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Contaminant Flow and Transport Simulation in Cracked Porous Media using Locally Conservative Schemes

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CONTAMINANT FLOW AND TRANSPORT SIMULATION IN CRACKED POROUS MEDIA USING LOCALLY CONSERVATIVE SCHEMES

A Dissertation
Presented to
the Graduate School of
Clemson University

In Partial Fulfillment
of the Requirements for the Degree
Master of Science
Mathematical Sciences

by
Pu Song
August 2010

Accepted by:
Dr. Shuyu Sun, Committee Chair
Dr. Leo Rebholz
Dr. Jeong-Rock Yoon

Abstract

The purpose of this paper is to analyze some features of contaminant flow passing through cracked porous media, such as the influence of fracture network on the advection and diffusion of contaminant species, the adsorption impact of contaminant wastes on the overall transport flow and so on. In order to precisely describe the whole process, we firstly need to build the mathematical model to simulate this problem numerically. Taking into consideration of the characteristics of contaminant flow, we employ two partial differential equations to formulate the whole problem. One is flow equation, the other is reactive transport equation. The first equation is used to depict the total flow of contaminant wastes, which based on Darcy law. The second one will characterize the adsorption, diffusion and convection behavior of contaminant species, which summarizes most features of contaminant flow we are interested in. After the construction of numerical model, we apply different tools to solve this mathematical model. There are two delicate measures for us to consider first. One is Mixed Finite Element (MFE) method, the other is Discontinuous Galerkin (DG) method. Both methods are locally conservative. MFE has a good convergence rate and numerical accuracy. DG is more flexible and can be used to deal with irregular meshes, as well as high-order accuracy. With these two numerical means, we investigate the sensitivity analysis of different features of contaminant flow in our model, such as diffusion, permeability, fracture density, K_d values which represent the distribution of contaminant wastes between the solid and liquid phases. We also make comparison of two different schemes and discuss advantages of both methods.

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Chapter 1

Introduction

In this paper, we are interested in simulating process in subsurface waste repositories. We have a solid concrete matrix to seal the radioactive wastes underground, however, there will be some fractures produced by the erosion of water, acid solute or other undetermined elements during the long time periods. Hence, we need to consider how these radioactive wastes leak through our concrete matrix from these apertures since the convection in fractures is much faster than that in matrix. Although this situation is complicated, we can simplify it as an easy-handle model. We shall construct a mathematical model like this way: we will consider the flow of an incompressible fluid through a homogenous saturated porous media, where the fluid is contaminated by solute, with concentration $c \geq 0$. We assume the flow is at steady state and that transport is describe by convection, molecular diffusion, mechanical dispersion, and chemical reaction (adsorption) between solute and the surrounding solid porous skeleton. There are lots of applications related to this model [2], [3], [5], [6], [12], [15].

The contaminant flow of fluids through fractures is a process that plays an important role for many areas of the geosciences. Research on fluid flow in fractures and in fractured porous media has a history that spans nearly four decades. This research can be classified as four principal aspects of fracture flow: 1) development of conceptual models, 2) development of analytical and numerical solution schemes, 3) description of fracture hydraulic characteristics in static and deforming media, and 4) development of stochastic techniques to describe fracture flow and hydro-geologic parameter distributions. In this paper, we will firstly build the mathematical model for the original problem, then apply different numerical schemes to solve this model and analyze the numerical results from

different methods in order to derive a better solution and accurate results.

Several conceptual models have been developed for describing contaminant fluid flow in fracture porous media. Fundamentally, each method can be distinguished on the basis of storage and flow capacities of the porous medium and the fracture. The storage characteristics are associated with porosity, and the flow characteristics are associated with permeability. There are four conceptual models which dominated the research so far: 1) dual continuum, 2) discrete fracture network, 3) single equivalent continuum. In addition, multiple-interacting continua and multi-porosity/multi-permeability conceptual models [11] saimi(1995) have recently been introduced into literature. Further distinctions can be drawn on the basis of spatial and temporal scales of integration, or averaging, of the flow regime. In our research, we will mainly focus on discrete fracture network [7], [8] which preserves the physics closely.

After we build the mathematical model, we need to solve it with numerical algorithms. There are lots of measures to implement it. For different parts of our models, we need to deal with them by specific methods in order to obtain best simulation. The movement of contaminants through the fractured porous medium is modeled by transport equations; that is, equations which describe the advection, diffusion and interaction of contaminants within the environment. These equations are often advection-dominated, and thus require special care when solved numerically. In recent years, there has been much interest in using upwind schemes for simulating such transport problems. These schemes are also referred to as high resolution or shock-capturing methods. In this paper, we employ an upwind-mixed finite element combining finite volume method to deal with transport and flow equation due to the advantage of Finite Volume Method (FVM) in dealing with advection part of transport equation and Mixed Finite Element (MFE) method in dealing with flow and diffusion , adsorption part of transport equation. On structured grids, using special numerical integration rules, the upwind-mixed method is equivalent to a cell-centered finite difference method, which is much easier to handle and code. We also investigate the Discontinuous Galerkin (DG) method [14], [13], [10] for advection part of transport equation since DG method can be locally conservative, stable, high-order accurate, flexible, less numerical cost and easy implemented method which can easily handle complex geometries, irregular mesh with hanging nodes and also can be easily coupled with other methods like conforming or mixed finite element methods.

Substantial research has been published in various aspects of the contaminant flow in fractured porous medium. For example, [9] Shinichi nakayama and Ikuji takagi et al.(1986) studied the

advection-diffusion migration of radionuclides through two-layer geological media; [4] Clint Dawson (1998) used upwind-mixed finite element method to solve nonlinear contaminant transport models; [1] Vandym Ayzinger and Dawson et al.(2001) used local DG to simulate contaminant flow models.

This paper is divided into following sections: First, the differential equations describing the contaminant diffusion and transport in the fractured cementitious matrix are presented. Second, a numerical model in saturated fractured media is described. We discuss in detail various components of our numerical approach, which include the MFE method and cell centered finite difference method for the flow equation, the combined FVM-MFE method and DG-MFE method for the transport equation and the numerical discretization in time. We then present numerical examples in fractured media with various fracture distributions. For each example, we provide and discuss simulated concentration profiles at different times, together with pressure and velocity fields, we also present some examples between MFE scheme and DG scheme to see the difference between two schemes. Finally, we numerically carry out a sensitivity analysis of parameters in our model and investigate the relationship between intrinsic K_d value and effective K_d value, also the relationship between fracture density and effective K_d value, impact of impulse concentration on our models, all of which will help to design barriers that are protective of the public environment.

Chapter 2

Mathematical model

When the contaminants leak through the porous medium, there will be adsorption, convection and diffusion brought by the movement of those contaminants. Therefore, we use reactive transport equation to describe these phenomenon during the time of contaminants passing through the medium. We also need to use flow equation to govern the fluid flow and give the pressure field and Darcy velocity field if the concentration of contaminants is given. Based on experimental data and above analysis, we construct mathematical models for contaminant species passing through the porous media, which include two coupled differential equations, one is flow equation (we know it is an elliptic equation for scalar unknown variable pressure if the concentration of contaminants is considered to be given), the other one is reactive transport equation which is a parabolic equation used for dealing with adsorption, diffusion and convection of contaminant flows.

Let Ω denotes a bounded domain in $R^d, (n = 2, 3)$. The classical equations governing the miscible displacement of contaminants in porous media is as follows.

2.1 Flow Equation

- Continuity equation

$$\nabla \cdot \mathbf{u} = q, \quad x \in \Omega$$

- Darcy velocity

$$\mathbf{u} = -\frac{\mathbf{K}}{\mu} \nabla p, \quad x \in \Omega$$

- Flow equation

$$-\nabla \cdot (\mathbf{u}) = -\nabla \cdot \left(\frac{\mathbf{K}}{\mu(c)} \nabla p \right) = q, \quad x \in \Omega$$

- Constitutive relation

$$\mu = \mu(c)$$

where p (the pressure in the fluid mixture), c (the concentration of contaminants measured in amount of species per unit volume of the fluid mixture) and $\mathbf{u}$ (the Darcy velocity of the mixture, i.e. the volume of fluid flowing cross a unit across-section per unit time) are unknowns. The permeability $\mathbf{K}$ of the medium measures the conductivity of the medium to fluid flow; the viscosity μ of the fluid measures the resistance to flow of the fluid mixture. The commonly used constitutive relation is the quarter- power mixing rule $\mu(c) = (c\mu_s^{-0.25} + (1-c)\mu^{-0.25})^{-4}$, but in this paper, we consider it as a constant. The imposed external total flow rate q is a sum of sources(injection) and sinks(extraction).

