Progress in Nuclear Energy 52 (2010) 282–291

Contents lists available at ScienceDirect

Progress in Nuclear Energy

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

A Lagrangian strategy for the numerical simulation of radionuclide transport problems

J. Aquino [a], A.S. Francisco [b], F. Pereira [c], T. Jordem Pereira [a], H.P. Amaral Souto [a,*]

[a] Departamento de Modelagem Computacional, Instituto Politécnico, Universidade do Estado do Rio de Janeiro, Caixa Postal 97282, 28601-970 Nova Friburgo, RJ, Brazil
[b] Departamento de Engenharia Mecânica, Escola de Engenharia Industrial Metalurgica de Volta Redonda, Universidade Federal Fluminense, Av. dos Trabalhadores, 420, 27255-250 Volta Redonda, RJ, Brazil
[c] Department of Mathematics and School of Energy Resources, University of Wyoming, 1000 E. University Ave., Laramie, WY 82071, USA

Keywords:
Heterogeneous porous medium
Lagrangian scheme
Local conservation
Tracer flow
Radionuclide transport

A B S T R A C T

In this work a new algorithm for the computational implementation of the Forward Integral Tracking (FIT) method, originally introduced in Aquino et al. (2007a), is presented and applied to the numerical solution of radionuclide transport problems in saturated heterogeneous porous media.

The FIT is a semi-discrete numerical method which is virtually free of numerical diffusion, does not use Riemann solvers, and is computationally very efficient. A new, locally conservative procedure for the inclusion and removal of tracked points that represent the particles of the radionuclide that are carried by the fluid flow is introduced.

Numerical results which indicate numerical convergence of the new procedure under mesh refinement are discussed.

1. Introduction

The field of reactive transport in geologic formations has expanded enormously in the last few decades and has contributed to the solution of many problems of environmental contamination (MacQuarrie and Mayer, 2005). Numerical models allow that coupled processes of transport and reactions of a contaminant be investigated over geologic time scales.

Currently, the problem of the storage of used nuclear fuel (or other radioactive substances) is of utmost importance for countries that possess nuclear power plants. One of the possibilities to deal with radioactive waste disposal consists of storing it in sealed recipients that must be emplaced in repositories located at great depths in rocky formations.

One of the major considerations when modeling multicomponent reactive transport is the wide range of spatial and time scales characterizing the various transport and reaction processes. The time scale related to the reaction process does not necessarily coincide with the time scale of advective and diffusive macroscopic transport. However each of these processes contributes to the overall transport of the radionuclide. The reaction time scale varies significantly depending on the type of reaction that we are considering. The time scales of advective transport processes are directly related to the groundwater flow rates, which can also vary over many orders of magnitude. diffusive transport time scales depend on the effective diffusive coefficients and the diffusion length scale of interest, and are equally variable.

In order to facilitate a discussion on comparison of time scales, if a reaction can be treated as an equilibrium reaction, we introduce the advective and diffusive Damköhler numbers (Bahr and Rubin, 1987). The advective Damköhler number, Da_a, relates the characteristic time of advection transport to the characteristic time of a reaction whereas the diffusive Damköhler number, Da_d, relates characteristic time of diffusion transport to the characteristic time of a reaction. In this work we consider that $Da_a/Da_d \gg 1$ so that we will neglect the macroscopic diffusion effects. In addition, for the current implementation of our numerical method we will not consider reactive transport; we focus on the development of a diffusion-free approximation for advective transport. Therefore, we consider radionuclide transport problems in saturated heterogeneous porous media, in the hypothetical case of a leakage of radioactive waste placed in a repository. In Aquino et al. (2007a) the authors introduced a new conservative Lagrangian scheme for solving pure-advection equations and we now present a new algorithm for the numerical implementation of this procedure. This new algorithm produces very accurate numerical results for the solution of the advective radionuclide transport problems in saturated, very heterogeneous porous media.

* Corresponding author. Tel.: +55 22 2533 2265; fax: +55 22 2533 2322.
E-mail address: helio@iprj.uerj.br (H.P. Amaral Souto).
URL: http://www.labtran.iprj.uerj.br

0149-1970/$ – see front matter © 2009 Elsevier Ltd. All rights reserved.
doi:10.1016/j.pnucene.2009.06.018

2. Mathematical modeling

The adopted mathematical model considers the flow of an incompressible fluid through heterogeneous porous medium $\Omega \subset \mathbb{R}^2$ with boundary $\partial\Omega$. We consider also that the porous medium is rigid and is saturated by fluid. Moreover, the gravitational and capillarity effects are not considered and the porosity of the medium is considered only a function of the space. A certain amount of a radionuclide is injected in the single-phase fluid that flows through the porous medium. The total concentration of radionuclide is sufficiently low such that the injected and resident fluids have, in practical terms, the same physical properties. The points of Ω are represented by the vector position $\mathbf{x}$, where $\mathbf{x} = (x, y) \in \mathbb{R}^2$.

2.1. Single-phase flow

Let Ω be an open and bounded domain in $\mathbb{R}^2$, with regular boundary $\partial\Omega$. The partial differential equations that govern single-phase flow transport in a rigid reservoir, Ω, on a time interval $I = [0, T] \subset \mathbb{R}$, $0 \le t \le T$, is described by Darcy's law

$$\mathbf{v} = -\frac{k(\mathbf{x})}{\mu}\nabla p, \tag{1}$$

together with

$$\nabla \cdot \mathbf{v} = 0 \tag{2}$$

which reflects the incompressibility of the fluid; in the above equations $\mathbf{v} = \mathbf{v}(\mathbf{x})$ and $p = p(\mathbf{x})$ are Darcy's velocity and fluid pressure. The coefficient μ represents the viscosity of the fluid phase and the scalar field $k(\mathbf{x})$ represents the absolute permeability of the rock.

