A TRANSPORT EQUATION IN POROUS MEDIA WITH AN OBLIQUE, EVOLUTIONARY BOUNDARY CONDITION

by

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In this thesis we consider a linear partial differential equation that models contaminant transport with sources in a fractured porous medium. The geometry we study consists of a single fracture bounded by semi-infinite porous blocks.

A general mathematical model describing contaminant flow in fractures is developed, and a careful scaling analysis is used to compare this model with some of the known models studied in the literature. A simplified model which serves as the focus for this paper is

$$u_t = u_{yy} - \lambda u + f(x, y, t), \quad x, y > 0, \ t > 0$$

$$u_t = -u_x + \gamma u_y - \lambda u \ \text{ on } \ y = 0; \quad u(0, 0, t) = u_0(t), \ t > 0$$

with zero initial data.

In the fracture, this simplified model assumes convection, decay, linear adsorption and loss to the porous matrix. In the porous medium, the model includes diffusion, decay, linear adsorption and sources. The governing equations are represented by a degenerate, linear, parabolic equation in a quarter-space with an oblique, evolutionary differential equation as a boundary condition.

We solve the problem using Laplace transforms to obtain the Green's function and determine how contaminant sources at the fracture inlet and in the porous media are propagated in time.

The one-dimensional diffusion assumed in the problem is common among models in the literature and results in the omission of a no-flux boundary condition along $x = 0$ (which in some physical problems may be incorrect). In this paper we also show that this simplifed problem is the outer problem for the correctly posed singular

perturbation problem

$$\begin{aligned} u_t &= \sqrt{\epsilon} u_{xx} + u_{yy} - \lambda u, \quad x, y > 0,\ t > 0 \\ u_t &= \epsilon u_{xx} - u_x + u_y - \lambda u \quad \text{on } \ y = 0 \\ u_x &= 0 \ \text{ on } \ x = 0 \\ u(0,0,t) &= u_0(t), \quad t > 0 \end{aligned}$$

with zero initial data, which includes two-dimensional diffusion and a no-flux boundary condition along $x = 0$.

Solution surfaces for the simplified problem are obtained in two ways: first, in the exact integral solution, the infinite limits of integration are mapped to a finite region to avoid truncation difficulties and a direct quadrature scheme is applied; second, the problem is solved numerically. An implicit, finite difference scheme is applied to the diffusion problem in the matrix while an explicit difference scheme is used to approximate the differential equation along the boundary. Finally, consistency and convergence of the scheme is proved subject to conditions on the discretization.

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Contents

Chapter 1

The Mathematical Model

1.1 Introduction

Studies of fractured porous media play an important role in the environmental sciences. Early studies were dominated by the field of petroleum engineering, but it has recently been an important topic in hydrogeology for purposes of waste storage. The subject's importance is illustrated by the following scenario: Certain rock formations and clay deposits are frequently chosen as sites for hazardous waste repositories because of their physical properties and low permeabilities. It is conjectured that minimal amounts of waste material can escape from repositories located in such formations, thereby avoiding return of the material to the ecosphere and limiting its leakage to nearby aquifers. Unfortunately, rock and clay deposits can be marred by fracture networks, which can allow for virtually unobstructed transport of the waste material away from the storage site, thereby increasing the chances of the waste returning to the ecosphere. Fortunately the porous medium surrounding the fracture network is susceptible to the mechanisms of diffusion. Some of the contaminant can diffuse into the surrounding porous block where it is stored (perhaps until it decays) and is removed from the flow, thereby lessening the extent of contaminant migration via the fracture network.

It is important, then, to study the mechanisms of contaminant flow through a system of fractures embedded in a porous medium to quantify the extent of contaminant migration, as well as to provide predictions for remediation processes. Frequently

such studies involve a highly idealized fracture network (as is the case in this paper) which is mathematically tractable and serve as a worst-case scenario to which more complicated networks can be compared. An example of a geometrical simplification is the consideration of a single, semi-infinite fracture separating two, semi-infinite, parallel blocks of porous material. This is the nature of problem studied in this thesis. Models of fracture-flow are often further simplified by the application of physical assumptions regarding the parameters characterizing fracture flow to the governing equations. One such assumption includes negligible diffusion in the direction of the fracture axis, resulting in one-dimensional diffusion orthogonal to the fracture in the porous medium. This assumption results in the exclusion of a no-flux condition on the vertical boundary of the porous matrix (see figure 1.1).

