Chapter 3

Forms of the Problem

3.1 An operator form of the problem

Let $\mathcal{U} = (p, c\phi, \phi)^t$, $M = \text{diag}(0, 1, 1)$, then the system of equations (2.2) - (2.5) can be written as:

$$M\frac{\partial}{\partial t}\mathcal{U} + L(\mathcal{U}) = 0 \tag{3.1}$$

where L is a nonlinear operator which is written as $L = L_1 + L_2 + L_3$ with

$$\begin{aligned} L_1 &= (\nabla \cdot (\phi\kappa(\phi)\nabla p) - f_1)e_1, \\ L_2 &= (\nabla \cdot [-c\phi\kappa(\phi)\nabla p - D\nabla(c\phi)] - f_2)e_2, \\ L_3 &= -f_1 e_3. \end{aligned}$$

Here $e_1 = (1, 0, 0)^T, e_2 = (0, 1, 0)^T, e_3 = (0, 0, 1)^T$ and

$$f_1(c, \phi) = -k(\phi_f - \phi)^{2/3}(c - c_{eq}), \quad f_2(c, \phi) = \rho f_1(c, \phi). \tag{3.2}$$

We also have that $L_2 = L_{21} + L_{22} + L_{23}$ with

$$\begin{aligned} L_{21} &= \nabla \cdot [-c\phi\kappa(\phi)\nabla p], \\ L_{22} &= -f_2, \\ L_{23} &= -\nabla \cdot [D\nabla(c\phi)]. \end{aligned}$$

Therefore, operator splitting method will be analyzed for the case of splitting into three nonlinear operators.

3.2 A weak form of the problem

Consider a polygonal domain $\Omega \subset \mathbb{R}^d$, $d = 2$ or 3, with a boundary $\partial\Omega = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$, where Γ_1 is the inflow, Γ_2 is the outflow, and Γ_3 is the no-flow part of the boundary. Let $\mathbf{u} = \bar{\mathbf{u}}\phi$, and let

$$\mathbf{F} = c\mathbf{u}, \quad \mathbf{q} = -D\nabla(c\phi), \tag{3.3}$$

f_1 and f_2 as in (3.2) above. We rewrite equations (2.2)–(2.5) as:

$$\nabla \cdot \mathbf{u} = -f_1(c,\phi), \qquad \mathbf{u} = -\phi\,\kappa(\phi)\nabla p, \tag{3.4}$$

$$\frac{\partial(c\phi)}{\partial t} + \nabla \cdot (\mathbf{F} + \mathbf{q}) = f_2(c,\phi), \tag{3.5}$$

$$\frac{\partial\phi}{\partial t} = f_1(c,\phi), \tag{3.6}$$

for $x \in \Omega, t \in J = (0,T]$. The system is completed with the boundary conditions

$$\mathbf{u}\cdot\nu = g_1 \text{ on } \Gamma_1, \quad p = g_2 \text{ on } \Gamma_2, \quad \mathbf{u}\cdot\nu = 0 \text{ on } \Gamma_3, \tag{3.7}$$

$$c = c_B \text{ on } \Gamma_1, \quad \mathbf{q} \cdot \nu = 0 \text{ on } \Gamma_2 \cup \Gamma_3, \tag{3.8}$$

and the initial condition

$$c(x,0) = c_0(x), \qquad\qquad x \in \Omega. \tag{3.9}$$

Let $\mathbf{V} = H(\text{div};\Omega)$ and define

$$\mathbf{V}^g = \{\mathbf{v} : \mathbf{v} \in H(\text{div};\Omega), \mathbf{v}\cdot\nu = g \text{ on } \Gamma_1 \text{ and } \mathbf{v}\cdot\nu = 0 \text{ on } \Gamma_3\},$$

$$\bar{\mathbf{V}} = \{\mathbf{v} : \mathbf{v} \in H(\text{div};\Omega), \mathbf{v}\cdot\nu = 0 \text{ on } \Gamma_2 \cup \Gamma_3\}, \qquad W = L^2(\Omega).$$

