Journal of King Saud University – Engineering Sciences (2016) **28**, 157–164

King Saud University

Journal of King Saud University – Engineering Sciences

www.ksu.edu.sa
www.sciencedirect.com

ORIGINAL ARTICLE

Spatial moment analysis of solute transport with Langmuir sorption in a fracture–skin–matrix coupled system

N. Natarajan [a,*], **G. Suresh Kumar** [b]

[a] *Department of Civil Engineering, Indian Institute of Technology-Madras, Chennai 600036, India*
[b] *Department of Ocean Engineering, Indian Institute of Technology-Madras, Chennai 600036, India*

Received 18 October 2013; accepted 10 April 2014
Available online 19 April 2014

KEYWORDS

Fracture;
Langmuir non-linear sorption;
Fracture–skin;
Spatial moments;
Effective solute velocity and dispersion

Abstract Sorption is one of the key processes that plays a major role in the transport of contaminants in fractured porous media. Extensive studies have been conducted on sorption isotherms in fracture matrix coupled system but studies pertaining to sorption in fractured porous media with fracture–skin are very limited. In this study, a numerical model is developed for analysing the influence of sorption intensities on velocity, macro dispersion coefficient and dispersivity using the method of spatial moments. Implicit finite difference numerical technique has been used to solve the coupled non-linear governing equations. A varying grid is adopted at the fracture and skin interface to capture the mass transfer at the interface. Results suggest that the role of non-linear sorption is dominant in comparison with that of advection and dispersion in deciding the final relative concentration within the fracture. The role of sorption partition coefficients is not always enhancing the mixing phenomena which lead to dilution of solutes. Furthermore, the role of sorption partition coefficients is extremely sensitive in the sense that the resultant magnitude of effective dispersivity may either get enhanced or mitigated depending on the magnitude of sorption partition coefficients.

1. Introduction

Contaminant transport in fractured porous media has been a topic of increasing interest in recent decades as the high permeability fracture provides a preferential pathway for the movement of fluids in the subsurface medium. The quantum of diffusive mass transport along the fracture walls decides the mobility and spreading of contaminants transported along the fracture (Renu and Suresh Kumar, 2012). It is well known that the transport of reactive solutes through porous media is affected by various rate limited processes, which mainly

---

[*] Corresponding author.
E-mail addresses: itsrajan2002@yahoo.co.in (N. Natarajan), gskumar@iitm.ac.in (G. Suresh Kumar).

Peer review under responsibility of King Saud University.

Production and hosting by Elsevier

http://dx.doi.org/10.1016/j.jksues.2014.04.003

include sorption, mass transfer between regions of different velocities and transformation (Srivastava et al., 2002). Many studies have been conducted on non-linear sorption of contaminants in the porous system (Weber et al., 1991; Brusseau, 1995; Srivastava and Brusseau, 1996; Abulaban et al., 1998; Abulaban and Nieber, 2000). Sekhar et al. (2006) numerically showed that in a single fracture with matrix diffusion, the ratio between dispersivities for linearly and non-linearly sorbing solutes varies exponentially at a very large time. Suresh Kumar (2008) performed spatial moment analysis to investigate the influence of non-linear sorption intensities on dispersivity and macro-dispersion coefficients, arising from marked heterogeneities between fracture and matrix transport parameters. Earlier studies on solute transport in a fractured formation generally did not consider the presence of fracture skins. Moench (1984, 1985) defined fracture skins to be a low permeability material deposited on the fracture walls which mitigates the diffusive mass transfer between high and low permeability materials. Sharp (1993) indicated the formation of skins in fractured porous media. Later studies concluded that the fracture skins can occur as clay filling (Driese et al., 2001), mineral precipitation (Fu et al., 1994) and organic material growth (Robinson and Sharp, 1997). Thus, the formation of fracture–skin can affect the contaminant transport mechanism in fractured porous media as the properties of the fracture–skin like porosity, diffusion coefficient and retardation factor can be significantly different from that of the surrounding rock-matrix. The variation in the properties of the fracture–skin from that of the associated rock-matrix causes the diffusive mechanisms at the fracture–skin interface to be different from that of the skin–matrix interface. The thickness of the fracture–skin is generally smaller when compared to that of the rock-matrix and therefore the sorption sites available in the fracture–skin can be significantly different compared to that of the rock-matrix. Renu and Suresh Kumar (2012) have performed moment analysis on solute transport in a fracture–skin–matrix system with Freundlich sorption. Although earlier studies have only dealt with Freundlich sorption, the adsorption of a variety of chemicals from the aqueous phase of the fracture onto the rock matrix can be described by the Langmuir equilibrium sorption, including surfactants and polymers (Satter et al., 1980). Further, in a coupled fracture–matrix system, the combined influence of matrix diffusion and non-linear sorption complicates the mixing behaviour along the fracture (Suresh Kumar, 2008). In Langmuir sorption isotherm, the number of sorption sites is considered to be limited compared to Freundlich sorption isotherm. The Langmuir sorption would presumably provide a better understanding of the sorption of contaminants in the fracture–skin–matrix system as the number of sorption sites in the fracture–skin can be limited due to its limited thickness compared to the rock-matrix. The aim of this study is to analyse the influence of Langmuir sorption intensities on effective solute velocity, dispersion and dispersivity in the fracture matrix coupled system in the presence of fracture–skin using the method of moments. The mobility and spreading of solutes cannot be obtained in a straight forward manner from the spatial and temporal distribution of concentration obtained from the fracture (Renu and Suresh Kumar, 2012) and thus requires a special tool. Field, experimental and analytical solutions have their limitations in carrying out this type of study. Field studies would be time consuming and quite costly, and thus not affordable. Moreover it would take many years before we can obtain tangible results. Experiments would last for many years if the long range transport processes need to be investigated and moreover it is difficult to obtain the non-linear behaviour in a coupled fracture matrix system under various conditions involving a range of fracture and solute transport parameters (Suresh Kumar, 2008). Analytical solutions for non-linear differential equations are difficult to solve. Thus, numerical modelling along with spatial moment analysis plays an important role in deducing the concentration distribution, and further aids in quantifying the mobility and spreading of solutes along the fracture.

