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An Analytical Solution for Contaminant Transport in Nonuniform Flow

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Abstract. We obtain an analytical solution for two-dimensional steady state mass transport in a trapezoidal embankment in a spatially varying velocity field through its replacement with a hydrologically equivalent rectangular embankment. Application of the Dupuit approximation and conform transformation allow for computation of the concentration field in the resulting rectangle in the complex potential plane. The latter allows deriving expression for the mass flow rate of contaminants, which is analogous to the Dupuit–Forchheimer discharge formula for volumetric water flow rate. Numerical simulation of advection-dispersion in the actual domain compares favorably with these analytical results, and provides limits of the ratio between transverse and longitudinal dispersivities within which the Dupuit approximation is applicable to mass transport problems.

Key words: hydrodynamic dispersion, nonuniform flow, analytical solution.

1. Introduction

'Cooling' or 'retention' ponds constructed for power and chemical plants, can cause environmental problems when polluted groundwater discharges through pond embankments into adjacent rivers and lakes. Solution of the convection-dispersion equation for contaminant transport through pond embankments is complicated by the presence of a free water-surface and the shape of the boundary. Although versatile, numerical approaches used to address this kind of problem have well-known drawbacks such as numerical dispersion (Bear and Verruijt, 1987, p. 323). Analytical solutions are helpful for rapid preliminary calculations, for verification of numerical results, and for understanding related physical phenomena.

For one-dimensional (1-D) problems, analytical solutions have been obtained for varying velocity and dispersivity functions. Among them are solutions to the convection-dispersion equation with: (i) velocity and dispersion coefficient varying in space by Serrano (1992); (ii) velocity varying as a function of cell concentration in an aquifer by Taylor and Jaffe (1991); and (iii) constant velocity but an exponential dispersivity function by Yates (1992). In some special cases, like three-dimensional (3-D) radial dispersion in a variable velocity flow field, it is possible

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to obtain an exact analytical solution by reducing the dimensionality of the problem (Yates, 1988). However, to obtain analytical solutions for multi-dimensional mass transport, the common approach is to assume an average velocity to represent the convection of the solute (see solutions to the 3-D problem by Ellsworth *et al*. (1993), Leij *et al*. (1991), and solutions to two-dimensional (2-D) problems by Latinopoulos *et al*. (1988), Cleary *et al*. (1978), Ogata (1976)).

A simplified analytical solution is derived here for the 2-D steady-state convection-dispersion equation with velocity and dispersion coefficient varying in space. To obtain this solution, which describes transport of a conservative contaminant in a homogeneous, isotropic, trapezoidal embankment, the Dupuit–Forchheimer approximation has been used. While the impact of, and limits for, this approximation are well-known when applied to hydraulic problems, it is not clear how the concentration field and integral characteristics of the mass transport are influenced by this approach. For example, the classical Dupuit–Forchheimer discharge formula is an *exact* expression (Bear, 1972, p. 367) even though it is obtained by neglecting the seepage face. Due to complexity of the convection-dispersion equation, the total mass flux through a domain of interest resulting from the Dupuit approximation cannot be compared readily with the actual flux. To address this problem, we compare our analytical solution with a numerical one obtained by using FREESURF 1 (Neuman and Witherspoon, 1970; Neuman, 1976) to calculate the real flow net and using the solute transport code ST1 (Istok, 1989) to calculate the actual concentration distribution and the total mass flux.

2. Statement of the Problem

Let us consider the transport of a conservative contaminant through a saturated, homogeneous, isotropic trapezoidal embankment (of height l_1 and upper width l_2) under steady-state flow with the free water-surface boundary AN (Figure 1a). The embankment rests on impermeable horizontal base FF'; the water levels are H $(H \leqslant l_1)$ and h_0 $(h_0 < H)$ in the upstream pond and downstream river, respectively; a is the initial pressure loss between the free surface in the pond and the embankment, and a_0 is the length of the seepage face.

The convection-dispersion differential equation governing 2-D steady-state transport of nonreactive dissolved contaminant in Cartesian coordinates has the following form (Bear, 1972, p. 617)

$$\nabla \cdot [\mathbf{D}(x,y)\nabla C(x,y)] - \mathbf{V}(x,y) \cdot \nabla C(x,y) = 0, \tag{1}$$

where $\nabla = (\partial/\partial x, \partial/\partial y)^T; C(x,y)$ is the concentration of a contaminant, (ML^{-2}); $\mathbf{V}(x,y)$ is the seepage velocity vector, equal to $(u(x,y), v(x,y))^T$, (LT^{-1}); and $\mathbf{D}(x,y)$ is the hydrodynamic dispersion coefficient, second-order tensor with four nonzero components $D_{ij}, (L^2T^{-1})$.

