A parallelizable procedure for contaminant diffusion in waste disposal

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Abstract

The contaminant transport problem is typically modeled by advection-diffusion equations. In this paper we apply a parallelizable iterative procedure to approximate the solution of the diffusion term of such equations. The spatial discretization is done by using mixed finite elements, and the resulting algebraic problems are handled by a domain decomposition procedure. This procedure permits one to implement the algorithm in distributed machines in order to save on computer memory and execution time. Numerical results are compared with experimental, which indicate that the numerical procedure is accurate and very efficient in a computational point of view.

Keywords: contaminant transport, parallelizable procedure, mixed finite elements, porous medium.

1 Introduction

The contaminant transport throughout the soil in waste disposal has been reasonably modeled considering the mechanisms of sorption, diffusion and advection of pollutants. We propose in this paper to investigate such transport taking into account the kinetic parameters of mass transfer that occur simultaneously along with the transport mechanisms. Here, we apply the parallelizable computational technique as an efficient numerical solver for resolution of the governing equation.

Contaminant transport is typically modeled by advection-diffusion equations. Pinto [1] developed a model that realizes simulations of environment impacts caused by deposition of solid waste in the soil. This model has considered the molecular diffusion as the main mechanism of contaminant transport in this
porous medium, and the sorption as the interaction process between the contaminant and soil. This model was constructed based on experimental data obtained by Ritter and Gatto [2] in molecular diffusion and equilibrium tests for soil and contaminant solution from a waste repository. Now we propose a parallelizable scheme for the numerical solution of the transport-diffusion equation, in which a mixed finite element method is applied for the spatial discretization. The resultant linear algebraic problems from this discretization are accomplished by an iterative procedure of domain decomposition [3]. This procedure permits to implement the parallel processing of a computational code in several machines, in order to obtain efficiency. It is naturally parallelizable in machines with distributed memory and allocates small memory space. Once it does not require the resolution of large linear equation systems, it is rapid. And it is of simple implementation concerning its code development.

In this paper we consider the process of soil-contaminant interaction described by a mass transfer coefficient of the contaminant, which values can be incorporated into the source/sink term of the mathematical model. Our investigation is conducted by comparing numerical simulations to experimental data of molecular diffusion tests.

2 Mathematical model

2.1 The contaminant solute

Solid wastes accumulated along the years in soil are not inactive. A contaminant solution of several chemical components is composed by physical, chemical and biological mechanisms. This solution moves into the groundwater, where takes place processes as such advection, diffusion, adsorption, degradation etc.

In order to investigate accurately the performance of our numerical solver we consider only one contaminant solute in the groundwater. The solute considered is the ammonium (\(\text{NH}_4^+\)). This contaminant ion suffers from adsorption process in the soil, and it has reliable experimental data available in the literature [4].

2.2 Governing equations

The objective of a contaminant transport model in a porous medium is to estimate the concentration of some solute as a function of the time and space. For this, the initial point is at the statement of the mass balance for the contaminant solute.

Let \(c_w\) be the contaminant mass fraction in the water phase and let \(c_s\) be the mass fraction in the soil phase. Then we can write two balance equations involving such variables; in the water phase:

\[
\frac{\partial}{\partial t} \left( \rho_w \varepsilon c_w \right) + \nabla \cdot \left( \bar{u}_w \rho_w \varepsilon c_w \right) + \nabla \cdot \left( -\rho_w \varepsilon D_w \nabla c_w \right) = -S ; \quad (1)
\]

and in the soil phase:
\[ \frac{\partial}{\partial t} \left( \rho_s (1 - \varepsilon) c_s \right) + \nabla \bullet \left( -\rho_s (1 - \varepsilon) D_s \nabla c_s \right) = S ; \]

where \( \rho_w \) is the water specific mass, \( \varepsilon \) the porosity, \( \bar{u}_w \) is the water velocity, \( D_w \) the diffusion coefficient in the water, \( S \) the sink term, \( \rho_s \) the solid specific mass, and \( D_s \) the diffusion coefficient in the soil.

