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Large scale cavity dissolution: From the physical problem to its numerical solution

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ABSTRACT

Dissolution of underground cavities by ground water (or solutions) may cause environmental problems and geological hazards. Efficient modeling and numerical solving of such phenomena are critical for risk analysis. To solve the cavity dissolution problems, we propose to use a porous medium based local non-equilibrium diffuse interface method (DIM) which does not need to track the dissolution fronts explicitly as the sharp front methods (such as ALE). To reduce the grid blocks when using the DIM method, an adaptive mesh refinement (AMR) method is used to have higher resolutions following the moving fronts. An efficient fully implicit scheme is used by taking care of the velocities across the gridblock interfaces on the AMR grid. Numerical examples of salt dissolution under different flow conditions were performed to validate the modeling and numerical solving. Core-scale and reservoir-scale cases were carried out to study the mass transport and the evolution of the profiles of the dissolution fronts. Gravity-driven physical instabilities are found to be more strong in the infinite channel with upper and lower planes than in the 3D tube configuration under the same condition. The implementations with the AMR method also showed a very good computational efficiency, while obtaining good agreement with the finest-grid solutions.

1. Introduction

Cavity dissolution problems are very common in fluid–solid systems, for instance, karstification [1], mining [2], CO2 storage [3,4], rock weathering by flowing groundwater or other chemical solutions [5,6], etc. In these cases, the growth of underground cavities may cause geological disasters and environmental problems [7–9]; thus, accurate description and prediction of such phenomena are crucial for risk analysis. In this paper, we focus on the study of the evolution of the fluid–solid fronts caused by dissolution, e.g., water flushing the halite deposit. Two types of cavities exist in the nature: (i) a region within a porous medium in which the soluble material has been dissolved, leaving a cavity formed of insoluble material with a large porosity; (ii) a true void cavern space created by the dissolving liquid into a purely soluble solid domain.

The type (i) cavity dissolution may be modeled by a macro-scale porous medium theory involving averaged equations and effective properties. Porous media dissolution models have been introduced and used widely on a heuristic basis. A thorough derivation may be achieved by using mathematical upscaling techniques. For example, volume averaging in [10–12] leads to different models, e.g., local equilibrium models, and local non-equilibrium models. In the latter models, the true dissolution front thickness, i.e., the region where porosity varies due to dissolution, is controlled mainly by a mass exchange term [13–16].

The type (ii) cavity dissolution may be modeled using either the sharp front methods [17–19] or the cellular automaton methods [20,21] and the diffuse interface methods[22]. In typical sharp front methods, like for instance those based on the Arbitrary Lagrangian–Eulerian (ALE) framework [17], the position of the interface with zero thickness is explicitly tracked and is part of the mesh boundaries. These methods are often inefficient in some applications, especially when the shape or the evolution in time and space of the interfaces is complex and not smooth, e.g., the peaks with sharp angles [23]. The geometrical singularities

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induced by differential dissolution can be overcome by using the transport of a phase indicator, like in a Volume Of Fluid (VOF) method [24]. However, in such cases numerical diffusion generates interface diffusion that must be controlled through the use of compressive schemes and reconstruction procedures. Complex mathematical reconstruction may be carried out using Level-set methods [25–27]. In contrary to requiring the special treatment to the interface by the sharp-front methods, the diffuse interface methods (DIM) generate global PDEs for the flow by smoothing the interface as a diffuse layer where some quantities, especially a scalar field that plays the role of the phase indicator, vary rapidly but continuously [28–30]. The continuous nature of the DIM equations solved is certainly an advantage since a dissolution problem can be solved on a fixed grid without a peculiar treatment of the equations in the neighborhood of the dissolution front. This feature is comprehensively discussed in [31], in which a DIM method was proposed based on the local non-equilibrium porous medium theories, such as those originally being used for the type (i) cavity dissolutions, to model the type (ii) cavity dissolutions. It was found out that if the mass exchange term becomes very large, the resulting dissolution front becomes thinner, thus reproducing the kind of sharp dissolution fronts encountered in the purely liquid–solid dissolution problem. Also, after a short transient regime, the thickness of the dissolution front becomes a constant and that the front velocity becomes close to the one of the sharp dissolution interface problem.

