A Level-Set Immersed Boundary Method for Reactive Transport in Complex Topologies with Moving Interfaces

Mehrdad Yousefzadeh, Ilenia Battiato

Energy Resources Engineering Department, Stanford University, Stanford, CA 94305, USA

Abstract

A simulation framework based on the level-set and the immersed boundary methods (LS-IBM) has been developed for reactive transport problems in porous media involving a moving solid-fluid interface. The interface movement due to surface reactions is tracked by the level-set method, while the immersed boundary method captures the momentum and mass transport at the interface. The proposed method is capable of accurately modeling transport near evolving boundaries in Cartesian grids. The framework formulation guarantees second order of accuracy. Since the interface velocity is only defined at the moving boundary, a physics-based interface velocity propagation method is also proposed. The method can be applied to other moving interface problems of the “Stefan” type. Here, we validate the proposed LS-IBM both for flow and transport close to an immersed object with reactive boundaries as well as for crystal growth. The proposed method provides a powerful tool to model more realistic problems involving moving reactive interfaces in complex domains.

Keywords: Immersed Boundary Method, Fluid-Solid Interaction, Level Set, Reactive Transport, Velocity Extrapolation

1. Introduction

Dissolution and/or precipitation of solid minerals due to heterogeneous reactions occurring at solid-fluid interfaces is important in a variety of geological [1, 2, 3] and engineered [4, 5] porous media. The dissolution of solid rock matrix due to acid injection into fractures and near wellbores leads to dramatic localized increases in permeability [6, 7, 8, 9]. During CO₂ sequestration into deep reservoirs, supercritical CO₂ reacts with water to form carbonic acid and leads to the dissolution of the carbonate host...
rock [10] [11] [12] [13]. Mineral precipitation is a vital process in the immobilization of heavy metals in contaminated soils and water resources [14] [15]. Dendrite growth on the electrode surface of a battery is another example of precipitation in reactive systems [4] [5].

Multiple approaches have been developed to numerically model reactive transport in complex porous structures. These approaches include direct numerical simulations (DNS), pore network models (PNM), micro-continuum models based on the coupling of Darcy-Brinkman-Stokes equations (DBS) [16], smoothed particle hydrodynamics (SPH) [17], lattice Boltzmann method (LBM) [18] [19] [20] and immersed boundary methods (IBM) [21]. The presence of precipitation and/or dissolution at fluid-solid interfaces poses additional challenges, since mass and momentum transfer are coupled through a moving boundary. Such a class of problems involving moving boundaries are generally referred to as “Stefan problems” and require an explicit treatment of the interface separating solid and fluid.

Numerical methods for problems involving interface phenomena are broadly categorized in two classes: sharp interface and diffusive interface methods. On the one hand, diffuse interface methods (e.g. the phase field method) smooth out any jump discontinuity across the interface over a range of grid cells (i.e. the support or width of the smoothed delta function). Diffuse interface methods are constructed such that in the limit of an infinitesimal interface width (the so-called ‘sharp interface limit’), the correct interfacial dynamics is recovered. On the other hand, sharp interface methods (e.g. VOF, IBM) preserve any sharp discontinuity in the variables across the interface. Generally, sharp interface methods are preferable over diffuse interface methods for interface problems: when mass, heat or flow boundary layers are thin, diffusive interface methods may encounter some difficulties, since the approximate width of the interface might be comparable to the boundary layer thickness. This would require very fine grids in proximity of the interface and will result in increased computational burden.

A number of methods have been proposed to handle moving boundaries [22]. In the front tracking method (FTM), introduced by Unverdi and Tryggvason [23], the interface is represented explicitly. Juric and Tryggvason [24] used FTM to model the solid boundary evolution in a dendrite solidification problem. Implicit models of the interface including the level set method (LSM) [25] [26], the volume of fluid (VOF) [27] and the phase field method (PFM) [28] [29] are preferable over explicit front tracking methods, since they are robust in handling complex topological changes. Xu et al. [29] used the phase field method to model the dynamics of a moving interface due to a surface chemical reaction. In the level set method (LSM),
first introduced by Osher and Sethian [25] for tracking the front propagation of a curvature dependent interface, the interface is represented as the zero contour of a higher dimensional function. LSM has been extensively used to model interfaces on static Cartesian grids and is used in both diffusive and sharp interface approaches, depending on how boundary conditions are enforced. In the context of fluid dynamic modeling, the LSM is primarily used for tracking fluid-fluid interfaces in multiphase flow problems [30, 31]. Li et al. [32, 33] proposed a level set method for precipitation and dissolution problems. Since the works by Li et al., the LSM has been broadly used for reactive transport problems involving moving interfaces [34, 35, 36].

Once the interface is properly captured, the boundary conditions associated with the interaction between the solid and fluid domains need to be imposed. The irregularity of the solid geometry imposes additional difficulties for Cartesian grids. Various Cartesian grid-based algorithms have been suggested for reactive type boundary conditions, including embedded boundary method (EBM) [37, 38] and immersed boundary methods (IBM) [21, 39]. Immersed boundary methods are powerful tools to capture boundary condition effects with Cartesian grids. They are based on modifying the discretization of governing equations for the grids near the interface to mimic the effect of the boundary conditions. Although few IBM formulations exist that involve moving interfaces, they do not have a general framework to capture the evolution of rigid boundaries as controlled by reactions (instead they may have a prescribed interfacial velocity). On the other hand, existing methods that have used LS for reactive transport problems have not taken advantage of an immersed boundary formulation to implement high order accuracy boundary conditions implicitly. For example, [33] used a first order interpolation to implement boundary conditions which is explicit in nature.

In this work we propose a framework that couples IBM and LS to model reactive transport in complex topologies with moving interfaces; we also propose a novel propagation formula for the interface velocity. The IBM formulation is based on the high-order method developed by Yousefzadeh and Battiato [21, 40]. The interface velocity propagation scheme of Li et al. [32] is improved and extended to ensure a consistent minimum second order of accuracy throughout the numerical framework.

The paper is organized as follows. In Section 2 we present the governing equations. The details of the numerical implementation of the proposed algorithm are presented in Section 3. In Section 4 we apply the proposed method to model, first, the dissolution of a calcite grain exposed to acid injection and, second, the diffusion-limited dendritic growth of a solid nucleus in an over-saturated solute. We conclude in Section 5 with a summary of
our work and main results.

