Chapter 1

Introduction

Many of the world's energy and environmental concerns can be addressed by modeling the flow of fluids and transport of dissolved materials beneath the earth's surface (e.g. oil and gas reservoirs, contaminated aquifers). The environments beneath the earth's surface act as open bio-geochemical reactors where chemical change is driven by the interactions between migrating fluids, solid phases, and organisms. Therefore, most of the geochemical and bio-geochemical phenomena of interest to earth scientists are the result of the coupling of some combination of fluid, heat, and solute transport with chemical reactions in the earth's crust. The use of numerical simulation provides a better understanding of the complex interplay of physical and chemical processes in geologic media.

In recent years there has been a great interest in the shape stability of the reaction interface for reactive flow in a porous medium. The porosity changes which occur due to reactions with the solid components may lead to fingering instabilities,

see Chadam et al [12]–[16]. We refer to this phenomenon as Reaction-Infiltration Instability. There are some important applications for understanding this shape stability to many geochemical situations (e.g. enhanced oil recovery, the dynamics of breakout from chemical and nuclear waste repositories [12, 11], and natural attenuation of a ground water plume at abandoned mining sites, see Zhu, Hu, and Burden [39, 40]). Since the time scale for a porosity change to occur in a porous medium is very long, laboratory experiments are very difficult to set. The most attractive and reliable method to understand the shape stability is numerical simulations.

This work concentrates on the numerical modeling of the Reaction-Infiltration Instability problem. A mathematical model of this phenomenon, which consists of a coupled nonlinear system of flow, transport, and reaction, was proposed and studied analytically in previous work [12, 14] using a complete linearized stability analysis in the setting of a free boundary model. The problem is studied for reactive flow in a homogeneous porous medium in [12]. Chadam et al [16] studied the flow of reactive fluids through layered porous media and analyzed the effects of the layering on the shape stability. The effect of coupling porosity and viscosity changes was investigated in [15], where it is allowed for the possibility that the solute can increase the viscosity of the fluid when it dissolves in the water. A velocity dependent hydrodynamic dispersion was included and studied in [13].

Here we develop a time-split and operator-split algorithm for the numerical solution of the nonlinear Reaction-Infiltration Instability model. The time-splitting is similar to the methods proposed by Dawson and Wheeler in [18, 17], and Arbogast in [2]. The added difficulty here is the nonlinear coupling between flow and transport due to the porosity change. Resolving this nonlinearity requires an additional iteration between the two equations on each time step. We also allow for advancing advection and reaction in time by a smaller time step than the one used for flow and diffusion/dispersion. This is needed for stability due to the explicit computations and difficult nonlinear couplings in the advection and reaction parts of the system.

The flow equation is discretized by the mixed finite element method [34], while the transport equation is discretized by the Godunov-mixed method [17]. The choice of the mixed finite element method is motivated by its local mass conservation property which is critical in porous media applications. We obtain optimal order $O(\Delta t + h)$ a priori error estimates for the coupled nonlinear system. The operator-splitting error is also analyzed and it is shown to be $O(\Delta t)$.

Numerical studies on the effect of the Peclet number and the dispersion on the stability of the front are presented. We also present some numerical studies on layered and heterogeneous porous medium. We apply our model to a real world example.

The rest of the thesis is organized as follows. In the next chapter we describe the physical problem and the mathematical model. An operator form of the problem along with a variational formulation suitable for our numerical scheme is given in Chapter 3. The semi-discrete numerical approximation is also presented in the third chapter. In Chapter 4 we give the error analysis for the flow and the transport equations, and the operator-splitting error. The numerical method is presented in Chapter 5, where a formal description of the algorithm is given. Computational results verifying analytical results and the effect of the Peclet number on the stability of the front are presented in Chapter 6. A summary of the above work and some suggestions for future research is given in Chapter 7.