

# The advective transport of a chemical from a cavity in a porous medium

A.P.S. Selvadurai\*

*Department of Civil Engineering and Applied Mechanics, McGill University, 817 Sherbrooke Street West, Montreal, QC, Canada H3A 2K6*

Received 10 October 2001; received in revised form 7 March 2002; accepted 7 March 2002

---

## Abstract

The paper examines the problem of advective transport of a chemical, which is introduced at the boundary of a spherical cavity contained in a fluid saturated non-deformable porous medium of infinite extent. The advective Darcy flow is caused by a hydraulic potential, maintained at a constant value at the boundary of the spherical cavity. Analytical results are developed for the time- and position-dependent distribution of the chemical concentration in the porous medium, in the presence of natural attenuation and time-dependent variability in the boundary chemical concentration. The analytical results for advective transport problems related to certain two-dimensional flows associated with an annular region are also presented. The analytical solutions provide valuable benchmarks for calibration of computational codes dealing with the advective transport problem. © 2002 Elsevier Science Ltd. All rights reserved.

---

## 1. Introduction

The transport of chemicals and other contaminants in porous geological media is a topic of fundamental importance to the general area of earth sciences and is of particular interest to geo-environmental engineering. The basic mechanisms of transport range from advective transport, which is dependent on an advective flow velocity, to diffusive transport that depends on a concentration gradient. Although the fundamental processes governing these basic modes of transport can be non-linear and highly dependent on the micro-structural morphology of the porous

---

\* Tel.: +1-514-398-6672; fax: +1-514-398-7361.

*E-mail address:* patrick.selvadurai@mcgill.ca (A.P.S. Selvadurai).

medium, the linear theories associated with these basic transport processes provide useful first approximations for the study of both advective and diffusive processes. The advective transport is related to the flow velocity, which, in its linearized form, is governed by Darcy flow and, similarly, the diffusive transport processes are governed by Fick's law. The extent to which one process or the other dominates depends primarily on the flow characteristics as opposed to the diffusive transport characteristics of the system, which consists of the porous medium, the pore fluid being transmitted and the chemical species that is being transported. There are, however, situations where the advective flow velocities are sufficiently large enough to transport the chemical species solely by advective transport. This paper investigates some elementary advective transport problems resulting from such a situation. The problem specifically focuses on transport from spherical cavities and annular regions, the boundaries of which are subjected to a hydraulic potential to induce steady flow through the porous medium. With this steady flow in place, the boundaries of the flow domains are subjected to a time-dependent chemical concentration that induces the advective transport of the chemical. It is shown that the potential flow resulting from a spherical cavity in an infinite space, an annular plane region and an annular sector region the boundaries of which are maintained at a constant potential can be evaluated in *exact closed form*. The advective transport problem is then solved using a Laplace transform technique. Specific *closed form* results for advective chemical migration from spherical and cylindrical cavities and annular sector regions are presented and the utility of these solutions as they relate to calibration of computational methodologies are also discussed.

## 2. Governing equations

The basic equation governing advective transport of a chemical species in a porous medium has been presented in a number of textbooks dealing with geoenvironmental transport processes [1–12]. The mathematical similarity between the partial differential equation governing advective transport of a chemical in a porous medium and partial differential equations governing the flow of vehicular traffic, movement of waves in shallow water, movement of charged particles such as electrons, gas dynamics, biological processes, salt movement in oceans and heat flow in heat exchangers is well documented [13–21]. For completeness, and for the sake of clarity, we shall document here the derivation of the basic partial differential equation governing advective flow of a chemical species through a non-deformable porous medium [21]. Consider an arbitrary region  $V$  of a porous medium with surface  $S$ . The porosity of the medium, defined by the ratio of the volume of pore space to the total volume, is denoted by  $n^*$ . The concentration of the chemical species per *unit volume of the fluid* contained in the pore space is defined by  $C(\mathbf{x}, t)$ , where  $\mathbf{x}$  is a position vector and  $t$  is time. We can also define a concentration  $\hat{C}(\mathbf{x}, t)$ , which is measured per *unit total volume* of the porous medium. At any given location at any time

$$\hat{C}(\mathbf{x}, t) = n^* C(\mathbf{x}, t). \quad (1)$$

The velocity vector defines the advective velocity averaged over the entire cross section of the medium  $\hat{\mathbf{v}}(\mathbf{x}, t)$ . The *flux* is defined as the mass of the chemical species either *entering* or *leaving* a unit area in unit time. The flux vector, or mass being transported by advection, per unit total area per unit time is given by

$$\mathbf{F}_a = \hat{\mathbf{v}}\hat{C}(\mathbf{x}, t) = n^*\hat{\mathbf{v}}C(\mathbf{x}, t). \quad (2)$$

The total mass of the chemical species transported into the volume  $V$  of surface  $S$  is given by

$$m_i = - \iint_S \mathbf{F}_a \mathbf{n} dS \quad (3)$$

where  $\mathbf{n}$  is the outward unit normal to the elemental surface area  $dS$ . Applying the divergence theorem, we can rewrite (3) as

$$m_i = - \iiint_V \nabla \cdot \{n^*\hat{\mathbf{v}}C\} dV. \quad (4)$$

The species is assumed to accumulate in the fluid within the void space of the porous medium. The rate of accumulation of the species is given by

$$m_a = \frac{d}{dt} \iiint_V n^* C dV = \iiint_V n^* \frac{\partial C}{\partial t} dV. \quad (5)$$

The rate of production/loss of the chemical species due to either generation (+) or decay (–) processes within the porous medium is given by

$$m_p = \pm \iiint_V n^* \xi C dV \quad (6)$$

where  $\xi$  is a specific generation/decay rate referred to the fluid volume (i.e. measured per unit time). For conservation of mass of the species we require  $m_a = m_i + m_p$ , which, when combined with the *Dubois-Reymond Lemma* for the existence of a local equation, gives the following first-order, linear partial differential equation of the hyperbolic-type, governing advective transport of a chemical species:

$$\frac{\partial C}{\partial t} + \nabla \cdot (\hat{\mathbf{v}}C) = \pm \xi C. \quad (7)$$

In this paper we restrict attention to flow fields characterized by Darcy flow. The flow velocities are governed by Darcy's law, which for a hydraulically isotropic medium is given by

$$\hat{\mathbf{v}} = -k\nabla\phi \quad (8)$$

where  $k$  is the hydraulic conductivity and  $\phi(\mathbf{x})$  is the reduced Bernoulli potential governing fluid flow through the porous medium, which includes only the datum potential and the pressure potential. For incompressible flow of the pore fluid and for non-deformability of the porous solid,

$$\nabla \cdot \hat{\mathbf{v}} = 0 \quad (9)$$

and the elliptic partial differential equation governing the flow potential is Laplace's equation

$$\nabla^2\phi(\mathbf{x}) = 0. \quad (10)$$

The partial differential equations governing the advective transport problem are therefore (7) and (10) respectively for the time-dependent chemical concentration  $C(\mathbf{x}, t)$  and for the flow potential  $\phi(\mathbf{x})$ . The initial boundary value problem governing  $C(\mathbf{x}, t)$  is subject to an initial condition and usually a Dirichlet type boundary condition are also prescribed on a given surface. The boundary value problem governing  $\phi(\mathbf{x})$  is subject to Dirichlet type boundary conditions on  $S_D$ , Neumann type boundary conditions on  $S_N$  and/or Robin type mixed boundary conditions on  $S_M$ , where the three separate surfaces are complementary sub-sets of  $S$ ; i.e.  $S = S_D \cup S_N \cup S_M$ .