2. Problem Formulation

The conservation of momentum of a Newtonian, viscous, incompressible fluid with constant properties flowing around an impermeable solid obstacle is governed by the dimensionless Navier-Stokes equations

\[
\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re} \frac{\partial}{\partial x_j} \left( \frac{\partial u_i}{\partial x_j} \right), \quad \frac{\partial u_i}{\partial x_i} = 0, \tag{1}
\]

where \( p [-] \) and \( u_i [-] \) are the dimensionless fluid pressure and velocity component in the coordinate direction \( i \). Also,

\[
Re = \frac{UL}{\nu} \tag{2}
\]

is the Reynolds number, where \( U [LT^{-1}] \), \( L [L] \) and \( \nu [L^2T^{-1}] \) are a characteristic velocity, a characteristic length and the fluid kinematic viscosity. Equations (1) are subject to the no-slip boundary condition at the fluid-solid interface, i.e. the immersed boundary, \( \Gamma_{IB} \).

\[
u = 0, \quad x \in \Gamma_{IB}. \tag{3}
\]

The transport of a species undergoing a heterogeneous reaction (dissolution or precipitation) on the boundary of an immersed solid object can be described by a dimensionless advection-diffusion equation for the species concentration \( C [ML^{-3}] \)

\[
\frac{\partial C}{\partial t} + \frac{\partial (u_j C)}{\partial x_j} = \frac{1}{Pe} \frac{\partial^2 C}{\partial x_j^2}, \tag{4}
\]

where \( Pe \) is the Péclet number and is defined as

\[
Pe = \frac{UL}{D} \tag{5}
\]

with \( D [L^2T^{-1}] \) the molecular diffusion coefficient. Equation (4) is subject to reactive boundary conditions on the solid-fluid interface, \( \Gamma_{IB} \)

\[-n_i \frac{\partial C}{\partial x_i} = Da C, \quad x \in \Gamma_{IB}, \tag{6}\]
where $Da$ $[\cdot]$ and $n_i$ are the Damköhler number and the component of the normal $\mathbf{n}$ to the solid-fluid interface in the $i$ direction. The Damköhler number is defined as

$$Da = \frac{KL}{D}$$

(7)

where $K$ $[LT^{-1}]$ is the reaction rate constant. The speed of the moving solid boundary due to precipitation/dissolution reaction is given by [34, 32],

$$u_\Gamma = -KC_\Gamma V_m, \quad \text{at } \Gamma_{IB}$$

(8)

where $V_m$ $[M^{-1}L^3]$ is the species molar volume, and $\mathbf{u}_\Gamma = u_\Gamma \mathbf{n}$ $[LT^{-1}]$ is the interface velocity vector. Equation (8) can be expressed in dimensionless form as

$$\mathbf{u}_\Gamma = -\frac{Da}{Pe} C_\Gamma V_mC_c \cdot \mathbf{n}, \quad \text{at } \Gamma_{IB}.$$  

(9)

where $C_c$ $[ML^{-3}]$ is the characteristic molar concentration. Without loss of generality, the dimensionless quantity $V_mC_c$ $[M^0L^0]$ is set to one in all simulations.

2.1. Level Set Representation of Evolving Reactive Interface

Accurately formulating and tracking the motion of an interface in reactive transport modeling at the pore-scale is critical to capture mass fluxes across a reactive and moving interface. The Level-set method [25] is a powerful approach to attain this objective, although mass losses associated with the nonconservative nature of LS formulation require a very fine grid near the interface. The GCIBM treatment of the boundary conditions preserves the discontinuous nature of the variables across the solid-fluid interface in a sharp manner. Such features are critical in applications where the mass, heat or momentum boundary layer is thin and comparable to the support thickness of the smoothed delta function used in diffuse interface methods.

The level-set method describes the interface, $\Gamma_{IB}$, as the zero-level contour of a higher dimensional function $\phi$. For practical reasons, the level-set function is defined as the signed distance function from the interface $\Gamma_{IB}$. Specifically, $\phi$ is equal to the minimum distance between each point in the domain and the interface, where such a distance is negative or positive if the points belong to the solid or fluid subdomains, respectively,

$$\phi(\mathbf{x}) = \begin{cases} 
  d & \mathbf{x} \in \Omega_{\text{fluid}} \\
  -d & \mathbf{x} \in \Omega_{\text{solid}} \\
  0 & \mathbf{x} \in \Gamma_{IB}
\end{cases}$$

(10)
where \( d \) is the minimum (Euclidean) distance between \( \mathbf{x} \) and the interface. The level-set function is also used to compute the normal to the interface as

\[
\mathbf{n} = \frac{\nabla \phi}{|\nabla \phi|}.
\]

(11)

The interface velocity, defined by (9) and due to the chemical reaction at the solid-fluid interface (6), satisfies the level-set equation

\[
\frac{\partial \phi}{\partial t} + \mathbf{u}_\Gamma \cdot \nabla \phi = 0
\]

(12)

where \( \mathbf{u}_\Gamma \) is the interface velocity. It is worth emphasizing that the computation of the normal vector (11), the interface velocity (9) and reactive boundary condition (6) at the interface all depend upon the level set function property to remain a signed distance function. However, in general, the level set function ceases to hold its signed distance function property as it evolves in time [26]. A reinitialization process is therefore adopted to project the new level set to a signed distance function, while preserving the zero level set location according to [41]

\[
\frac{\partial \phi}{\partial \tau} + \text{sgn}(\phi^0)(1 - |\nabla \phi|) = 0,
\]

(13)

where \( \tau \) is a pseudo-time step and \( \phi^0 \) is the level set function obtained after solving (12). Equation (13) needs to be solved up to the pseudo-time steady state.

3. Numerical Methodology

3.1. Finite Volume Discretization

Equations (1)-(4) are discretized using a finite-volume scheme [42, 43] on a structured Cartesian grid. A fully implicit Euler backward time integration scheme is used to avoid any stability problems associated with larger time steps.

The NS equations (1) are solved in the primitive variables (\( \mathbf{u}, p \)) formulation. The primitive variables are defined on a staggered grid. This avoids the checkerboard patterns in the solution [44]. In staggered grids, the velocities are stored at the grid faces and the scalar variables (e.g., pressure, temperature, concentration) are stored at the cell centers. Hence, a \( d + 1 \) Cartesian grid set is required in a \( d \)-dimensional problem. The PISO algorithm, a non-iterative method to solve the unsteady Navier-Stokes equation...
with large time steps, is adopted for pressure-velocity coupling and satisfies mass conservation using predictor-corrector steps. The convection and viscous terms in (1) are discretized using a third order upwinding (QUICK) and a second order central difference schemes, respectively. An identical spatial discretization is adopted to discretize the convection and diffusion terms in the scalar transport equation (4). Hamilton-Jacobi WENO scheme is used to discretize both the level set and the re-initialization equations in space. Their temporal discretization is performed by either TVD-RK3 or TVD-RK4. A comprehensive review of strategies to solve the level set and reinitialization equations is given in.

3.2. Immersed Boundary Treatment

The level set tracks the evolution of the interface, as well as the information about the normal to the interface. In order to implement equations (1) and (4) on Cartesian grids, their associated boundary conditions need to be properly treated. In this study, we use a variation of the ghost cell immersed boundary method (GCIBM) developed in to implement boundary conditions.

