Cairo University

SIMULATION OF REACTIVE TRANSPORT IN FRACTURED GEOLOGIC MEDIA USING RANDOM WALK PARTICLE TRACKING

By

Mohamed Mahmoud Khafagy Mahmoud

A Thesis Submitted to
the Faculty of Engineering at Cairo University
In Partial Fulfillment of the
Requirements for the Degree of
MASTER OF SCIENCE

In

IRRIGATION AND HYDRAULICS ENGINEERING

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Title of Thesis:

Simulation of Reactive Transport in Fractured Geologic Media Using Random Walk Particle Tracking

Key Words:
Reactive Transport in Fractured Media, Matrix Diffusion, Sorption in Matrix, Sorption on Fracture Walls.

Summary:

Modeling the mass transfer through the fracture-matrix interface is one of the critical issues in the simulation of transport in a fractured porous medium. A RWPT technique suitable for discrete fractured networks and capable of simulating conservative and reactive transport in fractured media is developed in this study. The particle tracking contaminant transport model, previously developed for simulating advection and dispersion processes in discrete fractures, is adapted to include matrix diffusion and reactive processes. Equations are developed to determine the relation between several controlling parameters to ensure model accuracy. The results indicate that the particle tracking model is performing well and provides an alternative to dual-porosity and dual-permeability models.

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Abstract

Transport through fractured porous media occurs in many subsurface systems and is of great importance in many scientific and engineering fields. In fractured porous media, the fractures generally occupy a tiny portion of the whole volume, but the pore water velocity in these fractures can be orders of magnitude higher than that in the matrix blocks surrounding these fractures. Modeling the mass transfer through the fracture-matrix interface is one of the critical issues in the simulation of transport in a fractured porous medium. Because conventional dual-continuum-based numerical methods may not be able to capture the transient features of the diffusion depth into the matrix, there is a need for a numerical approach to simulate the conservative as well as the reactive transport in fractured geologic media. A Random Walk Particle Tracking (RWPT) method is used for simulating contaminant transport in discretely modeled fractured system.

A RWPT technique suitable for discrete fractured networks and capable of simulating conservative and reactive transport in fractured media is developed in this study. The particle tracking contaminant transport model, previously developed for simulating advection and dispersion processes in discrete fractures, is adapted to include matrix diffusion and reactive processes. Matrix diffusion is incorporated into the technique using transfer probabilities. Reactive processes occurring in both the fractures and the matrix are incorporated into particle movements and transfer between the different phases.

Equations are developed to determine the relation between several controlling parameters to ensure model accuracy. The modified DFN–based model is verified by comparison to available analytical solutions for the case of a single fracture taking into account all processes. The model is also verified with SOLFRAC Program for the case of transport in a discrete fracture network taking into account the sorption process occurring along the fracture walls. Comparisons show good agreement between the modified DFN model and the other solutions.

The results indicate that the particle tracking model is performing well and provides an alternative to dual-porosity and dual-permeability models. However, for achieving accuracy and stability, the approach is limited to cases with diffusion coefficient values ranging between 1×10^{-11} and 1×10^{-8} m^2/sec. Also, the pore velocity values in fractures are limited to a maximum of 10 m/day for the approach to yield accurate results. Average fracture length should not exceed 100 m for the method to yield accurate simulations.

Chapter 1 : Introduction

1.1. Preface

Mass transport in fractured geological formation needs to be addressed in several areas of earth sciences such as groundwater resources, near-surface contaminant hydrology, petroleum engineering, and underground nuclear waste disposal. Mathematical modeling of hydrogeological processes in fractured rock formations is necessary for several of the above applications. One example concerns long-term predictions for solute migration that are required for underground nuclear waste repositories. In that case, fractures are preferential pathways for potential solute migration from the repository to the biosphere. Flow and mass transport processes need to be studied for a large variety of space and time scales, complicating field characterization and mathematical description.

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1.2. Problem Definition

In fractured geological formations, most fractures are located in consolidated rock; sedimentary, igneous or metamorphic, but they can also be present in some unconsolidated materials such as clays or glacial tills. A natural fracture will almost always have an irregular shape and its opening, also called width or aperture, is generally variable.

In a single fracture, a solute will migrate by advection along the fracture at a mean velocity. The solute will also undergo dispersion because of small-scale variations in the fracture aperture. One example of dispersion caused by variations in the fracture aperture is flow channeling in a fracture, where a solute tends to migrate through the portions of a fracture with the largest apertures. Such transport can be complex to describe because of the difficulty in characterizing channels in real fractures.