The boundary conditions for our domain Ω are:

- Dirichlet boundary

$$p = p_B, \quad x \in \Gamma_D$$

- Neumann boundary

$$\mathbf{u} \cdot \mathbf{n} = u_B, \quad x \in \Gamma_N$$

where $\partial\Omega = \Gamma_D \cup \Gamma_N$, Γ_D denotes the Dirichlet boundary and Γ_N denotes the Neumann boundary.

2.2 Reactive Transport Equations

The reactive transport equation is obtained from the mass conservation of considered contaminant species. It governs the convection, diffusion, and adsorption of movement of contaminants and gives the concentration profile provided the velocity field is given from flow equation. The contaminant concentrations in the fluid and in the solid as well as their relation can be described by:

$$\begin{cases} \frac{\partial \phi c}{\partial t} + \nabla \cdot (\mathbf{u}c - \mathbf{D}(\mathbf{u})\nabla c) = r(c, c_s), \\ \frac{\partial \rho c_s}{\partial t} = -r(c, c_s), \\ c_s = K_d c. \end{cases} \quad (x, t) \in \Omega \times (0, T]$$

Summation of the two concentration equations above (one in fluid and another one in solid) yields:

$$\frac{\partial \phi^{eff} c}{\partial t} + \nabla \cdot (\mathbf{u}c - \mathbf{D}(\mathbf{u})\nabla c) = 0,$$

where $\phi^{eff} = \phi + \rho K_d$ is the effective porosity and it is calculated separately for the matrix and for the fractures:

- In the matrix $\phi = \phi_{matrix}$
- In the fracture $\phi = 1, K_d = 0, \phi^{eff} = \phi = 1.0$

the unknown variable c is the concentration of the interested species within the fluid (i.e. the amount of the species per unit volume of the fluid mixture) and c_s is the concentration of the interested species in the solid. T is the final simulation time. The parameter K_d is the partitioning coefficient of the considered species between the fluid and the rock. We will talk about the details of K_d in chapter 4. ρ is the density of fluid mixture; the porosity ϕ is the fraction of the volume of the medium occupied by pores and is assumed to be time-independent, uniformly bounded above and below by positive numbers; the dispersion-diffusion tensor $\mathbf{D}(\mathbf{u})$ has contributions from molecular diffusion and mechanical dispersion, and can be calculated by:

- Dispersion/Diffusion tensor

$$\mathbf{D}(\mathbf{u}) = d_m \mathbf{I} + |\mathbf{u}| \{ \alpha_l \mathbf{E}(\mathbf{u}) + \alpha_t (\mathbf{I} - \mathbf{E}(\mathbf{u})) \}$$

where $d_m = \phi \tau D_m$ and is assumed to be strictly positive, τ is the tortuosity coefficient; $\mathbf{D}_m$ is the molecular diffusivity; α_l and α_t are the longitudinal and the transverse dispersivities, respectively; $\mathbf{E}(\mathbf{u})$ is the tensor that projects onto the $\mathbf{u}$ direction, whose (i, j) component is $\mathbf{E}(\mathbf{u})_{i,j} = \frac{u_i u_j}{|\mathbf{u}|^2}$. We assume our domain Ω has Lipschitz boundary $\partial\Omega = \Gamma_{in} \cup \Gamma_{out}$, where Γ_{in} is the inflow boundary and

Γ_{out} is the outflow boundary, defined as follows:

$$\begin{cases} \Gamma_{in} = \{x \in \partial\Omega : \mathbf{u}(x) \cdot \mathbf{n}_{\partial\Omega} < 0\}, \\ \Gamma_{out} = \{x \in \partial\Omega : \mathbf{u}(x) \cdot \mathbf{n}_{\partial\Omega} \geq 0\}. \end{cases}$$

where $\mathbf{n}_{\partial\Omega}$ is the unit outward normal vector to $\partial\Omega$. The boundary conditions for transport equation are following:

$$\begin{cases} (\mathbf{u}c - \mathbf{D}(\mathbf{u})\nabla c) \cdot \mathbf{n} = c_B \mathbf{u}(x) \cdot \mathbf{n}, & x \in \Gamma_{in}, t \in (0, T], \\ (-\mathbf{D}(\mathbf{u})\nabla c) \cdot \mathbf{n} = 0, & x \in \Gamma_{out}, t \in (0, T]. \end{cases}$$

We specify an initial concentration in the following:

$$c(x, 0) = c_0(x).$$

Chapter 3

Numerical Algorithms

In this paper, the system contains two parts: a flow equation involving the pressure (scalar variable) and Darcy velocity (vector variable), and a reactive transport equation for describing the evolution of contaminant concentrations. We first solve the flow equation by a MFE method; then we solve the reactive transport equation semi-implicitly (explicitly for convection and implicitly for diffusion and adsorption) in time by using a combination of FVM and MFE method, and also employing a combination of DG and MFE method for advection and diffusion parts respectively.

3.1 Mixed Finite Element Method

Mixed finite element method was initially introduced by engineers in the 1960's (Fraeijns de Veubeke, 1965; Hellan, 1967; Hermann, 1967) for solving problems in solid continua, which is a generalized finite element method. The advantage for using the mixed method is that it can be used to approximate both vector variable (flux velocity) and scalar variable (pressure) simultaneously and to give a high order approximation of both variables. Compared with traditional finite element method, mixed method employs two different spaces to treat the two variables mentioned above, and these two spaces must satisfy inf-sup condition for the mixed method to be stable, which avoids to work with conventional finite element space, something which is difficult to use low order polynomials.

For simplicity, we consider only two dimensional rectangular domain and we only consider rectangular mesh, However, the results can be directly extended to logically rectangular do-

main/mesh by conforming mapping. Although we can employ different domain partitions for flow and transport problems respectively, the same non-uniform rectangular partition is considered for both of flow and transport equations. Also the permeability tensor K is assumed to be invertible and uniformly positive definite and uniformly bounded and the viscosity μ is considered to be constant 1 in our simulation.

Before giving out the variational form of our problem, we first introduce some abstract spaces, which are used to formulate mixed finite element scheme:

$$\begin{aligned} W &= L^2(\Omega) = \{v; \int_{\Omega} v^2 dx < \infty\}, \\ \mathbf{V} &= \mathbf{H}(\text{div}; \Omega) = \{\mathbf{v} \in (L^2(\Omega))^d : \nabla \cdot \mathbf{v} \in L^2(\Omega)\}, \\ \mathbf{V}^0 &= \{\mathbf{v} \in \mathbf{H}(\text{div}; \Omega) : \mathbf{v} \cdot \mathbf{n} = 0 \text{ on } \partial\Omega\}, \\ \mathbf{V}_N^0 &= \{\mathbf{v} \in \mathbf{H}(\text{div}; \Omega) : \mathbf{v} \cdot \mathbf{n} = 0 \text{ on } \Gamma_N\}, \end{aligned}$$

where

$$\nabla \cdot \mathbf{v} = \frac{\partial v_1}{\partial x_1} + \frac{\partial v_2}{\partial x_2} + \cdots + \frac{\partial v_d}{\partial x_d}.$$

The norms of the two spaces $W = L^2(\Omega)$ and $\mathbf{V} = \mathbf{H}(\text{div}; \Omega)$ are respectively defined by:

$$\|w\| \equiv \|w\|_{L^2(\Omega)} = (\int_{\Omega} w^2 dx)^{1/2}, w \in W,$$

and

$$\|\mathbf{v}\|_V \equiv \|\mathbf{v}\|_{H(\text{div}; \Omega)} = \{\|\mathbf{v}\|^2 + \|\nabla \cdot \mathbf{v}\|^2\}^{1/2}, \mathbf{v} \in W.$$

3.2 MFE for flow equation

We first give the weak formulation of flow equation. The mixed variational form of the flow equation is to find $\mathbf{u} \in V_N^0 + E(u_B)$, $p \in W$ such that:

$$\begin{cases} (K^{-1}\mathbf{u}, \mathbf{v}) - (\nabla \cdot \mathbf{v}, p) = - \int_{\Gamma_D} p_B \mathbf{v} \cdot \mathbf{n} ds, & \forall \mathbf{v} \in V_N^0, t \in (0, T], \\ (\nabla \cdot \mathbf{u}, w) = (q, w), & \forall w \in W, t \in (0, T]. \end{cases}$$

Here $E(u_B)$ is the velocity extension such that its normal component agrees with u_B on Γ_N .