The method is based on a pre-classification of the type of cell: fluid, solid or ghost. Fluid cells are the cells whose centers are located inside the flow domain; solid cells have their centers inside the solids and are not directly adjacent to a fluid cell; ghost cells are the cells inside the solid with at least one neighboring fluid cell. A flag variable is constructed to assign each cell to a specific class (liquid, solid, ghost). The values of state variables inside solids, fluid and ghost cells are treated differently.

Instead of using more classical approaches, e.g. the ray-casting algorithm, we note that the Level Set function itself provides a natural framework for cell classification. In particular, if the cell center is in the flow domain then it will have a negative level set value \( \phi < 0 \). In solid cells, \( \phi > 0 \). If the level set has a zero value, then the cell center lays on the boundary. The ghost cells are identified as the solid cells with at least one fluid cell neighbor. The detailed steps of the identification process are outlined in Algorithm 1. Once the tagging process is completed (see Figure 1), an appropriate formulation for each class of the cells will be used to update the state variables. The algebraic equation for each variable in the fluid cells will be obtained by discretizing the governing PDEs. The values of all state variables in the solid cells are set to be constant, however, one may prefer to exclude the solid cells from the computations as they are completely decoupled from the rest of the domain. Finally, the algebraic equation for the ghost cell values are constructed in such a way that their coupling with the
Algorithm 1 Point Identification Algorithm

1: function PointID(X, Y, φ) ▷ The type of each grid point
2: for all \((x_i, y_j) \in \{(X, Y)\}\) do
3: \(\phi(x_i, y_j) \leftarrow \) level set value at \((x_i, y_j)\)
4: if \(\phi(x_i, y_j) > 0\) then
5: \(F(i, j) \leftarrow 1\) ▷ flag value 1 is for fluid points
6: \((x_i, y_j) \in (X_f, Y_f)\)
7: else if \(\phi(x_i, y_j) < 0\) then
8: \(F(i, j) \leftarrow -1\) ▷ flag value −1 is for solid points
9: \((x_i, y_j) \in (X_s, Y_s)\)
10: for all \((x_i, y_j) \in (X_s, Y_s)\) do
11: if \(F(i + 1, j) + F(i - 1, j) + F(i, j + 1) + F(i, j - 1) \neq -4\) then
12: \(F(i, j) \leftarrow 0\) ▷ flag value 0 is for ghost points
13: \((x_i, y_j) \in (X_g, Y_g)\)
14: return \(F\)

fluid cells will result in correct boundary condition implementation. Details of the implementation can be found in [21, 40]. Specifically, the GCIBM developed in [21] is capable of treating the general boundary condition of the form

\[
- \mathbf{n} \cdot \alpha \frac{\partial \psi}{\partial r_n} = \beta \psi + q, \quad r_n = 0, \quad (14)
\]

for a generic state variable \(\psi\). Both a Dirichlet boundary condition in the NS Equation (3) and a reactive boundary condition in the transport equation (6) can be modeled through (14) by defining the proper values for \(\alpha, \beta\) and \(q\). For a more detailed discussion on the implementation of GCIBM, we refer the interested reader to [21, 40].

3.3. Level Set-Immersed Boundary Method

A level set function is used to implicitly capture the interface separating the fluid and solid \((\Gamma_{ib})\). The evolution of the interface (boundary) is governed by Eq. (12), with Eq. (9) defines the velocity of the interface in the normal direction to \(\Gamma_{ib}\).

Once the interface velocity, \(u_n\) is found, the level set function is advanced in time from \(t^n\) to \(t^{n+1}\) by solving equation (12). Subsequently, the reinitialization equation (13) is solved to ensure that the updated level set remains a signed distance function. The new level set defines the current location of the interface at time \(t^{n+1}\), and can be used to obtain the normal vector...
The flow and transport equations are finally solved to 

Figure 1: A 2D schematic representation of different type of the points in the domain.
update velocity, pressure and concentrations using the GCIBM.

It is worth to emphasize that Eqs. (12) and (13) need to be solved only within a narrow region in proximity of the interface, $|\phi| \leq \varepsilon$, where $\varepsilon$ is larger than the stencil required for WENO scheme, i.e. $\varepsilon \geq 5\Delta x$.

3.3.1. Interface Velocity Propagation

Although Eq. (12) assumes the velocity field $u_n$ is defined in the entire computational domain, the velocity is only properly defined at the interface. This calls for propagating (extrapolating) the velocity to the narrowband around the interface ($\phi = 0$). A common approach to propagate the interface velocity is multidimensional ghost fluid method \[31\]. Fedkiw et al. \[31\] write

$$\frac{\partial \lambda}{\partial \tau} \pm n_i \frac{\partial \lambda}{\partial x_i} = 0,$$

(15)

to propagate a generic variable $\lambda$, where the plus and minus signs are used when $\phi > 0$ and $\phi < 0$, respectively. Aslam \[51\] extended this method by introducing the concept of PDE extrapolation, where a higher order PDE is solved to perform extrapolation with higher order of accuracy. Li et al. \[32, 33\] employed the ghost fluid method to propagate the interface velocity in a narrowband of the interface inside the solid domain. In the fluid domain, instead of solving the extrapolation equation (15), they derive an explicit expression for the interface velocity field at point $a$ (see Fig. 2)

$$u_a^n = \frac{Da}{Pe} \left( \frac{1}{1 + \phi_a Da} \right) C_a.$$

(16)

The velocity field in the fluid domain serves as the boundary condition for equation (15). Equation (16) is derived based on the fact that the equation (15) is solved to the steady state, (i.e. $n_i \frac{\partial \lambda}{\partial x_i} = 0$). They used a first order approximation of the derivative to do the constant extrapolation as shown in the Figure 2. However, the interface velocity propagation algorithm by \[32\] employs two separate approaches for the solid and fluid sub-domains. Moreover, Equation (16) has a first order of accuracy. The formula does not suggest a local formulation for the points farther from the interface. The later issue becomes critical specially for the cases where there is a high concentration gradient near the interface. Here, we improve upon the formulation of \[32, 33\] by (i) deriving a new expression for interface velocity to include both the fluid and solid domain and (ii) employing a different stencil in the extrapolation to obtain a higher order of accuracy while ensuring a more local formulation.
The steady state solution of the equation (15) for the interface velocity can be expressed as,

\[ n_i \frac{\partial u_i}{\partial x_i} = 0. \] (17)

Equation (17) indicates that the normal velocity should be constant along the normal vectors to the interface. Therefore, for any grid point \( X = (x, y) \) in the neighborhood of the interface \(|\phi| < \varepsilon\) we need to find the corresponding boundary points (i.e. the intersection of the interface and the line passing through \( X \) with its slope equal to the normal vector \( n_X \)). The boundary points can be obtained as follows

\[ X_{IB} = (x_{IB}, y_{IB}) = (x - n_x \phi(x,y), y - n_y \phi(x,y)). \] (18)

