Numerical Simulations of Miscible Channel Flow with Chemical Reactions

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Approval Sheet

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To my parents and brother
Nomenclature

Roman Letters

\( x \) : horizontal coordinate
\( y \) : vertical coordinate
\( t \) : time
\( H \) : height of the channel
\( L \) : length of the channel
\( V \) : average velocity
\( Q \) : total flow rate
\( M \) : mass fraction
\( E \) : activation energy
\( R \) : universal gas constant
\( \mathcal{H} \) : discrete convection
\( \mathcal{L} \) : discrete diffusion
\( Q \) : dimensionless heat of reaction
\( T_1 \) : temperature of the initial fluid
\( T_2 \) : temperature of the injected fluid
\( \phi_m \) : volume fraction of the reactant
\( \phi_p \) : volume fraction of the product
\( u \) : velocity field
\( p \) : pressure field of the fluid
\( m \) : viscosity ratio
\( D_m \) : diffusion coefficient for reactant
\( D_p \) : diffusion coefficient for product
\( r_T \) : dimensionless temperature of the invading fluid
\( \kappa_o \) : pre-exponential factor
\( R_m \) : log-mobility ratios of reactant
\( R_p \) : log-mobility ratios of reactant
\( Re \) : Reynolds number
\( Sc \) : Schmidt number
\( Pe \) : Peclet number
\( Pr \) : Prandtl number
\( Da \) : Damköhler number
\( C_p \) : specific heat at constant pressure
\( n \) : time steps
\( u^* \) : intermediate velocity
\( V_f \) : velocity of the tip
\( q \) : heat of the reaction
Greek Letters

$\alpha$ : thermal diffusivity

$\beta$ : dimensionless activation energy

$\rho$ : density of the fluid

$\mu$ : dimensionless viscosity of the fluid

$\kappa$ : rate of the reaction
Abstract

We investigate the pressure-driven miscible displacement of one fluid by another in a horizontal channel in the presence of an exothermic chemical reaction. We solve the continuity, Navier-Stokes, and energy conservation equations coupled to convective-diffusion equations of the reactant and product. The viscosity is assumed to depend on the volume fraction of the reactant and product as well as the temperature. The effects of relevant parameters such as the Reynolds number, Schmidt number, Damköhler number and the viscosity ratio of the reactant and product are investigated. Our results indicate that increasing the intensity of chemical reaction by increasing Damköhler number and decreasing dimensionless activation energy increases the displacement rate. We found that increasing Reynolds number leads to more pronounced instabilities and roll-up phenomena, which in turn provides rapid displacement of the resident fluid inside the channel. However, heat of reaction and the Schmidt numbers of the reactant and product have a negligible influence on the displacement rates for the parameter range considered.
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Chapter 1

Introduction

1.1 Introduction

The dynamics of two-fluid flows is an active research area due to their central importance to a number of industrial applications, which include enhanced oil recovery, fixed bed regeneration, hydrology and filtration, transportation of crude oil in pipelines [1], and mixing of liquids using, for instance, static mixers [2]. In food and drink industrial plants, cleaning involves the removal of a highly viscous fluid by high-speed flow of water pumped through the plant [3]. Thus in the latter case, achieving fundamental understanding of these flows permits the determination of the degree of mixing between the fluids and minimization of the amount of waste-water utilized.

The stability of two-phase flows in a channel or pipe have been widely investigated both theoretically [4–6] and experimentally [1, 7–9] in the context of immiscible [9–16] and miscible [17–21] fluids. By conducting a linear stability analysis, Ern et al. [19] has shown that for rapidly-varying viscous stratification, diffusion can be destabilising. However, Govindarajan [18] has demonstrated that three-layer Poiseuille flow is unstable at high Schmidt numbers and low Reynolds numbers. In neutrally-buoyant, core-annular flows, Selvam et al. [6] have shown that, above a critical viscosity ratio, the flow is unstable even when the less viscous fluid is at the wall (although it should be noted that the range of parameters over which this is true is limited). This is in contrast to the studies of Joseph et al. [1] and Malik and Hooper [22], who found stable flow in this configuration. Several authors [23–27] also experimentally studied miscible core-annular flows and investigated the thickness of the remnant fluid layer, left on the pipe walls and the speed of the propagating “finger” tip. The development of different instability patterns, like axisymmetric “corkscrew” patterns in miscible flows, have also been investigated [2, 28-31]. d’Olce et al [32] observed axisymmetric “pearl” and “mushroom” patterns in neutrally-buoyant, core-annular horizontal pipe flow at high Schmidt numbers and Reynolds numbers in the range $2 < \text{Re} < 60$.

