show that this method is able to follow the moving of both the solid-liquid and liquid-gas interfaces. The solid-air interface will not move due to the absence of dissolution. Adaptive mesh refinement method can be also applied to this kind of problems with sharp fronts to improve the computational efficiency.

References

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