The level set velocity at \( X = (x, y) \) is equal to the velocity at its corresponding \( X_{IB} = (x_{IB}, y_{IB}) \),

\[ u_{\Gamma}(x,y) = u_{IB} = -\frac{Da}{P_e} V_m C_{IB} \cdot n. \] (19)

The concentration at the interface, \( C_{IB} \), is needed to fully describe the velocity at \( X \) and it is reconstructed using two mirror points in the fluid domain and a one-sided second-order finite difference expression for the concentration derivative in the normal direction. A second order approximation of the derivative requires the values at three points. Equation (6) is employed to close the system. If the mirror point does not coincide with a grid point, its value is obtained by a bilinear interpolation. The two mirror points are defined as

\[ X' = (x', y') = (x_{IB} + dn_x, y_{IB} + dn_y) \]
\[ X'' = (x'', y'') = (x' + dn_x, y' + dn_y) \] (20)

where \( d = \sqrt{2} \Delta x \) ensures that the mirror point is surrounded by 4 points in the fluid domain as shown in Figures 3 and 4. The concentration value at the interface is obtained as

\[ C_{IB} = \frac{4C_{X'} - C_{X''}}{-dDa + 3}. \] (21)

Finally the level set velocity vector can be calculated as

\[ u_{\Gamma}(x,y) = -\frac{Da}{P_e} V_m \left( \frac{4C_{X'} - C_{X''}}{Dad + 3} \right) (n_x, n_y). \] (22)

The current formulation provides a general expression for both solid and fluid points.
3.4. Discussion on the Practical Aspects of LS-IBM

The IBM flow and transport solver is based on an implicit method. As a result, there is no severe restriction on the time step. Yet, a reasonably small time step, close to the viscous (diffusive) and CFL time steps, is recommended for faster convergence. This choice also honors the physical time scales. The GCIBM requires that the grid Damköhler number \( (Da_{\Delta x} = K \Delta x / D) \) be less than 2, (see the derivation of GCIBM in [21, 40]). This poses restrictions on the grid size close to the interface. Table 1 summarizes the time step and grid size restrictions, where the value of \( \lambda_{cfl} \) in Table 1 is between 0 and 1.

| Time Step       | Restriction                              |
|-----------------|------------------------------------------|
| Viscous time step | \( \Delta t \leq \Delta t_v = \frac{Re}{\Delta x^2 + \Delta y^2} \) |
| CFL time step    | \( \Delta t \leq \Delta t_{cfl} = \frac{\Delta x}{u_{max}} \)         |
| Diffusion time step | \( \Delta t \leq \Delta t_D = \frac{Pe}{\Delta x^2 + \Delta y^2} \) |
| IBM grid size   | \( \Delta x \leq \Delta x_{IBM} = \frac{2K}{D} \)               |
| LS time step    | \( \Delta t \leq \Delta t_{LS} = \frac{\lambda_{cfl} \Delta x_{min} Pe}{Da} \) |

It is worth emphasizing that, since the movement of the interface due to reaction is much smaller than flow and transport processes, one may not solve the level set equation (i.e. update the boundary geometry) at every flow and transport time step, i.e. the time step in Eq. (12) is a multiple of the time step in equations (1) and (4), namely, \( \Delta t_{LS} = m \Delta t \), with \( m \) an integer.
4. Numerical Implementation

In the following, we validate the scheme against two benchmark problems: a 2D cylindrical calcite grain dissolution problem \[35\] and a precipitation-driven dendrite growth problem.

4.1. Dissolution of a Cylindrical Grain

We consider flow and transport around a 2D cylindrical calcite grain, fully immersed in an acidic fluid. The reaction at the solid-fluid interface dissolves the grain. We consider the benchmark problem setup of Molins et al. \[35\]. The total length and width of the computational domain is $5d$ and $2.5d$ respectively, where $d$ is the initial diameter of the grain. The grain is placed at the center of the domain as shown in Figure 5. The simulation parameters are summarized in Table 2.

![Figure 5: Computational domain and BCs for reacting grain](image)

\[ u = u_{in}, \quad v = 0, \quad C = C_{in} \]

\[ p = 0, \quad \frac{\partial C}{\partial x} = 0 \]

\[ u = 0, \quad v = 0, \quad \frac{\partial C}{\partial y} = 0 \]

Table 2: Simulation parameters for dissolving grain

| Parameter       | Value          |
|-----------------|----------------|
| Reynolds number | $Re = 0.1$     |
| Inlet velocity  | $u_{in} = 1$  |
| Inlet concentration | $C_{in} = 1$ |
| Reynolds number | $Re = 0.1$     |
| Grid size       | $\Delta x = 0.005$ |
| Time step       | $\Delta t = 1e^{-4}$ |
| Grain diameter  | $d = 0.4$     |
4.1.1. Grid convergence, accuracy and stability analysis

The grid size is chosen after a grid convergence study for the shape and volume of the grain. Figure 6 shows the grain shape convergence as the grid is refined. The required grid size for accurate simulation strongly depends on the Damkohler and Peclet number. A more refined grid is needed for high Damkohler and Peclet numbers, as seen in Fig. 6 (III and IV) the coarse grid size fails to even predict a physical shape. We chose \( \Delta x = 0.005 \).

\[
\begin{array}{c}
\Delta x = 0.02 \\
\Delta x = 0.01 \\
\Delta x = 0.005 \\
\Delta x = 0.0025
\end{array}
\]

Figure 6: Grid shape convergence for different grid sizes at several transport regimes at different times. I) : \((\text{Da, Pe, t}) = (6, 0.178, 5)\), II) : \((\text{Da, Pe, t}) = (6, 178, 0.75)\), III) : \((\text{Da, Pe, t}) = (600, 178, 5)\), IV) : \((\text{Da, Pe, t}) = (6, 17800, 6)\)

In figures 7-10, \(L_1\), \(L_2\) and \(L_\infty\) errors of the grain volume (area) at various Peclet and Damkohler numbers are plotted vs the grid size. The solutions at the finest grid, \(\Delta x = 0.0025\) is set as the reference solution. The convergence rate shows at least second order of accuracy for all the norms of the error. In figures 8 and 10 a higher convergence rate is observed, in both cases the ratio of Damkohler and Peclet (\(\text{Da}_I\)) is higher than the other two cases.
Figure 7: The grid convergence for \((Da, Pe) = (6, 0.178)\).

Figure 8: The grid convergence for \((Da, Pe) = (6, 178)\).
In Figure 11, the volume convergence versus different time step sizes are plotted. All error norms show first order of accuracy in time. This aligns with the first order implicit time integration method that we have used. Although not implemented, the proposed GCIBM and LSIBM methods can be accompanied with higher order explicit temporal integration schemes to achieve higher temporal accuracy.
The numerical stability of LSIBM is examined for flow and reactive transfer around both a dissolving circular grain. The test cases consist of a wide range of $Pe$ and $Da$ and are performed for multiple time steps ($\Delta t$).