Sahu et al. [20] studied the stability of neutrally-buoyant, two-fluid miscible channel flows for large viscosity contrasts. They carried out a generalized spatio-temporal linear stability analysis [33–35] for the case of a three-layer flow and determined the boundaries between convectively and absolutely unstable flows in the space of the Reynolds number and viscosity ratio, for parameterically-varying Schmidt numbers. The vertical gradients of viscosity perturbations were found to be the main destabilizing influence. In order to understand the flow dynamics in the nonlinear regime, the
Navier-Stokes equations coupled to a convective-diffusion equation for the concentration of the more viscous fluid were solved. These transient numerical simulations demonstrated the development of complex dynamics characterized by ‘roll-up’ and convective mixing, which increase in intensity with increasing viscosity ratio, Reynolds and Schmidt numbers. Selvam et al. [36] also conducted a similar analysis in miscible core annular flows at high Schmidt numbers. This system was also studied experimentally by d’Olce et al. [37]. They observed absolute instabilities for a range of core radii for high viscosity ratios when the less viscous fluid is in the core. The work of Sahu et al. [20] has been extended to account for buoyancy effects in inclined channels [38], and non-isothermal effects in pressure-driven miscible displacement flow [5] in the nonlinear regime. The results of Sahu et al. [5, 38] demonstrated that the rates of mixing and displacement of the more viscous fluid are promoted by the development of Rayleigh-Taylor instabilities, and enhanced with increasing density ratio, Froude number and viscous heating. The mixing rates were also shown to increase with increasing inclination angles when the displaced fluid is also the denser one.

In spite of the large volume of research on two-fluid flows, very few studies have considered the effects of chemical reactions on the flow dynamics in pressure-driven displacement flows although their effects on viscous fingering in porous media have been examined extensively by several authors [39–43]. Nagatsu et al. [44, 45] have studied experimentally the reactive viscous fingering in a Hele-Shaw cell and found that fingering becomes more pronounced when the product is more viscous than the reactant; the reverse trend was observed for reactions generating a less viscous product. For relatively slow reactions, these authors have also shown that fingering becomes more vigorous in the reactive than in the non-reactive case.

In the present work, we examine the stability of miscible, pressure-driven displacements in horizontal, rectangular channels in the presence of exothermic chemical reactions via direct numerical simulations. We solve the mass and energy conservation equations coupled to convective-diffusion equations of the reactant and product, and, in contrast to previous studies [39, 40], the full Navier-Stokes equations (rather than Darcy’s equations, appropriate for Hele-Shaw flow). The viscosity is assumed to vary with temperature and the volume fraction of the reactant and product; the density is assumed to remain constant. The governing equations are parameterised by the Reynolds, Schmidt, and Damköhler numbers, and the viscosity ratio of the reactant and product. Our numerical results demonstrate that increasing the intensity of chemical reaction by increasing Damköhler number and decreasing dimensionless activation energy increases the displacement of the resident fluid present inside the channel. We also found that increasing Reynolds number leads to more pronounced instabilities and roll-up phenomena, which increases the displacement rates of the resident fluid.

The rest of this thesis is organized as follows. The problem is formulated in chapter 2, the method of solution using a finite volume approach is explained in chapter 3 and the results of the numerical simulations are presented in chapter 4.Concluding remarks are provided in chapter 5.
Chapter 2

Formulation

2.1 Governing equations

We consider the two-dimensional miscible channel flow, wherein, initially, the horizontal channel is occupied by a stationary, viscous fluid of viscosity \( \mu_1 \). Another liquid, with viscosity \( \mu_2 \), is injected into the channel with an average velocity, \( V \equiv Q_f/H \), where \( Q_f \) denotes the total flow rate. The initially resident and invading fluids are labelled ‘1’ and ‘2’, as shown in Fig. 1, and their initial temperatures are denoted by \( T_1 \) and \( T_2 \), respectively. A volume fraction, \( \phi_m \), is also defined so that it is equal to unity and zero for fluids ‘1’ and ‘2’, respectively. An exothermic chemical reaction takes place in the mixed region separating the two fluids that alters the viscosity of the fluid in this region. Initially, the volume fraction of the product of this reaction, \( \phi_p \), equals to zero. We assume that the densities of all fluids to be the same. A rectangular coordinate system, \((x,y)\), is used to model the flow dynamics, where \( x \) and \( y \) denote the horizontal and vertical coordinates, and the channel inlet and outlet are located at \( x = 0 \) and \( x = L \), respectively. The channel walls, which are rigid and impermeable, are located at \( y = 0 \) and \( y = H \), respectively.

![Figure 2.1: Schematic diagram showing the initial flow configuration: fluid ‘1’ occupies the entire channel, and is about to be displaced by the in-flowing fluid. The symbols are defined in the text.](image)

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The equations governing the problem can be written as:

\[ \nabla \cdot \mathbf{u} = 0, \quad (2.1) \]

\[ \rho \left[ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right] = -\nabla p + \nabla \cdot \left[ \mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \right], \quad (2.2) \]

\[ \frac{\partial \phi_m}{\partial t} + \mathbf{u} \cdot \nabla \phi_m = D_m \nabla^2 \phi_m - k \phi_m (1 - \phi_m), \quad (2.3) \]

\[ \frac{\partial \phi_p}{\partial t} + \mathbf{u} \cdot \nabla \phi_p = D_p \nabla^2 \phi_p + k \phi_m (1 - \phi_m), \quad (2.4) \]

\[ \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \alpha \nabla^2 T + k \phi_m (1 - \phi_m) q, \quad (2.5) \]

where \( \mathbf{u}, p \) and \( T \) denote the velocity, pressure and temperature fields of the fluid, respectively; \( D_m \) and \( D_p \) are the diffusion coefficients of the reactant and product, respectively; \( \alpha \) denotes the thermal diffusivity and \( q \) is the heat of reaction. In the above equation, the rate of reaction is defined as

\[ k(T) = k_0 \exp(-E/RT), \quad (2.6) \]

where \( k_0 \) is the pre-exponential factor, \( E \) is the activation energy, and \( R \) is the universal gas constant.