Although a more thorough review of the current literature appears in Section 1.4, the issues above are highlighted to assist in identifying the aspects of this dissertation which distinguish it from previous works. The topics addressed in this thesis which make it unique among the literature are 1) the inclusion of sources within the porous matrix, 2) the arrival at a simplified model via thorough scaling analyses of the parameters involved in contaminant flow, and 3) a reconciliation, using singular perturbation theory, of the no-flux boundary condition omitted from simplified models.

1.2 Formulation of the Problem

The geometry we consider (figure 1.1) is an idealized fracture network consisting of a single fracture channel in an infinite porous domain; it is the same as that studied by Tang *et al* (1981), Fogden *et al* (1981), and others. Contaminant enters into the system at the inlet of the fracture, is transported along the fracture channel, and is diminished only by the diffusion of some of the contaminant into the surrounding porous block. As noted in the introduction, examination of such a model provides insight into transport mechanisms in fractured media by serving as an example to which transport in more complicated fracture networks can be compared.

In the fracture, which we assume is of uniform width b, we consider advection, dispersion and loss to the porous medium. The average velocity v in the fracture is

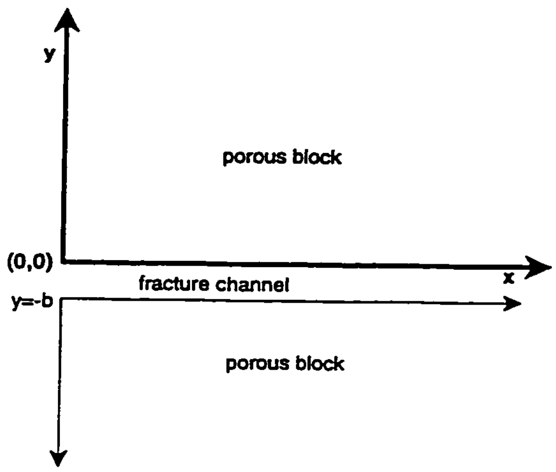

Figure 1.1: Single fracture system.

assumed constant in the direction of the fracture axis. Due to the effects of transverse dispersion and the small magnitude of b, we also assume perfect mixing of the concentration across the width of the fracture. The assumption of uniformity in y within the fracture is also made by Tang *et al* (1981), and it is shown to be valid in the case of small fracture apertures by Fogden *et al* (1988). This allows for a one-dimensional treatment of the contaminant flow in the fracture.

In the porous matrix, velocity is assumed to be negligible (due to low permeability) so that molecular diffusion is the primary source of transport. We will also include a source term in the porous domain. The source term can be representative of contaminant deposits that have leaked into the porous media (perhaps into fissures with small penetration depth) or representative of noninstantaneous sorption of the contaminant by the porous media (this will be addressed more fully in the next section) and is part of what sets our model apart from those previously studied in the literature.

Lastly, in both the fracture and the porous domain the contaminant will be subject to decay. The decay rate is given by $\Lambda = \ln 2/t_{1/2}$, where $t_{1/2}$ is the half-life of the contaminant.

Let $c(x,t)$ denote the contaminant concentration in the fracture (in mass of contaminant per unit volume of water). To derive the governing equation in the fracture channel we take a small section of the fracture of length Δx, width b, and unit thick-

ness. We apply mass balance (for example see DeMarsily (1988)) to this section to obtain

$$\frac{\partial}{\partial t}(cb\Delta x) = b(F(x,t) - F(x+\Delta x,t)) - (b\Delta x)\Lambda c - (2\Delta x)q - (2\Delta x)s_t$$