Let $a(\phi) = (\phi\kappa(\phi))^{-1}$. Multiplying each equation by a test function from the proper space and integrating, the weak solution of (3.3)–(3.9) is $\mathbf{u}(\cdot,t) \in \mathbf{V}^{g_1}$, $p(\cdot,t) \in W$, $\mathbf{q}(\cdot,t) \in \bar{\mathbf{V}}$, $c(\cdot,t) \in W$, and $\phi(\cdot,t) \in W$ such that

$$\begin{aligned}
(a(\phi)\mathbf{u},\mathbf{v}) &= (p,\nabla\cdot\mathbf{v}) - < g_2, \mathbf{v}\cdot\nu >_{\Gamma_2}, & \mathbf{v} \in \mathbf{V}^0, \quad &(3.10)\\
(\nabla\cdot\mathbf{u}, w) &= (-f_1, w), & w \in W, \quad &(3.11)\\
(D^{-1}\mathbf{q},\mathbf{v}) &= (c\phi,\nabla\cdot\mathbf{v}) - < c_B, \mathbf{v}\cdot\nu >_{\Gamma_1}, & \mathbf{v} \in \bar{\mathbf{V}}, \quad &(3.12)\\
(\frac{\partial(c\phi)}{\partial t}, w) + (\nabla\cdot\mathbf{q}, w) &= -(\nabla\cdot\mathbf{F}, w) + (f_2, w), & w \in W, \quad &(3.13)\\
(\frac{\partial\phi}{\partial t}, w) &= (f_1, w), & w \in W. \quad &(3.14)
\end{aligned}$$

where Green's Formula (2.8) is used to obtain (3.10) and (3.12).

3.3 Discretization in space

For $h > 0$, (3.11) - (3.14) are discretized in space on a finite element partition of Ω, $\mathcal{T}_h$, with elements of diameter $\leq h$. Let $\mathbf{V}_h \subset \mathbf{V}$ and $W_h \subset W$ be the lowest order Raviart-Thomas spaces (RT0) defined as follows [34].

For an element $\mathcal{T} \in \mathcal{T}_h$, define

$$P_k(\mathcal{T}) = \{\text{polynomials of degree} \leq k \text{ on } \mathcal{T}\},$$

$$P_{k_1,k_2}(\mathcal{T}) = \{p(x_1, x_2) : p(x_1, x_2) = \sum_{i \leq k_1, j \leq k_2} a_{i,j} x_1^i x_2^j\}.$$

Then we define

$$Q_k(\mathcal{T}) = \begin{cases} P_{k,k}(\mathcal{T}) & \text{for } d = 2, \\ P_{k,k,k}(\mathcal{T}) & \text{for } d = 3. \end{cases}$$

For a rectangular element the Raviart-Thomas velocity spaces (RT) are defined as

$$\text{RTk} = \begin{cases} P_{k+1,k} \times P_{k,k+1} & \text{for } d = 2, \\ P_{k+1,k,k} \times P_{k,k+1,k} \times P_{k,k,k+1} & \text{for } d = 3, \end{cases}$$

with

$$\dim \text{RTk} = \begin{cases} 2(k+1)(k+2) & \text{for } d = 2, \\ 3(k+1)^2(k+2) & \text{for } d = 3. \end{cases}$$

Therefore, for RT0 the degrees of freedom of a vector $\mathbf{v} \in \mathbf{V}_h$ are the values of $\mathbf{v} \cdot \nu$ at the centers of the element edges (faces),see Figure 3.1. For $\mathcal{T} \in \mathcal{T}_h$ we have

$$\mathbf{V}_h(\mathcal{T}) = P_{1,0}(\mathcal{T}) \times P_{0,1}(\mathcal{T}).$$

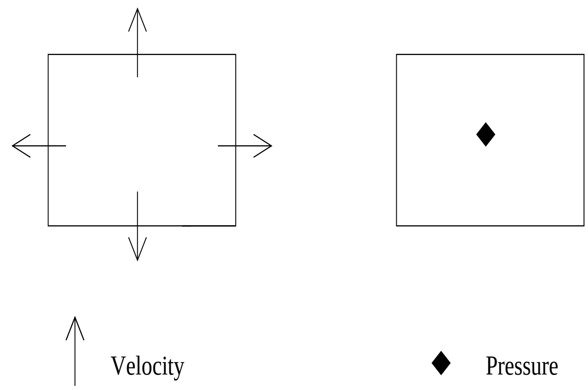

Figure 3.1: RT0

In the RT0 pressure space a function $w \in W_h$ is constant on each element $E \in \mathcal{T}_h$, therefore