In order to investigate the mixed finite element scheme, we need to introduce Raviart-Thomas (RT) space (Raviart, R.A. 1977) to discretize the above weak formulation.

For a two-dimensional domain with non-uniform rectangular partitions ε_h , the r -th order RT space is defined by:

$$W_h = \{w \in L^2(\Omega) : w|_E \in Q_{r,r}(E), E \in \varepsilon_h\},$$

$$\mathbf{V}_h = \{v \in H(\text{div}; \Omega) : v|_E \in Q_{r+1,r}(E) \times Q_{r,r+1}(E), E \in \varepsilon_h\},$$

where $Q_{r,s}(E)$ is the space of polynomials of degree less than or equal to r and s in the first and second variables restricted to the element E . Clearly, $V_h \subset V$ and $W_h \subset W$. In our numerical examples below we use RT_0 space. The MFE scheme for flow equation is to find $p_h \in L^\infty((0, T], W_h)$ and $\mathbf{u}_h \in L^\infty((0, T], \mathbf{V}_h^0)$ where $\mathbf{V}_h^0 = \mathbf{V}^0 \cap \mathbf{V} + E_h(u_B)$, such that,

$$\begin{cases} (K^{-1}\mathbf{u}_h, \mathbf{v}) - (\nabla \cdot \mathbf{v}, p_h) = - \int_{\Gamma_D} p_B \mathbf{v} \cdot \mathbf{n} ds, & \forall \mathbf{v} \in V_h, t \in (0, T], \\ (\nabla \cdot \mathbf{u}_h, w) = (q, w), & \forall w \in W_h, t \in (0, T]. \end{cases}$$

3.2.1 MFE and FVM for reactive transport equation

Like above, we first give the weak formulation of transport equation. The weak formulation of transport equation is to find the concentration solution $c \in W$ and the diffusive flux solution $\mathbf{v} \in \mathbf{V}^0$ such that:

$$\begin{cases} (\frac{\partial \phi^{\text{eff}} c}{\partial t}, w) + (\nabla \cdot \mathbf{v}, w) + \sum_E \int_{\partial E} w \mathbf{u} c^* \cdot \mathbf{n} ds - \sum_E (c^* \mathbf{u}, \nabla w) = 0, & \forall w \in W, t \in (0, T], \\ (-D^{-1} \mathbf{v}, \hat{\mathbf{v}}) + (c, \nabla \cdot \hat{\mathbf{v}}) = 0, & \forall \hat{\mathbf{v}} \in V^0, t \in (0, T], \\ (c, w) = (c_0, w), & \forall w \in W, t = 0. \end{cases}$$

here c^* denotes the upwind value of the concentration of contaminants on an edge. We will introduce its definition in the DG schemes.

The continuous-in-time MFE method for approximating the transport equation is to find $c_h \in L^\infty((0, T), W_h)$, $\mathbf{v}_h^\infty((0, T), V_h^0)$ such that:

$$\left\{ \begin{array}{ll} (\frac{\partial \phi^{\text{eff}} c_h}{\partial t}, w) + (\nabla \cdot \mathbf{v}_h, w) + \sum_E \int_{\partial E} w \mathbf{u} c_h^* \cdot \mathbf{n} ds - \sum_E (c_h^* \mathbf{u}, \nabla w) = 0, & \forall w \in W_h, t \in (0, T], \\ (-D^{-1} \mathbf{v}_h, \hat{\mathbf{v}}) + (c_h, \nabla \cdot \hat{\mathbf{v}}) = 0, & \forall \hat{\mathbf{v}} \in V_h^0, t \in (0, T], \\ (c_h, w) = (c_0, w), & \forall w \in W_h, t = 0. \end{array} \right.$$

Then we will give the fully discretized algorithm for the transport equation. We partition the simulation time $(0, T]$ into m subintervals: $0 = t_0 < t_1 < \dots < t_{m-1} < t_m = T$. We let $\Delta t_k = t_k - t_{k-1}$, $\Delta t = \max \Delta t_k$. Assuming that there exists a constant C satisfying that $\Delta t \leq C \min \Delta t_k$, the transport equation can be solved by semi-implicit Euler method in time and the combined FVM-MFE method in space. The fully discretized approximation is to find $c_{h,k} \in W_h$ and $\mathbf{v}_{h,k} \in V_h^0$, for $k = 0, 1, 2, \dots, m$ such that

$$\left\{ \begin{array}{ll} (\frac{\partial \phi^{\text{eff}} c_{h,k} - \phi^{\text{eff}} c_{h,k-1}}{\Delta t}, w) + (\nabla \cdot \mathbf{v}_{h,k}, w) + \sum_E \int_{\partial E} w \mathbf{u} c_{h,k-1}^* \cdot \mathbf{n} ds - \sum_E (c_{h,k-1}^* \mathbf{u}, \nabla w) = 0, & \forall w \in W_h, t \in (0, T], \\ (-D^{-1} \mathbf{v}_{h,k}, \hat{\mathbf{v}}) + (c_{h,k}, \nabla \cdot \hat{\mathbf{v}}) = 0, & \forall \hat{\mathbf{v}} \in V_h^0, t \in (0, T], \\ (c_{h,0}, w) = (c_0, w), & \forall w \in W_h, t = 0. \end{array} \right.$$

3.3 Discontinuous Galerkin(DG) Method

Traditional Continuous Galerkin (CG) finite element method has been around for more than 60 years. It is widely used for solving practical problems due to its simple implementation comparing with MFE method and DG method. However, with more requirements on the accuracy of solutions and high efficient computation, CG method can not meet the needs of most problems. Thus, the investigation of MFE method and DG method draws lots of attention in recent years.

The DG method has many attractive features compared with CG method. First of all, in terms of problem size, the total number of degrees of freedom is proportional to the number of elements in the mesh for DG. However, for CG, the degrees of freedom not only depends on the number of elements but also on the number of vertices in the mesh. Therefore, CG method is more expensive than DG. Secondly, the DG method can easily handle complex geometries, irregular meshes with hanging nodes, and approximations that have polynomials of different degrees in different elements, but CG method cannot use non-conforming or irregular meshes with any order. Actually,

because of no continuity constraints between the elements of DG, we can use many hanging nodes per face as we need, but for CG methods, we can only have at most one hanging node per edge, and special continuous basis functions have to be used to fit this condition. Moreover, the DG method does not need auxiliary variables such as those used in hybrid and mixed method. Also, it is locally mass conservative at the element level while CG method only satisfies a global mass balance over the whole computational domain. The property of mass conservation is crucial in flow and transport problems, especially in convection-dominated problems. In addition, it has less numerical diffusion and provides more local approximation than most conventional logarithms. The success of this method is mainly due to three facts. First, the nonlinear conservation laws are enforced locally; second, when the approximate solution is not piecewise constant, the stability of the method does not follow from the form the numerical fluxes anymore and has to be enforced by means of flux or slope limiter; third, both the approximate solution and associated fluxes can experience discontinuities across inter-element boundaries due to its discontinuous function space. But for CG methods or other traditional logarithms, they must enforce continuity condition when crossing the inter-element boundaries. Furthermore, DG method can be used to handle rough coefficient problems and is particular convenient for time-dependent problems, because the global mass matrix is block diagonal with uncoupled blocks, but not for conforming methods. This makes the cost of computation is relatively smaller than other logarithms. Actually, because of local property of DG method, the trial and test spaces are easier to construct than conforming methods, which render the code shorter and more efficient for DG method. Unlike mixed finite element methods or traditional continuous Galerkin methods which not only care about information of interface and elements but also include vertices of each element, DG method just needs to handle the information of elements and interfaces, which help us save lots of CPU time and costs. For DG methods, a priori error estimates are derived so that the parameters affecting the rate of convergence and limitations of the method are established. For instance, in terms of smooth convection-diffusion problems, DG method with varying P can yield nearly exponential convergence rates. Also, the flexibility of DG method makes the implementation of h-p adaptivity more easier than other conventional approaches as a result.

All the features listed above makes DG method will be a good candidate for solving convection-dominated problems, especially for the problem of contaminants leaking through porous media. There are only two popular families of DG methods. One is primal DG method, namely variations

of interior penalty methods which include symmetric interior penalty Galerkin (SIPG), incomplete interior penalty Galerkin (IIPG,) and non-symmetric interior penalty Galerkin (NIPG) methods; the other is local DG method which is systematically investigated by Cockburn B and Shu CW. Both methods have their attractive features, but we will use the primal DG in this paper due to it reduce costs of computation and handle the diffusion tensor more easily than the local DG methods.

