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The numerical modelling of advective transport in the presence of ”uid pressure transients

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SUMMARY

Conventional modelling of transport problems for porous media usually assumes that the Darcy ”ow velocities are steady. In certain practical situations, the ”ow velocity can exhibit time-dependency, either due to the transient character of the ”ow process or time dependency in the boundary conditions associated with potential ”ow. In this paper, we consider certain one- and three-dimensional problems of the advective transport of a chemical species in a ”uid-saturated porous region. In particular, the advective ”ow velocity is governed by the piezo-conduction equation that takes into account the compressibilities of the pore ”uid and the porous skeleton. Time- and/or mesh-re“ning adaptive schemes used in the computational modelling are developed on the basis of a Fourier analysis, which can lead to accurate and optimal solutions for the advective transport problem with time- and space-dependent advective ”ow velocity distributions.

KEY WORDS : advective transport; piezo-conduction equation; stabilized numerical methods; time- and mesh-adaptive schemes; transport from cavities

1. INTRODUCTION

The problem that deals with the movement of hazardous chemicals and other contaminants in ”uid-saturated porous media is of considerable importance to geoenvironmental engineering [1…6]. The assessment of the distribution of the concentration of a chemical or a contaminant within the porous medium in”uences the environmental decision-making process. It is rarely possible to conduct large-scale experiments to determine the location of contaminant plumes within the geosphere. In the event of either an accidental chemical spill or a geological disposal of the chemical, recourse must be made to a plausible model to establish the spatial and between the porous medium and the chemical species that is being transported. Purely advective transport is perhaps the simplest approach to the modelling of the movement of a contaminant of a chemical species in the porous medium that can provide useful “rst approximations of engineering value. The absence of both di usion e ects and natural attenuation can lead to the estimation of the location of contaminant plumes with the strongest concentration, which can then be used to assess the most adverse e ects.

In the conventional modelling of the advective transport problem it is invariably assumed that where x is a position vector, t is time, $v(x, t)$ is the averaged advective flow velocity in the pore space. The third term on the LHS of (1) is non-zero if the fluid is considered to be compressible. The advective flow velocity in the porous medium is assumed to be governed by Darcy's law, which for an isotropic porous medium can be expressed by

$$v = -k\nabla\phi \qquad (2)$$

convection term has the adjoint form of the advection term in the equation, which gives rise to computational schemes that are symmetric [21]. Alternatively, their choice can be based on a Fourier analysis to ensure that numerical modelling gives rise to an 'optimal' solution of the transient advection equation [22], such as the one in streamline upwind Petrov–Galerkin method proposed by Hughes and Brooks [17]. The upwind function can also take different values to generate different stabilized methods, such as the Taylor–Galerkin method [23].

3.2. The modified LS method

Since the LS method can generate a symmetric matrix form for the advection equation, the method has significant potential for the examination of the non-linear problem. Wendland and Schmid [21] proposed the 3S scheme (Symmetrical Streamline Stabilization) for the numerical modelling of the advection-dominated transport problem, in which a parameter was introduced into the upwind term of the LS scheme to obtain optimal computational performance. This approach is equivalent to using different perturbation parameters in the weighting functions for the temporal and spatial terms of the advection equation in the LS method: i.e.

$$\int_V [w + \theta \Delta t\, \mathbf{v} \cdot \nabla w] \frac{\partial C}{\partial t} \, dV + \int_V [w + \alpha \theta \Delta t\, \mathbf{v} \cdot \nabla w](\mathbf{v} \cdot \nabla C^{n+\theta}) \, dV = 0 \tag{6}$$

and therefore this scheme can be referred to as the modified LS (MLS) method. The parameter α in (6) accounts for the upwind effect, which can be determined from a Fourier analysis to achieve a better numerical performance of the MLS scheme for the advection equation.