$$W_h(\mathcal{T}) = Q_0(\mathcal{T}).$$

These spaces possess the approximation properties [10, 21]:

$$(A_p) \qquad \begin{aligned} \inf_{\mathbf{v}\in\mathbf{V}_h} \quad & \|\mathbf{q}-\mathbf{v}\| \le K\|\mathbf{q}\|_1 h, \\ \inf_{\mathbf{v}\in\mathbf{V}_h} \quad & \|\mathbf{q}-\mathbf{v}\|_{H(\mathrm{div})} \le K(\|\mathbf{q}\|_1 + \|\nabla\cdot\mathbf{q}\|_1)h, \\ \inf_{w\in W_h} \quad & \|\varphi - w\| \le K\|\varphi\|_1 h. \end{aligned}$$

Here and in the rest of the thesis K denotes a generic positive constant independent of h. Let

$$\mathbf{V}_h^g = \{\mathbf{v}\in\mathbf{V}_h; <\mathbf{v}\cdot\nu - g, \mu >= 0 \ \forall\mu\in\mathbf{V}_h\cdot\nu|_{\Gamma_1}, \text{ and } \ \mathbf{v}\cdot\nu = 0 \text{ on } \Gamma_3\},$$

$$\bar{\mathbf{V}}_h = \{\mathbf{v}\in\mathbf{V}_h : \mathbf{v}\cdot\nu = 0 \ \text{ on } \ \Gamma_2\cup\Gamma_3\},$$

In the semidiscrete mixed finite element approximation to (3.10)–(3.14) we seek $\mathbf{U}(\cdot,t) \in \mathbf{V}_h^{g_1}$, $P(\cdot,t) \in W_h$, $\mathbf{Q}(\cdot,t) \in \bar{\mathbf{V}}_h$, $C(\cdot,t) \in W_h$, and $\Phi(\cdot,t) \in W_h$ such that

$$(a(\Phi)\mathbf{U},\mathbf{v}) = (P,\nabla\cdot\mathbf{v}) - < g_2, \mathbf{v}\cdot\nu >_{\Gamma_2}, \qquad \mathbf{v} \in \mathbf{V}_h^0, \tag{3.15}$$

$$(\nabla\cdot\mathbf{U}, w) = (-f_1, w), \qquad w \in W_h, \tag{3.16}$$

$$(D^{-1}\mathbf{Q},\mathbf{v}) = (C\Phi,\nabla\cdot\mathbf{v}) - < c_B, \mathbf{v}\cdot\nu >_{\Gamma_1}, \qquad \mathbf{v} \in \bar{\mathbf{V}}_h, \tag{3.17}$$

$$(\frac{\partial(C\Phi)}{\partial t}, w) + (\nabla\cdot\mathbf{Q}, w) = -(\nabla\cdot\mathbf{F}_h, w) + (f_2, w), \qquad w \in W_h, \tag{3.18}$$

$$(\frac{\partial\Phi}{\partial t}, w) = (f_1, w), \qquad w \in W_h. \tag{3.19}$$

Here $\mathbf{F}_h$ is a numerical approximation to the advective flux $\mathbf{F} = c\mathbf{u}$ which can be obtained by an appropriate advection method.

3.4 Discretization in time

Let $\{t_n\}_{n=0}^N$ be a monotone partition of $[0,T]$ with $t_0 = 0$ and $t_N = T$, let $\Delta t_n = t_n - t_{n-1}$, and let $f^n = f(t_n)$. Let $\Delta t = \max_n \Delta t_n$. Our time discretization scheme is based on operator-splitting and Godunov method for the advection part $(\widetilde{\phi c})_t + \nabla\cdot\mathbf{F} = 0$ of the transport equation. Let $(C\Phi)^{n-1}$ be given approximations at time level t_{n-1}. Godunov method is based on conservation of mass element-by-element. Let $\mathcal{T}$ be a generic element in $\mathcal{T}_h$. Integrate over $\mathcal{T}\times[t^{n-1},t^n]$ to get

$$\int_{\mathcal{T}} \widetilde{(c\phi)}^n = \int_{\mathcal{T}} (C\Phi)^{n-1} - \int_{t^{n-1}}^{t^n} \int_{\partial\mathcal{T}} \mathbf{F}\cdot\nu$$