### 3. Advective transport from a spherical cavity

We first consider the problem of a non-deformable porous medium of infinite extent, which is bounded internally by a spherical cavity of radius  $a$ . The steady fluid flow into the porous medium is caused by a flow potential that is constant at the boundary of the prolate cavity and reduces uniformly to zero at large distances from the cavity. When steady flow is maintained, the boundary of the cavity is subjected to a chemical concentration  $C_0F(t)$ , where  $C_0$  is a constant and  $F(t)$  is some arbitrary function (Fig. 1). Since the flow potential is constant ( $\phi_0$ ) at the boundary of the spherical cavity, the flow problem is radially symmetric and the flow potential is governed by Laplace's equation in its spherically symmetric form; i.e.

$$\nabla^2\phi(R) = \frac{d^2\phi}{dR^2} + \frac{2}{R}\frac{d\phi}{dR} = 0 \quad (11)$$

with the single boundary condition  $\phi(a) = \phi_0$  and the regularity condition  $\phi(R) \rightarrow 0$  as  $R \rightarrow \infty$ . The exact solutions for the distribution of potential and the radial flow velocity are given by

$$\phi(R) = \frac{\phi_0 a}{R}; \quad v_R = \frac{ka\phi_0}{R^2}. \tag{12}$$

Assuming that the porous medium contributes to the decay of the chemical with a constant decay rate  $\xi$ , the appropriate form of the governing partial differential Eq. (7) now reduces to

$$\frac{\partial C}{\partial t} + \frac{\phi_0 ka}{R^2} \frac{\partial C}{\partial R} = -\xi C. \tag{13}$$

The partial differential Eq. (13) needs to be solved, subject to a single boundary condition and a single initial condition. Although the boundary conditions can vary depending on the nature of the problem that is being discussed, we shall, throughout this presentation, implicitly assume that the porous medium is initially at zero chemical concentration; i.e.

$$C(\mathbf{x}, 0) \equiv 0 \tag{14}$$

While there are a number of procedures that have been proposed in the literature [2,21–23] for the solution of first-order partial differential equations of the type (13), we shall adopt a procedure, which involves the use of Laplace transforms [24,25]. The use of Laplace transforms is both convenient and adequate. We define the Laplace transform of  $C(R, t)$  with respect to the time variable as

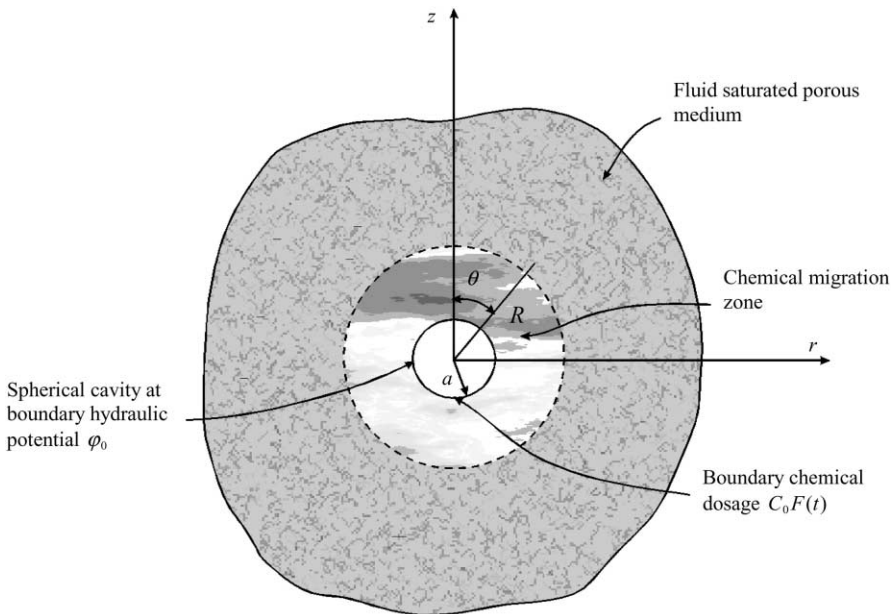


Fig. 1. Advective chemical transport from a spherical cavity.

$$\bar{c}(R, s) = L\{C(R, t)\} = \int_0^{\infty} \exp(-st)C(R, t)dt \quad (15)$$

and since the initial chemical concentration in the porous medium is zero [see e.g. (14)], we have

$$L\left\{\frac{\partial C}{\partial t}\right\} = s\bar{c}(R, s) \quad (16)$$

Applying the Laplace transform to (13) we obtain an ordinary differential equation for the transformed dependent variable  $\bar{c}(R, s)$ , the solution of which is

$$\bar{c}(R, s) = A \exp\left(-\frac{(s + \xi)R^3}{3k\phi_0 a}\right) \quad (17)$$

where  $A$  is an arbitrary constant that needs to be determined by considering the time dependent chemical dosage at the boundary of the spherical cavity. i.e.

$$C(a, t) = C_0 F(t) \quad (18)$$

the Laplace transforms of which gives

$$\bar{c}(a, s) = C_0 f(s) \quad (19)$$

where  $f(s)$  is the Laplace transform of  $F(t)$ . The exact form of  $F(t)$  is not important to the discussion that follows; it is only sufficient to require that the Laplace transform of  $F(t)$  exists. Using (19) we can solve for the arbitrary constant  $A$ , and by the inverting the resulting expression for  $\bar{c}(R, s)$ , we obtain the following expression for the time-dependent spatial distribution of the chemical from the spherical source:

$$\frac{C(R, t)}{C_0} = L^{-1}\left\{f(s)\exp\left(-\frac{(s + \xi)(R^3 - a^3)}{3\phi_0 ka}\right)\right\} \quad (20)$$

where  $L^{-1}$  refers to the inverse Laplace transform. The general result (20) for the advective transport involving spherical symmetry can be evaluated by specifying plausible time variations defined by  $F(t)$  along with the use of the convolution theorem for Laplace transforms defined by

$$L^{-1}\{f(s)g(s)\} = F * G = \int_0^t F(u)G(t - u)du. \quad (21)$$

Alternatively, the inversion can be carried out by appeal to Tables of Integral Transforms [24], or through the use of symbolic mathematical manipulation software such as MAPLE<sup>®</sup> or MATHEMATICA<sup>®</sup> [26] or through the use of numerical inversion techniques. In the ensuing we shall present some analytical results for three

specific forms of chemical dosage histories at the boundary of the spherical cavity.

We consider the case where the boundary of the spherical cavity is subjected to a chemical concentration, which is in the form of a Heaviside step function: i.e.

$$F(t) = \begin{cases} 0 & ; \quad -\infty > t \geq 0 \\ 1 & ; \quad 0 \leq t < \infty \end{cases} \quad (22)$$

In this case the result (20) gives

$$\frac{C(R, t)}{C_0} = \exp(-\xi\lambda(\rho))H[t - \lambda(\rho)] \quad (23)$$

where  $H[t - \lambda(\rho)]$  is the Heaviside step function with the time shift

$$\lambda(\rho) = \frac{a^2}{3\phi_0 k} \left\{ \left( \frac{R}{a} \right)^3 - 1 \right\}; \quad \rho = \frac{R}{a}. \quad (24)$$

The relevant solutions for situations involving *no natural attenuation* of the chemical concentration during its migration through the porous medium can be obtained by setting  $\xi = 0$ , in (23).