The left side of the equation is the time rate of change of the mass in the section; the first term on the right is the net flux through the cross sections at x and $x + \Delta x$ (F is the flux); the second term is the decay rate and the third term represents the diffusive loss of contaminant to the porous blocks through the upper and lower faces ($q = q(x,t)$ is measured in mass per unit area per unit time). The last term on the right-hand side of the equation describes the rate of sorption of the contaminant to the fracture walls, where $s = s(x,y,t)$ is given in mass of contaminant per unit area. The constitutive relation for the flux F consists of a dispersive flux term and a convection term; that is

$$F = -Dc_x + vc$$

Here v is the average velocity (it is the same as the Darcy velocity in the fracture since a channel has a porosity of one). The hydrodynamic dispersion coefficient D [L^2/T] is taken to be a constant satisfying the constitutive relation

$$D = \alpha_L v + D^*$$

where α_L is the longitudinal dispersivity and D^* is the molecular diffusion coefficient of a solute in a free solution (Bear (1972)). Dividing the mass balance law by $b\Delta x$, taking the limit as Δx goes to zero, and using the definitions above yields the partial differential equation

$$c_t = Dc_{xx} - vc_x - \frac{2q}{b} - \Lambda c - \frac{2s_t}{b}, \quad x > 0,\ t > 0 \tag{1.1}$$

which describes contaminant flow in the fracture.

In the porous matrix we let $m(x,y,t)$ denote the concentration of the contaminant (also in mass of contaminant per unit volume of water). We apply mass balance in a similar manner to obtain

$$m_t = D^x m_{xx} + D^y m_{yy} - \Lambda m - \frac{\rho}{\theta}\sigma_t + \Phi, \quad x,y > 0,\ t > 0 \tag{1.2}$$

where ρ is the bulk density [M/L^3], θ (dimensionless) is the average porosity of the matrix, and $\sigma = \sigma(x,y,t)$ is the total sorption of the concentration in the matrix

measured in mass of solute per mass of soil. The effective diffusion coefficients D^x and D^y [L^2/T] are equivalent in an isotropic medium and are given by $D^x = D^y = \tau D^*$ where τ is the matrix tortuosity (Bear (1972)). The mass source term $\Phi = \Phi(x, y, t)$ is assumed to be symmetric about the fracture. That is to say it satisfies

$$\Phi(x, -(y+b), t) = \Phi(x, y, t), \quad y > 0$$

which defines the source in the half-space $y < -b$. Thus, we are analyzing a problem whose solution in the half-space $y < -b$ is the mirror image of the solution in the half-space $y > 0$. It is clearly sufficient, by our symmetry assumption, to formulate and solve the problem in the quarter-space $y > 0$, $x > 0$. Generally, we further assume that Φ is bounded, continuously differentiable in each variable, and $\Phi(x, y, 0) = 0$.

The diffusive flux q across the fracture-matrix interface in equation (1.1) occurs only in the y direction (perpendicular to the fracture flow) and is assumed proportional to the gradient of the matrix concentration in the y direction. We describe this with Fick's first law:

$$q(x, t) = -\theta D^y m_y(x, 0, t) \tag{1.3}$$

Assuming that first order kinetics govern the instantaneous sorption, we can take s and σ to be at equilibrium (i.e. the sorption is instantaneous) and describe them by the linear isotherms

$$s = k_f c \quad \text{and} \quad \sigma = k_m m \tag{1.4}$$

where k_f and k_m are the distribution coefficients with dimensions [L] and [L^3/M], respectively (Freeze and Cherry (1979)). If, for example, more complicated kinetics were to govern the processes of sorption in the matrix, then σ could be written as the sum of two types of sorption: the sorption σ_1 governed by the linear isotherm and the sorption σ_2 governed by a nonlinear isotherm (Van Genuchten *et al* (1981)). While σ_1 could still take the form of (1.4), σ_2 could only be described by a rate law, say

$$\frac{\partial \sigma_2}{\partial t} = k_1 \Phi(c, \sigma_2)$$

where k_1 is the (finite) reaction rate. Then σ_t would satisfy

$$\sigma_t = k_f c_t + k_1 \Phi(c, \sigma_2)$$

Substituting this into the equation

$$m_t = D^x m_{xx} + D^y m_{yy} - \Lambda m - \frac{\rho}{\theta}\sigma_t$$

would yield, in linear form, a source term much like the one presently being considered in equation (1.2). For our purposes, however, we will consider the sorption in the matrix to be instantaneous and governed by a linear isotherm and view $\Phi(x,y,t)$ as the source term previously described.