4. TIME- AND SPACE-ADAPTIVE PROCEDURES

4.1. Fourier analysis

The mathematical performance of stabilized semi-discrete Eulerian methods for the advection equation can be demonstrated via a Fourier analysis in the frequency domain by means of the algorithmic amplitude and the phase velocity of the numerical scheme [24, 25]. Selvadurai and Dong [26] performed a Fourier analysis of the MLS scheme for the advection equation and obtained the following analytical expressions for the algorithmic amplitude ξ^h and the relative phase velocity $\bar{u}/u$ of the MLS method applicable for the one-dimensional advection equation with the application of the trapezoidal rule

$$\xi^h = |\xi(\omega)| = \frac{\sqrt{[2 + \cos(\omega h) - 6\alpha Cr^2 \theta (1-\theta)(1-\cos(\omega h))]^2 + 9Cr^2 \sin^2(\omega h)}}{2 + \cos(\omega h) + 6\alpha Cr^2 \theta^2 (1 - \cos(\omega h))} \tag{7a}$$

$$\frac{\bar{u}}{u} = \frac{\Omega^h}{\omega} = -\frac{\arg(\xi(\omega))}{\omega \Delta t} = \frac{1}{Cr\,\omega h} \arctan\left(\frac{3Cr \sin(\omega h)}{2 + \cos(\omega h) - 6\alpha Cr^2 \theta (1-\theta)(1 - \cos(\omega h))}\right) \tag{7b}$$

where $\xi(\omega)$ is the spectral function of the MLS numerical operator for the advection equation with the application of the trapezoidal rule, $Cr\ (= u\Delta t/h)$ is the Courant number, u is the one-dimensional flow velocity, h is the length of the piecewise element, ωh is dimensionless wave number andy

the solution is located through an error indicator $E(e)$, based on the first derivative of the solution for each element [27]

$$E(e) = \left(\frac{1}{2}\sum_{j\in\partial e} h_j^2 [n_j \cdot \nabla C]^2\right)^2 \qquad (10)$$

where n_j is the unit normal to the edge j of the element with the length h_j and ∂e is the boundary of the element. The term in square brackets in (10) represents the jump in the flux across the element edge. The locations (or elements) of the steep front are determined by satisfying $E(e) > \beta$ and β is a parameter, which can be defined by the half of the maximum of $E(e)$, i.e. $\beta = 0.5 \max(E(e))$

In the ensuing sections, the time- and mesh-adaptive procedures will be used in conjunction with the MLS scheme to examine the advective transport problems associated with one- and three-dimensional axisymmetric configurations where the advective flow velocities are both time- and space-dependent and derived from the transient pressure potential governed by the piezo-conduction equation (3).

5. A ONE-DIMENSIONAL ADVECTIVE TRANSPORT PROBLEM

5.1. The transport equation with the analytical transient flow velocity

From (12), the flow velocity in the semi-infinite porous region is given by

$$v(x,t) = -k\frac{\partial \phi_p}{\partial x} = k\phi_0 \frac{1}{\sqrt{\pi D_p t}} \exp\left(-\frac{x^2}{4D_p t}\right) \tag{14}$$

Therefore, the one-dimensional problem of advective transport in the semi-infinite porous region is governed by the following PDE:

$$\frac{\partial C}{\partial t} + k\phi_0\left(\frac{\exp(-x^2/4D_p t)}{\sqrt{\pi D_p t}}\right)\frac{\partial C}{\partial x} - k\phi_0\left(\frac{x\exp(-x^2/4D_p t)}{2\sqrt{\pi}(D_p t)^{3/2}}\right)C = 0 \tag{15}$$

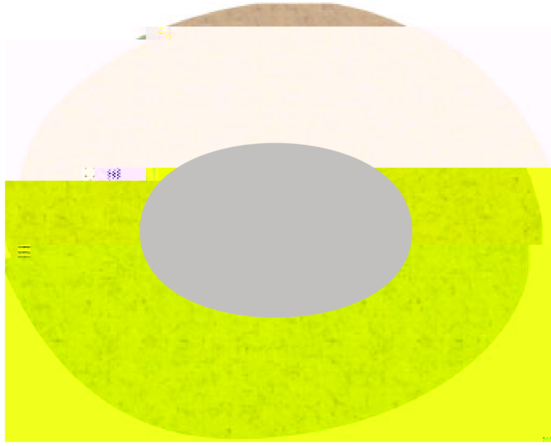
The solution of (15) is subject, respectively, to the following initial and boundary conditions:

$$C(x,0) = 0, \quad x \in [0,\infty) \tag{16a}$$

$$C(0,t) = C_0 H(t) \tag{16b}$$

The IBVP defined by (15) and (16) is well-posed. In the computational modelling of the velocity; the time-adaptive MLS scheme, on the other hand, gives oscillation-free and non-diffusive computational results for the concentration profile resulting from one-dimensional advective transport with transient flow velocities. In the computational scheme associated with the time-adaptive technique, the initial time step of $\Delta t = 0.2$ days finally increases to $\Delta t = 33$ days to satisfy constraint (9) imposed by the Courant number criterion.