Next consider the case where the boundary of the spherical cavity is subjected to a chemical concentration with a time-dependent decay of the form

$$C(a, t) = C_0 \exp(-\zeta t) \quad (25)$$

where  $\zeta$  is a non-negative constant. In this case, the time-dependent spatial variation in the chemical concentration in the porous medium is given by

$$\frac{C(R, t)}{C_0} = \exp(-\zeta t - (\xi - \zeta)\lambda(\rho))H[t - \lambda(\rho)] \quad (26)$$

We also consider the case where the boundary of the spherical cavity is subjected to a time-dependent chemical concentration of the form

$$F(t) = C_0[1 + \sin(\omega t)] \quad (27)$$

where  $\omega$  is a circular frequency. The relevant solution for the time and position dependent variation of chemical concentration within the porous medium is given by

$$\frac{C(R, t)}{C_0} = \exp\{-\xi\lambda(\rho)\}H[t - \lambda(\rho)]\{1 + \sin(\omega[t - \lambda(\rho)])\}. \quad (28)$$

Solutions for other forms of time variations in the boundary concentration  $C_0F(t)$

can be obtained by considering the basic procedures outlined in the preceding equations. It is worth noting that approximate solutions to any arbitrary time variation in the chemical concentration at the boundary of the spherical cavity can also be obtained by considering the time variation as a summation of solutions, over discrete time intervals, of the solution involving *constant* boundary concentrations applied over a finite time interval. Other *spectral methods* can also be used for this purpose but this does not add any new fundamental developments. For example, consider the case where the boundary is subjected to a constant chemical dosage over a finite time interval  $t \in (0, t^*)$  such that the time-dependent chemical concentration in the porous medium

$$F(t) = \begin{cases} 0 & ; -\infty > t \geq 0 \\ 1 & ; 0 \leq t < t^* \\ 0 & ; t > t^* \end{cases} \quad (29)$$

In this case the result (20) gives

$$\frac{C(R, t)}{C_0} = \exp(-\xi\lambda(\rho)) [H[t - \lambda(\rho)] - H[t - t^* - \lambda(\rho)]] \quad (30)$$

with the Heaviside step functions being interpreted appropriately.

#### 4. Advective transport in a plane circular region

We now focus attention on certain problems related to advective transport of a chemical in a plane, with specific reference to an annular region. The in-plane advective transport can be visualized as being a suitable model for contaminant migration in either fractures with narrow aperture or thin porous seams contained between relatively impermeable media, and the hydraulic conductivity is related to the either the aperture of the fracture or the hydraulic conductivity of the seam [27,28].

We first consider the problem of an annular porous region with internal radius  $a$  and external radius  $b$ . The inner boundary of the annular region is maintained at a constant hydraulic potential  $\phi_0$ , and the outer boundary is maintained at zero hydraulic potential (Fig. 2). This induces radially symmetric in-plane flow, governed by

$$\frac{d^2\phi}{dr^2} + \frac{1}{r} \frac{d\phi}{dr} = 0 \quad (31)$$

and the resulting solution for the velocity field is given by



$$v_r = \frac{k\phi_0}{r \ln(b/a)}. \tag{32}$$

Since the velocity field is singular at the origin, the location  $r = 0$  is excluded from the solution domain. The velocity field is thus valid for  $0 < r < \infty$  and  $0 < \theta < 2\pi$ . When this steady in-plane radial flow is established, the inner boundary of the annular region is maintained at a chemical concentration  $C_0F(t)$ , where  $F(t)$  is an arbitrary function, but again with the proviso that its Laplace transform,  $f(s)$ , exists. We shall also assume that the natural attenuation of the chemical as it migrates through the porous medium has a decay rate  $\xi$  per unit time. Following (7), the advective transport in the annular region is now governed by the partial differential equation

$$\frac{\partial C}{\partial t} + \frac{k\phi_0}{r \ln(b/a)} \frac{\partial C}{\partial r} = -\xi C. \tag{33}$$

We can proceed to solve the above equation, using the basic procedures outlined previously. The time-dependent movement of the chemical within the porous medium is now given by

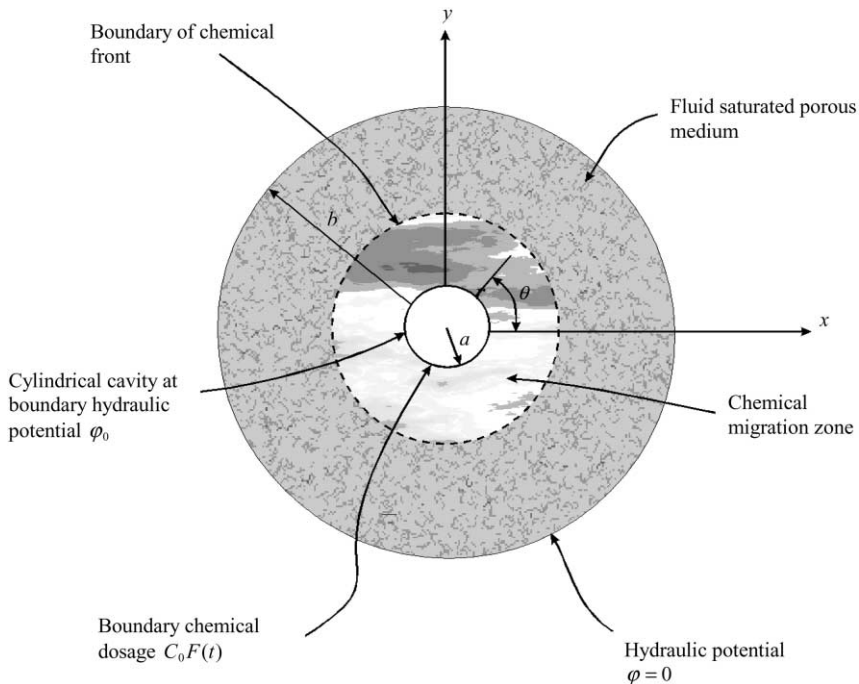


Fig. 2. Advective chemical transport from a cylindrical cavity.

$$\frac{C(r, t)}{C_0} = \exp(-\xi\mu(\eta))L^{-1}\{f(s)\exp(-s\mu(\eta))\} \tag{34}$$

where

$$\mu(\eta) = \frac{a^2(\eta^2 - 1)\ln(b/a)}{2k\phi_0}; \quad \eta = \frac{r}{a}. \tag{35}$$

The specific solutions for the time-dependent chemical concentration within the porous medium can now be obtained by prescribing the variation  $F(t)$ . For the specific case when the function has a time dependency in the form of a Heaviside step function defined by (22), the time and spatial distribution of the chemical concentration is given by a result similar to (23) obtained for the problem involving spherically symmetric migration from a spherical cavity: i.e.

$$\frac{C(r, t)}{C_0} = \exp(-\xi\mu(\eta))H[t - \mu(\eta)]. \tag{36}$$

Results for other time-dependent variations of chemical concentration at the boundary of the cavity can be obtained in a similar manner.

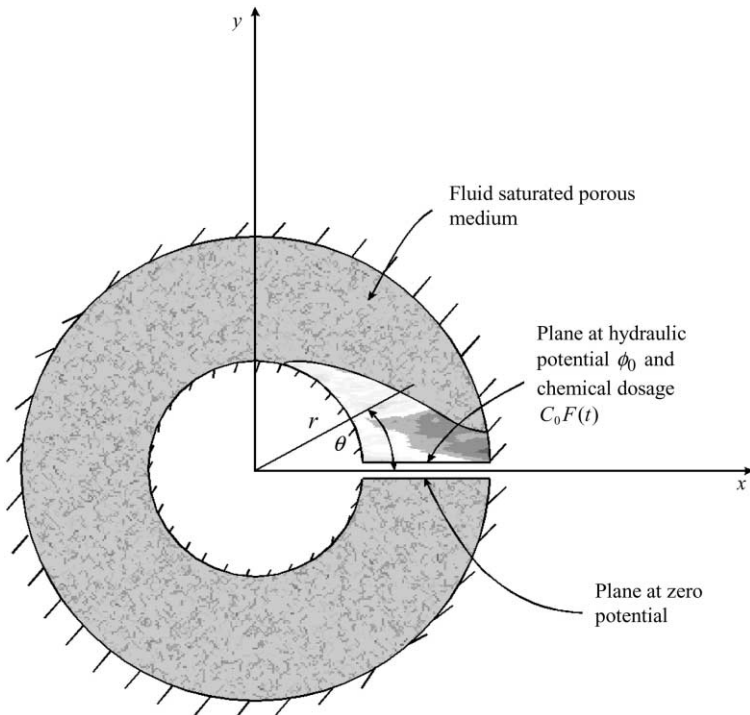


Fig. 3. Advective chemical transport in porous medium due to circular flow.