Finally, substituting (1.3) and (1.4) into equations (1.1) and (1.2) we obtain

$$Rc_t = Dc_{xx} - vc_x - \Lambda c + \frac{2\theta}{b} D^y m_y(x,0,t), \quad x > 0, \quad t > 0 \tag{1.5}$$

$$\bar{R}m_t = D^x m_{xx} + D^y m_{yy} - \Lambda m + \phi, \quad x, y > 0, \quad t > 0 \tag{1.6}$$

where $\phi = \frac{\rho}{\theta}\Phi$ and R, $\bar{R}$ are the (dimensionless) retardation factors given by

$$R = 1 + \frac{2k_f}{b} \quad \text{and} \quad \bar{R} = 1 + \frac{\rho}{\theta}k_m \tag{1.7}$$

(Freeze and Cherry (1979)).

The concentration equations in the two regions are coupled by an assumption of continuity along the interface

$$c(x,t) = m(x,0,t), \qquad x > 0, \quad t > 0 \tag{1.8}$$

We apply a contaminant source function at the fracture opening, assume a no-flux condition along the vertical boundary of the matrix, and assume no contaminant is present in the system at time $t = 0$. These conditions are written as follows:

$$\begin{aligned} c(0,t) &= g(t), & t \geq 0 \qquad (1.9)\\ m_x(0,y,t) &= 0, & y > 0, \quad t > 0 \qquad (1.10)\\ c(x,0) &= m(x,y,0) = 0, & x > 0, \quad y > 0 \qquad (1.11) \end{aligned}$$

Equations (1.5)–(1.6) and (1.8)–(1.11) model the contaminant transport problem that will be the focus of this paper.

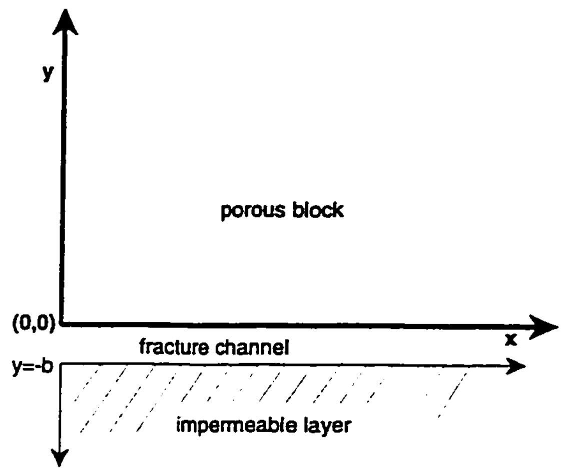

Figure 1.2: Single fracture network with lower impermeable layer.

1.3 Other Models

The above model can easily be adapted to describe other simple fracture networks. For example, a network consisting of a single fracture in which the lower face is an impermeable block (see figure 1.2) is governed by essentially the same model with two minor exceptions: first, diffusive loss of the contaminant to the porous block occurs through only one of the fracture faces; second the mass source term $\Phi(x,y,t)$ no longer needs to be defined below the fracture (i.e. for $y < -b$). Thus, removing the factor of 2 from the last term of equation (1.5) and lifting the symmetry condition on $\Phi(x,y,t)$ yields a model which describes this system.

Another network to which (1.5)–(1.6), (1.8)–(1.11) can be adapted is a system of parallel fractures. To arrive at a model for such a system, we again assume the fractures to be of uniform width b and of infinite length. We further assume that these fractures are uniformly spaced and separated by porous blocks of finite width h, where h is generally taken to be much larger than b. See figure 1.3. In order to incorporate a source term $\Phi(x,y,t)$ in the porous block, it must satisfy rather strict symmetry conditions; within the porous block between $y = 0$ to $y = h$, Φ must be symmetric about the half-block line $y = h/2$. Specifically,

$$\Phi\left(x, \frac{h}{2} + y, t\right) = \Phi\left(x, \frac{h}{2} - y, t\right), \quad y \in \left[0, \frac{h}{2}\right]$$

