Chapter 5

The Numerical Algorithm

A fully implicit fully coupled time discretization of the Reaction-Infiltration Instability system (3.15)–(3.19) would lead at each time step to a large and difficult to solve algebraic nonlinear system. To avoid this difficulty we develop a sequential (time-split) algorithm which also uses operator splitting. Time splitting is used to isolate the flow part, the transport part, and the porosity update part. Operator splitting is used to isolate the advection part, reaction part and the diffusion part in the transport equation. By doing so we can use a numerical method which is particularly suited for each piece of the computation. Due to the close coupling between the equations, several outer iterations which include flow, transport, and porosity update are performed. We note that the velocity $\mathbf{u}$, but not the pressure p, appears explicitly in the transport equation (2.4). We first employ the mixed finite element procedure (3.15)–(3.16) to solve for flow and obtain a direct locally mass conservative approximation to $\mathbf{u}$. Next, in the transport solve, we first alternate between advection and reaction (including porosity update), taking a series of smaller time steps. This is needed to ensure stability in the presence of nonlinearities and to satisfy a CFL constraint. All of the computations in this loop are explicit and the cost is relatively small. At each small time step the advection part of the transport equation is solved using a higher-order Godunov method [17]. The advection-reaction solution is then used as an initial value for the diffusion/dispersion part, which is solved using a mixed finite element method. This completes the outer iteration loop. If the porosity change from the previous iteration is larger than a specified tolerance, the algorithm returns to the beginning of the loop using the new porosity value to compute an updated velocity field. We now give a formal description of the algorithm.

5.1 Algorithm

Let m denote the old time level and Δt the current time step size.

$$l = 0, \quad \phi^{m,0} \leftarrow \phi^{m}, \quad c^{m,0} \leftarrow c^{m}$$

While $\| \phi^{m,l+1} - \phi^{m,l} \| >$ Tol and $l <$ max

1. Solve the flow equation (Mixed Finite Element Method):

$$\nabla \cdot \mathbf{u} = k(\phi_f - \phi^{m,l})^{2/3}(c^{m,l} - c_{eq}), \quad \mathbf{u} = -\kappa(\phi^{m,l})\nabla p$$

2. Solve the transport equation

$$\Delta\tilde{t} = \frac{\Delta t}{\mathrm{imax}}, \quad c_1 \leftarrow c^{m}, \quad \phi_1 \leftarrow \phi^{m}$$

for $i = 1, \mathrm{imax}$

<u>Advection:</u> Solve (Godunov)

$$\phi_1 \frac{\bar{c} - c_1}{\Delta \tilde{t}} + \nabla \cdot (c_1 \mathbf{u}) = 0 \Longrightarrow \bar{c}$$

<u>Reaction:</u> Solve

$$\phi_1 \frac{\hat{c} - \bar{c}}{\Delta \tilde{t}} \quad = \quad -(\rho - \bar{c}) k (\phi_f - \phi_1)^{2/3} (\bar{c} - c_{eq}) \Longrightarrow \hat{c}$$

Update porosity: Solve

$$\frac{\tilde{\phi} - \phi_1}{\Delta \tilde{t}} = -k(\phi_f - \tilde{\phi})^{2/3} (\hat{c} - c_{eq}) \Longrightarrow \tilde{\phi}$$

$$c_1 \leftarrow \hat{c}, \quad \phi_1 \leftarrow \tilde{\phi}$$

End for

<u>Diffusion/Dispersion:</u> Solve (Mixed Finite Element Method)

$$\tilde{\phi} \frac{\tilde{c} - \hat{c}}{\Delta t} - \nabla \cdot D \nabla \tilde{c} = 0 \Longrightarrow \tilde{c}$$

3. Update variables

$$\phi^{m,l+1} \leftarrow \tilde{\phi}, \quad c^{m,l+1} \leftarrow \tilde{c}, \quad \kappa = \kappa(\phi^{m,l+1}), \quad l = l + 1$$

End while

$$\phi^{m+1} \leftarrow \phi^{m,l}, \quad c^{m+1} \leftarrow c^{m,l}$$