In some cases, this system of equations is conveniently solved assuming that there is no diffusion in the soil phase and considering that the solute concentration in both water and soil phases are in equilibrium. Thus we could derive a model based only on the sorption isothermal, in which is defined a parameter called distribution coefficient.

Otherwise, we solve the contaminant problem using a model for the sink term as a function of a mass transfer coefficient that represents the dissolution rate of the contaminant solute in the soil and the water. Here, the sink term is associated to the mass transfer kinetic of the contaminant solute as a function of time. This model permits to solve the contaminant problem treating only the eqn. (1). Once we are simulating molecular diffusion tests, in which the advection can be neglected, the contaminant transport is then described by

\[ \frac{\partial}{\partial t} \left( \rho_w \varepsilon c_w \right) + \nabla \bullet \left( -\rho_w \varepsilon D_w \nabla c_w \right) = -S . \]

The mass transfer rate, \( S \), of the contaminant ion (NH\(_4^+\)) between the soil and water phases can be written by the following equation [5, 6]:

\[ S = k \beta_e A_{sw} \rho_w \varepsilon \left( c_w - c_{eq} \right) \eta c_w , \]

where \( k \) is a kinetic constant, \( \beta_e \) the mass transfer coefficient, \( A_{sw} \) the contact area between the soil and water phases, \( c_{eq} \) the equilibrium concentration of the contaminant ion in the leakage within the granular soil, and \( \eta \) an exponent of the equation.

The contact area is calculated by

\[ A_{sw} = \frac{6(1 - \varepsilon)}{d_s \varphi_s} , \]

where \( d_s \) is the average diameter of soil particle, and \( \varphi_s \) the form factor of soil particle.

The mass transfer coefficient is calculated by

\[ \beta_e = \frac{S_h D_w}{d_s \varphi_s} . \]
where \( S_h \) is the Sherwood number.

The Sherwood number represents the non-dimensional concentration gradient on the soil surface [7] and is determined by

\[
S_h = 1.17 Re^{0.585} Sc^{1/3} + 2, \tag{7}
\]

where \( Re \) is the Reynolds number, and \( Sc \) is the Schmidt number. The Reynolds and Schmidt numbers can be determined by the respective equations:

\[
Re = \frac{\rho_w (1 - \varepsilon)|\vec{u}_w|d_s}{\mu_w}, \tag{8}
\]

and

\[
Sc = \frac{\mu_w}{\rho_w D_w}, \tag{9}
\]

where \( \mu_w \) is the water viscosity.

### 3 Mixed finite element approximation

#### 3.1 Numerical solution

For the contaminant transport eqn. (3), a parabolic problem, we employ an implicit time discretization along with mixed finite elements in the spatial discretization (see references [8–10]). This technique is appropriate to obtain accurate diffusion flux computations. A domain decomposition procedure is applied towards the solution of the resulting algebraic problems.

#### 3.2 Time and space discretization

We write a discretized form for the contaminant transport equation as

\[
\rho_w \varepsilon \frac{C_{w}^{n+1} - C_{w}^{n}}{\Delta t} + \nabla \cdot (\vec{d}^{n+1}) = -S^{n+1}, \tag{10}
\]

in which \( \vec{d}^{n+1} = -\rho_w \varepsilon D_w \nabla C_{w}^{n+1} \).