In order to investigate DG scheme, let us firstly give broken Sobolev spaces which are natural spaces to work with the DG methods. These spaces depend strongly on the partition of the domain. Let ε_h be a quasi-uniform family and possibly non-conforming partitions of our bounded polygonal domain, which is composed of triangles or quadrilaterals in 2D, or a tetrahedron or hexahedron in 3D. We also require that these partitions are regular. This means that every element is convex, and if h_E denotes the diameter of the element $E \in \varepsilon_h$ and h denotes the maximum diameter of a ball inscribed in each element $E \in \varepsilon_h$, there exists a constant $\rho > 0$ such that h/h_E for every element $E \in \varepsilon_h$. We assume no element crosses the boundaries $\Gamma_{in}, \Gamma_{out}$ of our domain.

The broken Sobolev Space for any real number s is defined as follows:

$$H^s(\varepsilon_h) = \{\phi \in L^2(\Omega) : \phi|_E \in H^s(E), E \in \varepsilon_h\},$$

where $H^s(\Omega)$ is known as Sobolev space for any dimension (may be Hausdorff dimension).

And the broken Sobolev norm is defined as follows:

$$|||\phi|||_{H^s(\varepsilon_h)} = \left(\sum_{E \in \varepsilon_h} \|\phi\|_{H^s(E)}^2 \right)^{1/2}.$$

In particular, we will use the broken gradient semi-norm:

$$|||\nabla\phi|||_{H^0(\varepsilon_h)} = \left(\sum_{E \in \varepsilon_h} \|\nabla\phi\|_{L^2(E)}^2 \right)^{1/2}.$$

Clearly, we have

$$H^s(\Omega) \subset H^s(\varepsilon_h), H^s(\varepsilon_h) \subset H^{s+1}(\varepsilon_h).$$

Next, we will introduce the jumps and averages for DG schemes, which are crucial concepts in DG method. Let Γ_h be the set of all interior edges (for 2D domain) or faces (for 3D domain) for the sub-division ε_h . The set of all edges or faces on the boundaries Γ_{in} and Γ_{out} are denoted by $\Gamma_{h,in}$ and $\Gamma_{h,out}$. On each edge or face $\gamma \in \Gamma_h$, we associate a unit normal vector n_γ . If edge or face

is on the boundary of our domain, then n_γ is taken to be the unit normal outward vector to the boundary of our domain. If $\phi \in H^1(\varepsilon_h)$, then the trace of ϕ along the side of each element is well defined. But for two elements E_i and E_j which are neighbors and share one common side, there will be two traces of ϕ along the edge or face $\gamma = \partial E_i \cap \partial E_j$. Then we need to give the definition of jumps and averages.

The average and the jump for $\phi \in H^s(\varepsilon_h), s > 1/2$ is defined as follows: Let $E_i, E_j \in \varepsilon_h$ and $\gamma = \partial E_i \cap \partial E_j \in \Gamma_h$ with n_γ exterior to E_i . Denote

$$\{\phi\} = 1/2((\phi|_{E_i})|_\gamma + (\phi|_{E_j})|_\gamma),$$

$$[\phi] = (\phi|_{E_i})|_\gamma - (\phi|_{E_j})|_\gamma.$$

For the one dimensional case, we extend the definition of jump and average to sides that belong to the boundary :

$$\{\phi\} = [\phi] = (\phi|_{E_j})|_\gamma, \quad \forall \gamma = \partial E_i \cap \Omega.$$

The discontinuous finite element space is taken to be

$$D_r(\varepsilon_h) \equiv \{\phi \in L^2(\Omega) : \phi|_E \in P_r(E), E \in \varepsilon_h\},$$

where $P_r(E)$ denotes the space of polynomials of (total) degree less than or equal to r on E .

The inner product in $(L^2(\Omega))^d$ or $L^2(\Omega)$ is indicated by $(\cdot, \cdot)$ and the inner product in the boundary function space $L^2(\gamma)$ is indicated by $(\cdot, \cdot)_\gamma$. The norm $(L^2(\Omega))^d$ for a vector-value function is defined as

$$\|\mathbf{u}\|_{(L^2(\Omega))^d} = \| |\mathbf{u}| \|_{L^2(\Omega)},$$

where $|\cdot|$ is the standard vector norm defined by $|\mathbf{u}| = (\mathbf{u}, \mathbf{u})^{1/2}$. For simplicity, the norms $\|\cdot\|_{(L^2(\Omega))}$ and $\|\cdot\|_{(L^2(\Omega))^d}$ are also written as $\|\cdot\|_0$ for scalar-value and vector-value functions, respectively. The norm of $(L^p(\Omega))^{d \times d}$ for a matrix-value function is defined as

$$\|A\|_{(L^p(\Omega))^{d \times d}} = \| \|A\|_2 \|_{L^p(\Omega)},$$

where $\|\cdot\|_2$ is the matrix 2-norm defined by $\|A\|_2 = \sup_{|\mathbf{u}|=1} |A\mathbf{u}|$.

3.4 DG for transport equation

Next, we will give the continuous in time formulation for transport problem. We first define the bilinear form $B(c, \omega; \mathbf{u})$ as

$$\begin{aligned} B(c, \omega; \mathbf{u}) = & \sum_{E \in \mathcal{E}_h} \int_E (\mathbf{D}(\mathbf{u}) \nabla c - c\mathbf{u}) \cdot \nabla \omega - \int_{\Omega} cq^- \omega - \sum_{\gamma \in \Gamma_h} \int_{\gamma} \{\mathbf{D}(\mathbf{u}) \nabla c \cdot n_{\gamma}\} [\omega] \\ & - S_{transp} \sum_{\gamma \in \Gamma_h} \int_{\gamma} \{\mathbf{D}(\mathbf{u}) \nabla c \cdot n_{\gamma}\} [c] + \sum_{\gamma \in \Gamma_h} \int_{\gamma} c^* \mathbf{u} \cdot n_{\gamma} [\omega] + \sum_{\gamma \in \Gamma_{h,out}} \int_{\gamma} c^* \mathbf{u} \cdot n_{\gamma} \omega + J_0^{\sigma, \beta}(c, \omega) \end{aligned}$$

where the upwind value of concentration $c^*|_{\gamma}$ is defined as follows:

$$c^*|_{\gamma} = \begin{cases} c|_{E_i} & \text{if } \mathbf{u} \cdot n \geq 0 \\ c|_{E_j} & \text{if } \mathbf{u} \cdot n < 0 \end{cases}$$

for $\gamma = \partial E_i \cap \partial E_j$ and n_{γ} is a unit normal vector pointing from E_i to E_j . Notice $\mathbf{u}_{\gamma}$ is continuous on the direction n_{γ} , thus has well-defined value at the interface. $S_{transp} = -1$ for NIPG, $S_{transp} = 1$ for SIPG and $S_{transp} = 0$ for IIPG. Here q^+ is the injection source term and q^- is the extraction source term, i.e., $q^+ = \max(q, 0)$, $q^- = \min(q, 0)$. By definition, we have $q = q^+ + q^-$. (actually in our model $q = 0$, thus we can omit the term relative to q in both bilinear and linear form). Because of the mixed boundary condition, the jump term penalizes the interior face only. $J_0^{\sigma, \beta}(c, \omega)$ is the interior penalty term,

$$J_0^{\sigma, \beta}(c, \omega) = \sum_{\gamma \in \Gamma_h} \frac{\sigma_{\gamma}}{h_{\gamma}^{\beta}} \int_{\gamma} c[\omega],$$

where σ is a discrete positive function that takes constant value σ_{γ} on the edge or face γ and have upper and lower bound $\sigma^*, \sigma_* > 0$, h_{γ} denotes the size of γ and $\beta \geq 0$ is a real number.

The linear functional $L(\omega; \mathbf{u}, c)$ is defined as

$$L(\omega; \mathbf{u}, c) = \int_{\Omega} c_{\omega} q^+ \omega - \sum_{\gamma \in \Gamma_{h,in}} \int_{\gamma} c_B \mathbf{u} \cdot n_{\gamma} \omega.$$

The continuous in time DG scheme for approximating transport equation is as follows: we seek $\mathbf{u}_h \in L^\infty((0, T]; V_h^0(\varepsilon_h))$, $c_h \in L^\infty((0, T]; D_r(\varepsilon_h))$ satisfying,

$$\begin{cases} (\phi^{eff} \frac{\partial c_h}{\partial t}, \omega) + B(c_h, \omega; \mathbf{u}_h) = L(\omega; \mathbf{u}_h, c_h) & \forall \omega \in D_r(\varepsilon_h), \forall t \in (0, T] \\ (\phi^{eff} c_h, \omega) = (\phi^{eff} c_0, \omega) & \forall \omega \in D_r(\varepsilon_h), t = 0 \end{cases}$$

Actually, in our simulation, we split the whole transport equation into two sub-equations, one is advection equation, and the other one is diffusion equation. Because the mass matrices are different, we need to deal with them separately for the convenience of implementation. Also we can deal with two sub-equations with two different schemes, which will be more convenient for coding and more accurate for the final solution. For instance, in our simulation, we apply DG scheme to advection problem and use MFE or CCFD to deal with diffusion problem, which will render a better solution for the whole problem.