Currently, most previous studies on type (ii) dissolutions are limited to pore-scale problems, but few are for large scales. Also, simulations of three-dimensional dissolution cases are rarely in the literature. However, the practical cavity dissolutions are often found with large scales, for instance, large caverns due to dissolution are reported in various countries [32,33], which belong to the type (ii) cavity dissolutions. Therefore, it is desirable for this paper to attempt a study for the modeling of the large-scale cavity dissolution and the efficient numerical simulation of the processes in both time and space. Of course, the DIM models are preferred for numerical implementations because of the continuous nature of the equations. Also, cavities often have locally non-differentiable surfaces which are difficult to be handled with an explicit interface (sharp front) treatment. Nevertheless, inherently to the DIM approaches, the dissolution front is characterized by a strong porosity gradient in the dissolution front area; thus, accurate numerical solutions would require fine grids in the regions where the dissolution fronts are likely to progress. This need for fine grids is also enforced by the fact that the dissolution boundary layer may be thin because of the low liquid diffusion/dispersion coefficient and large length-scale involved. These requirements may lead to the use of quite homogeneous fine grids, thus counter balancing the advantage of DIM. To tackle this limitation, an efficient solution is the use of Adaptive Mesh Refinement (AMR), in which the refinement will take into account, at least, the porosity gradient, in order to follow the dissolution front, and the concentration gradient, to have an accurate estimate of the mass fluxes and hence the dissolution velocity.

The applications of AMR have covered lots of physical problems, such as shock hydrodynamics analysis [34,35], compressible flow [36], turbulent flow [37], flow in porous media [38–40], and oil displacement [41,42]. The AMR methods can be distinguished into two categories: patch-based and cell-based. The patch-based AMR methods solve the problem separately on different patches of the domain under different grid refinement levels, and the solutions are coupled through the interior boundaries using interpolations in space and time [34,43,44]. They are often used to solve the Navier–Stokes equations and hyperbolic equations. The cell-based AMR methods, which are frequently applied to porous media flows [39,42], use one-coupled system (one grid) for all the grid blocks under different levels. The cell-based methods are efficient when the problems are solved implicitly, because the time step is not so restricted by the size of the fine grid blocks.

In this paper, we use the cell-based AMR for the DIM model with a fully implicit solving, considering that the mass exchange terms have strong impact on all the balance equations and the unknown variables are strongly coupled. We develop a new cell-based AMR algorithm, which is more advantageous to solve fully implicitly the balance equations to ensure the mass conservation. An important aspect of the cell-based AMR is to calculate accurate fluxes across the block interfaces when blocks from different AMR levels are involved. Nevertheless, some of the cell-based AMR algorithms are relatively inaccurate when computing the velocity flux (with Darcy's Law) across the cell interfaces as the cell-centered nodes of different levels are not along the same straight line. For example, Forsyth and Sammon [41] computed the interface velocity with Darcy's Law using the pressure (or potential) difference evaluated at two cell-centered nodes, which was pointed out that the truncation error is large. Durbin and Iaccarino [37,39] improved the accuracy using the reconstruction and bi-linear extrapolation of solutions of hanging nodes with anisotropic refinement. It showed globally $O(h^2)$ errors where h represents the characteristic length of the grid block. In this paper, to respect the physical pressure drop along the coarse blocks, we develop an accurate scheme to compute the flux on the interfaces by performing an integration to the pressure along the path between the central and auxiliary points of a coarse block with the help of Darcy's Law. More details can be found in Section 4.

The paper is organized as follows. First the original dissolution model and the diffuse interface dissolution model based on porous medium theory are introduced briefly, since it has been discussed elsewhere in the literature. Then, the AMR algorithm is presented, the focus being more on the problems specific to dissolution models. Finally, simulation examples are provided which give some insight on the use of DIM–AMR models.

2. Solid–liquid dissolution model

The original mathematical dissolution problem is characterized by the existence of separate fluid and solid phases, denoted by l and s. The solid chemical species dissolves into the fluid phase. As a minimal example, we will consider a single component in the solid phase, denoted A, and a binary mixture in the liquid phase. The total mass balance equation for the liquid phase of density ρ_l flowing at velocity $\boldsymbol{v}_l$ is written as follows

$$\frac{\partial \rho_l}{\partial t} + \nabla \cdot (\rho_l \boldsymbol{v}_l) = 0, \tag{1}$$

and the mass balance equation for chemical species A in the liquid phase is

$$\frac{\partial (\rho_l \omega_{Al})}{\partial t} + \nabla \cdot (\rho_l \omega_{Al} \boldsymbol{v}_l - \rho_l D_{Al} \nabla \omega_{Al}) = 0 \tag{2}$$

where ω_{Al} represents the mass fraction of species A in the liquid phase and D_{Al} is the liquid binary diffusion coefficient.

The mass balance equation for the solid phase of density ρ_s is the following:

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \boldsymbol{v}_s) = 0 \tag{3}$$

where the solid velocity, $\boldsymbol{v}_s$, is normally regarded as zero in most cases (in a non moving reference frame).

In the case under consideration, we suppose that the solid dissolution is mainly controlled by thermodynamic equilibrium at the solid–liquid interface. In such a case, this translates into