The viscosity of the fluid is assumed to depend on temperature and the volume fractions of the reactant and product as follows:

\[ \mu = \mu_2(T_1) e^{[R_m \phi_m + R_p \phi_p, \frac{T - T_1}{T_1}]} , \quad (2.7) \]

where \( R_m (\equiv \ln(\mu_1/\mu_2)) \) and \( R_p (\equiv \ln(\mu_p/\mu_2)) \) are the log-mobility ratios of the reactant and product, respectively.

The following scaling is employed in order to render the governing equations dimensionless:

\[ (x, y) = H (\tilde{x}, \tilde{y}), \]

\[ t = \frac{H}{V T}, \]

\[ (u, v) = V (\tilde{u}, \tilde{v}), \]

\[ p = \rho V^2 \tilde{p}, \]

\[ \mu = \tilde{\mu} \mu_2(T_1), \]

\[ T = \tilde{T} T_1 + T_1, \]

where the tildes designate dimensionless quantities. After dropping tildes from all non-dimensional terms, the governing dimensionless equations are given by

\[ \nabla \cdot \mathbf{u} = 0, \quad (2.8) \]

\[ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \frac{1}{Re} \nabla \cdot \left[ \mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \right], \quad (2.9) \]
\[
\frac{\partial \phi_m}{\partial t} + \mathbf{u} \cdot \nabla \phi_m = \frac{1}{\text{ReSc}_m} \nabla^2 \phi_m - Da e^{-\beta/(T+1)} \phi_m (1 - \phi_m), \tag{2.10}
\]

\[
\frac{\partial \phi_p}{\partial t} + \mathbf{u} \cdot \nabla \phi_p = \frac{1}{\text{ReSc}_p} \nabla^2 \phi_p + Da e^{-\beta/(T+1)} \phi_m (1 - \phi_m), \tag{2.11}
\]

\[
\frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla T = \frac{1}{\text{RePr}} \nabla^2 T + Da Q e^{-\beta/(T+1)} \phi_m (1 - \phi_m), \tag{2.12}
\]

where \(\text{Re} \equiv \rho V H/\mu_2(T_1)\) denotes the Reynolds number, \(\text{Sc}_i \equiv \mu_2(T_1)/\rho D_i (i = m, p)\) represent the Schmidt numbers of the reactant and product; \(Q \equiv q/T_1 \rho c_p\) is the dimensionless heat of reaction, and \(Da \equiv k_0 H/V\) and \(\text{Pr} \equiv \mu_2(T_1)/\rho \alpha\) are the Damköhler number and the Prandtl number, respectively, wherein \(c_p\) is the specific heat at constant pressure. The dimensionless activation energy is given by \(\beta = E/RT_1\), while the dimensionless temperature of the invading fluid is expressed by \(r_T = (T_2 - T_1)/T_1\). Finally, the dimensionless viscosity, \(\mu\) has the following dependence on \(T, \phi_m\) and \(\phi_p\):

\[
\mu = \exp (R_m \phi_m + R_p \phi_p - T). \tag{2.13}
\]
Chapter 3

Numerical Methods

The convective-diffusion equation is a nonlinear fourth order partial differential equation, and its numerical solution is complicated. Several methods have been proposed previously to solve this equation. We use a finite-volume approach similar to the one developed by Ding et al. [46] in order to solve the system of Eqs. (2.8)-(2.13). These equations are discretized using a staggered grid; the scalar variables (pressure, temperature and volume fraction) are defined at the center of each cell and the velocity components are defined at the cell faces.

![Staggered grid with flow variables](image)

Figure 3.1: Two-dimensional staggered grid with flow variables

The discretized advection-diffusion equations for the reactant and product and the energy equation are given by:

\[
\begin{align*}
\frac{1.5\phi_m^{n+1} - 2\phi_m^n + 0.5\phi_m^{n-1}}{\Delta t} &= \frac{1}{\text{ReSc}_m} \nabla^2 \phi_m^{n+1} - 2 \nabla \cdot (u^n \phi_m^n) + D_{\alpha e}^{-\beta/(T+1)} \phi_m (1 - \phi_m), \\
\nabla \cdot (u^n \phi_m^{n-1}) &= D_{\alpha e}^{-\beta/(T+1)} \phi_m (1 - \phi_m), \\
\frac{1.5\phi_p^{n+1} - 2\phi_p^n + 0.5\phi_p^{n-1}}{\Delta t} &= \frac{1}{\text{ReSc}_p} \nabla^2 \phi_p^{n+1} - 2 \nabla \cdot (u^n \phi_p^n) + D_{\alpha e}^{-\beta/(T+1)} \phi_m (1 - \phi_m), \\
\nabla \cdot (u^n \phi_p^{n-1}) &= D_{\alpha e}^{-\beta/(T+1)} \phi_m (1 - \phi_m),
\end{align*}
\]
\[
\frac{1.5T^{n+1} - 2T^n + 0.5T^{n-1}}{\Delta t} = \frac{1}{\text{RePr}} \nabla^2 T^{n+1} - 2 \nabla \cdot (u^n T^n) + \\
\nabla \cdot (u^{n-1} T^{n-1}) + Da \Phi e^{-\beta/(T+1)} \phi_m (1 - \phi_m), \tag{3.3}
\]

where \(\Delta t = t^{n+1} - t^n\) and the superscript \(n\) signifies the discretized \(n^{th}\) step. In order to discretize the advective terms in the Eqs. (3.1)-(3.3), a weighted essentially non-oscillatory (WENO) scheme is used, while a centered-difference scheme is used to discretize the diffusive terms on the right-hand-sides of these equations.