Next, we will give the semidiscrete formulation for the advection problem. We apply an upwind discretization. The upwind value of concentration function c^* is denoted above. The bilinear form for advection problem is denoted by $b(c, \omega; \mathbf{u})$:

$$b(c, \omega; \mathbf{u}) = - \sum_{E \in \varepsilon_h} \int_E c \mathbf{u} \cdot \nabla \omega + \sum_{\gamma \in \Gamma_h} \int_{\gamma} c^* \mathbf{u} \cdot n_{\gamma} [\omega] + \sum_{\gamma \in \Gamma_{h,out}} \int_{\gamma} c^* \mathbf{u} \cdot n_{\gamma} \omega.$$

The continuous in time DG scheme for approximating advection equation is as follows: we seek $\mathbf{u}_h \in L^\infty((0, T]; V_h^0(\varepsilon_h))$, $c_h \in L^\infty((0, T]; D_r(\varepsilon_h))$ satisfying,

$$\begin{cases} (\phi^{eff} \frac{\partial c_h}{\partial t}, \omega) + b(c_h, \omega; \mathbf{u}_h) = 0 & \forall \omega \in D_r(\varepsilon_h), \forall t \in (0, T] \\ (\phi^{eff} c_h, \omega) = (\phi^{eff} c_0, \omega) & \forall \omega \in D_r(\varepsilon_h), t = 0 \end{cases}$$

For single element, the DG scheme is simplified as follows:

$$\int_{E \in \varepsilon_h} \phi^{eff} \frac{\partial c_h}{\partial t} \omega dx + \int_{\partial E \in \Gamma_h} c_h^* \omega \mathbf{u} \cdot n_{\gamma} ds - \int_{E \in \varepsilon_h} c_h \mathbf{u} \cdot \nabla \omega, \forall \omega \in D_r(\varepsilon_h), \forall t \in (0, T].$$

After computing local matrix on each element, we assemble local matrix into stiff matrix then apply backward Euler method to compute solution for advection part.

3.5 Cell Centered Finite Difference method

We firstly solve the flow equation with cell centered finite difference method , then plug our solved velocity into reactive transport equation using FVM and CCFD deal with advection and diffusion part respectively. As we all known that "Finite volume" refers to the small volume surrounding each node point on a mesh. In the finite volume method, volume integrals in a partial differential equation that contain a divergence term are converted to surface integrals, using the divergence theorem. These terms are then evaluated as fluxes at the surfaces of each finite volume. Because the flux entering a given volume is identical to that leaving the adjacent volume, these methods are conservative. Another advantage of the finite volume method is that it is easily formulated to allow for unstructured meshes. The method is used in many computational fluid dynamics packages.

We denote $\delta_x \times \delta_y$ as a possibly non-uniform rectangular mesh:

$$\begin{aligned}\delta_x : 0 = x_0 < x_1 < \dots < x_M = L_x, \\ \delta_y : 0 = y_0 < y_1 < \dots < y_M = L_y.\end{aligned}$$

We partition the simulation time $[0, T]$ into K subintervals: $0 = t_0 < t_1 < \dots < t_{K-1} < t_K = T$. We First define center point of each subintervals :

$$\begin{aligned}x_{i+1/2} &= 1/2(x_i + x_{i+1}), \\ y_{j+1/2} &= 1/2(y_j + y_{j+1}).\end{aligned}$$

where $i = 0, 1, 2, \dots, M-1$ and $j = 0, 1, 2, \dots, N-1$.

We simply denote the approximate solution of $c(x_{i+1/2}, y_{j+1/2}, t_k)$ as

$$c_{i+1/2, j+1/2}^k \quad \text{for } i = 0, 1, 2, \dots, M-2, \text{ and } j = 0, 1, 2, \dots, N-2$$

for the convenience to discretize flow and transport equations respectively Therefore the CCFD scheme for our problem is defined as follows:

For flow part, we have following discretezied cell-centered finite difference scheme

$$-\left(\frac{1}{x_{i+1} - x_i} \left(K_{xx} \frac{P_{i+3/2, j+1/2} - P_{i+1/2, j+1/2}}{x_{i+3/2} - x_{i+1/2}} - K_{xx} \frac{P_{i+1/2, j+1/2} - P_{i-1/2, j+1/2}}{x_{i+1/2} - x_{i-1/2}} \right)\right)$$

$$+ \frac{1}{y_{i+1} - y_i} (K_{yy} \frac{P_{i+1/2,j+3/2} - P_{i+1/2,j+1/2}}{y_{j+3/2} - y_{j+1/2}} - K_{yy} \frac{P_{i+1/2,j+1/2} - P_{i+1/2,j-1/2}}{y_{j+1/2} - y_{j-1/2}})) = q$$

For transport part, the discreteized cell-centered finite difference scheme is defined as follows:

$$\begin{aligned} & \frac{\phi_{i+1/2,j+1/2} c_{i+1/2,j+1/2}^{k+1} - \phi_{i+1/2,j+1/2} c_{i+1/2,j+1/2}^k}{t^{k+1} - t^k} + \left(\frac{u_{xx} c_{i+1,j+1/2}^{k+1} - u_{xx} c_{i,j+1/2}^{k+1}}{x_{i+1} - x_i} \right. \\ & + \frac{u_{yy} c_{i+1/2,j+1}^{k+1} - u_{yy} c_{i+1/2,j}^{k+1}}{y_{j+1} - y_j} \left. \right) - \left(\frac{1}{x_{i+1} - x_i} (D_{xx} \frac{c_{i+3/2,j+1/2}^{k+1} - c_{i+1/2,j+1/2}^{k+1}}{x_{i+3/2} - x_{i+1/2}} \right. \\ & - D_{xx} \frac{c_{i+1/2,j+1/2}^{k+1} - c_{i-1/2,j+1/2}^{k+1}}{x_{i+1/2} - x_{i-1/2}}) + \frac{1}{y_{i+1} - y_i} (D_{yy} \frac{c_{i+1/2,j+3/2}^{k+1} - c_{i+1/2,j+1/2}^{k+1}}{y_{i+3/2} - y_{i+1/2}} \\ & \left. - D_{yy} \frac{c_{i+1/2,j+1/2}^{k+1} - c_{i+1/2,j-1/2}^{k+1}}{y_{i+1/2} - y_{i-1/2}}) \right) = q c_{i+1/2,j+1/2}^{k+1} \end{aligned}$$

where K_{xx} , K_{yy} are the x -component and y -component of permeability tensor at cell centers respectively; D_{xx} , D_{yy} are the x -component and y -component of diffusion coefficient tensor at cell centers respectively; u_{xx} , u_{yy} are the computed x -direction and y -direction Darcy velocity(flux) respectively from flow equation; q is a constant. For general case, q in the transport part does not equal to 0, but in our simulation, we simplify it as 0 in transport because of our models. After discretization, we need to put in boundary condition, then we can formulation matrix for both flow and transport equations and finish implementation.

Chapter 4

Numerical Results on Rectangular Meshes

4.1 Simulation Examples (MFE scheme)

According to experimental data, we construct a computational domain of $(0, 0.6 \text{ m}) \times (0, 0.6 \text{ m})$ for all numerical examples. We also use non-uniform rectangular mesh to discretize a $(0, 0.6 \text{ m}) \times (0, 0.6 \text{ m})$ rectangular domain with random fractures for our simulation.

Among our simulation examples, example 1 is the base case to be compared with other examples. In this base case, we use a set of standard parameters from laboratory (see Table 1). In other examples we vary the fractures with different lengths and distributions, but maintain the same parameters with base case. In all examples, we assume no-flow boundary conditions on both top ($y=0 \text{ m}$) and bottom boundaries ($y=0.6 \text{ m}$). We also specify a constant pressure of 0 (gauge pressure against a reference pressure) on the right boundary ($x=0.6 \text{ m}$). Contaminant species is injected on the inflow boundary located on the left ($x=0 \text{ m}$), where a higher pressure condition of 1 m-H₂O is imposed. The medium is initially saturate with clean water.