6. THREE-DIMENSIONAL AXISYMMETRIC ADVECTIVE TRANSPORT PROBLEMS



cavity also exhibits symmetry about the plane $z = 0$, attention can be restricted to the consideration of a quarter-domain where suitable Neumann boundary conditions are imposed to satisfy requirements of symmetry. The boundary conditions corresponding to a cavity region with $a = 8$ m and $b = 1$ m are shown in Figure 5. The outer boundary is fixed at a radius $R(= \sqrt{r^2 + z^2}) = 30$ m where a Neumann boundary condition is applied to $C(x, t)$ in order to achieve the required regularity condition at infinity. The Dupuit–Forchheimer measure of hydraulic conductivity of the porous medium is taken as $k = 0.03$ m/day. The boundary of the cavity is subject to a potential $\phi_0 H(t)$ and the far field potential is maintained at a zero value as shown in Figure 5.

6.1. Mesh-refining adaptive scheme

The computations presented in Section 5 indicate that the MLS scheme with the chosen values of $\alpha = 3/2$ and $\theta = 1/3$ can generate an accurate solution for the advection equation when the such a mesh-adaptive scheme, the mesh at the locations of the steep front of the solution can be re“ned quantitatively with the Courant number criterion (9) based on the magnitude of the ”ow velocity. Since the size of the element will be decreased during the mesh re“nement, the elemental Courant number will be increased. Therefore, in order to avoid high elemental Courant numbers, the criterion ðCrÞ$_{ie}$ 4 0.5 should be used in the mesh-adaptive algorithm, such that the Courant numbers in the re“ned elements do not exceed unity. In such a mesh-re“ning approach, only the elements where the high gradient of the solution is encountered need be re“ned by reducing the dimensions of all the edges or the longest edge of the selected triangles into half their original length. This mesh-re“ning adaptive scheme will be used in the ensuing section to develop computational results for the advective transport of a contaminant from the boundary of an oblate spheroidal cavity, induced by both steady ”ow and unsteady ”ow.

6.2. The advective transport with a steady ”uid ”ow

First, the steady-state problem of the advective transport from the oblate spheroidal cavity in a non-deformable porous medium is considered (i.e. the pore ”uid is considered to be incompressible and the porous skeleton is assumed to be non-deformable). In this case, the piezo-conduction equation reduces totthisedred9-40

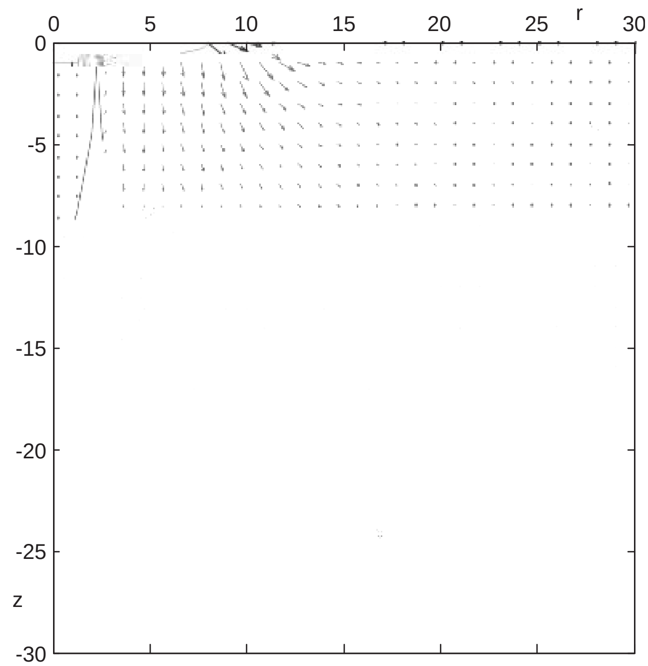


Figure 7. The ”ow velocity pattern in the computational domain containing an oblate cavity.

