Applied Mathematics and Computation 219 (2013) 7127–7138

Contents lists available at SciVerse ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Dual permeability variably saturated flow and contaminant transport modeling of a nuclear waste repository with capillary barrier protection

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ARTICLE INFO

Keywords:
Richards equation
Convection dispersion reaction equation
Distinct unsaturated hydraulic properties
Problem conditionality
Matrix balancing

ABSTRACT

This paper presents a new release of the DRUtES computer program, a finite element numerical solver in one and two dimensions of flow and contaminant transport in a dual porosity variably saturated porous medium.

The main part of this paper evaluates the capillary barrier based structure on the Richard – Litoměřice nuclear waste facility in the Czech Republic. The barrier structure is evaluated for various cases under normal regime flow conditions and under emergency conditions caused by intense infiltration. The capillary barrier is based on the unsaturated hydraulic properties of gravel. A failure of the barrier function due to saturation is successfully simulated, and is presented here.

1. Introduction

The problem of predicting fluid movement in an unsaturated/saturated zone is important in many fields, ranging from agriculture, via hydrology to technical applications of dangerous waste disposal in deep rock formations.

The mathematical model of unsaturated flow was originally published by Richards [1]. Together with the convection–dispersion–reaction equation a full contaminant transport model is formed.

The Richards equation problem has undergone various investigations and numerical treatments. Its finite element solution was originally published by Neuman in 1970 for several engineering applications, e.g. dam seepage modeling, see [2,3]. The existence and the uniqueness of its solution was discovered 10 years later, by Alt and Luckhaus [4]. A fundamental work analyzing a mass conservation numerical method for the Richards equation was published in 1990 by Celia et al. [5]. A new technique for adaptive time discretization was recently published by Kuráž et al. [6].

A new version of the DRUtES [7] computer code, a finite element numerical solver of contaminant transport in a dual porosity variably saturated porous medium, was recently released by Kuráž. This code was already presented in [6]. Compared to the previous release, the current version supports the two dimensional problem of variably saturated flow and soluble contaminant transport. The code is written in F-language – a subset of Fortran programming language, including the recent Fortran 2008 standard – coarrays (parallel computing support).

The aim of this paper is to present the application of DRUtES to a real technical problem – an evaluation of an engineering barrier on the Richard – Litoměřice nuclear waste repository. The barrier is evaluated for two distinct cases – under a normal flow regime (pseudo-steady-state flow conditions) – for a simulation time of 200 years, and under intense infiltration into an

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doi:10.1016/j.amc.2011.08.109

initially dry medium – for a simulation time of 200 days. The former case is a simulation of the barrier efficiency in a long time scale, and the latter case is a simulation of a certain emergency state, when there is sudden and intense infiltration into an initially dry repository barrier. Based on the material properties of the barrier, the protection is efficient only for an unsaturated state, and thus infiltration, as considered in the second case, finally caused the barrier function to collapse. A simple matrix balancing method is presented here, and its application offers a dramatic improvement of conditionality for all evaluated cases. A positive repository protection effect is proven, and the code successfully simulates the failure of the capillary barrier effect.

Earlier models used for the safety assessment of the site are summarized in the most recent report by Baloun et al. [8] from 2002. As the barrier design was proposed after the release of the report, the barrier effect was not considered. The Baloun report also assumed the dual permeability concept, but the fast medium properties considered here originate from a new and original mathematical model of fractures analyzed by Kuráž et al. [6], and thus a new and improved estimate of a possible preferential flow effect is considered here.

2. Mathematical model

The problem of Darcian flow in a tectonically fractured rock medium is usually expressed by the dual permeability conceptual approach. The governing equations for variably saturated Darcian flow and contaminant transport in the dual flow regime were originally published by Gerke and van Genuchten [9].

The following section introduces the strong and weak formulation of dual permeability variably saturated flow and contaminant transport. A very brief description of the constitutive relations and coefficients involved in this problem is given, however an interested reader can find more information in the references provided below.

2.1. Strong and weak formulations

The mathematical problem to be solved is the Richards equation with the dual porosity conceptual approach and the convection–dispersion–reaction equation.