The stability of LSIBM highly depends on the LS CFL condition mentioned in Table 1. In order to better test the stability we defined the initial concentration equal to 1 ($C_0 = 1$). This will ensure that the concentration at the interface is high, so the interface will move with a higher speed. Two important factors in the interface velocity expression are the Da and Pe ratio as well as the concentration near the interface. We noticed that for two cases with the same Da and Pe ratio the one with higher Da is more stable at larger time steps. This is due to the fact that the higher reaction rate will decrease the concentration more, therefore the interface velocity is lower. The stability tests for multiple Da and Pe are listed in Table 3. For each transport two time steps are reported, the critical time step value for a stable solution lies between these two values.
Table 3: Stability of LSIBM for different Pe, Da and time steps ($\Delta x = 0.005$)

| $\Delta t$ | $Da$ | $Pe$ | stable/unstable |
|------------|------|------|-----------------|
| 5E-4       | 178  | 6    | stable          |
| 8E-4       | 178  | 6    | unstable        |
| 5E-5       | 178  | 0.6  | stable          |
| 8E-5       | 178  | 0.6  | unstable        |
| 1E-2       | 178  | 600  | stable          |
| 4E-2       | 178  | 600  | stable          |
| 5E-3       | 17800| 600  | stable          |
| 3E-2       | 17800| 600  | unstable        |
| 1E-2       | 1.78 | 6    | stable          |
| 3E-2       | 1.78 | 6    | unstable        |

Figure 12 (I-IV) shows the evolution of the concentration as well as the grain interface at times, $t = 3, 4, 5, 6$, respectively. These overall dissolution pattern shows a good agreement with the simulations in [52] and [16]. In Figures 13-15 the solid mineral shape is plotted along with the results in [52] for a more quantitative comparison. Due to the non-symmetric concentration field along the x-axis the grain surface evolves in a non-uniform manner. The diamond (petal) shape of the solid grain is a results of higher dissolution rate at the upstream (far left) side of the grain, while the downstream (far right) side of the grain is exposed to less reactive acid ions and dissolves with a lower rate and moving much less.
Figure 12: The concentration for \((Da, Pe) = (178, 600)\) at times I): \(t = 3\), II): \(t = 4\), III): \(t = 5\), IV): \(t = 6\). The solid white line shows the grain interface.

The grain shape for \(Da = 178\) and \(Pe = 600\) at different time steps is compared to the results from several methods in the benchmark paper by Molin et. al [52] in Figs 13-15. The grain dissolution pattern is close and in good agreements with the benchmark results. Our results shows a closer match to the results from Chombo-Crunch. This is due to the fact that both methods are based on an Eulerian finite-volume framework.
Figure 13: The solid grain shape for $(Da, Pe) = (178, 600)$ at dimensional time $t = 15$ minutes from different methods.

Figure 14: The solid grain shape for $(Da, Pe) = (178, 600)$ at dimensional time $t = 30$ minutes from different methods.
To validate the method quantitatively we have considered the evolution of the total surface area (perimeter in 2D) of the calcite grain with time. In Figures 16 and 17, we show simulation results corresponding to two scenarios with \((Da = 178, Pe = 600)\) and \((Da = 0.178, Pe = 6)\). The surface evolution for both cases is in agreement with the results presented in [35] where five different numerical algorithms were compared.

In first case \((Da = 178\) and \(Pe = 600)\), the grain starts changing to a petal shape from its initial circular shape during the dissolution. This is due to the lower acid concentration at the stagnation point on right side of the cylinder and thus, lower local dissolution rate at the right side of the grain (see Fig. 18 (V)). In second case, the \(Da\) and \(Pe\) are much smaller \((Da = 0.178\) and \(Pe = 6)\), and the grain shape stays circular throughout the dissolution process. According to phase diagram (Fig. 19 and 16), at smaller Damkohler \((Da < 1)\) the solid grain is surrounded by same amount of reactive acid ions, which will dissolve the grain surface homogeneously. Figs. 16 and 17 shows that our results and those reported by Combo-Crunch are closer to each other than other methods. This is expected because both methods use a finite volume scheme along with level-set to update the geometry.
Figure 16: Grain surface area temporal evolution for $Pe = 600$ and $Da = 178$: comparison between LS-IBM and the methods in [35].
In order to test the robustness and capabilities of the LSIBM we performed the dissolution of the solid grain at a multiple $Pe$ and $Da$. The table summarizes the dimensionless groups used in the simulation.

| Case | $Da$  | $Pe$ | $Da_Pe^{-1}$ |
|------|-------|------|--------------|
| (I)  | 0.178 | 6    | 0.03         |
| (II) | 17.8  | 0.6  | 296.67       |
| (III)| 1.78  | 6    | 0.3          |
| (IV) | 1780  | 6    | 296.67       |
| (V)  | 178   | 600  | 0.3          |
| (VI) | 17800 | 600  | 29.67        |

The simulation results and the grain shape pattern agrees with the $Pe/Da$ diagram for dissolution regime reported in [16]. Similar to Soulaine...
and et. al [16], three distinct grain shape pattern is observed. As in Fig. [18] (a), once the reaction rate is small (i.e. $Da \leq 1$) the grain dissolves in a uniform manner, the grain center almost stays unchanged and the initial cylindrical shape is preserved. However for larger $Da$ numbers, the grain shape starts deviating from its initial cylindrical shape and the grain center of mass moves due to the non uniform dissolution. For moderate to low Peclet number ($Pe \leq 10$) the grain surface stays smooth (Fig. [18] II -IV). Unlike, Soulaine and et. al we noticed three different sub-regimes. For very small Peclet numbers ($Pe \leq 1$), the grain elongation is perpendicular to the flow direction (Fig. [18] II). Indeed, because of the low Peclet number the right side of the grain is exposed to very small amount of acid ions, and since the $Da$ is not very large the reaction rate near the top and bottom of the grain is smaller when compared to case (IV), the low dissolution rate at top and bottom and high rate at the left side of the grain, causes a horizontally skewed shape. As the $Pe$ increases, the right side of the grain is exposed to more reactive acid ions and an elongation in the flow direction is observed (III), however, this elongation becomes less apparent when the Damkohler is very large ($Da \geq 10$). Finally for large Peclet numbers the diamond (petal) pattern of the grain (Fig. [18]) corresponding to the third regime in Soulaine et. al [16], is observed.
Figure 18: The concentration contour for simulation cases according to table 4 at different time snapshots ($t_I = 6$, $t_{II} = 0.2$, $t_{III} = 1.5$, $t_{IV} = 0.9$, $t_{V} = 6$ and $t_{VI} = 8$). The solid and dotted white lines show the evolved and initial grain surface respectively.