Example 1. Three horizontal and two vertical fractures (Base Case)

We use parameters listed in table 1 for our base case and the total simulation time is 10,000 years. The fracture network involves three horizontal and two vertical fractures that are interconnected (Figure 1). We generate non-uniform rectangular mesh for this fractured media due

to efficiency. As described before, we apply MFE for the flow equation, and semi-implicit FVM-MFE for the transport equation using a uniform time step of 100 years. The simulated pressure field (Figure 2) clearly indicates the influence of the fractures on the flow. We could see that there is a sharp peak when the inlet and outlet of fracture network does not touch the matrix boundary. If the inlet of fracture network extends to the boundary of our domain, then contaminant species pass through the fracture immediately, the pressure field will be a little bit same as in the matrix. Velocity fields are displayed in the streamline/quiver plot (Figure 2). As expected, the magnitude of the velocity is much smaller in the matrix as compared to it in the fracture. Moreover, it can be observed that streamlines tend to converge into fractures in the left part of the domain but diverge from the fractures in the right part, which suggests that fractures are the main pathways for transporting contaminants via convection. Figure 3 are results of simulated concentration profiles at different times (100 years, 300 years, 1000 years, 2000 years, 5000 years, and 10,000 years). At 100 years to 1000 years, the contaminant transports mainly through the convection within fractures. This is clearly demonstrated by the concentration plume formed quickly at the fracture outlets while the matrix closer to the inflow boundary is still quite clean. After 2,000 years, diffusion and convection via the matrix also start to play a significant role in the overall contaminant transport behavior. The average effluent concentration in effluent fluid as a function of time is provided in Figure 4. We note that the effluent concentration quickly increases to 0.999, and then slowly approaches to 1. This is because the fracture network here connects inflow and outflow boundaries, which creates a flow shortcut and leads to almost all fluid exiting from the cracks rather than from the matrix.

Example 2. Five horizontal and three vertical fractures (within medium interior)

Similar to Example 1, we employ the model parameters listed in table 1 and we also simulate up to 10,000 years. We impose Neumann boundary condition (10^{-4} m/year) on the left boundary and Dirichlet boundary condition (0 m-H₂O) on the right boundary. Unlike previous crack setting, the fracture network in this case involves five horizontal and three vertical fractures that are interconnected, but do not extend to the boundary (Figure 5). We apply RT0-MFE on rectangular meshes for the flow equation, and semi-implicit FVM-MFE for the transport equation using a uniform time step of 100 years. The simulated pressure field (Figure 6) clearly indicates the influence of the fractures on the flow. The velocity fields are displayed in the streamline/quiver plot (the right panel of Figure 6). Again, the magnitude of the velocity is much smaller in the matrix as compared to it in the fracture. Moreover, it can be observed that streamlines tend to converge into fractures

near the inflow boundary but diverge from the fractures close to the outflow boundary. Obviously, we observe one more time that fractures are the main pathways for transporting contaminants via convection. Figure 7 are results of simulated concentration profiles at different times (100 years, 300 years, 1000 years, 2000 years, 5000 years, 10 000 years) from rectangular mesh simulation. At early simulation times, the contaminant transports mainly through the convection within fractures. This is clearly demonstrated by the concentration plume formed quickly at the fracture outlets while the matrix closer to the inflow boundary is still quite clean. At later simulation times, diffusion and convection via the matrix also start to play a significant role in the overall contaminant transport behavior. Figure 8 depicts the relationship between average effluent concentration and time. We note that the effluent concentration does not quickly increase to 0.999 within a short time, cause our fracture network does not extend to the inflow and outflow boundaries, thus it leads our curve smoothly increasing before the contaminant species reaches the fracture network and also increasing smoothly when it comes out from fracture network, therefore we can see a breakthrough curve (a smooth step function) in this example. In about ten thousand years, the average normalized concentration on outflow boundary reaches about 99 percent.

Example 3. Random generated fracture network without touching boundary

The model parameters employed in this base case are listed in table 1 and we attempt to simulate up to 10,000 years. The fracture network is randomly generated but not extending to the boundary (Figure 9) and the fracture density is 16.36081. We generate non-uniform rectangular mesh for this fractured media due to efficiency. As described before, we apply RT0-MFE for the flow equation, and semi-implicit FVM-MFE for the transport equation using a uniform time step of 100 years. The simulated pressure field (Figure 10) clearly indicates the influence of the fractures on the flow. In particular, two inlets of the fracture network have corresponding local pressure irregularities. The velocity fields are displayed in the streamline/quiver plot (Figure 10). As expected, the magnitude of the velocity is much smaller in the matrix as compared to it in the fracture. Moreover, it can be observed that streamlines tend to converge into fractures in the left part of the domain but diverge from the fractures in the right part, which suggests that fractures are the main pathways for transporting contaminants via convection. Figure 11 are results of simulated concentration profiles at different times (100 years, 300 years, 1000 years, 2000 years, 5000 years, and 10,000 years). At 100 years to 1000 years, the contaminant transports mainly through the convection within fractures. This is clearly demonstrated by the concentration plume formed quickly at the fracture outlets while

the matrix closer to the inflow boundary is still quite clean. After 2,000 years, diffusion and convection via the matrix also start to play a significant role in the overall contaminant transport behavior. The average effluent concentration in effluent fluid as a function of time is provided in Figure 12. We note that the effluent concentration quickly increases to 0.999, and then slowly approaches to 1. This is because the fracture network here connects inflow and outflow boundaries, which creates a flow shortcut and leads to almost all fluid exiting from the cracks rather than from the matrix.

Example 4. Random generated fracture network extending to boundary

In this example, we still employ the model parameters listed in table 1 and we also simulate up to 10,000 years. We apply RT0-MFE on rectangular meshes for the flow equation, and semi-implicit FVM-MFE for the transport equation using a uniform time step of 100 years. The fracture network (Figure 13) in this example is extending to the boundary and the fracture density is 24.49502. The simulated pressure field (Figure 14) clearly indicates the influence of the fractures on the flow. The velocity fields are displayed in the streamline/quiver plot (the right panel of Figure 14). Obviously, we observe one more time that fractures are the main pathways for transporting contaminants via convection. Figure 15 are results of simulated concentration profiles at different times (100 years, 300 years, 1000 years, 2000 years, 5000 years, 10,000 years) from rectangular mesh simulation. At early simulation times, the contaminant transports mainly through the convection within fractures. This is clearly demonstrated by the concentration plume formed quickly at the fracture outlets while the matrix closer to the inflow boundary is still quite clean. At later simulation times, diffusion and convection via the matrix also start to play a significant role in the overall contaminant transport behavior. Figure 16 depicts the relationship between average effluent concentration and time. We note that the effluent concentration does not quickly increase to 0.999 within a short time, cause our fracture network does not extend to the inflow and outflow boundaries, thus it leads our curve smoothly increasing before the contaminant species reaches the fracture network and also increasing smoothly when it comes out from fracture network, therefore we can see a breakthrough curve (a smooth step function) in this example. In about ten thousand years, the average normalized concentration on outflow boundary reaches about 99 percent. Through observing two graphs of average effluent concentration versus time (Figure 12 and Figure 16), we find that even if in the random fracture network, provided that there's one side of our fracture network touching the boundary, S-curve will increasing to 99 percent quickly, therefore, our fracture network plays an import role in transporting contaminant species and can not be neglected in the reality and

simulation process.

4.2 Simulation examples(DG)

Example 5. Four horizontal and two vertical fractures

We still use the same parameter as previous numerical examples and also attempt to simulate up to 10,000 years. The fracture network in this case involves four horizontal and two vertical fractures that are interconnected and does not extend to the boundary (Figure 17). We first apply RT0-MFE for the flow equation, and semi-implicit FVM-MFE for the transport equation using a uniform time step of 100 years. Figure 18 are results of simulated concentration profiles at different times (100 years, 300 years, 1000 years, 2000 years, 5000 years, and 10,000 years). Then we apply RT0-MFE for the flow equation, and semi-implicit DG-MFE for the transport equation using a uniform time step of 100 years. Figure 19 are results of simulated concentration profiles at different times under DG schemes with same simulation time. In order to specify the advantage of DG scheme, we use original concentration file not the post-processed data file, although it looks not so beautiful, but we can see the difference between two schemes. In Figure 19, at simulation time 100 years, we can see that there is a gradual change in the matrix region (outside the fracture network), but in Figure 18, this gradual change does not show up very obviously in the matrix region, also, when the contaminant species approaches fracture network, this gradual change will be more sharp contrasting with picture in Figure 18 (that is MFE scheme), furthermore, in the fracture network, we can still see the gradual change is better than the picture under MFE scheme, all these demonstrate one result: that is DG scheme will present more detailed stuff than MFE scheme and therefore made our numerical result will be more accurate to the real problem. Under DG scheme, we can see detailed variation of contaminant species passing through the fracture network and matrix, unlike MFE and CCFD scheme, which cover lots of detailed stuff and therefore made the result inaccurate. Figure 20 and 21 are the pictures of the average effluent concentration on the outflow boundary versus time under both MFE and DG scheme, from two pictures, we can observe that under DG scheme, S-curve will be closer to a step function which is real solution to our problem. All these once again confirm the priority of DG schemes.