In order to achieve second-order accuracy in the temporal discretization, the Adams-Bashforth and Crank-Nicolson methods are used for the advective and second-order dissipation terms in Eq. (2.9), respectively. This results in the following discretized equation:

\[
\frac{u^* - u^n}{\Delta t} = \frac{1}{\rho^{n+1/2}} \left\{ -1.5H(u^n) - 0.5H(u^{n-1}) \right\} + \frac{1}{2\text{Re}} \left\{ L(u^*, \mu^{n+1}) + L(u^n, \mu^n) \right\}, \tag{3.4}
\]

where \(u^*\) is the intermediate velocity, and \(H\) and \(L\) denote the discrete convection and diffusion operators, respectively. The intermediate velocity \(u^*\) is then corrected to \((n + 1)^{th}\) time level as follows

\[
\frac{u^{n+1} - u^*}{\Delta t} = \nabla p^{n+1/2}. \tag{3.5}
\]

The pressure distribution is obtained from the continuity equation at time step \(n + 1\) using

\[
\nabla \cdot \left( \nabla p^{n+1/2} \right) = \frac{\nabla \cdot u^*}{\Delta t}. \tag{3.6}
\]

At the top and bottom walls, solutions of the above discretized equations are subject to no-slip, no-penetration conditions for the velocity, and no-flux condition for the temperature and the volume fractions of the reactant and product. A fully-developed velocity profile with a constant flow rate taken to be unity is imposed at the inlet \((x = 0)\), and Neumann boundary conditions is used at the outlet \((x = L)\).

The following steps are employed in our numerical solver in order to solve Eqs. (2.8)-(2.12):

- The temperature field and volume fractions of the reactant and product are updated by solving Eqs. (2.10)-(2.12) with the velocity field at time steps \(n\) and \(n - 1\);
- The velocity field is then updated to time-step \(n + 1\) by solving Eqs. (2.9) and (2.8).

The numerical procedure described above was originally developed by Ding et al. [46] in the context of interfacial flows.

Sahu et al. [20, 38] then modified this procedure to simulate pressure-driven, neutrally-buoyant miscible channel flow with high viscosity contrast. The results are presented next.
Chapter 4

Results and Discussion

4.1 Grid independence test

We begin the presentation of our results by conducting mesh refinement test to show the convergence of the numerical method. The temporal evolution of a dimensionless measure of the mass of the displaced fluid ‘1’, \( M_{0.95}/M_0 \), is plotted in Fig.4.1(a) for \( Re = 100, Pr = 7, Sc_m = 100, Sc_p = 50, Da = 0.1, r_T = 1, \beta = 1, Q = 100, R_m = 2.3026 \) and \( R_p = -1.609 \). Here, \( M_{0.95} \) and \( M_0 \) denote the mass of fluid with \( \phi_m \geq 0.95 \), and that of fluid ‘1’ initially occupying the channel, respectively. The parameter values chosen are characteristic of a situation where a cold fluid is displaced by a hot fluid, of lower viscosity and the viscosity of the product due to the chemical reaction is lower than those of the reactants.

![Figure 4.1](image)

Figure 4.1: (a) Mass fraction \( M_{0.95}/M_0 \) of \( \phi_m \), and (b) temporal evolution of the position of the leading front separating the two fluids, \( x_{tip} \) for different grid densities. The rest of the parameter values are \( Re = 500, Pr = 7, Sc_m = 100, Sc_p = 50, Da = 0.1, r_T = 1, \beta = 1, Q = 100, R_m = 2.3026 \) and \( R_p = -1.609 \). The dotted lines in panel (a) and (b) represent the limiting case given by \( M_{0.95}/M_0 = 1 - tH/L \) and \( x_{tip} = t \), respectively.

Inspection of Fig.4.1(a) reveals that \( M_{0.95}/M_0 \) undergoes an almost linear decrease at the earlier stages of the flow due to its displacement by fluid ‘2’. The slope of the curve during this linear stage (before the ‘front’ separating the fluids has reached the channel exits) is considerably steeper than that of the line represented by \( 1 - tH/L \) which corresponds to the plug flow displacement of fluid ‘1’.
by fluid ‘2’. At approximately $t = 30$ for this set of parameters, when the ‘front’ of the displacing fluid ‘2’ reaches the end of simulation domain, a transition to another linear regime occurs; the slope of the $M_{0.95}/M_0$ versus time plot in this regime is much smaller than the previous one. At this later stage, the flow dynamics is controlled by diffusion. The temporal variation of the spatial location of the leading ‘front’, or ‘finger’, separating the two fluids, $x_{\text{tip}}$ is plotted in Fig. 4.1(b); this exhibits a linear dependence on time, the slope of which provides an estimate of the front speed [5,20,38]. The results in Fig. 4.1(b) are obtained using different grid points for the same computational domain. It is evident that convergence of the results has been achieved upon mesh refinement as the curves are virtually indistinguishable for different mesh sizes. The front velocity of the finger, obtained using different sets of grid points, is also compared in Table 4.1. In view of this observed small effect of the grid, the rest of the computations presented in this thesis were performed using $41 \times 701$ grid points, in a channel of aspect ratio of 1 : 40.