2. Physical system and governing equations

The conceptual model illustrating a coupled fracture–skin–matrix system (Robinson et al., 1998) is illustrated in Fig. 1. A set of parallel fractures having fracture aperture of 2b is separated by a distance of 2H. In between fracture and rock-matrix fracture–skin having thickness d–b has been considered. The principal transport mechanisms considered within the fracture include advection, hydrodynamic dispersion, sorption, and mass transfer to the adjacent skin by diffusion. Molecular diffusion, sorption and radioactive decay have been considered within the fracture–skin and rock-matrix.

The governing equation for contaminant transport in a fracture in given below (Robinson et al., 1998)

$$\frac{\partial C_f}{\partial t} + \frac{1}{b}\frac{\partial S}{\partial t} + v\frac{\partial C_f}{\partial x} - D\frac{\partial^2 C_f}{\partial x^2} - \frac{\theta_s D_s}{b}\frac{\partial C_s}{\partial y}\bigg|_{y=b} = 0 \tag{1}$$

The most commonly used expression for Langmuir sorption Isotherm is given below (Singh and Srivastava, 2001; Patnaik and Das, 1995):

$$S = \frac{S_{maxf} K_a C_f}{1 + K_a C_f} \tag{2}$$

where C_f is the concentration in the fracture, S_{maxf} is the maximum sorption capacity of the contaminants on the fracture wall surface, K_a is the sorption partition coefficient.

$$\frac{1}{b}\cdot\frac{\partial S}{\partial t} = \frac{1}{b}\cdot\frac{\partial S}{\partial C_f}\cdot\frac{\partial C_f}{\partial t} = \frac{1}{b}\cdot\left[\frac{S_{maxf} K_a}{1 + K_a C} - \frac{S_{maxf} K_a^2 C}{(1 + K_a C)^2}\right]\cdot\frac{\partial C_f}{\partial t} \tag{3}$$

Substituting Eq. (3) into Eq. (1)

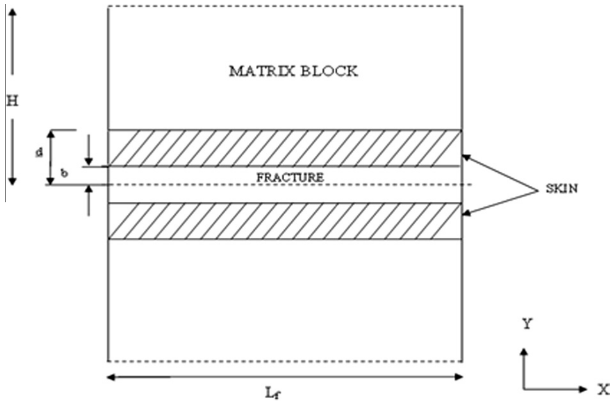

Figure 1 Schematic representation of the coupled fracture–skin–matrix system.