Example 6. Single fracture (without extending to the boundary)

We consider a single fracture in our domain with fracture inlet/outlet not touching the

domain boundary. The fracture network is depicted in Figure 22. We still give out the simulated concentration profiles at different times under two different schemes (Figure 23 and 24), from those pictures (1000 years, 2000 years, 3000 years, 5000 years, 8000 years, 10000 years), we can clearly see the difference between two schemes, the simulated concentration profile under MFE scheme obviously looks more coarsely than DG scheme and covers lots of details no matter in the fracture net work or in the matrix region. In addition, we can see the picture of the average effluent concentration on the outflow boundary versus time under DG scheme will be more accurate than MFE scheme (Figure 25 and 26), since it looks more like a step function, which is our real solution to our problem, and the break through time is shorter under DG scheme than MFE scheme. All these once again corresponds our previous conclusion: DG scheme will more accurate than MFE scheme.

Example 7. Single fracture (without extending to the boundary)

Continuing above example, we found an interesting result: that is when both ends of our single fracture network approach the matrix boundary (Figure 27), we observe that the graph of the average effluent concentration on the outflow boundary versus time does not looks like a strict S-curve, it seems that there are two break through during the whole simulation process. The reason for this result is that if single fracture network will be more closer to the matrix boundary, then the contaminant species will quickly leak through the fracture network to the other boundary of matrix and therefore formulate first breakthrough, when other contaminant species transport from matrix to the boundary of matrix, it will form a second breakthrough, all these illustrate one result: if there are any fracture in our matrix, contaminant species will leak through from fracture network firstly and quickly, provided diffusivity and permeability is not large in the matrix region. We still use two schemes to present the results of this case. Figure 28 is the graph of the average effluent concentration on the outflow boundary versus time under MFE scheme. Figure 29 is under DG scheme. Once more, we could see that DG scheme will be more accurate than MFE scheme, because of less break through time.

Example 8. Single fracture (outlet extending to the boundary)

We consider a single fracture in our domain with fracture inlet not touching the domain boundary. The fracture network is depicted in Figure 30. In this case, we will see that the graph of the average effluent concentration on the outflow boundary versus time (Figure 31) still have two break through point, also there is a sharpen increase at first break through, this is because our fracture network touches the outflow boundary and therefore made the average effluent concentration on

the outflow boundary increase quickly, when other contaminant species reaches the outflow boundary through matrix it will form a second shallow break through. Figure 32 is under DG scheme. Although it has same shape, it will be closer to real problem.

4.3 Sensitivity Analysis under MFE scheme

In all sensitivity analysis, we use average effluent concentration to test the influence of different parameters to our model, the average effluent concentration $\bar{c}$ is defined as follows:

$$\bar{c} = \frac{\int_{\Gamma_{outflow}} \mathbf{u} \cdot \mathbf{n} c ds}{\int_{\Gamma_{outflow}} \mathbf{u} \cdot \mathbf{n} ds}$$

Effect of K_d Values

The parameter K_d value, which represents the distribution of contaminant between the solid and liquid phases, is defined as follows

$$K_d = c_s/c = \frac{\text{mass of solute on the solid phase per unit mass of solid phase}}{\text{concentration of solute in solution}}$$

The effect of the K_d expresses as a retardation in the breakthrough curve of a contaminant. Retardation of dissolved contaminant element is due to sorption, chemical reactions with porous media or fracture walls, and movement into dead-end pores by diffusion. As a result, contaminant element will not move as fast as average advective velocity of ground water which carries it. The retardation coefficient in porous media is expressed as (Freeze and Cherry,1979;Prickett et al.1981)

$$K_d = \frac{v}{v_c},$$

$$K_d = 1 + \frac{\rho_b R_d}{n},$$

and in fracture media(Burkholder, 1976) as

$$K_d = 1 + AR_a,$$

where v = average ground-water velocity; v_c = average velocity of the contaminant mass; ρ_b = bulk mass density of the porous medium; n = effective porosity; R_d = distribution coefficient

of porous medium; R_a = fracture-rock distribution coefficient; and A = ratio of fracture-wall surface area to void space(volume). To analyze the effect of K_d values, we test three cases. Different K_d values are employed and the concentrations on outflow boundary versus time are depicted in Figure 33. Clearly, the contaminant exits the system earlier in a fractured medium with low K_d than with high K_d value.

Effect of Conductivity

We simulate contaminant transport with three different conductivity values. The breakthrough curves for these cases are depicted in Figure 34. From the picture we see that the exiting time of the contaminant reduces slightly in fractured medium with high conductivity values as compared to the one with lower conductivity.

Effect of diffusion coefficient

To analyze the effect of diffusion coefficient, we again test three cases. Different diffusion coefficient is employed and the concentrations on outflow boundary versus time are depicted in Figure 35. Contaminant reaches the outflow boundary more quickly with a lower diffusion coefficient.

Effect of fracture density

We modulate various fracture density to investigate its influence. Different fracture density is employed and the concentrations on outflow boundary versus time are described in Figure 36. Clearly and also as expected, concentration on the outflow boundary increases to 0.5 more quickly in a fractured medium with higher fracture density at in our simulation.

4.4 Sensitivity Analysis under DG scheme

Effect of diffusion coefficient

We use multi-fracture media in Example 1 to analyze the effect of diffusivity under DG scheme. We use average effluent concentration on the outflow boundary to test the influence of diffusion coefficient under DG scheme. The saturated effective diffusion coefficient is changed from the low value $5 \times 10^{-12} m^2/s$ to the high value $5 \times 10^{-11} m^2/s$ (Figure 37). It will spend more time to reach 50 % concentration with higher diffusivity, however, it takes less time to reach a higher value like 90 % concentration. In order to see the difference of two schemes, we also give the graph of MFE scheme (Figure 38).

4.5 Lumping an entire fracture network into one equivalent crack via effective K_d

We first use our flow and contaminant transport simulator to obtain the relationship between 50 % concentration time and real K_d values (Figure 39). Here we use polynomials to fit this relationship. The resultant correlation is $y = 5000x + 8000$, (y is 50 % concentration time, x is real K_d). In the second step, we get the relationship between 50 % concentration time and effective K_d values (Figure 40) for a single-fracture network: $y = 12500x + 1080$, (y is 50% concentration time, x is effective K_d). Finally, we use 50 % concentration time to match relationship between effective K_d and real K_d . The final relationship we obtained is: $12.5u + 1.08 = 5v + 8$, (u denotes effective K_d , v denotes real K_d). Apparently, the relationship between the effective K_d and the real K_d is a linear relationship (also shown in Figure 41).

4.6 Relationship between lumped effective K_d and fracture density

In order to find this relationship between lumped effective K_d and fracture density, we first get the relationship between 50% concentration time and fracture density (Figure 42) under multi-fracture network. Like above, we still use polynomials to fit this relationship. From Figure 42 we can see that this relationship is kind of linear relationship, although there's some discrepancy around real curves, it can be considered as a linear relation due to the numerical errors of our simulator. The resultant correlation is $y = 62.7x + 1527.3$, (y is 50% concentration time, x is fracture density). In the second step, we get the relationship between 50% concentration time and effective K_d values (Figure 43) for a single-fracture network: $y = 38588x + 3477$, (y is 50% concentration time, x is effective K_d). Finally, we use 50% concentration time to match relationship between effective K_d and fracture density. The final relationship we obtained is: $38.588u + 3.477 = 0.0627v + 1.5273$, (u denotes effective K_d , v denotes fracture density). Apparently, the relationship between the effective K_d and fracture density is a linear relationship (also shown in Figure 44).