We now focus on the problem of advective transport of a chemical resulting from circular flow in an annular domain  $r \in (a, b)$  and  $\theta \in (0 + \varepsilon, 2\pi - \varepsilon)$ , where  $\varepsilon$  is a small parameter. Consider the flow problem where the circular boundaries  $r = a$  and  $r = b$  of the annular domain are subjected to Neumann-type no flow boundary conditions and the plane boundaries  $\theta = 0 + \varepsilon$  and  $\theta = 2\pi - \varepsilon$  are maintained at constant potentials  $\phi_0$  and 0 respectively (Fig. 3). The boundary value problem resulting from flow in the porous medium is governed by the partial differential equation

$$\frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r} \frac{\partial \phi}{\partial r} + \frac{1}{r^2} \frac{\partial^2 \phi}{\partial \theta^2} = 0 \tag{37}$$

subject to the boundary conditions

$$\phi(r, 0) = \phi_0; \phi(r, 2\pi) = 0 \tag{38}$$

$$\left[ \frac{\partial \phi}{\partial r} \right]_{r=a} = 0; \left[ \frac{\partial \phi}{\partial r} \right]_{r=b} = 0. \tag{39}$$

Considering the complete general solution for Laplace’s equation [21], given by

$$\phi(r, \theta) = A \ln r + B \theta \ln r + C \theta + D + \sum_{n=1,2,\dots}^{\infty} \left[ A_n r^n + \frac{B_n}{r^n} \right] [C_n \sin n \theta + D_n \cos n \theta] \tag{40}$$

where  $A, B, C, D, A_n, B_n$ , etc., are arbitrary constants, it can be shown that the solution to the boundary value problem is given by

$$\phi(r, \theta) = \phi_0 \left( 1 - \frac{\theta}{2\pi} \right). \tag{41}$$

The circular flow in the annular region is given by the velocity vector

$$\mathbf{v} = \frac{k\phi_0}{2\pi r} \mathbf{i}_\theta. \tag{42}$$

Since the velocity field is singular at the origin, the location  $r = 0$  can be excluded from the solution domain. The velocity field is thus valid for  $0 < r < \infty$  and  $0 \leq \theta < 2\pi$ . The advective transport in the annular domain is governed by the partial differential equation

$$\frac{\partial C}{\partial t} + \frac{k\phi_0}{2\pi r^2} \frac{\partial C}{\partial \theta} = -\xi C \tag{43}$$

The partial differential Eq. (43) can be solved using a Laplace transform technique

and employing the boundary condition

$$C(r, 0, t) = C_0 F(t). \quad (44)$$

Avoiding details, it can be shown that the time-dependent distribution of chemical concentration in the porous domain is given by

$$\frac{C(r, \theta, t)}{C_0} = \exp(-\xi\tau(\eta)) L^{-1} \{f(s) \exp(-s\tau(\eta))\} \quad (45)$$

where

$$\tau(\eta) = \frac{2\pi a^2}{k\phi_0} \eta^2 \theta; \quad \eta = \frac{r}{a}. \quad (46)$$

In the particular instance when the boundary of the region  $\theta = 0$  is subjected to a chemical dosage in the form of a Heaviside step function of time, (45) gives

$$\frac{C(r, \theta, t)}{C_0} = \exp(-\xi\tau(\eta)) H[t - \tau(\eta)]. \quad (47)$$

Again, specific expressions for situations involving other forms of time-dependent variations in the chemical concentration at the boundary  $\theta = 0$ ;  $r \in (a, b)$  can be obtained by specifying the appropriate variations for the function  $F(t)$ . It is also worth noting that since the flow in the region corresponds to circular flow and the chemical concentration is maintained constant on the plane  $0 < x < \infty$ ;  $y = +\varepsilon$  and zero along  $0 < x < \infty$ ;  $y = -\varepsilon$ , where  $\varepsilon$  is a small parameter, the solution is applicable to the entire domain but which *excludes* the origin.

## 5. Numerical results

Since the final results for the time-dependent variation of chemical concentration in the porous medium induced by the advective flow process can be evaluated in exact closed form it is not necessary to provide extensive numerical results. It is nonetheless instructive to present some typical numerical results to illustrate the pattern of migration of the chemical mainly for the case involving a boundary chemical dosage in the form of a Heaviside step function of constant intensity  $C(t) = C_0$ . In all cases, the general form of the time- and position-dependent chemical concentration can be evaluated in the form

$$\frac{C(R, t)}{C_0} = \exp(-\zeta t - (\xi - \zeta)\Omega(\rho)) H[t - \Omega(\rho)] \quad (48)$$

where  $\xi$  is the attenuation factor associated with the porous medium,  $\zeta$  is the decay

factor associated with the boundary chemical flux and  $\Omega(\rho)$  is a function which depends on the hydraulic conductivity of the porous medium, the radius of the cavity, the hydraulic potential inducing Darcy flow and the normalized radial distance  $\rho$ .

For purposes of illustration, we first consider the problem of a spherical cavity of radius  $a = 3$  m, which is located in a porous medium of hydraulic conductivity  $k =$

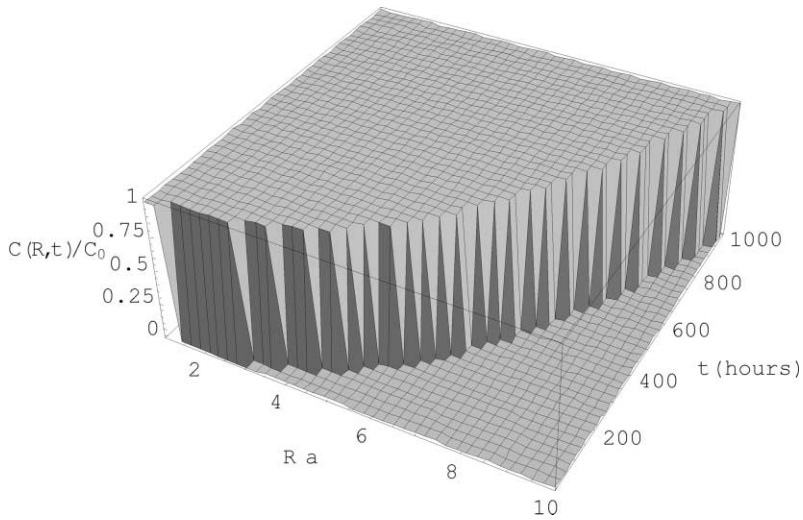


Fig. 4. Spherically symmetric advective chemical transport from a spherical cavity. Location of the chemical front  $C(R, t)/C_0$  in the absence of attenuation effects in the porous medium.