Table 4.1: The velocity of the finger tip, $V_f$, for different grid densities. The rest of the parameter values are the same as those used to generate Fig. 4.1.

<table>
<thead>
<tr>
<th>Grid</th>
<th>$V_f$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$41 \times 701$</td>
<td>1.68</td>
</tr>
<tr>
<td>$61 \times 701$</td>
<td>1.68</td>
</tr>
<tr>
<td>$41 \times 1001$</td>
<td>1.61</td>
</tr>
</tbody>
</table>

The spatio-temporal evolution of $\phi_m$, $\phi_p$, $T$ and $\mu$ fields for the same parameter values as those used to generate Fig. 4.1 is shown in Fig. 4.2(a), (b), (c) and (d), respectively. Panel (a) of this figure shows that the displacement of fluid ‘1’ by a finger of the less viscous and warmer fluid ‘2’ leaves behind virtually no trace of the latter adhering to the channel walls. It is also seen that mild Kelvin-Helmholtz-type ‘roll-up’ phenomena become apparent at the diffuse ‘interface’ separating the two fluids at later times; these phenomena become pronounced at higher viscosity ratios, Re, and Sc [20,32]. The volume fraction of the product of the chemical reaction that takes place between fluids ‘1’ and ‘2’, depicted in Fig. 4.2(b), is highest in the diffuse interfacial region at early times; at later times, the convective mixing brought about by the roll-up phenomena entrain the product from the wall region into the core. The mixing action of the roll-up instabilities is also clearly seen in the case of the temperature within the channel shown in Fig. 4.2(c). In contrast, very little mixing can be seen in the case of the viscosity, $\mu$, which exhibits very similar patterns to those associated with the dynamics of fluids ‘1’ and ‘2’, as shown in Fig. 4.2(d); this is due to the dependence of $\mu$ on $\phi_m$ through the term $\exp(R_m \phi_m)$ in Eq. (2.13), which, for the parameter values used to generate Fig. 4.2, is the dominant contribution to that equation. To compare this dynamics to a reference case, the spatio-temporal evolution of $\phi_m$, $\phi_p$, $T$ and $\mu$ fields for $r_T = 0$, with the rest of the parameter values remaining the same as in Fig. 4.1, is shown in Fig. 4.3(a), (b), (c) and (d), respectively. In this case, there is no imposed temperature gradient, i.e the system is isothermal at $t = 0$. However, at later times, a temperature gradient arises due to heat generation by the exothermic chemical reaction. It can be clearly seen in Fig. 4.3(c) that the temperature is maximum at the interfacial region where the reaction takes place.
Figure 4.2: Spatio-temporal evolution of the contours of (a) $\phi_m$ (b) $\phi_p$ (c) $T$ (d) $\mu$ at successive times (from top to bottom: $t = 10, 20$ and $25$). The rest of the parameter values are the same as those used to generate Fig. 4.1. The color-maps are shown at the bottom.
Figure 4.3: Spatio-temporal evolution of the contours of (a) $\phi_m$ (b) $\phi_p$ (c) $T$ (d) $\mu$ at successive times (from top to bottom: $t = 10, 20$ and $25$) for $r_T = 0$ (at $t = 0$ flow is isothermal). The rest of the parameter values are the same as those used to generate Fig. 4.1. The color-maps are shown at the bottom.
4.2 Effects of Damköhler number

Next, we examine the parametric dependence of the temporal variation of $M_{0.95}/M_0$ on $Da$, which provides a dimensionless measure of the relative importance of chemical reactions in this flow; this is shown in Fig. 4.4 with the rest of the parameters remaining unaltered from those used to generate Figs. 4.1 and 4.2. Inspection of panel (a) of this figure shows that increasing the relative intensity of chemical reaction by increasing the value of $Da$ leads to more rapid displacement in comparison to the displacement without chemical reactions ($Da = 0$). It can be seen that all the curves in Fig. 4.4(a) lie below the $1 - tH/L$ curve that corresponds to a ‘plug-flow’-type displacement in which the ‘interface’ separating the fluids remains vertical throughout; the curves closest to the $1 - tH/L$ line are those associated with $Da = 0$. In Fig. 4.4(b), it is clearly seen that increasing $Da$ leads to an increase in the speed of the penetrating front.