In Fig. 19 the updated Da-Pe regime diagram for grain shape is presented. We have summarized the characteristics of each regime and subregime in table 5.
Figure 19: The concentration contour for simulation cases according to table 4 at different time snapshots ($t_{I} = 6$, $t_{II} = 0.2$, $t_{III} = 1.5$, $t_{IV} = 0.9$, $t_{V} = 6$ and $t_{VI} = 8$). The solid and dotted white lines show the evolved and initial grain surface respectively.

Table 5: Dissolution regime characteristics

| Regime | grain center | grain shape   |
|--------|--------------|---------------|
| (I)    | unchanged    | cylindrical   |
| (II)   | moves to the left | horizontally skewed |
| (III)  | moves to the left | vertically skewed |
| (IV)   | moves to the left | cylindrical   |
| (V)    | moves to the left | diamond (petal) |

4.2. Diffusion limited precipitation and unstable dendritic growth

In order to further investigate the capability of the proposed LS-IBM to handle complicated interface dynamics, we compute both the symmetric and unstable dendritic growth of a small circular nucleus with initial radius of $r_0$. The growth occurs due to the surface precipitation of a solute with initial value of $c_{\infty}$. The dynamic of the solid-fluid interface and resulting growth pattern can be anticipated as a moving boundary (Stefan problem)
The Damköhler number of the problem is high and therefore the transport is under diffusion limited condition.

The crystal growth problem due to diffusion limited precipitation is extensively studied in the reactive transport research community. Lattice Boltzmann method [55], smoothed particle hydrodynamics (SPH) [56], level set method [32] and phase field method [28] have all been used, among others, to model stable and unstable crystal growth.

We consider the initial radius of a solid nucleus to be \( r_0 = 0.005 \), placed in a unit square domain. The concentration at radius \( r_\infty = 0.5 \) is held constant and equal to the initial concentration \( c(r_\infty) = c_\infty \). Two values for the initial concentrations \( c_\infty = \{0.1, 1\} \) and four values for Damköhler number \( Da = \{10, 100, 1000, 10000\} \) are considered. The domain is discretized in a 600 × 600 uniform grid.

The growth patterns for \( c_\infty = 1 \) at two different instances in time are shown in Figures 20 and 21. The effect of Damköhler number is depicted in each Figure. The process is more reaction-limited at smaller Damköhler numbers (\( Da \approx O(1) \)) and results in a stable uniform growth with a smooth interface, see Figures 20(i) and 21(i). As the Damköhler number increases the diffusion rate becomes less and less adequate to sustain a uniform concentration around the boundary and the interface becomes increasingly less smooth, see Figures 20(ii) and 21(ii). Ultimately, at very high Damköhler numbers (\( Da = 10^3, 10^4 \)), the reaction rate is much faster than the diffusion rate and the process is diffusion limited: as a result, any small perturbation will lead to a dendritic growth pattern, see Figures 20(iii, iv) and 21(iii, iv).

The growth of a solid crystal by super saturated solute precipitation under high absorption rate is governed by the Mullins-Sekerka instability [57].
Figure 20: The growth pattern for $c_\infty = 1$ at time $t = 0.001$ at different Damkohler numbers: (i) $Da = 10$, (ii) $Da = 10^2$, (iii) $Da = 10^3$, (iv) $Da = 10^4$. 
Figure 21: The growth pattern for $c_\infty = 1$ at time $t = 0.003$ at different Damkohler numbers: (i) $Da = 10$, (ii) $Da = 10^2$, (iii) $Da = 10^3$, (iv) $Da = 10^4$.

In order to investigate the effects of $c_\infty$ on the growth pattern, we have simulated the problem at $c_\infty = 0.1$. The results for various Damkohler numbers at two time snapshots are presented in figures 22 and 23. A more branched growth compared to the case with $c_\infty$ is evident. The branches perish as they advance to the far field due to the competition with their adjacent branches to absorb mass. The lack of initial mass stops the growth of branches and unlike the previous case the pattern will have thinner branches.
Figure 22: The growth pattern for $c_\infty = 0.1$ at time $t = 0.1$ at different Damköhler numbers: (i) $Da = 10$, (ii) $Da = 10^2$, (iii) $Da = 10^3$, (iv) $Da = 10^4$. 
Figure 23: The growth pattern for $c_\infty = 0.1$ at time $t = 0.3$ at different Damköhler numbers: (i) $Da = 10$, (ii) $Da = 10^2$, (iii) $Da = 10^3$, (iv) $Da = 10^4$.

Further, we compare the effective fractal dimension obtained in the previous simulations with those in the literature. The effective fractal dimension, $D_f$, characterizes the volume (or area in 2D) of the crystal within a radius $r$ and can be determined through the power law relationship

$$M_r \sim r^{D_f},$$

where $M_r$ is the volume (area in 2D) of the solid. We use the box-counting method to measure the fractal dimension for different Damköhler numbers.
In Figure 24 we plot the area of the solid $M_r$ versus the radius $r$ in a logarithmic scale for different Damköhler numbers. As expected from Eq. 23, $\log(M_r)$ increases linearly with $\log(r)$. 

Figure 24: $M_r$ vs. $r$ for dendritic growth for $c_\infty = 0.1$

The effective fractal dimensions are reported in Table 6. The fractal dimension measured by SPH method [54], LBM [55], large scale off-lattice diffusion limited aggregation (DLA) model [53] and level set method of Li.eta al [32] at extremely high reaction rate ($Da = O(10^3 \sim 10^4)$) are $D_f = 1.66$, 1.715 and 1.75 are 1.82, respectively.

We obtained $D_f = 1.74$, Our results shows close agreement with the previously cited values.
Table 6: Comparison of fractal dimension $D_f$ for dendritic growth with different Damkohler numbers

| $Da$ | 10  | 100 | 1000 | 10000 |
|------|-----|-----|------|-------|
| Kang et. al (2004) [55] | -   | -   | 1.715 | -     |
| Kang et. al (2004) [55] | 2.0 | 1.88 | 1.75  | -     |
| Tartakovsky et. al (2007) [56] | 2.0 | 1.74 | 1.66  | -     |
| Li et. al (2008) [32] | 2.0 | 2.0  | 1.85  | 1.82  |
| current | 2   | 1.99 | 1.81  | 1.74  |

In most cases, we want to trigger these instabilities anyway, so perturbations induced by the grid are not necessarily undesirable.

In these simulations, we use a 600 $\times$ 600 grids. The grid size has a noticeable effect on the solution. For the largest grid size the interface main branches are greater in numbers (16) compared to higher resolution solutions (8 main branches). On the other hand the two higher resolution solutions are more similar and each have 8 large branches. While the solutions in Figures 25 (ii, iii) are not fully converged in the sense that the two solutions are completely identical, we believe that the physical phenomena are fully resolved for both grids. Starting from an initially perturbed (non circular) interface will reduce this differences resulting from the grid size. These observation are similar to those of Juric and Tryggvason [24]. Despite the differences in interface shape at the three grid resolution, the fractal dimension and the overall trend remains unchanged Fig 26.