Let Ω be a bounded domain in $\mathbb{R}^n$ $(n = 1, 2)$, with a Lipschitz boundary $\partial\Omega$ for $n = 2$. Let $\Gamma^h_{D,m}$ and $\Gamma^h_{N,m}$ be smooth open disjoint subsets of $\partial\Omega$ (not necessarily connected) such that $\partial\Omega = \overline{\Gamma^h_{D,m}} \cup \overline{\Gamma^h_{N,m}}$, $\mathrm{meas}_{n-1}\left(\partial\Omega \setminus \left(\Gamma^h_{D,m} \cup \Gamma^h_{N,m}\right)\right) = 0$ and $\mathrm{meas}_{n-1}(\Gamma_D) > 0$ and $\mathrm{meas}_{n-1}(\Gamma_N) > 0$. Let the same hold for the pairs $\Gamma^h_{D,f}, \Gamma^h_{N,f}$ and $\Gamma^c_{D,m}, \Gamma^c_{N,m}$ and $\Gamma^c_{D,f}, \Gamma^c_{N,f}$. Let $\boldsymbol{n}$ denotes the outer unit normal to $\partial\Omega$. For positive T let $Q_T = \Omega \times [0, T)$.

The Richards equation in the dual regime was presumed by Gerke and van Genuchten [9] as

$$\begin{aligned} C_m(h_m)\frac{\partial h_m}{\partial t} &= \nabla.(K_m(h_m)\nabla h_m) + \frac{\partial K_m(h_m)}{\partial z} + \frac{\Gamma_w}{1-\omega_f} \quad (x,t) \in \Omega \times [0,T) \\ C_f(h_f)\frac{\partial h_f}{\partial t} &= \nabla \cdot (K_f(h_f)\nabla h_f) + \frac{\partial K_f(h_f)}{\partial z} - \frac{\Gamma_w}{\omega_f} \quad (x,t) \in \Omega \times [0,T), \quad \Gamma_w = \alpha_w(h_f - h_m) \end{aligned} \tag{1}$$

the subscripts f and m denote the subsystem of fractures (macropores) and matrix blocks (micropores), h is the capillary pressure head function [L], $K(h)$ is the unsaturated hydraulic conductivity [L T^{-1}], $C(h)$ is the water retention capacity [L^{-1}], usually defined as $C(h) = \frac{d\theta}{dh} + \frac{\theta(h)}{\theta_S} S_s$, where $\theta(h)$ is the water content function [–], S_s is the specific aquifer storage [L^{-1}], θ_S is the saturated water content [–], and α_w is the first order mass transfer coefficient [L^{-1} T^{-1}] presumed as

$$\alpha_w = \frac{\beta}{\alpha_{DP}^2} K_a \gamma_w, \tag{2}$$

where β is the dimensionless geometry coefficient, α_{DP} is the characteristic half width [L] of the matrix block, K_a is the effective hydraulic conductivity [L T^{-1}] of the matrix at or near the fracture/matrix interface, and γ_w is the dimensionless scaling factor. Constitutive relation for function $\theta(h)$ was supplied by van Genuchten's law [10], and for the $K(h)$ function it was supplied by Mualem's law [11], see Fig. 2 for a plot of these functions.

The Darcian flux (a convective term required by the transport equation) is obtained from the Darcy–Buckingham law.

$$q_m = -K_m(h_m)(\nabla h_m + \nabla z), \quad q_f = -K_f(h_f)(\nabla h_f + \nabla z), \tag{3}$$

where ∇z is a geodetic gradient, if positive upwards, then in $\mathbb{R}^1$ $\nabla z = 1$, and in $\mathbb{R}^2$ $\nabla z = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

The initial conditions are stated as

$$h_m(x,0) = h^0_m(x) \quad x \in \Omega, \quad h_f(x,0) = h^0_f(x) \quad x \in \Omega$$

and the boundary conditions

$$\begin{aligned} h_m(x,t) &= h^D_m(x,t) \quad (x,t) \in \Gamma^h_{D,m} \times [0,T), \quad \frac{\partial h_m}{\partial \boldsymbol{n}} = h^N_m(x,t) \quad (x,t) \in \Gamma^h_{N,m} \times [0,T), \\ h_f(x,t) &= h^D_f(x,t) \quad (x,t) \in \Gamma^h_{D,f} \times [0,T), \quad \frac{\partial h_f}{\partial \boldsymbol{n}} = h^N_f(x,t) \quad (x,t) \in \Gamma^h_{N,f} \times [0,T). \end{aligned}$$