2.2. Radionuclide transport equation

We assume that a non-volatile radionuclide is transported only by the water phase. Let c_w be the concentration of the radionuclide in the water phase and let c_s be the concentration in the solid matrix. Then we can write two balance equations involving c_w and c_s (Bear, 1979). Within the water phase

$$\frac{\partial}{\partial t}(\theta_w c_w) + \nabla \cdot (\mathbf{v} c_w) - \nabla \cdot (\theta_w \mathbf{D} \nabla c_w) + \gamma \theta_w c_w = -f(c_w, c_s) \tag{3}$$

and on the solid matrix

$$\frac{\partial}{\partial t}(\theta_s \rho_s c_s) + \gamma \theta_s \rho_s c_s = f(c_w, c_s), \tag{4}$$

where θ_w is the volumetric water content $\theta_w = \phi$, ϕ is the porosity, γ is the radioactive decay constant, $\mathbf{D}$ is the dispersion tensor, θ_s is the volumetric content of solid matrix ($\theta_s = 1 - \phi$), ρ_s is the density of the solid matrix, and $f(c_w, c_s)$ is the sorption term.

Assuming that c_w and c_s concentrations are always in equilibrium, it implies that

$$c_s = k_d c_w, \tag{5}$$

where k_d is a distribution coefficient.

Equations (3) and (4) may now be simplified by adding them:

$$\frac{\partial}{\partial t}[R(\theta_w) c_w] + \nabla \cdot (\mathbf{v} c_w) - \nabla \cdot (\theta_w \mathbf{D} \nabla c_w) + R(\theta_w) \gamma c_w = 0, \tag{6}$$

where $R(\theta_w) = \theta_w + \theta_s \rho_s k_d$ is defined as the retardation factor.

In this paper we assume, as mentioned before, that the diffusion and decay processes are negligible to study only the effect of pure advection. Then, we consider the following transport equation:

$$\frac{\partial}{\partial t}[R(\theta_w) c_w] + \nabla \cdot (\mathbf{v} c_w) = 0, \tag{7}$$

where

$$\theta_w = \phi$$

for the problem considered here.

2.3. Boundary and initial conditions

In our numerical studies Equations (1), (2) and (7) are defined in a bounded rectangular domain $\Omega = [0, L_x] \times [0, L_y] \subset \mathbb{R}^2$ for time interval $I = [0, T]$, subject to the following boundary and initial conditions:

$$\begin{aligned} &\mathbf{v} \cdot \mathbf{n} = -q, \quad \text{on } x = 0;\ y \in [0, L_y] \\ &p = 0, \quad \text{on } x = L_x;\ y \in [0, L_y] \\ &\mathbf{v} \cdot \mathbf{n} = 0, \quad \text{on } y = 0, L_y;\ x \in [0, L_x] \end{aligned} \tag{8}$$

and

$$c_w(\mathbf{x}, 0) = c_{w0}(\mathbf{x}) \quad \text{in } \Omega. \tag{9}$$

The conditions represented by Equations (8) determine an injection of water from the left to the right. This injection is done by a constant rate – q through the vertical boundary on $x = 0$; $y \in [0, L_y]$ of Ω and there is no flow through the horizontal boundaries on $y = 0, L_y$; $x \in [0, L_x]$.

3. Permeability fields

Reservoir rock properties such as permeability and porosity vary in space and may be characterized by their distributions. Random fields provide a natural description of rock heterogeneities in the typical case in which the geological knowledge of rock is much less detailed than is necessary to predict flow properties through it deterministically (Glimm and Sharp, 1991).

Random field generators are used as a tool to model heterogeneities in porous media for applications in hydrocarbon recovery and groundwater flow (Bruining et al., 1997). Many realizations of such fields are used in studies aiming at the quantification and reduction of uncertainty of multiphase flows in porous media (Karniadakis and Glimm, 2006; Douglas et al., 2006).

A number of methods have been employed to generate random fields: Turning Bands Method (Mantoglou and Wilson, 1982; Oh, 1998), Successive Random Addition (Oh, 1998), Spectral Methods (Bruining et al., 1997), and Successive Sum of Independent Gaussian Fields (Borges et al., 2009) among others. In this work we use the method of Borges et al. (2009) which is based on a hierarchical sum of independent random fields.

In particular, we focus on correlated random fields with a power-law covariance structure. This characterization consists in adopting a log–normal theoretical probabilistic model for $k(\mathbf{x})$, such that it reproduces realistically the statistics distribution of the permeability field. In such a way, we consider a Gaussian field $\xi(\mathbf{x}) = \ln k(\mathbf{x})$ characterized by its statistics average $\langle \xi(\mathbf{x}) \rangle = 0$ and its covariance function (Furtado and Pereira, 2003; Borges et al., 2009)

$$C(\mathbf{x}, \mathbf{y}) = \langle \xi(\mathbf{x}), \xi(\mathbf{y}) \rangle. \tag{10}$$

Therefore, the random scalar permeability field $k(\mathbf{x})$ with log–normal distribution is given by