Figure 25: The growth pattern for $c_\infty = 1$ and $Da = 10^4$ at time $t = 0.001$ at different grid resolutions: (I) $\Delta x = \frac{1}{400}$, (II) $\Delta x = \frac{1}{600}$ and (III) $\Delta x = \frac{1}{800}$.
5. Conclusions

We introduced a Level Set-Immersed Boundary Method (LS-IBM) for reactive transport involving moving boundaries. The proposed method extends the GCIBM by [21] to problems with moving boundaries. The level set method keeps track of the evolving interface, while the immersed boundary captures the reactive boundary condition. To the best of our knowledge, this is the first method to couple level set with the immersed boundary method for reactive transport problems involving a moving boundary. The proposed method also ensures at least second-order accuracy throughout the process as well as a more accurate formulation to propagate the interface velocity in a narrow band near the interface. Moreover, a consistent formulation

Figure 26: $M_r$ vs. $r$ for dendritic growth for $c_\infty = 1$ and $Da = 10^4$ at three different grid resolutions.
is used to propagate the velocity for both fluid and solid regions. This is different from Li et al. [32] where for each subdomain a separate method is used: the solution of a PDE for the solid subdomain and the ghost fluid method for fluid subdomain. The new method uses local grid points to propagate the interface velocity, and therefore is suitable for problems involving interface phenomena. Validation studies for a cylindrical reactive calcite grain and dendritic solid growth have been successfully implemented. Further improvements, such as extensions to three dimensional geometries and inclusion of multicomponent transport, are straightforward and subject of current research.

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References

[1] J. W. Morse, R. S. Arvidson, A. Lüttge, Calcium carbonate formation and dissolution, Chemical reviews 107 (2) (2007) 342–381.

[2] P. C. Lichtner, C. I. Steefel, E. H. Oelkers, Reactive transport in porous media, Vol. 34, Walter de Gruyter GmbH & Co KG, 2018.

[3] M. Yousefzadeh, I. Battiato, Physics-based hybrid method for multiscale transport in porous media, Journal of Computational Physics 344 (2017) 320–338.

[4] E. M. Ryan, K. Ferris, A. Tartakovsky, M. Khaleel, Computational modeling of transport limitations in li-air batteries, ECS Transactions 45 (29) (2013) 123–136.

[5] J. Tan, E. M. Ryan, Computational study of electro-convection effects on dendrite growth in batteries, Journal of Power Sources 323 (2016) 67–77.

[6] M. Pournik*, D. Tripathi, Effect of acid on productivity of fractured shale reservoirs, in: Unconventional Resources Technology Conference, Denver, Colorado, 25-27 August 2014, Society of Exploration Geophysicists, American Association of Petroleum..., 2014, pp. 1811–1823.
[7] T. W. Teklu, H. H. Abass, R. Hanashmooni, J. C. Carratu, M. Ermila, Experimental investigation of acid imbibition on matrix and fractured carbonate rich shales, Journal of Natural Gas Science and Engineering 45 (2017) 706–725.

[8] M. Pournik, D. Tripathi, I. El-Monier, Productivity of hydraulically fractured calcite rich shale reservoirs enhanced by acid, Journal of Petroleum Engineering & Technology 6 (1) (2019) 54–68.

[9] H. Deng, M. Voltolini, S. Molins, C. Steefel, D. DePaolo, J. Ajo-Franklin, L. Yang, Alteration and erosion of rock matrix bordering a carbonate-rich shale fracture, Environmental science & technology 51 (15) (2017) 8861–8868.

[10] T. Rathnaweera, P. Ranjith, M. Perera, Experimental investigation of geochemical and mineralogical effects of co2 sequestration on flow characteristics of reservoir rock in deep saline aquifers, Scientific reports 6 (2016) 19362.

[11] Y. Xiao, T. Xu, K. Pruess, The effects of gas-fluid-rock interactions on co2 injection and storage: insights from reactive transport modeling, Energy Procedia 1 (1) (2009) 1783–1790.

[12] T. Xu, J. A. Apps, K. Pruess, Reactive geochemical transport simulation to study mineral trapping for co2 disposal in deep arenaceous formations, Journal of Geophysical Research: Solid Earth 108 (B2).

[13] N. J. Huerta, M. A. Hesse, S. L. Bryant, B. R. Strazisar, C. Lopano, Reactive transport of co2-saturated water in a cement fracture: Application to wellbore leakage during geologic co2 storage, International Journal of Greenhouse Gas Control 44 (2016) 276–289.

[14] R. A. Wuana, F. E. Okieimen, Heavy metals in contaminated soils: a review of sources, chemistry, risks and best available strategies for remediation, Isrn Ecology 2011.

[15] F. Guo, C. Ding, Z. Zhou, G. Huang, X. Wang, Stability of immobilization remediation of several amendments on cadmium contaminated soils as affected by simulated soil acidification, Ecotoxicology and environmental safety 161 (2018) 164–172.

[16] C. Soulaine, S. Roman, A. Kovscek, H. A. Tchelepi, Mineral dissolution and wormholing from a pore-scale perspective, Journal of Fluid Mechanics 827 (2017) 457–483.
[17] A. M. Tartakovsky, P. Meakin, T. D. Scheibe, B. D. Wood, A smoothed particle hydrodynamics model for reactive transport and mineral precipitation in porous and fractured porous media, Water resources research 43 (5).

[18] C. Huber, B. Shafei, A. Parmigiani, A new pore-scale model for linear and non-linear heterogeneous dissolution and precipitation, Geochimica et Cosmochimica Acta 124 (2014) 109–130.

[19] A. Parmigiani, C. Huber, O. Bachmann, B. Chopard, Pore-scale mass and reactant transport in multiphase porous media flows, Journal of Fluid Mechanics 686 (2011) 40–76.

[20] N. Prasianakis, E. Curti, G. Kosakowski, J. Poonoosamy, S. Churakov, Deciphering pore-level precipitation mechanisms, Scientific reports 7 (1) (2017) 13765.

[21] M. Yousefzadeh, I. Battiato, High order ghost-cell immersed boundary method for generalized boundary conditions, International Journal of Heat and Mass Transfer 137 (2019) 585–598.

[22] S. Molins, Reactive interfaces in direct numerical simulation of pore-scale processes, Reviews in Mineralogy and Geochemistry 80 (1) (2015) 461–481.

[23] S. O. Unverdi, G. Tryggvason, A front-tracking method for viscous, incompressible, multi-fluid flows, Journal of computational physics 100 (1) (1992) 25–37.