4.7 Impact of impulse concentration on our model

In the previous numerical examples, we have assumed that the concentration of contaminant species is a constant on the boundary of our matrix. However, in the practical case, concentration on the boundary may be changed with time. Thus, it is interesting to investigate the case that concentration varies with different time. To see the difference between two different cases, we still observe the picture of average effluent concentration on the right boundary versus time in each case and then do some analysis between two cases. We have already known that in the former case the graph of effluent concentration versus time looks like a smooth S-curve because our fracture network and different permeability between fracture and matrix make contaminant species reach the right export at different time, and in this case our concentration on the left boundary is still a constant (Figure 45). Then we have a question that if the concentration on the left boundary is not a constant, how the graph of average effluent concentration versus time changes? In order to figure out this problem, we vary our concentration on the left boundary from a constant function into a impulse (Figure 46), then we use our simulator producing the graph of average effluent concentration versus time (Figure 46). We have seen that this curve does not look like a S-curve, indeed it looks more like a picture of normal distribution, also you can consider it as a smoothed step function of left boundary concentration. In this graph we can see that this curve reaches its peak at 5000 years, and its peak's value is about 85 percent, which is just consistent with picture of constant concentration on the left boundary at 5000 years (Figure 46). In Figure 45, S-curve increases smoothly into about one with time elapsing due to the constant concentration on the left boundary, however, In Figure 46, we have seen that after 5000 years, the curve drops smoothly from 85 percent into about 0 with time reaching our final simulation time, because we set our impulse function of left boundary concentration, after 5000 years, into zero. Thus, we can see that our average effluent concentration curve is related to the concentration on the boundary, and also we have test several cases if our boundary pressure changed. From Figure 46, we know that with the boundary pressure increasing, peak point will approximate into one and also curve become more smooth, but when the boundary pressure change a lot, it will looks more like a step function, the reason may be considered as the high pressure makes velocity of contaminant species become huge and therefore makes no difference between fracture and matrix. Hence the picture of average effluent concentration is related to many reasons such as boundary concentration, pressure, also the permeability, K_d values and so on.

Chapter 5

Conclusions and future work

In this paper, an efficient and robust simulator has been developed for the solution of contaminant species passing through a fractured cementitious matrix. We first presented our mathematical model consisting of two differential equations, i.e. the flow equation and the reactive transport equation. A numerical scheme based on the mixed finite element (MFE) method is developed to approximate the second-order partial derivate terms in the flow and transport equations. The convection term in the transport equation is treated using an upwind finite volume method (FVM) and discontinuous galerkin method (DG). With the MFE method, the fluxes through fractures are accurately approximated using non-uniformed rectangular mesh cause rectangular grids have the advantages of efficient vector computation. Various patterns of fractures are simulated and compared. In the rectangular simulations, we employ non-uniform meshes with small elements representing cracks. Sensitivity analysis has been carried out for the analysis of each parameter's impact on our models. The effective K_d calculation for lumping an entire crack network to an equivalent single-fracture system has been proposed and carried out using our contaminant transport simulator on rectangular meshes. We also investigate the relationship between lumped effective K_d and fracture density on rectangular meshes, which we believe is meaningful and useful to our applications because the fracture network plays a crucial rule in the contaminant transport system and it tightly interacts with many other parameters in our mathematics model such as conductivity, porosity and intrinsic K_d , thus affecting the lumped effective K_d . At last, we exert an impulse concentration to our clean matrix, we saw an interesting result as described in section 4.5. In the near future, we may use multi-scale scheme to implement our model, this is meaningful to our project. Since it has

practical meaning in the real models, for instance, the time step used in fracture must be different with matrix, this may be challenging, but it deserve to investigate at the next step.

Appendices

Appendix A

Tables

Conductivity, $K_s(cm/s)$	Diffusion , $D_e(cm^2/s)$	Effective Porosity (%)	$K_d(ml/g)$
1.0E-12	5.0E-11	18.4	0

Table A.1: Standard parameters

Appendix B

Figures

Figure B.1: Fracture and conductivity distribution for base case

Pressure distribution

Velocity field

Figure B.2: Pressure distribution and Velocity field for example 1

Concentration distribution at 100 year

Concentration distribution at 300 year

Concentration distribution at 1000 year

Concentration distribution at 2000 year

Concentration distribution at 5000 year

Concentration distribution at 10000 year

Figure B.3: Concentration at different time within ten thousand years

Figure B.4: Average effluent concentration versus time for example 1

Figure B.5: Fracture and conductivity distribution for example 2

Figure B.6: Pressure distribution and Velocity field for example 2

Concentration distribution at 100 year

Concentration distribution at 300 year

Concentration distribution at 1000 year

Concentration distribution at 2000 year

Concentration distribution at 5000 year

Concentration distribution at 10000 year

Figure B.7: Concentration at different time within ten thousand years

Figure B.8: Average effluent concentration versus time for example 2

Figure B.9: Fracture and conductivity distribution for example 3

Pressure distribution

Velocity field

Figure B.10: Pressure distribution and Velocity field for example 3

Concentration distribution at 100 year

Concentration distribution at 300 year

Concentration distribution at 1000 year

Concentration distribution at 2000 year

Concentration distribution at 5000 year

Concentration distribution at 10000 year

Figure B.11: Concentration at different time within ten thousand years

Figure B.12: Average effluent concentration versus time for example 3

Figure B.13: Fracture and conductivity distribution for example 4

Pressure distribution

Velocity field

Figure B.14: Pressure distribution and Velocity field for example 4

Concentration distribution at 100 year

Concentration distribution at 300 year

Concentration distribution at 1000 year

Concentration distribution at 2000 year

Concentration distribution at 5000 year

Concentration distribution at 10000 year

Figure B.15: Concentration at different time within ten thousand years

Figure B.16: Average effluent concentration versus time for example 4

Figure B.17: Fracture and conductivity distribution for example 5

Concentration distribution at 100 year

Concentration distribution at 300 year

Concentration distribution at 1000 year

Concentration distribution at 2000 year

Concentration distribution at 5000 year

Concentration distribution at 10000 year

Figure B.18: Concentration at different time within ten thousand years for example 5(MFE)

Concentration distribution at 100 year

Concentration distribution at 300 year

Concentration distribution at 1000 year

Concentration distribution at 2000 year

Concentration distribution at 5000 year

Concentration distribution at 10000 year

Figure B.19: Concentration at different time within ten thousand years for example 5(DG)

Figure B.20: the average effluent concentration versus time for example 5 (MFE)

Figure B.21: the average effluent concentration versus time for example 5 (DG)

Figure B.22: Fracture and conductivity distribution for example 6

Concentration distribution at 1000 year

Concentration distribution at 2000 year

Concentration distribution at 3000 year

Concentration distribution at 5000 year

Concentration distribution at 8000 year

Concentration distribution at 10000 year

Figure B.23: Concentration at different time within ten thousand years for example 6(MFE)

Concentration distribution at 1000 year

Concentration distribution at 2000 year

Concentration distribution at 3000 year

Concentration distribution at 5000 year

Concentration distribution at 8000 year

Concentration distribution at 10000 year

Figure B.24: Concentration at different time within ten thousand years for example 6(DG)

Figure B.25: The average effluent concentration versus time for example 6 (MFE)

Figure B.26: The average effluent concentration versus time for example 6 (DG)

Figure B.27: Fracture and conductivity distribution for example 7

Figure B.28: The average effluent concentration versus time for example 7 (MFE)

Figure B.29: The average effluent concentration versus time for example 7 (DG)

Figure B.30: Fracture and conductivity distribution for example 8

Figure B.31: The average effluent concentration versus time for example 8 (MFE)

Figure B.32: The average effluent concentration versus time for example 8 (DG)

Figure B.33: Sensitivity analysis for parameter K_d under MFE scheme

Figure B.34: Sensitivity analysis for parameter conductivity under MFE scheme

Figure B.35: Sensitivity analysis for parameter diffusion coefficient under MFE scheme

Figure B.36: Sensitivity analysis for fracture density under MFE scheme

Figure B.37: Average effluent concentration versus time with different diffusivities (DG)

Figure B.38: Average effluent concentration versus time with different diffusivities (MFE)

Figure B.39: Relationship between 50% concentration time and real K_d

Figure B.40: Relationship between 50% concentration time and effective K_d

Figure B.41: Effective K_d versus real K_d

Figure B.42: Relationship between 50% concentration time and fracture density

Figure B.43: Relationship between 50% concentration time and effective K_d

Figure B.44: Effective K_d versus fracture density

Step function of left boundary concentration

Average effluent concentration versus time

Figure B.45: standard case

Step function of left boundary concentration

Average effluent concentration versus time

Left boundary pressure at 3 mH₂O

Left boundary pressure at 10 mH₂O

Left boundary pressure at 50 mH₂O

Left boundary pressure at 100 mH₂O

Figure B.46: Average effluent concentration versus time at different boundary pressure

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