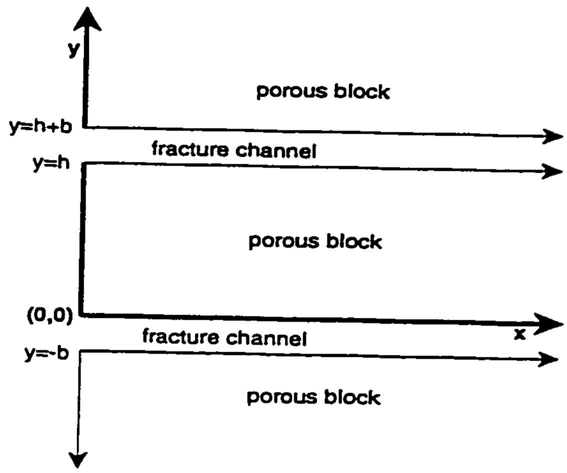

Figure 1.3: Parallel fracture network.

which defines Φ on $[0, h]$. A similar condition must be satisfied by Φ for each of the remaining blocks in the system. Then, the symmetry of the network allows us to consider the problem over a region including only one fracture and one adjacent half-block of the surrounding porous medium.

To formulate the equations describing this problem we again let $c(x,t)$ denote the contaminant concentration in the fracture and $m(x,y,t)$ the contaminant in the matrix. We apply mass balance and the same constitutive relations as described above to arrive at

$$Rc_t = Dc_{xx} - vc_x - \Lambda c + \frac{2\theta}{b} D^y m_y(x,0,t), \qquad x > 0, \;\; t > 0 \qquad (1.12)$$

$$\bar{R}m_t = D^x m_{xx} + D^y m_{yy} - \Lambda m + \phi, \qquad x > 0, \;\; t > 0, \;\; 0 < y < h/2 \qquad (1.13)$$

Note that these differ from equations (1.5) and (1.6) in that equation (1.13) is valid only when the variable y satisfies $0 < y < h/2$. The coupling assumption of continuity across the interface, the no-flux condition along $x = 0$, and the inlet and initial conditions still apply:

$$c(x,t) \;\; = \;\; m(x,0,t), \qquad x > 0, \;\; t > 0 \qquad (1.14)$$

$$
\begin{aligned}
m_x(0,y,t) &= 0, && 0 < y < h/2, \;\; t > 0 && (1.15)\\
c(0,t) &= g(t), && t \geq 0 && (1.16)\\
c(x,0) &= m(x,y,0) = 0, && x > 0, \;\; 0 < y < h/2 && (1.17)
\end{aligned}
$$

We now include the additional requirement of a no-flux condition at $y = h/2$ (due to the symmetry of the problem). Thus the complete model of a parallel-fracture network consists of equations (1.12)–(1.17) above, and (1.18) below:

$$m_y(x,h/2,t) = 0, \qquad x > 0, \;\; t > 0 \qquad (1.18)$$

1.4 Review of the Literature

Two important works regarding flow in fractured porous media include Grisak and Pickens (1980) and Neretnieks (1980). These works among the first to firmly establish matrix diffusion as a significant factor in fracture flow. Prior to these works its effects had been suggested by Foster (1975) and Day (1977). Garrels *et al* (1949) and Peck (1967) had demonstrated the role of matrix diffusion in ore deposition, while Foster (1975) showed that the tritium profile of the Chalk Aquifer in England was also a likely consequence of matrix diffusion. Skopp and Warrick (1974) studied a similar interaction between mobile and stationary flow phases and its effect on miscible solutes. Grisak and Pickens (1980) summarized these works in a parameter sensitivity analysis on flow in fractured media which used a numerical finite element method to examine the effects of diffusion into the matrix from the fracture, aperture size of the fracture and the groundwater velocity, dispersivity, porosity, and the distribution coefficient. The model used by the authors included adsorption by the medium (described by a linear isotherm), hydrodynamic dispersion, advection, diffusion and first order reactions (decay). Their results indicated that even with large aperture sizes, fast velocities and low matrix porosities (which weaken the effects of matrix diffusion) it is seldom appropriate to view matrix diffusion as negligible. Neretnieks (1980) reiterated this result with an analytical solution to a single fracture model of a single nuclide that incorporated matrix diffusion into the surrounding infinite porous block (though it omitted dispersion in the fracture). This model was extended by Rasmuson and Neretnieks (1981) to include axial dispersion in a fracture network formed