The Godunov method approximates $\mathbf{F}$ by a discontinuous, piecewise polynomial. The normal advective flux $\mathbf{F}\cdot\nu$ is approximated by a constant on element edges. On the boundary of each element the flux is approximated numerically by first calculating left and right states w^L and w^R, and then using the Godunov flux to determine the solution of a one-dimensional Riemann problem in the direction normal to the boundary [23]. The Godunov flux $H_\omega(w^L, w^R)$ for a given flux function $\omega(s)$ is given by [17]

$$H_\omega(w^L, w^R) = \begin{cases} \min_{w^L\le s\le w^R}\omega(s) & \text{if } w^L \le w^R, \\ \max_{w^R\le s\le w^L}\omega(s) & \text{otherwise.}\end{cases}$$

Now, let $\mathbf{G}^{n-1}$ be the Godunov approximation to $\mathbf{F}$ and define $(\widetilde{C\Phi})^n \in W_h$ by

$$(\widetilde{C\Phi})^n|_{\mathcal{T}} = (C\Phi)^{n-1}|_{\mathcal{T}} - \frac{\Delta t}{m(\mathcal{T})}\int_{\partial\mathcal{T}} \mathbf{G}^{n-1}\cdot\nu$$

where $m(\mathcal{T})$ is the measure of $\mathcal{T}$. A CFL (Courant, Friedrichs, and Lewy) stability constraint is assumed. Thus, if $\mathbf{F} = \mathbf{F}(c,\phi)$, then the time-step satisfies

$$\sup|\mathbf{F}|\Delta t \le h.$$

Next, we solve the reaction part $(\widehat{c\phi})_t = f_3(c,\phi)$ with initial condition $(\widetilde{C\Phi})^n \in W_h$. Applying backward differencing in time to get

$$\frac{(\widehat{C\Phi})^n - (\widetilde{C\Phi})^n}{\Delta t} = f_2(C^n,\Phi^n) = \tilde{f}_2^n$$

and then substituting the value for $(\widetilde{C\Phi})^n$ we get

$$(\widehat{C\Phi})^n|_{\mathcal{T}} = (C\Phi)^{n-1}|_{\mathcal{T}} + \Delta t\tilde{f}_2^n|_{\mathcal{T}} - \frac{\Delta t}{m(\mathcal{T})}\int_{\partial\mathcal{T}} \mathbf{G}^{n-1}\cdot\nu.$$

Finally we solve the diffusion/dispersion part

$$(c\phi)_t + \nabla \cdot \mathbf{q} = 0, \qquad \mathbf{q} = -D\nabla c$$

with initial condition $(\widehat{C\Phi})^n$. Applying backward differencing in time to get

$$\frac{(C\Phi)^n - (\widehat{C\Phi})^n}{\Delta t} + \nabla \cdot \mathbf{q} = 0,$$

and then substituting the value for $(\widehat{C\Phi})^n$ we get:

$$\frac{(C\Phi)^n - (C\Phi)^{n-1}}{\Delta t} - \tilde{f}_2^n + \frac{1}{m(\mathcal{T})}\int_{\partial\mathcal{T}} \mathbf{G}^{n-1} \cdot \nu + \nabla \cdot \mathbf{q} = 0.$$

The approximation $(C\Phi)^n \in W_h$ and $\mathbf{Q}^n \in \bar{\mathbf{V}}_h$ to $(c\phi)^n$ and $\mathbf{q}^n$, respectively, are determined by

$$(D^{-1}\mathbf{Q}^n, \mathbf{v}) - ((C\Phi)^n, \nabla \cdot \mathbf{v}) =< c_B, \mathbf{v} \cdot \nu >_{\Gamma_1}, \quad \mathbf{v} \in \bar{\mathbf{V}}_h \tag{3.20}$$

$$(\partial_t((C\Phi)^n), w) + (\nabla \cdot \mathbf{Q}^n, w) = -(\nabla \cdot \mathbf{G}^{n-1}, w) + (\tilde{f}_2^n, w), \quad w \in W_h \tag{3.21}$$

where

$$\partial_t (C\Phi)^n = \frac{(C\Phi)^n - (C\Phi)^{n-1}}{\Delta t_n}.$$

For the time discretization of (3.19) we employ Euler method

$$\left(\frac{\Phi^{n+1} - \Phi^n}{\Delta t_n}, w\right) = (f_1(\Phi^n, C^n), w), \quad w \in W_h. \tag{3.22}$$