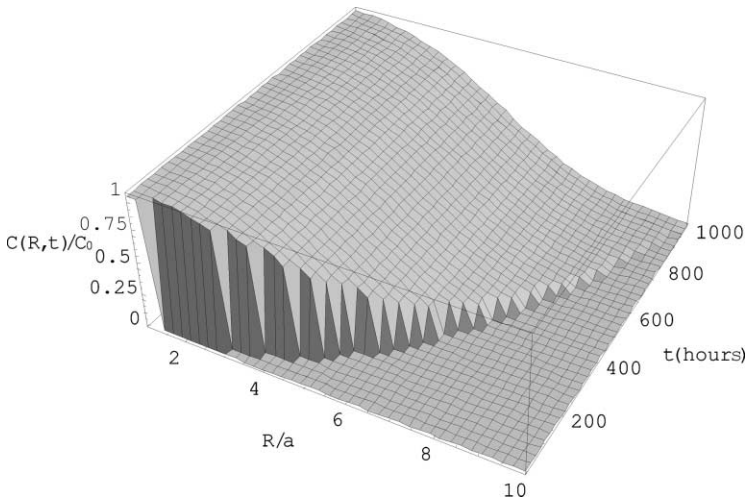


Fig. 5. Spherically symmetric advective chemical transport from a spherical cavity. Location of the chemical front  $C(R, t)/C_0$  in the presence of attenuation effects in the porous medium.

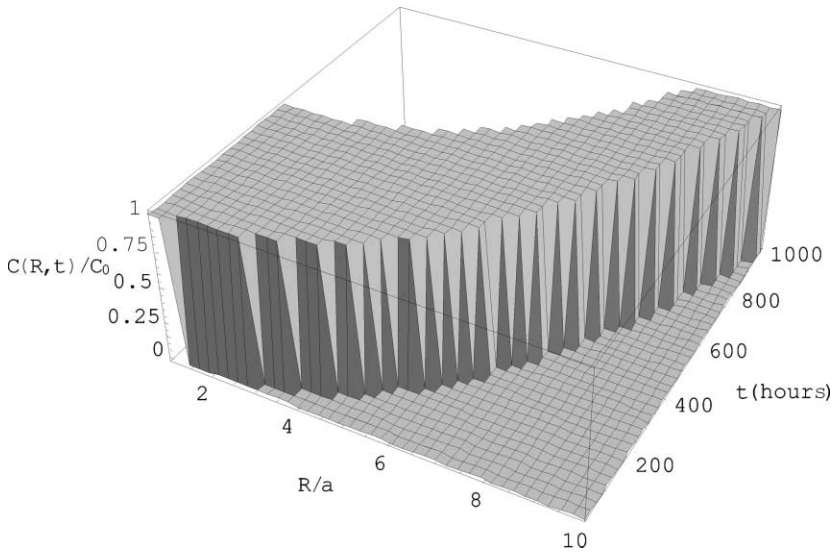


Fig. 6. Spherically symmetric advective chemical transport from a spherical cavity, due to a pulse of constant concentration. Location of the chemical front  $C(R, t)/C_0$  in the absence of attenuation effects in the porous medium.

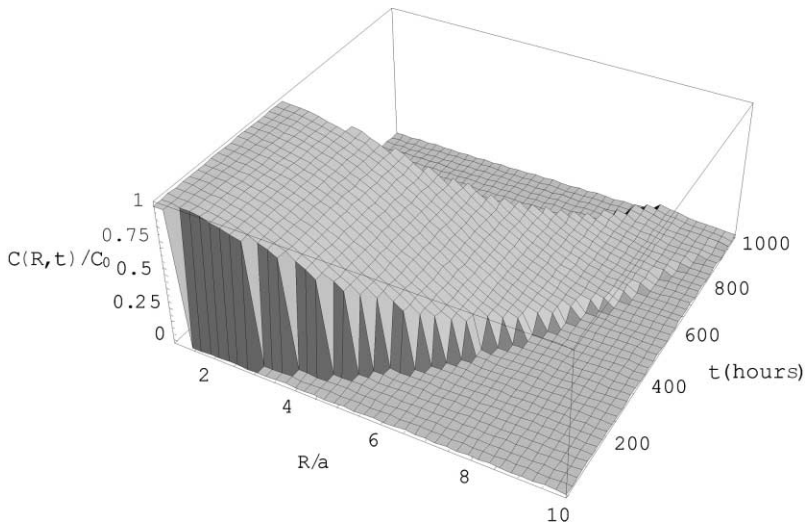


Fig. 7. Spherically symmetric advective chemical transport from a spherical cavity, due to a pulse of constant concentration. Location of the chemical front  $C(R, t)/C_0$  in the presence of attenuation effects in the porous medium.

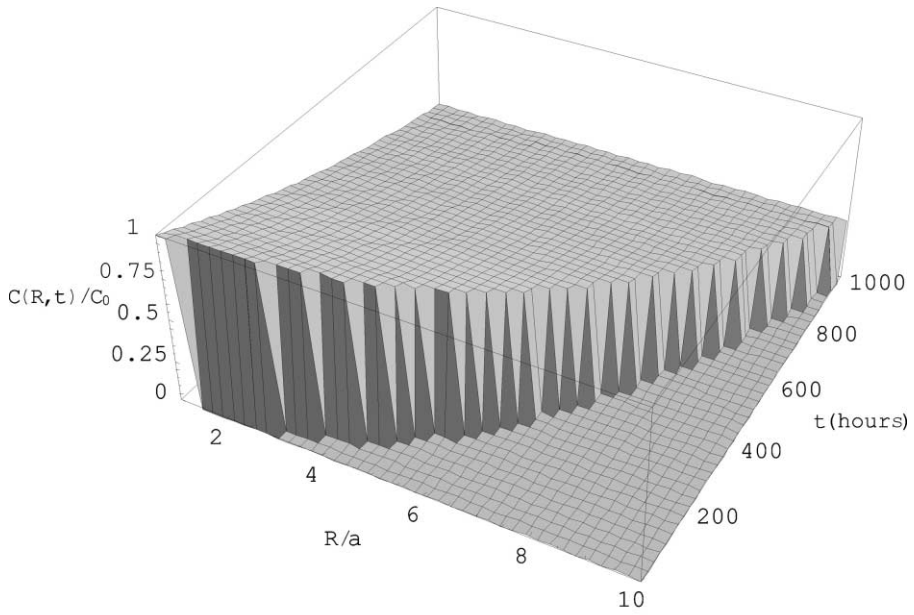


Fig. 8. Spherically symmetric advective chemical transport from a spherical cavity; influence of a time-dependent boundary flux. Location of the chemical front  $C(R, t)/C_0$  in the absence of attenuation effects in the porous medium.

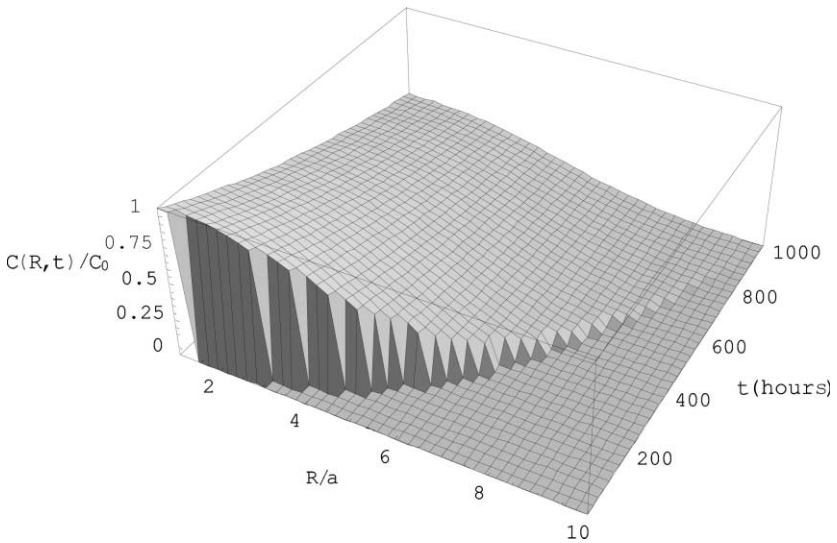


Fig. 9. Spherically symmetric advective chemical transport from a spherical cavity; influence of a time-dependent boundary flux. Location of the chemical front  $C(R, t)/C_0$  in the presence of attenuation effects in the porous medium.