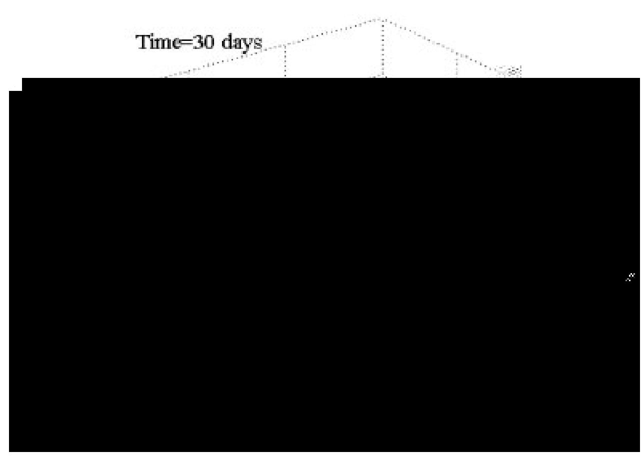


Figure 8. The analytical solution of the advective transport from an oblate spheroidal cavity (a/b ¼ 0.125) [10].

located remote from the cavity, due to the small magnitude of the ”ow velocity, which induces the low Courant number and the large discrepancy between the phase velocity and the ”ow velocity. If the time step is increased, the numerical oscillations will be introduced into the solution at the early stages of the transport process (i.e. the steep front is located in the vicinity of the cavity) due to the high Courant number resulting from the large magnitude of the ”ow velocity. In the transport processes where the ”ow “eld exhibits spatial variations of the type indicated in Figure 7, it is di cult to choose a constant time step with an almost uniform mesh (similar to that shown in Figure 5) to ensure that the elemental Courant number is unity over the entire computational domain. For this reason, adaptive procedures should be used during the computations to satisfy the Courant number criterion (9) at all times. This conclusion can be veri“ed through a numerical computation obtained from a time-adaptive scheme.

The application of the time-adaptive procedure is based on the consideration that the advective ”ow “eld along the steep front of the solution is almost uniformly distributed (see

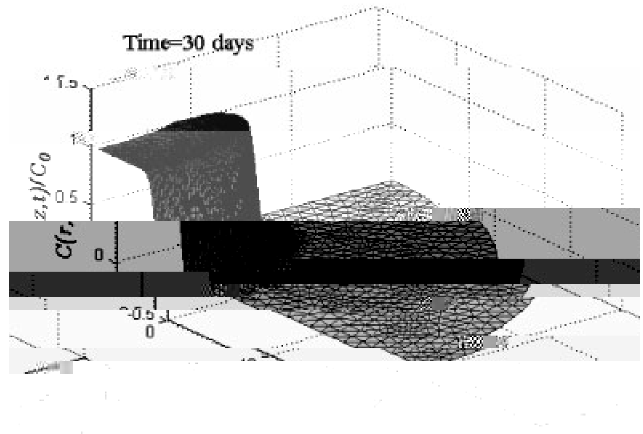


Figure 11. Numerical results at $t = 30$ days for the advective transport from the oblate cavity obtained from the mesh-adaptive CN-MLS scheme with $\Delta t = 1.0$ days.

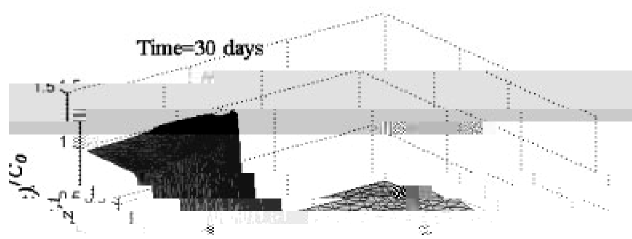


Figure 12. Numerical results at $t = 30$ days for the advective transport from the oblate cavity obtained from the mesh-adaptive MLS scheme with $\alpha = 3/2$ and $\psi = 1/3$.

step of $\Delta t = 1.0$ day adaptively increases to $\Delta t = 5.5$ days at the end of the computation. With the increase in the time step, the mesh refinement is performed on a coarser level than that used in the mesh-adaptive scheme. From this point of view, the combined time- and mesh-adaptive scheme is computationally more efficient than the purely mesh-adaptive scheme. However, because of the use of the coarser refined mesh, the numerical solution obtained from the combined time- and mesh-adaptive scheme is more diffusive than that obtained from the mesh-adaptive scheme.