Figure 4.4: (a,c) Mass fraction $M_{0.95}/M_0$ of $\phi_m$, and (b,d) temporal evolution of the position of the leading front separating the two fluids, $x_{tip}$ for different values of $Da$. Here panels (a and b) and (c and d) correspond to the parameters ($R_m = 2.3026$ and $R_p = -1.609$) and ($R_m = 1.609$ and $R_p = 2.3026$), respectively. The rest of the parameter values are Re = 500, Pr = 7, Sc_m = 100, Sc_p = 50, $r_T = 1$, $\beta = 1$ and $Q = 100$. The dotted lines in panels (a,c) and (b,d) represent the limiting case given by $M_{0.95}/M_0 = 1 - tH/L$ and $x_{tip} = t$, respectively.
The spatio-temporal evolution of the $\phi_m$ fields associated with $Da = 0$ and 0.5 is shown in Fig. 4.5(a) and (b), respectively. It can be seen in Fig. 4.5(a) that for $Da = 0$ the remnants of $\phi_m$ assume the form of thin layers adjacent to the upper and lower channel walls. Also evident are roll-up instabilities that lead to vigorous, convective mixing of the two fluids. In the reactive flow case ($Da = 0.5$), however, shown in Fig. 4.5(b), the flow dynamics are markedly different: the ‘interfacial’ region remains essentially parabolic, with a well-defined ‘nose’, and there is little evidence of instability.

Figure 4.5: Spatio-temporal evolution of the contours of $\phi_m$ for (a) $Da = 0$ and (b) $Da = 0.5$ at successive times (from top to bottom in each panel: $t = 5, 10, 15$ and 20) for $R_m = 2.3026$ and $R_p = -1.609$. The rest of the parameter values are the same as those used to generate Fig. 4.17. The color-map is shown at the bottom.
It can also be seen that reactive displacements appear to be faster and more efficient than non-reactive ones, with very little fluid ‘1’ left at the walls. This is because the viscosity of the wall layers is significantly lower in the case of reactive displacements (see Fig. 4.6), which facilitates their removal. Thus the displacement rate increases with increasing the value of \( Da \) (shown in Fig. 4.4(a)).

Figure 4.6: Spatio-temporal evolution of the contours of \( \mu \) for (a) \( Da = 0 \) and (b) \( Da = 0.5 \) at successive times (from top to bottom in each panel: \( t = 5, 10, 15 \) and 20) for \( R_m = 2.3026 \) and \( R_p = -1.609 \). The rest of the parameter values are the same as those used to generate Fig. 4.17. The color-map is shown at the bottom.
Interestingly, we have found that even for $R_p > 0$, i.e., when $\mu_2 < \mu_p < \mu_1$, the chemical reaction helps in the cleaning process by increasing the displacement rate as shown in Fig. 4.4(c), generated for $R_m = 1.609$ and $R_p = 2.3026$ with the rest of the parameter values remaining unaltered from Fig. 4.4(a). Close inspection of the $\phi_m$ field in Fig. 4.7(b), however, shows that the parabolic ‘nose’ shape, characteristic of the ‘interfacial’ region in the $R_p < 0$ case (shown in Fig. 4.5(b)), has given way to a sharper structure whose tip becomes increasingly elongated with time. In case of miscible flow without chemical reaction, this type of finger of the invading fluid with sharp ‘nose’ was observed experimentally by Petitjeans and Maxworthy [25] and numerically by Rakotomalala et al. [47]. The viscosity fields for $Da = 0$ and $Da = 0.5$ with the rest of the parameter values same as Fig. 4.4(c) and (d) are shown in Fig. 4.8(a) and (b), respectively. In this case, it can be seen that the viscosity of the fluid in front of the invading finger becomes significantly lower as compared to that of the fluid initially present in this region, which accelerates the displacement process.

![Figure 4.7: Spatio-temporal evolution of the contours of $\phi_m$ for (a) $Da = 0$ and (b) $Da = 0.5$ at successive times (from top to bottom in each panel: $t = 5, 10, 15$ and $20$) for $R_m = 1.609$ and $R_p = 2.3026$. The rest of the parameter values are the same as those used to generate Fig. 4.17. The color-map is shown at the bottom.](image-url)
Figure 4.8: Spatio-temporal evolution of the contours of $\mu$ for (a) $Da = 0$ and (b) $Da = 0.5$ at successive times (from top to bottom in each panel: $t = 5, 10, 15$ and $20$) for $R_m = 1.609$ and $R_p = 2.3026$. The rest of the parameter values are the same as those used to generate Fig. 4.17. The color-map is shown at the bottom.
4.3 Effects of dimensionless activation energy

The effect of varying the dimensionless activation energy, $\beta$, on the displacement process is shown in Fig. 4.9. The temporal evolutions of the dimensionless mass of the displaced fluid ‘1’, $M_{0.95}/M_0$, and the position of the leading ‘front’ separating the two fluids, $x_{tip}$, are plotted for different values of $\beta$ in Fig. 4.9(a) and (b), respectively; the rest of the parameters remain unaltered from Fig. 4.1. As expected, increasing the values of $\beta$, which raises the activation energy barrier for the chemical reaction, decreases the displacement rate (refer to Fig. 4.9(a)). Inspection of Fig. 4.9(b) reveals that the velocity of the leading front also decreases with increasing $\beta$.