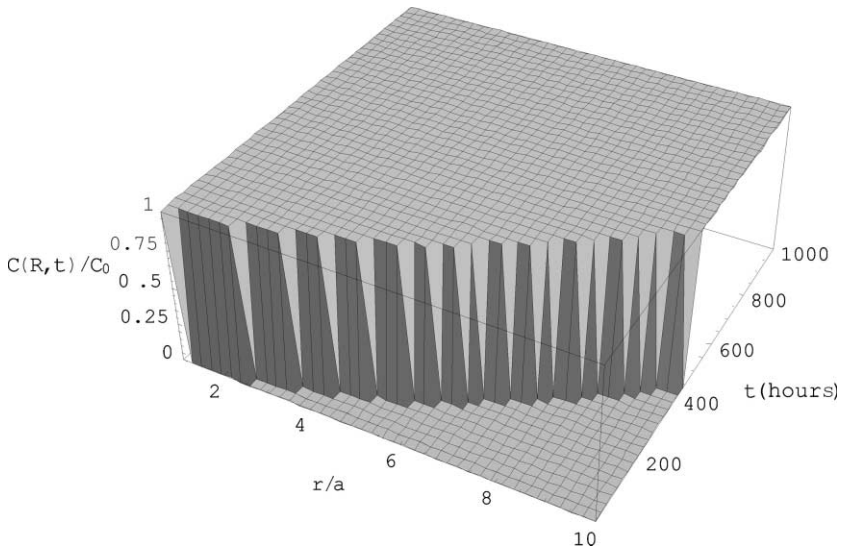


Fig. 10. Radially symmetric in-plane advective chemical transport from a cylindrical cavity. Location of the chemical front  $C(r, t)/C_0$  in the absence of attenuation effects in the porous medium ( $b/a = 100$ ).

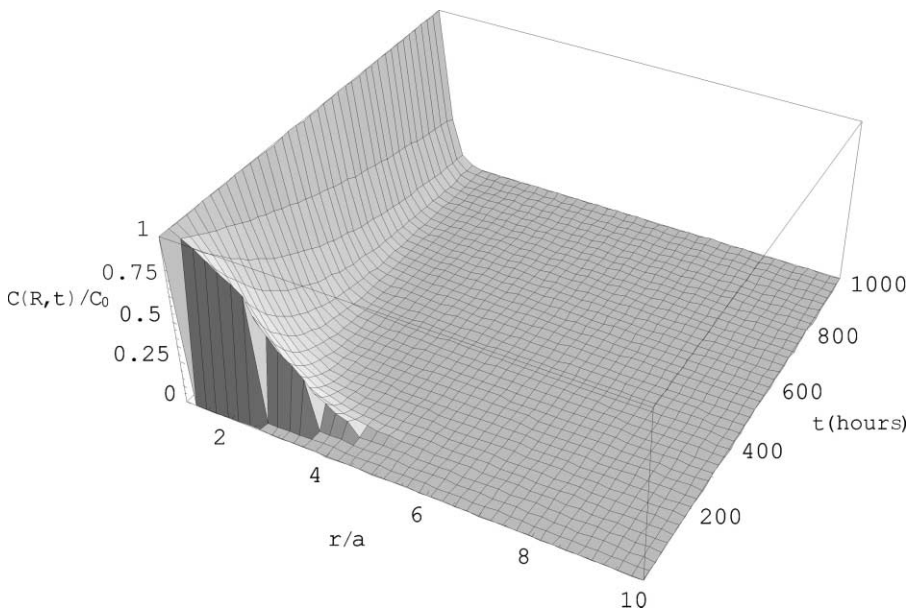


Fig. 11. Radially symmetric in-plane advective chemical transport from a cylindrical cavity. Location of the chemical front  $C(r, t)/C_0$  in the presence of attenuation effects in the porous medium ( $b/a = 100$ ).



$3 \times 10^{-2}$  m/day. The advective flow is induced under a boundary hydraulic potential of  $\phi_0 = 100$  m and the natural attenuation factor for the chemical in the porous medium is taken as  $\xi = 0.005/\text{day}$ . The analytical results have been evaluated by using the symbolic mathematical manipulation software MATHEMATICA<sup>®</sup>. Other software with similar capabilities can also be used to display the results. Fig. 4 illustrates the time- and position-dependent variation of the chemical concentration within the porous medium for the simple case involving migration without the natural attenuation. It is evident that, unlike for the case of purely one-dimensional column reactor-type problem [21], the spatial position of the migration front is not a linear function of the independent variables. Fig. 5 shows the case when the porous medium exhibits natural attenuation  $\xi = 0.005/\text{day}$ . As a further illustration we consider the problem where the surface of the spherical cavity is subjected to a constant chemical concentration of finite strength for a limited duration. The solution to this problem is given by the result (30), and the duration of the chemical dosage is set at  $t^* = 500$  h. The dimensions of the cavity, the hydraulic conductivity of the porous medium, the hydraulic potential  $\phi_0$  and the attenuation factor  $\xi$  are exactly the same as those used previously. Figs. 6 and 7 illustrate, respectively, the time- and position-dependent variation in the chemical concentration within the

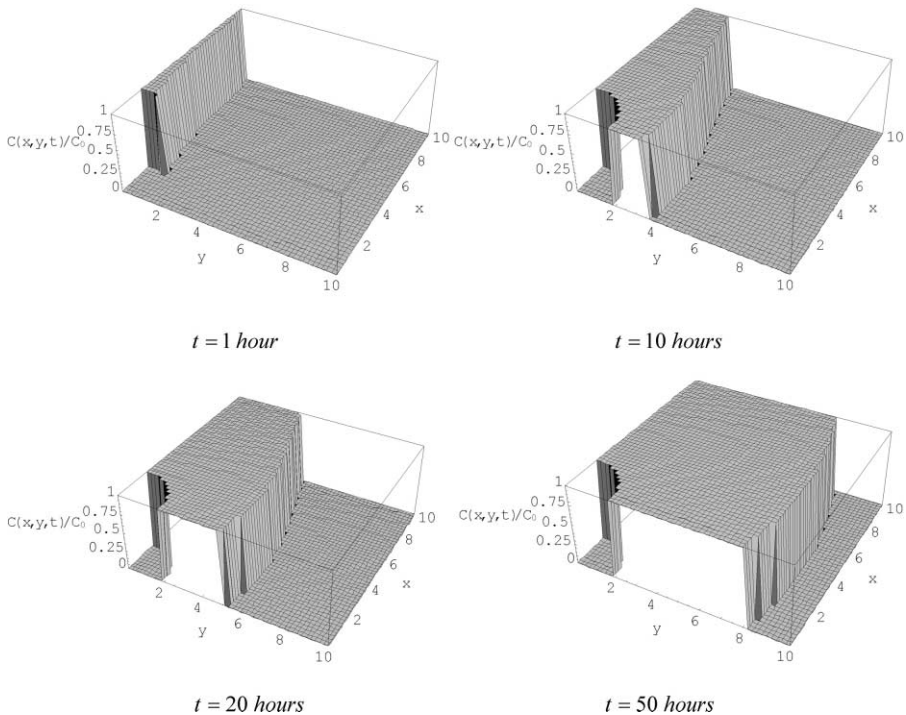


Fig. 12. Advective chemical transport in a quarter-plane region of a porous medium, which exhibits no attenuation effects. (The visual presentation of the results is limited to the region  $r > 2$ ,  $x < 10$  and  $y < 10$ .)

porous medium either in the absence or presence of attenuation. We next consider the case where the chemical dosage at the boundary of the spherical cavity exhibits a decay rate  $\zeta = 0.001/\text{day}$ . Fig. 8 presents results for the case where advective chemical transport takes place in the absence of attenuation effects in the porous medium and Fig. 9 presents results for the case where attenuation effects are present.

