

Chapter 2

Reaction-Infiltration Instability Problem

2.1 The mathematical model

The mathematical model was developed by Chadam, Hoff, Merino, Ortoleva and Sen [12]. It is based on a simplified geological situation where an aquifer consists of an insoluble porous matrix with a soluble mineral component partially filling the pores. As flow passes through, the mineral dissolves out, leading to an increase of the porosity and the permeability. Across the dissolution zone the soluble mineral content, and hence the porosity, changes from its original downstream value to the altered value upstream. If a protrusion in the porosity level curves occurs, dissolution is enhanced at the tip of the protrusion and the flow focuses there, leading to a fingering effect. On the other hand, diffusion from the sides of the tip slows the reaction rate there and consequently decelerates the advancement of the dissolution front (see Figure

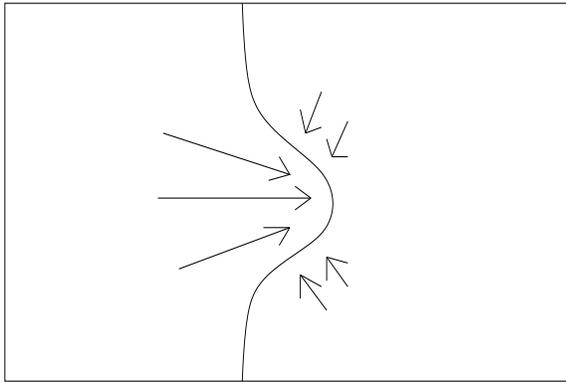


Figure 2.1: Reaction-Infiltration Instability

2.1). As a result of the competition of these two mechanisms the reaction zone could restabilize, go back to the original planar front, or develop fingering.

The Reaction-Infiltration Instability problem is modeled by a system of partial differential equations. If we denote by ϕ the porosity then the flow equation, representing conservation of water, is

$$\nabla \cdot (\bar{\mathbf{u}}\phi) = -\frac{\partial \phi}{\partial t},$$

where the flow velocity $\bar{\mathbf{u}}$ is given by Darcy's law,

$$\bar{\mathbf{u}} = -\kappa(\phi)\nabla p.$$

Here ∇p is the pressure gradient and $\kappa(\phi)$ is a porosity-dependent permeability function. The exact relationship between permeability and porosity is complex and poorly known. It depends on a complex interplay of many factors, such as pore size distribution, pore shapes, and connectivity [37]. It is predicted that $\kappa(\phi)$ is a power function

of porosity. We use the linear function

$$\kappa(\phi) = \left(\frac{\kappa_0}{\phi_0}\right)\phi \quad (2.1)$$

where κ_0 and ϕ_0 are the initial permeability and porosity, respectively. Some of the equations found in the literature are given below.

- P.C. Lichtner [7]

$$\kappa(\phi) = \kappa_0 \left(\frac{\phi}{\phi_0}\right)^3 \frac{1.001 - \phi_0^2}{1.001 - \phi^2}$$

- Kozeny-Carman equation [19]

$$\kappa(\phi) = \frac{\omega\phi^3}{(1 - \phi)^2}$$

where ω is a rock-dependent constant which varies between 10^{-4} and 10^{-10} cm^2 .

- Walder and Nur [30]

$$\kappa(\phi) = \kappa_0 \frac{\phi^n - \phi_c^n}{\phi_0^n - \phi_c^n},$$

where ϕ_c is the critical porosity for through flow.

If we denote by c the concentration of the soluble component then the mass transport equation takes the form

$$\frac{\partial(c\phi)}{\partial t} + \nabla \cdot [c\phi\bar{\mathbf{u}} - D\nabla c\phi] = \rho \frac{\partial\phi}{\partial t},$$

where the right-hand side is the reaction term due to dissolution of the grains comprising the medium and ρ is the molar density of the mineral being dissolved. The

first term in the bracket on the left side of the equation expresses the convection of the solute, and the second term represents both mechanical and diffusive flux.

Let ϕ_f be the final porosity after complete dissolution and c_{eq} be the equilibrium concentration. The rate of increase in porosity is given by [12]

$$\frac{\partial\phi}{\partial t} = -k(\phi_f - \phi)^{\frac{2}{3}}(c - c_{eq}),$$

where k is the reaction rate constant. For moderately reactive chemicals k is between 0.0025 and 0.001 day^{-1} and for highly reactive chemicals k is greater than 0.0025 day^{-1} [31]. The $2/3$ power in the above equation is typical of a simplified surface dissolution [13]. Note that the above equation also represents the rate of dissolution of soluble minerals. The details of its derivation are given in [12]. There are some other equations that represent the change in porosity [29, 32].