Let \( \Omega \subset \mathbb{R}^2 \) be a bonded domain with a Lipschitz boundary \( \partial \Omega \). Let \( \{ \Omega_j, j = 1, \ldots, M \} \) be a partition of \( \Omega \) with

\[
\Gamma = \partial \Omega, \Gamma_j = \Gamma \cap \partial \Omega_j, \Gamma_{jk} = \Gamma_{kj} = \partial \Omega_j \cap \partial \Omega_k.
\]
We consider decomposing eqn. (10) over partition \( \{ \Omega_j \} \). In addition to requiring that \( \{ c_w, d_j \} \) be a solution of eqn. (10) for \( \Omega_j \), it is necessary to impose the consistency conditions

\[
c_w = c_w, \quad \text{on } \Gamma_{jk},
\]

(11)

and

\[
d_j \cdot v_j + d_k \cdot v_k = 0, \quad \text{on } \Gamma_{jk},
\]

(12)

where \( v_j \) is the unit outer vector normal to \( \partial \Omega_j \).

In order to define an iterative method for solving the above algebraic problems, it is convenient to replace eqn. (11) and (12) by Robin transmission boundary conditions. Thus, consistency conditions for the contaminant concentration will be given by

\[
\chi d_j \cdot v_j + l_{jk} = \chi d_k \cdot v_k + l_{kj}, \quad \text{on } \Gamma_{jk},
\]

(13)

\[
\chi d_k \cdot v_k + l_{kj} = \chi d_j \cdot v_j + l_{jk}, \quad \text{on } \Gamma_{kj},
\]

(14)

where \( \chi \) is a positive function on \( \cup \Gamma_{jk} \), and \( l_{jk} \) is a Lagrange multiplier defined on \( \Gamma_{jk} \).

We shall consider lowest index Raviart-Thomas spaces for the spatial discretization with square elements of size \( h \). Then the discretized form of the system of equations can be written as

\[
\frac{\rho_w e}{\Delta t} c_w^{n+1} + \frac{1}{h} \sum_{\beta} d_{\beta}^{n+1} = -S^{n+1} + \frac{\rho_w e}{\Delta t} c_w^n,
\]

(15)

\[
d_{\beta}^{n+1} = -2 \frac{\rho_w e D_w}{h} (l_{\beta}^{n+1} - c_w^{n+1})
\]

(16)

where \( d_{\beta} \) denote the value of the outgoing diffusive flux on the edge \( \beta \), \( \beta = L, R, U, D \) (see the fig. 1).

All the variables which appear in the above system refer to a single element. In order to define an iterative scheme, we use eqn. (11) and (12) in the above system to express all Lagrange multipliers in terms of the Lagrange multipliers and the fluxes of the adjacent elements. We introduce the superscript “~” to denote variables of adjacent elements, and let \( \beta' \) denote the edge \( \beta \) of the element under consideration. Then, the eqn. (16) takes the form
where \( \xi = 2 \frac{\rho_w \varepsilon D_w}{h} \). See the Douglas et al [11] for details about the iterative scheme.

Substituting eqn. (17) into eqn. (15), we have

\[
\frac{\rho_w \varepsilon}{\Delta t} c_{w}^{n+1} + \frac{1}{h} \sum_{\beta} \frac{\xi}{1 + \chi \xi} c_{w}^{n+1} = -S^{n+1} + \frac{\rho_w \varepsilon}{\Delta t} c_{w}^{n} + \frac{1}{h} \sum_{\beta} \frac{\xi}{1 + \chi \xi} \left( \chi \tilde{d}_{\beta'}^{n} + \tilde{I}_{\beta'}^{n} \right). \tag{18}
\]

If we take a linear scheme for the discretization of the mass transfer rate, then it results that

\[
S^{n+1} = k \beta_v A_{sw} \rho_w \varepsilon \left( c_{w}^{n} - c_{eq} \right)^{\eta} c_{w}^{n+1}. \tag{19}
\]