Figs. 10 and 11 relate to the problem of advective in-plane transport of a chemical that is induced by radially symmetric flow in an annular region. The inner radius of the annular region is taken as 2 m and the radii ratio  $b/a = 100$ . For the purposes of illustration, the attenuation factor for the porous medium is set equal to  $\xi = 0.0005/\text{day}$ , which is an order of magnitude lower than that used previously in connection with the numerical evaluation of the results applicable to the case of the spherical cavity. Fig. 10 is applicable to the case involving no natural attenuation in the porous medium and Fig. 11 gives results that account for the attenuation.

Finally we consider the problem of the advective chemical transport induced by circular flow in a plane region. Since the result is applicable to the complete plane, which excludes the origin, it is possible to display the results in relation to the quadrant of the quarter-plane, occupying the entire region  $r \geq 0$ . Also, for purposes of visual presentation, only the quadrant region where  $r > 2$ ,  $x < 10$  and  $y < 10$  is considered. [Also, in this case, the factor  $2\pi$  occurring in the first equation of (46)

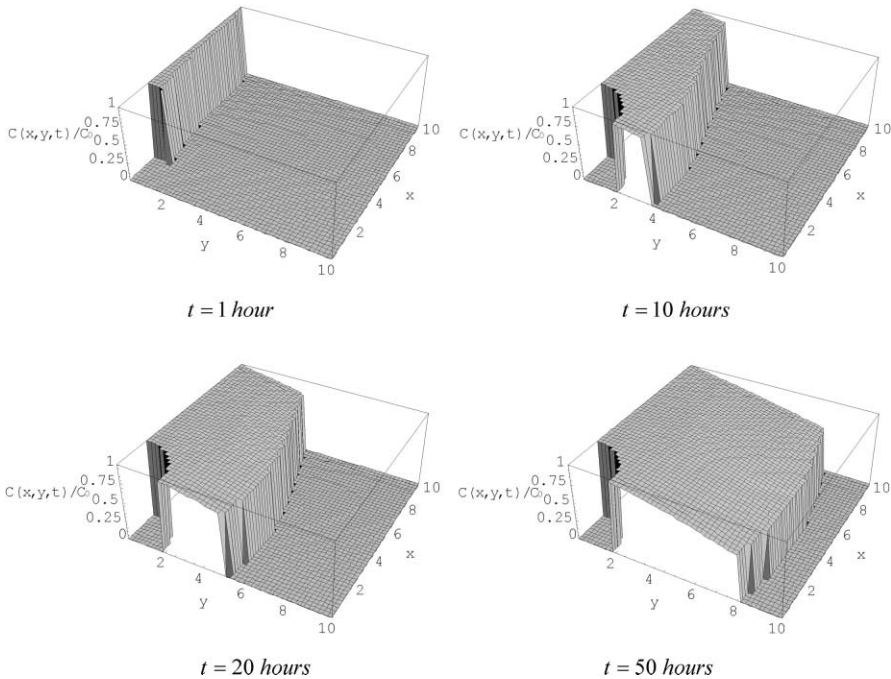


Fig. 13. Advective chemical transport in a quarter-plane region of a porous medium, which exhibits attenuation effects. (The visual presentation of the results is limited to the region  $r > 2$ ,  $x < 10$  and  $y < 10$ .)

should be replaced by  $\pi/2$ ]. The requirement is that any boundary that is placed to define a specific domain should satisfy the requirement for the existence of circular flow within the region. Two concentric circles of arbitrary radii will always satisfy this condition. In this sense, the solution developed has wider applicability for description of the in-plane transport processes. Also for the purposes of illustration, the length parameter  $a = 2$  m, the hydraulic conductivity  $k = 3 \times 10^{-2}$  m/day, the hydraulic potential  $\phi_0 = 100$  m and the attenuation parameter for the porous medium is taken as  $\xi = 0.01$ /day. The boundary  $y = 0$  is subjected to a constant chemi-

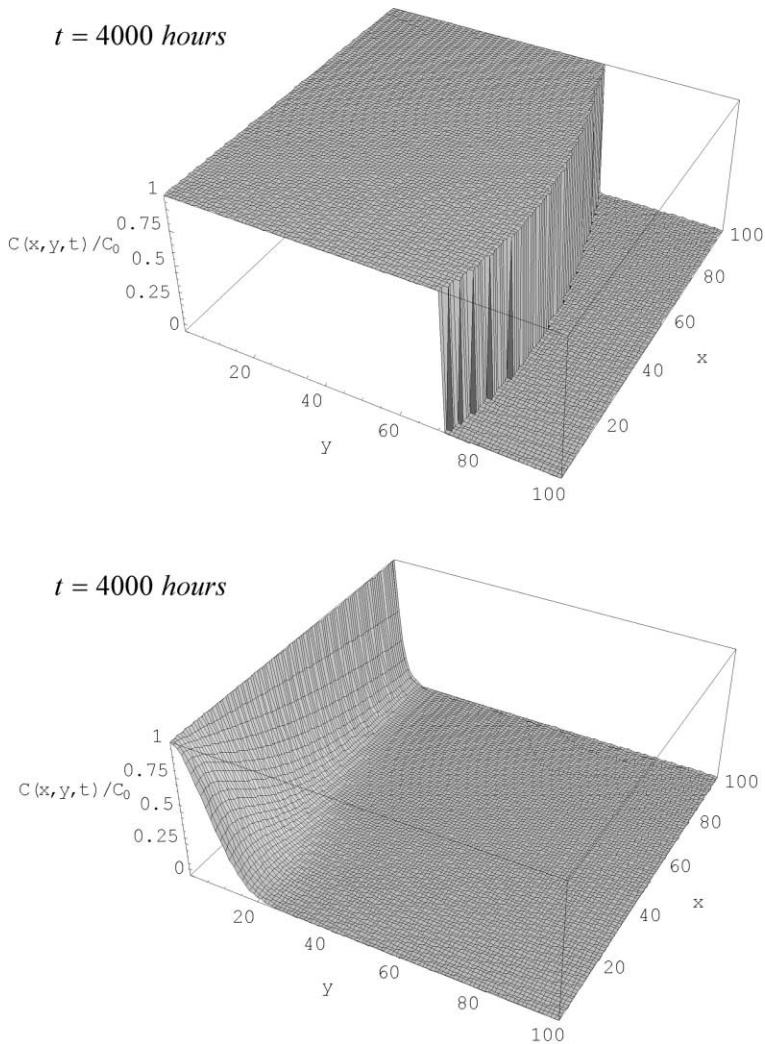


Fig. 14. Advective chemical transport in a quarter-plane region of a porous medium: an illustration of the influence of attenuation. (The visual presentation of the results is limited to the region  $0.001 < x < 100$  and  $0.001 < y < 100$ .)

cal concentration with a time dependency in the form of a Heaviside step function. The appropriate solution is given by (47). Fig. 12 illustrates the spatial variation of the chemical concentration, for selected times as indicated, for the case where there is no attenuation of the chemical as it migrates through the quarter-plane region (i.e.  $\xi = 0$ ). Similarly, the results shown in Fig. 13, account for effects of attenuation in the porous medium. Finally, Fig. 14 illustrates the significant influences of the effects of attenuation on the spatial distribution of chemical concentration over an extensive region, where  $a = 0.01$  m,  $0.01 < x < 100$  and  $0.01 < y < 100$ , and for a relatively long duration of 4000 h. In the case a medium with no attenuation, a significant part of the region of interest is occupied by the chemical.