Modeling flow and contaminant transport in fractured geological systems is a challenging problem. These two coupled processes deal with the main characteristics of the transmitting fractures. Most of these characteristics are described using statistical distributions because of the limited field data. Each fracture parameter has many approaches in simulation and the more convenient approach is selected according to field data.

The vast majority of studies on solute transport in fractured media have emphasized the behavior of conservative chemicals. And yet, a wide range of reactive transport mechanisms are often present – including adsorption/desorption, dissolution and precipitation, interactions among chemical species, radionuclide decay, organic reactions and volatilization, and/or biotransformations – all within a fracture, along the fracture walls, and/or within the adjacent porous host rock (Berkowitz, 2002). Incorporating all these processes into the mathematical models based on the Advection Dispersion Equation (ADE) for a discrete fracture network is apparently a formidable task. There is thus a need for a more tractable approach for incorporating these reactive processes into models of flow and transport in fractured geologic media.

An efficient technique was developed over the past four decades for modeling flow and transport in the fractured media which is the Discrete Fracture Network (DFN) technique. The DFN technique is considered the most accurate technique in simulating the network domain for solving the flow and transport. It simulates the fractures in the network as a connected pipe network and around it there is an impermeable media which is the porous matrix. DFN deals with the main fracture properties as the fracture orientation, aperture size (width of flow channel), hydraulic conductivity, and the fracture length. These properties can be efficiently presented as stream tubes (interconnected lines) in the domain of interest.

In earlier studies, the focus was on simulating the transport problem in DFN taking into account the advection process only with little consideration of other processes such as the diffusion process inside the matrix and reactive processes between contaminants and fractured media. Little attention was given to simulating the transport problem taking into account all processes.

1.3. Research Objectives

The main research objective of this study is to develop a numerical technique which can simulate conservative and reactive contaminant transport in two dimensional DFN using the Random Walk Particle Tracking method (RWPT)

To achieve this general objective, the following specific objectives are considered:

1. Adapting an existing RWPT technique for simulating advection and dispersion processes in discrete fractures
2. Incorporating matrix diffusion into the RWPT technique using some form of transfer probabilities
3. Incorporating reactive processes occurring in the fractures and in the matrix into the RWPT technique
4. Investigating the effect of changing the main parameters on contaminant transport

1.4. Dissertation Scope and Methodology

To achieve the studied research objectives, several research tasks have been undertaken and they are divided into two parts:

- Tasks for incorporating chemical processes and matrix diffusion in single fracture:
    1. Modifying the existing RWPT model (originally developed by Ismaiel, 2016) to incorporate the matrix diffusion process and the reactive processes in the matrix and along fracture walls
    2. Solving contaminant transport in a single fracture taking into consideration all processes such as advection and dispersion processes, sorption in the matrix, matrix diffusion and sorption along fracture walls
    3. Comparing the results with single-fracture analytical solution provided by Sudicky and Frind (1982)
    4. Quantifying the error resulting from comparing the model and the analytical solution
    5. Applying equations for overcoming the difference between the results of the model and the analytical solution
- Tasks for incorporating chemical processes and matrix diffusion in discrete fracture network:
    1. Solving the DFN flow problem (mass balance at fracture joints and Darcy's low along each fracture) using the approach developed by Botros et al. (2008)
    2. Solving contaminant transport for the generated DFN
    3. Solving contaminant transport for the generated DFN using the numerical solution (SOLFRAC program) by Bodin et al. (2007)
    4. Comparing the results of the generated model with the numerical solution by Bodin et al. (2007)
    5. Solving contaminant transport for a generated DFN and investigating the effect of changing the parameters on the contaminant transport process

1.5. Thesis Outline

Chapter (1) gives an introduction including problem definition, objectives of the study, thesis scope and methodology, and thesis outline.

Chapter (2) presents a brief background on analytical solutions, studies carried out on contaminant transport from the literature, diffusion process of contaminant in the matrix, reactive processes in the matrix and along fracture walls and the random walk particle tracking method.

Chapter (3) discusses the methodology and the model development for the contaminant transport in Single Fracture and Discrete Fracture Networks.

Chapter (4) presents the results of the contaminant transport in Discrete Fracture Networks and the discussion of these results.

Chapter (5) presents a summary of the work carried out in this study, general conclusions, and some recommendations for future research work.