Figure 4.9: (a) Mass fraction $M_{0.95}/M_0$ of $\phi_m$, and (b) temporal evolution of the position of the leading front separating the two fluids, $x_{tip}$ for different values of $\beta$. The rest of the parameter values are $Re = 500$, $Pr = 7$, $Sc_m = 100$, $Sc_p = 50$, $r_T = 1$, $Da = 0.1$, $Q = 100$, $R_m = 2.3026$ and $R_p = −1.609$. The dotted lines in panel (a) and (b) represent the limiting case given by $M_{0.95}/M_0 = 1 - tH/L$ and $x_{tip} = t$, respectively.
The spatio-temporal evolutions of the $\phi_m$ and $\mu$ fields associated with $\beta = 0.5$ and 10 are shown in Fig. 4.10(a) and (b), and Fig. 4.11(a) and (b), respectively. As expected, it can be seen that the flow dynamics associated with higher $\beta$ value is qualitatively similar to that associated with smaller $Da$ value considered.

Figure 4.10: Spatio-temporal evolution of the contours of $\phi_m$ for (a) $\beta = 0.5$ and (b) $\beta = 10$ at successive times (from top to bottom in each panel: $t = 5$, 10, 15 and 20). The rest of the parameter values are the same as those used to generate Fig. 4.9. The color-map is shown at the bottom.
Figure 4.11: Spatio-temporal evolution of the contours of $\mu$ for (a) $\beta = 0.5$ and (b) $\beta = 10$ at successive times (from top to bottom in each panel: $t = 5, 10, 15$ and $20$). The rest of the parameter values are the same as those used to generate Fig. 4.9. The color-map is shown at the bottom.
4.4 Effects of dimensionless temperature of the invading fluid

Next, in Fig. 4.12 we study the effect of \( r_T \), the dimensionless temperature of the invading fluid (fluid ‘2’) on the displacement characteristics for \( Da = 0.05 \), \( Q = 200 \) and \( \beta = 5 \). The rest of the parameter values remain unaltered from Fig. 4.1. It can be seen in Fig. 4.12(a) that increasing \( r_T \) progressively from \( r_T = 0 \) to \( r_T = 5 \) leads to more rapid displacement of fluid ‘1’ in comparison to the isothermal case. In Fig. 4.12(b), it can be seen that the position of the leading ‘front’ separating the two fluids, \( x_{tip} \), is very weakly-dependent on variations in \( r_T \) values. It can also be seen that all the curves in Fig. 4.12(a) lie below \( 1 - tH/L \) (and these in Fig. 4.12(b) are above \( x_{tip} = t \)) which corresponds to plug flow’ displacements. This is due to the presence of instabilities which enhance mixing and increase the displacement rate.

![Figure 4.12](image)

Figure 4.12: (a) Mass fraction \( M_{0.95}/M_0 \) of \( \phi_m \), and (b) temporal evolution of the position of the leading front separating the two fluids, \( x_{tip} \) for different \( r_T \) values. The rest of the parameter values are \( Re = 500 \), \( Pr = 7 \), \( Sc_m = 100 \), \( Sc_p = 50 \), \( Da = 0.05 \), \( \beta = 5 \), \( Q = 200 \), \( R_m = 2.3026 \) and \( R_p = -1.609 \). The dotted lines in panel (a) and (b) represent the limiting case given by \( M_{0.95}/M_0 = 1 - tH/L \) and \( x_{tip} = t \), respectively.

The above results are rationalized by examining the spatio-temporal evolution of \( \phi_m \) contours for \( r_T = 0 \) and \( r_T = 5 \) in Fig. 4.13(a) and (b), respectively. The rest of the parameter values remain unchanged from those used to generate Fig. 4.12. \( r_T = 5 \) corresponds to the case when a warmer fluid displaces a cooler one. For \( r_T = 0 \) (isothermal flow at \( t = 0 \)), it can be seen that fluid ‘1’ is penetrated by a relatively stable ‘finger’ of fluid ‘2’. Similar observations were made by Sahu et al. [5] who studied the displacement flow without chemical reaction. In contrast to the \( r_T = 0 \) case, for \( r_T = 5 \), the flow appears to be considerably more unstable due to the associated increase in viscosity contrasts. As a result, the region separating fluids ‘1’ and ‘2’ is highly diffuse and hence a higher displacement rate is observed for \( r_T = 5 \) as compared to \( r_T = 0 \).
Figure 4.13: Spatio-temporal evolution of $\phi_m$ for (a) $r_T = 0$ and (b) $r_T = 5$ at successive times (from top to bottom in each panel: $t = 5, 10, 20$ and $25$). The rest of the parameter values are the same as those used to generate Fig. 4.12. The color-map is shown at the bottom.
4.5 Effects of Reynolds number

Finally, we have investigated the effect of varying the Re on the flow dynamics. As shown in Fig. 4.14, increasing Re leads to more pronounced roll-up phenomena, highly convective mixing, and rapid displacement rates.