[24] D. Juric, G. Tryggvason, A front-tracking method for dendritic solidification, Journal of computational physics 123 (1) (1996) 127–148.

[25] S. Osher, J. A. Sethian, Fronts propagating with curvature-dependent speed: algorithms based on hamilton-jacobi formulations, Journal of computational physics 79 (1) (1988) 12–49.

[26] S. Osher, R. P. Fedkiw, Level set methods: an overview and some recent results, Journal of Computational physics 169 (2) (2001) 463–502.

[27] C. W. Hirt, B. D. Nichols, Volume of fluid (vof) method for the dynamics of free boundaries, Journal of computational physics 39 (1) (1981) 201–225.
[28] Z. Xu, P. Meakin, Phase-field modeling of two-dimensional solute precipitation/dissolution: Solid fingers and diffusion-limited precipitation, The Journal of chemical physics 134 (4) (2011) 044137.

[29] Z. Xu, H. Huang, X. Li, P. Meakin, Phase field and level set methods for modeling solute precipitation and/or dissolution, Computer Physics Communications 183 (1) (2012) 15–19.

[30] S. Osher, R. Fedkiw, K. Piechor, Level set methods and dynamic implicit surfaces, Appl. Mech. Rev. 57 (3) (2004) B15–B15.

[31] R. P. Fedkiw, T. Aslam, B. Merriman, S. Osher, A non-oscillatory eulerian approach to interfaces in multimaterial flows (the ghost fluid method), Journal of computational physics 152 (2) (1999) 457–492.

[32] X. Li, H. Huang, P. Meakin, Level set simulation of coupled advection-diffusion and pore structure evolution due to mineral precipitation in porous media, Water Resources Research 44 (12).

[33] X. Li, H. Huang, P. Meakin, A three-dimensional level set simulation of coupled reactive transport and precipitation/dissolution, International Journal of Heat and Mass Transfer 53 (13-14) (2010) 2908–2923.

[34] S. Molins, D. Trebotich, G. H. Miller, C. I. Steefel, Mineralogical and transport controls on the evolution of porous media texture using direct numerical simulation, Water Resources Research 53 (5) (2017) 3645–3661.

[35] S. Molins, C. Soulaine, N. Prasianakis, A. Abbasi, P. Poncet, A. Ladd, V. Starchenko, S. Roman, D. Trebotich, H. Tchelepi, et al., Simulation of mineral dissolution at the pore scale with evolving fluid-solid interfaces: Review of approaches and benchmark problem set.

[36] M. Chai, K. Luo, C. Shao, H. Wang, J. Fan, A finite difference discretization method for heat and mass transfer with robin boundary conditions on irregular domains, Journal of Computational Physics (2019) 108890.

[37] D. Trebotich, D. Graves, An adaptive finite volume method for the incompressible navier–stokes equations in complex geometries, Communications in Applied Mathematics and Computational Science 10 (1) (2015) 43–82.
[38] D. Trebotich, M. F. Adams, S. Molins, C. I. Steefel, C. Shen, High-resolution simulation of pore-scale reactive transport processes associated with carbon sequestration, Computing in Science & Engineering 16 (6) (2014) 22–31.

[39] K. Luo, Z. Zhuang, J. Fan, N. E. L. Haugen, A ghost-cell immersed boundary method for simulations of heat transfer in compressible flows under different boundary conditions, International Journal of Heat and Mass Transfer 92 (2016) 708–717.

[40] M. Yousefzadeh, Numerical simulation of fluid - mineral interaction and reactive transport in porous and fractured media, Stanford University, 2020.

[41] M. Sussman, P. Smereka, S. Osher, A level set approach for computing solutions to incompressible two-phase flow, Journal of Computational physics 114 (1) (1994) 146–159.

[42] J. H. Ferziger, M. Peric, Computational methods for fluid dynamics, Springer Science & Business Media, 2012.

[43] H. K. Versteeg, W. Malalasekera, An introduction to computational fluid dynamics: the finite volume method, Pearson Education, 2007.

[44] F. H. Harlow, J. E. Welch, Numerical calculation of time-dependent viscous incompressible flow of fluid with free surface, The physics of fluids 8 (12) (1965) 2182–2189.

[45] R. I. Issa, Solution of the implicitly discretised fluid flow equations by operator-splitting, Journal of computational physics 62 (1) (1986) 40–65.

[46] B. P. Leonard, A stable and accurate convective modelling procedure based on quadratic upstream interpolation, Computer methods in applied mechanics and engineering 19 (1) (1979) 59–98.

[47] T. Hayase, J. Humphrey, R. Greif, A consistently formulated quick scheme for fast and stable convergence using finite-volume iterative calculation procedures, J. Comput. Phys. 98 (1) (1992) 108–118.

[48] X.-D. Liu, S. Osher, T. Chan, Weighted essentially non-oscillatory schemes, Journal of computational physics 115 (1) (1994) 200–212.
[49] C.-W. Shu, S. Osher, Efficient implementation of essentially non-oscillatory shock-capturing schemes, Journal of computational physics 77 (2) (1988) 439–471.

[50] F. Gibou, R. Fedkiw, S. Osher, A review of level-set methods and some recent applications, Journal of Computational Physics 353 (2018) 82–109.

[51] T. D. Aslam, A partial differential equation approach to multidimensional extrapolation, Journal of Computational Physics 193 (1) (2004) 349–355.

[52] S. Molins, C. Soulaine, N. I. Prasianakis, A. Abbasi, P. Poncet, A. J. Ladd, V. Starchenko, S. Roman, D. Trebotich, H. A. Tchelepi, et al., Simulation of mineral dissolution at the pore scale with evolving fluid-solid interfaces: Review of approaches and benchmark problem set, Computational Geosciences (2020) 1–34.

[53] P. Meakin, Fractals, scaling and growth far from equilibrium, Vol. 5, Cambridge university press, 1998.

[54] P. Meakin, J. Deutch, Monte carlo simulation of diffusion controlled colloid growth rates in two and three dimensions, The Journal of chemical physics 80 (5) (1984) 2115–2122.

[55] Q. Kang, D. Zhang, P. C. Lichtner, I. N. Tsimpanogiannis, Lattice boltzmann model for crystal growth from supersaturated solution, Geophysical Research Letters 31 (21).

[56] A. M. Tartakovsky, P. Meakin, T. D. Scheibe, R. M. E. West, Simulations of reactive transport and precipitation with smoothed particle hydrodynamics, Journal of Computational Physics 222 (2) (2007) 654–672.

[57] W. W. Mullins, R. Sekerka, Stability of a planar interface during solidification of a dilute binary alloy, Journal of applied physics 35 (2) (1964) 444–451.
Figure 2: The classification of points and stencil used in Li et al. [32]
Figure 3: The stencil used in velocity extrapolation for fluid points
Figure 4: The stencil used in velocity extrapolation for solid points