Finally, the numerical scheme to solve the contaminant transport is given by

\[
c_{w}^{n+1} = \frac{\sum_{\beta} \frac{\xi}{1 + \chi \xi} \left( \chi \tilde{d}_{\beta'}^{n} + \tilde{I}_{\beta'}^{n} \right) + \frac{\rho_w \varepsilon h}{\Delta t} c_{w}^{n}}{\sum_{\beta} \frac{\xi}{1 + \chi \xi} + \frac{\rho_w \varepsilon h}{\Delta t} + k \beta_v A_{sw} \rho_w \varepsilon h \left( c_{w}^{n} - c_{eq} \right)^{\eta}}. \tag{20}
\]
4 Numerical simulations

In this section we apply our numerical procedure for simulating the experimental results of a molecular diffusion test [2]. This laboratory experiment were performed with samples of soil and leachate of a solid waste landfill, conform the model presented by [12]. According this model, such samples with distinct concentrations are put into an experimental cell in order to measure the diffusion coefficient. At the top, we have a leachate repository where occurs the diffusion of the ammonium in free solution. And at the bottom, we have the effective diffusion of the ammonium over through the interstices of a soil column due to the tortuosity and porosity effects.

Our numerical experiments are performed in a two-dimensional square domain $\Omega = (0, L_x) \times (0, L_y)$, with boundary conditions $d \cdot v = 0$, on $x = 0, L_x$ and $y = 0, L_y$. The domain has $0.1 \text{ m} \times 0.1 \text{ m}$ discretized by $50 \times 50$ computational grid, and we use a time-step length of 60 s. We have as initial condition the ammonium ($\text{NH}_4^+$) concentration of $9.2 \times 10^{-2} \text{ kg/m}^3$ in the leachate repository and the concentration of $1.815 \text{ kg/m}^3$ in the soil column. The following data are held fixed in our experiments: porosity $\varepsilon = 0.76$, diffusion coefficient in the water $D_w = 6.342 \times 10^{-10} \text{ m}^2/\text{s}$, water velocity $u_w = 1.0 \times 10^{-6} \text{ m/s}$, kinetic constant $k = 2.5 \times 10^{-2}$, equilibrium concentration $c_{eq} = 7.544 \times 10^{-1} \text{ kg/m}^3$, exponent number $\eta = 1.75$, soil particle average diameter $d_s = 5.0 \times 10^{-6} \text{ m}$, and soil particle form factor $\varphi_s = 1.0$.

The numerical results are presented in fig. 2 at 72 hours. A concentration profile of the ammonium can be observed as a result of the solute transport that takes place in the experimental cell. The diffusion process tends to smooth the sharp concentration discontinuity at the interface between the leachate repository and the soil column. Our numerical solver is able to capture such physical behavior, even near that interface. In this figure, experimental results are also depicted. We can note that our results are in good agreement with the experimental results.

In order to investigate the evolution in time of the concentration profile, we simulate the experiment at different times: 18, 36 and 72 hours. Fig. 3 shows the respective concentration profiles. Also, we can confirm that our numerical solver duplicates the physical behavior along the time quite well.

5 Discussions

A two-dimensional method for the simulation of the contaminant transport in experimental cell is developed by combining a sorption model to determine the rate of mass transfer of the contaminant with a numerical scheme to solve accurate and efficiently the transport problem.
Figure 2: Concentrations of the ammonium as a function of the height at the experimental cell, at 72 hours.

Figure 3: Profiles of the concentrations of the ammonium at times $t = 18$, $36$ and $72$ hours.
We conclude that the model with a sink term representing the sorption process describes adequately the behavior of the contaminant concentration in the experimental cell. Others models of sorption process do not take into account the rate of mass transfer that takes place on the interface between the soil and the contaminant solution. In reference [4] several simulation results are obtained for different models of sorption process, where is evidenced the advantage of the sorption model that we have applied in this paper.

The accuracy of the parallelizable iterative procedure is tested against observed values for this transport problem. Such procedure permits to implement the algorithm in distributed machines in order to save on computer memory and execution time. This parallel computation can also be an efficient way to simulate the transport in the experimental cell considering the soil and leachate regions separately, at which we can use distinct diffusion coefficients.

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References