Figure 4.14: (a) Mass fraction $M_{0.95}/M_0$ of $\phi_m$, and (b) temporal evolution of the position of the leading front separating the two fluids, $x_{tip}$, for different values of Re (c) spatio-temporal evolution of $\phi_m$ at $t = 20$ for different Reynolds numbers (from top to bottom in each panel: Re = 50, Re = 100, Re = 500 and Re = 1000). The rest of the parameter values are Pr = 7, $Sc_m = 100$, $Sc_p = 50$, $r_T = 1$, $Da = 0.1$, $\beta = 5$, $Q = 100$, $R_m = 2.3026$ and $R_p = -1.609$. The dotted lines in panel (a) and (b) represent the limiting case given by $M_{0.95}/M_0 = 1 - tH/L$ and $x_{tip} = t$, respectively.
4.6 Effects of Schmidt number of reactant and product

Variation of $Sc_m$ and $Sc_p$ were also found to have a negligible effect on the displacement rates, as shown in Figs. 4.15.

Figure 4.15: (a,c) Mass fraction $M_{0.95}/M_0$ of $\phi_m$, and (b,d) temporal evolution of the position of the leading front separating the two fluids, $x_{tip}$. The panels (a,b) and (c,d) are plotted for different values of $Sc_m$ for $Sc_p = 50$, and $Sc_p$ for $Sc_m = 100$, respectively. The rest of the parameter values are $Re = 500$, $Pr = 7$, $r_T = 1$, $Da = 0.1$, $\beta = 1$, $Q = 100$, $R_m = 2.3026$ and $R_p = -1.609$. The dotted lines in panel (a) and (b) represent the limiting case given by $M_{0.95}/M_0 = 1 - tH/L$ and $x_{tip} = t$, respectively.
4.7 Effects of heat of the reaction

Variation of $Q$ also found to have a negligible effect on the displacement rates, as shown in Figs. 4.16.

Figure 4.16: (a) Mass fraction $M_{0.95}/M_0$ of $\phi_m$, and (b) temporal evolution of the position of the leading front separating the two fluids, $x_{tip}$ for different values of $Q$. The rest of the parameter values are $Re = 500$, $Pr = 7$, $Sc_m = 100$, $Sc_p = 50$, $r_T = 1$, $Da = 0.1$, $\beta = 1$, $R_m = 2.3026$ and $R_p = -1.609$. The dotted lines in panel (a) and (b) represent the limiting case given by $M_{0.95}/M_0 = 1 - tH/L$ and $x_{tip} = t$, respectively.
4.8 Effects of Damköhler number with variable diffusivity

In this section, the effects of variable diffusivity is discussed. It can be seen that results remain mostly similar to those of the constant diffusivity case which is discussed in the previous section. The comparison of the flow dynamics shown in Figure 4.7 (Constant diffusivity case) with that shown in Figure 4.20 (variable diffusivity case) reveals that the thin layers adjacent to the wall are evident, which is absent in the constant diffusivity case. However, these effects are very little.

Figure 4.17: (a,c) Mass fraction $M_{0.95}/M_0$ of $\phi_m$, and (b,d) temporal evolution of the position of the leading front separating the two fluids, $x_{tip}$ for different values of Da. Here panels (a and b) and (c and d) correspond to the parameters ($R_m = 2.3026$ and $R_p = -1.609$) and ($R_m = 1.609$ and $R_p = 2.3026$), respectively. The rest of the parameter values are $Re = 500$, $Pr = 7$, $Sc_m = 100$, $Sc_p = 50$, $r_T = 1$, $\beta = 1$ and $Q = 100$. The dotted lines in panels (a,c) and (b,d) represent the limiting case given by $M_{0.95}/M_0 = 1 - tH/L$ and $x_{tip} = t$, respectively.
Figure 4.18: Spatio-temporal evolution of the contours of $\phi_m$ for (a) $Da = 0$ and (b) $Da = 0.5$ at successive times (from top to bottom in each panel: $t = 5, 10, 15$ and $20$) for $R_m = 2.3026$ and $R_p = -1.609$. The rest of the parameter values are the same as those used to generate Fig. 4.17. The color-map is shown at the bottom.
Figure 4.19: Spatio-temporal evolution of the contours of $\mu$ for (a) $Da = 0$ and (b) $Da = 0.5$ at successive times (from top to bottom in each panel: $t = 5, 10, 15$ and 20) for $R_m = 2.3026$ and $R_p = -1.609$. The rest of the parameter values are the same as those used to generate Fig. 4.17. The color-map is shown at the bottom.
Chapter 5

Conclusions

Pressure-driven displacement of one fluid by another in a horizontal channel in the presence of an exothermic chemical reaction is studied numerically. In our simulations, the continuity, Navier-Stokes and energy equations coupled to two convective-diffusion equations the reactant and product are solved using a finite-volume approach. The viscosity is assumed to be an exponential function of the temperature as well as the volume fraction of the reactant and product. In order to isolate the effects of viscosity contrast, the density is assumed to be constant. The effects of relevant parameters such as the Reynolds number, Schmidt number, Damköhler number and the viscosity ratio of the reactant and product are investigated. The results of the present study indicate that increasing the intensity of chemical reaction by increasing Damköhler number and decreasing dimensionless activation energy increases the displacement rate. More pronounced instabilities and roll-up phenomena are observed with increasing Reynolds number, which increases the displacement rates of the resident fluid inside the channel. For the parameter range considered, we found that the heat of reaction and the Schmidt numbers of the reactant and product have a negligible influence on the displacement characteristics.
References