## 6. Concluding remarks

The modelling of transport processes by appeal to purely advective processes is, of course, a highly idealized theoretical framework for examining very complex phenomena involving the movement of chemicals in porous media. The primary purpose of this paper is to illustrate the basic features of the advective transport process by appeal to some elementary problems for which exact closed form solutions are possible. It is shown that, owing to the closed form nature of the potential flow problem in the situations considered, the solutions for the advective transport problem can also be obtained in explicit closed form. The analytical solutions presented here have several important attributes; first, from an educational perspective, they form ideal vehicles for introducing the subject in terms of the study of a well-posed initial boundary value problem in mathematical modelling, albeit, for the linearized problem in advective transport in a porous medium. An appreciation of fundamental aspects of the advective transport problem is better gained by examining relatively elementary problems rather than complex ones that are burdened by numerical rigour. Second, the treatment of the chemical source as, say, a spherical cavity, gives the problem an all-important physical dimension of length which is absent if one were to consider the problem simply as a *point source* of prescribed strength. In this sense the problems are multi-dimensional. Third, despite their simplicity, the solutions can be used to significant advantage to conduct preliminary scoping calculations for advective transport problems that can be encountered in geoenvironmental engineering practice; the advective flow problem essentially gives plausible times for the arrival of the chemical and its most concentrated form, without the benefits of diffusive processes, which will invariably “smear out” the concentration profile without a definable discontinuous “migrating front”. Fourth, as the spatial dimensions of the region of transport increases and as the time of the chemical dosing persists, the solution for, say, the spherical cavity problem will closely approximate the chemical transport pattern that could be applicable to a *cavity source of arbitrary shape*, the boundary of which is maintained at a constant, but time-variable concentration. Finally, analytical solutions, however elementary they may be, serve as all important benchmarks for the calibration of computational procedures that are increasingly being used, somewhat unhesitatingly, to model

practical engineering problems involving both linear and non-linear advective chemical transport in porous media. Although the analytical solutions presented in the paper are deceptively simple, they have associated with them solutions that display discontinuities. Furthermore these discontinuities are “propagating discontinuities” or from a mathematical perspective they are “shock structures” in the solution. These aspects are difficult to handle numerically, and the robustness of a computational scheme, in terms of the competing influences of accurate modelling of a discontinuous front, numerical damping and stability of time-integration schemes [19,29–31] can be adequately assessed through the use of analytical solutions of the type described in this paper. The methodologies presented in the paper can be further extended to include effects such as non-classical time variations in the boundary chemical concentration and time-dependency in both the hydraulic conductivity and the attenuation coefficient. Such extensions are left for further exercises.

## Acknowledgements

The work described in this paper was completed during the tenure of a *Killam Research Fellowship* awarded by the Canada Council for the Arts. The author gratefully acknowledges this support and wishes to thank the Alexander von Humboldt Foundation for the *Senior Researcher Award* and the Institut A fuer Mechanik, Universitaet Stuttgart, for the hospitality during the preparation of the paper. The author is grateful to the referees for their constructive and critical comments.

## References

- [1] Bear J. Dynamics of fluids in porous media. New York: Dover Publications; 1972.
- [2] Lapidus L, Pinder GF. Numerical solution of partial differential equations in engineering. New York: John Wiley; 1982.
- [3] Bear J, Veruijt A. Modeling of groundwater flow and pollution. Dordrecht, The Netherlands: D. Reidel Publ. Co; 1990.
- [4] Philips OM. Flow and reactions in permeable rocks. Cambridge: Cambridge University Press; 1991.
- [5] Bear J, Bachmat Y. Introduction to the modelling of transport phenomena in porous media. Dordrecht, The Netherlands: D. Reidel Publ. Co; 1992.
- [6] Shutie X, editor. Flow and transport in porous media. New York: World Scientific Publ. Co, 1992.
- [7] Chung TJ. Applied continuum mechanics. Cambridge: Cambridge University Press; 1993.
- [8] Banks RB. Growth and diffusion phenomena: mathematical frameworks and applications. Berlin: Springer-Verlag; 1994.
- [9] Vukovich M. Groundwater dynamics: steady flow. Littleton, Colorado: Water Resources Publications; 1997.
- [10] David I. Grundwasserhydraulik: Stromungs-und Transportvorgange, Friedr.. Weisbaden, Germany: Vieweg & Sohn; 1998.
- [11] Nield DA, Bejan A. Convection in porous media. Berlin: Springer-Verlag; 1999.
- [12] Zijl W, Nawalany M. Natural groundwater flow. Boca Raton: Lewis Publishers, CRC Press; 2000.

- [13] Bird RB, Stewart HE, Lightfoot EN. Heat, mass and momentum transfer. Englewood-Cliffs, New Jersey: Prentice-Hall; 1960.
- [14] Haight FA. Mathematical theory of traffic flow. New York: Academic Press; 1963.
- [15] Whitham GB. Linear and non-linear waves. New York: John Wiley; 1976.
- [16] Gill AE. Atmosphere-ocean dynamics, international geophysics Series Vol. 30. New York: Academic Press; 1982.
- [17] Carroll JE. Rate equations in semiconductor electronics. Cambridge: Cambridge University Press; 1985.
- [18] Edelstein-Keshet L. Mathematical models in biology, Birkhauser Mathematics Series. New York: Random House; 1988.
- [19] Segol G. Classic groundwater simulations: proving and improving numerical models. New Jersey: Prentice-Hall; 1994.
- [20] Sun N-Z. Mathematical modelling of groundwater pollution. Berlin: Springer-Verlag; 1996.
- [21] Selvadurai APS. Partial differential equations in mechanics: Vol. 1. Fundamentals, Laplace's equation, diffusion equation, wave equation. Berlin: Springer-Verlag; 2000.
- [22] Ayers Jr. F. Theory and problems of differential equations. New York: Schaum Publ. Co; 1952.
- [23] Hill JM. Differential equations and group methods for scientists and engineers. Boca Raton, Florida: CRC Press; 1992.
- [24] Erdelyi A, et al. Tables of integral transforms. Vols. 1 and 2. New York: McGraw-Hill; 1954.
- [25] Sneddon IN. The use of integral transforms. New York: McGraw-Hill; 1972.
- [26] Wolfram S. The mathematica book, 4th ed., Mathematica Version 4. Cambridge: Cambridge University Press; 1999.
- [27] Tsang C-F, editor, Coupled processes associated with nuclear waste repositories. New York: Academic Press, 1987.
- [28] Selvadurai APS. Partial differential equations in mechanics: Vol. 2. The biharmonic equation, Poisson's equation. Berlin: Springer-Verlag; 2000.
- [29] Cushman JH, editor, Dynamics of fluids in hierarchical porous media. New York: Academic Press, 1990.
- [30] Corapcioglu MY, editor, Advances in porous media, Vol. 2. Amsterdam, The Netherlands: Elsevier Scientific Publ. Co, 1994.
- [31] Hornung U, editor, Homogenization and porous media. Berlin: Springer-Verlag, 1997.