Summarizing the above, the governing equations that model the above phenomenology in terms of the variables ϕ , c , and p -the porosity, solute concentration, and pressure, respectively, may be written as:

$$\nabla \cdot (\bar{\mathbf{u}}\phi) = -\frac{\partial\phi}{\partial t}, \quad (2.2)$$

$$\bar{\mathbf{u}} = -\kappa(\phi)\nabla p, \quad (2.3)$$

$$\frac{\partial(c\phi)}{\partial t} + \nabla \cdot [c\phi\bar{\mathbf{u}} - D\nabla c\phi] = \rho\frac{\partial\phi}{\partial t}, \quad (2.4)$$

$$\frac{\partial\phi}{\partial t} = -k(\phi_f - \phi)^{\frac{2}{3}}(c - c_{eq}). \quad (2.5)$$

To incorporate both diffusive and convective mass transport processes the coefficient of hydrodynamical dispersion D is defined by

$$D_{ij} = D_1(\phi)\delta_{ij} + a_T|\bar{\mathbf{u}}|\delta_{ij} + (a_L - a_T)\frac{\bar{u}_i\bar{u}_j}{|\bar{\mathbf{u}}|},$$

where a_L and a_T are called the *longitudinal* and *transversal dispersivities*, respectively, D_1 is the coefficient of purely molecular diffusion, and δ_{ij} is the Kronecker delta function.

To analyze the method two forms of the problem will be given in the next chapter, an operator form and a weak form. In the analysis below we assume that

$$\phi_0 \leq \phi \leq \phi_f - \delta \tag{2.6}$$

for small fixed $\delta > 0$. Under this assumption the right hand side of (2.5) is Lipschitz continuous function of ϕ .

2.2 Some notation

For Ω , a bounded, open subset of \mathbb{R}^d , with $d = 2$ or $d = 3$, having a sufficiently smooth boundary Γ , we define the following Sobolev spaces which are based on the space of square integrable functions on Ω :

$$L^2(\Omega) = \left\{ v : \int_{\Omega} |v|^2 dx = \|v\|_{L^2(\Omega)}^2 < +\infty \right\}$$

For an integer $m \geq 0$ we define

$$H^m(\Omega) = \{ v : D^\alpha v \in L^2(\Omega), |\alpha| \leq m \}$$

where

$$D^\alpha v = \frac{\partial^{|\alpha|} v}{\partial x_1^{\alpha_1} \dots \partial x_n^{\alpha_n}}, \quad |\alpha| = \alpha_1 + \dots + \alpha_n,$$

with derivatives being taken in the sense of distributions. On this space we have the semi-norm

$$|v|_{m,\Omega}^2 = \sum_{|\alpha|=m} |D^\alpha v|_{L^2(\Omega)}^2,$$

and the norm

$$\|v\|_{m,\Omega} = \sum_{k \leq m} |v|_{k,\Omega}^2.$$

In particular, $L^2(\Omega)$ is the space $H^0(\Omega)$ and we shall usually write $\|v\|$ to denote its norm. We also define the special vector-function space

$$H(\text{div}; \Omega) = \{\mathbf{v} : \mathbf{v} \in (L^2(\Omega))^d, \nabla \cdot \mathbf{v} \in L^2(\Omega)\},$$

with a norm

$$\|\mathbf{v}\|_{H(\text{div})} = (\|\mathbf{v}\|^2 + \|\nabla \cdot \mathbf{v}\|^2)^{\frac{1}{2}}.$$

We shall omit the subscript Ω from the notation of the norms.

The standard inequality,

$$ab \leq \frac{\epsilon}{2} a^2 + \frac{2}{\epsilon} b^2, \quad a, b, \epsilon \in R, \epsilon > 0 \quad (2.7)$$

will be used repeatedly in the analysis.

We shall also make use of the following version of Green's formula:

$$\int_{\Omega} (v \nabla \cdot \mathbf{u} + \nabla v \cdot \mathbf{u}) dx = \int_{\Gamma} v \mathbf{u} \cdot \nu dn \quad (2.8)$$

for all $v \in H^1(\Omega)$ and $\mathbf{u} \in H(\text{div}; \Omega)$ and where ν is the unit outward normal along Γ [25].