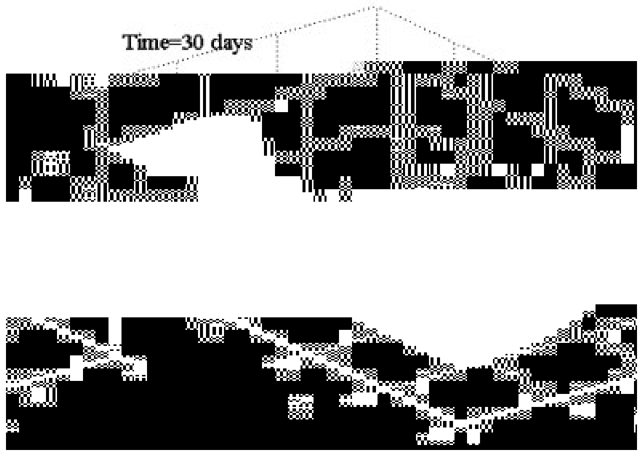


Figure 13. Numerical results at $t = 30$ days for the advective transport from the oblate cavity obtained from the time- and mesh-adaptive CN-MLS scheme (the initial time step $\Delta t = 1.0$ days is increased to $\Delta t = 5.5$ days).

6.3. Advective transport from an oblate spheroidal cavity induced by pressure transients

In this section, we consider the advective transport problem where the flow velocities are governed by the piezo-conduction equation, which takes into consideration the compressibilities of the pore fluid and the soil skeleton. Attention is focused on the advective transport of a chemical from an oblate spheroidal cavity located in an extended porous medium where the boundary of the cavity is simultaneously subjected to pressure and chemical pulses in the form of Heaviside step function. The material and physical parameters governing hydraulic conductivity, compressibilities and porosity are kept the same as those used in Section 5. The mesh-refining adaptive as well as the combined time- and mesh-refining adaptive CN-MLS schemes are used to solve the pressure transient-induced advective transport problem. Figure 14 illustrates the numerical results obtained from the two adaptive schemes. In the combined time- and mesh-refining adaptive scheme, the initial time step commences with $\Delta t = 1.0$ day and increases to $\Delta t = 5.5$ days at the end of the computation corresponding to $t = 30$ days. Again, the mesh-adaptive scheme generates a more accurate solution, but the combined time- and mesh-adaptive scheme is considered to be more efficient.

6.4. Advective transport from a cylindrical cavity

As a final example, we consider the problem of advective transport from a cylindrical cavity located in an extended porous medium. The chemical is introduced at the boundary of the borehole and its migration through the porous medium is as a result of a time- and space-dependent velocity field. Figure 15(a) illustrates the axisymmetric computational domain and its discretization as well as the boundary conditions applicable to the piezo-conduction equation and the advection equation. Figure 15(b) illustrates the flow field over the computational domain corresponding to $t = 30$ days, which is determined from the piezo-conduction equation and the potential boundary conditions. The computational results and the refined mesh for the advective transport from the borehole corresponding to $t = 30$ days, obtained from the

Figure 16. Numerical results for $t = 30$ days for the advective transport from a borehole with pressure transient obtained using a mesh-adaptive CN-MLS scheme: (a) 3D concentration profile; and (b) the corresponding refined mesh.

Figure 17. Computational results for $t = 30$ days of the advective transport from a borehole with pulsed potential boundary, obtained using the mesh-adaptive CN-MLS scheme: (a) 3D concentration profile; and (b) the corresponding refined mesh.

The computational results and the refined mesh corresponding to $t = 30$ days, obtained from the mesh-refining CN-MLS scheme with $\Delta t = 1.0$ day, are shown in Figure 17. A mesh gap can be clearly seen in the refined mesh, which corresponds to an increase of the flow velocity caused by a rise in the potential pulse applied at the boundary of the borehole. This increase of the flow velocity has the effect of accelerating the transport process (see e.g. the results shown in Figures 16(a) and 17(a)).

7. CONCLUSIONS

In this paper, certain advective transport problems for ”uid-saturated porous media are examined using a computational approach, where, due to the presence of ”uid pressure transients, the ”ow velocity “eld is both time- and space-dependent. The piezo-conduction equation is used in the study to determine the pore ”uid pressure transients in a ”uid-saturated porous medium. The time- and mesh-adaptive numerical schemes are proposed, respectively, for the modelling of one- and multi-dimensional advective transport problems with time- and space-dependent ”ow velocity to achieve an optimum computational performance. The computational results for one-dimensional semi-in“nite domains as well as three-dimensional axisymmetric domains are presented to illustrate the need for adaptive procedures, for handling a non-classical hyperbolic conservation equation with time- and position-dependent advective ”ow velocities and with steep advective transport fronts.

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