Additional assumptions are: (1) the contaminant concentration C_0 in the pond is constant; (2) the flow in the river is sufficient to carry away all of the seeping

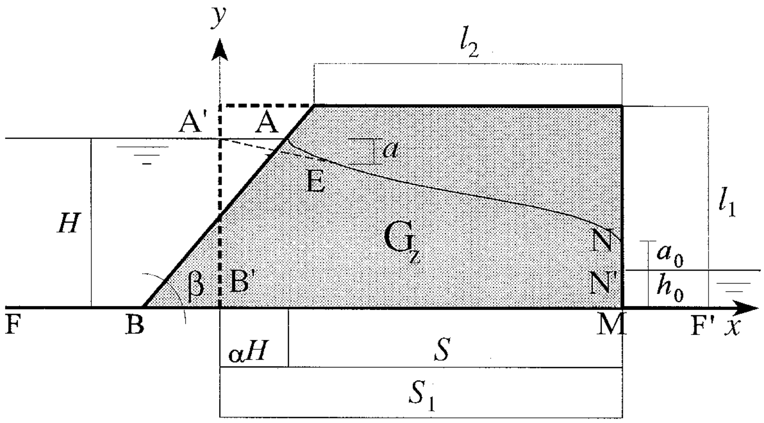

Figure 1(a). Domain geometry.

pollutant; (3) there is no mass flux through either the impermeable base of the embankment, BM, or the free surface, AN. These boundary conditions are stated as

$$C(x,y) = C_0 \text{ along } AB; \qquad C(x,y) = 0 \text{ along } N'M; \tag{2}$$

$$\frac{\partial C(x,y)}{\partial y} = 0 \text{ along } BM; \qquad \frac{\partial C(x,y)}{\partial \mathbf{n}} = 0 \text{ along } AN;$$

$$\frac{\partial C(x,y)}{\partial x} = 0 \text{ along } NN', \tag{3}$$

where $\mathbf{n}(x,y)$ is the outward unit normal vector of the free surface.

Under the stated boundary conditions, and particularly the last of (2), the total amount of contaminant $Q_c, (MT^{-1})$, passing through the lower slope of the embankment per unit time and width is defined by Fick's law as follows

$$Q_c = -\int_M^N D_L \frac{\partial C}{\partial x}\, \mathrm{d}y, \tag{4}$$

where D_L is the longitudinal dispersion coefficient.

The seepage velocity distribution $\mathbf{V}(x,y)$ in (1) is determined by solving Darcy's equation and continuity equation

$$\mathbf{V}(x,y) = -K\nabla h(x,y) = \nabla\varphi(x,y), \qquad \nabla\cdot\mathbf{V}(x,y) = 0, \tag{5}$$

where K is the constant hydraulic conductivity, (LT^{-1}); $h(x,y)$ is the hydraulic head, (L); and $\varphi(x,y) = -Kh(x,y)$ is the velocity potential function.

Equations (5) are subject to the following boundary conditions (Polubarinova–Kochina, 1962, p. 33)

$$\varphi = -KH \text{ along } AB, \qquad \varphi = -Kh_0 \text{ along } N'M, \tag{6}$$

$$\varphi(x, y) + Ky = \text{Constant}, \qquad \psi = Q \text{ along } AN, \tag{7}$$

$$\psi = 0 \text{ along } BM, \tag{8}$$

$$\varphi + Ky = \text{Constant along } NN', \tag{9}$$

where Q is the total water discharge per unit width through the embankment, (L^2T^{-1}); and $\psi(x, y)$ is the streamfunction related to φ by the Cauchy–Riemann equations.

3. Domain Transformation and Hydraulic Approach

Geometry of the domain $ABMN$ in a complex potential domain, $w = \varphi + i\psi$, makes it impossible to obtain the exact analytical solutions of (5)–(9) and (1)–(3). To overcome this difficulty, we, following Grishin (1982, p. 87), replace the upper wedge AB of our trapezoidal embankment by an equivalent (from the seepage viewpoint) rectangle with the width $AA' = \alpha H$ and the height H (Figure 1a). By equivalent rectangle, we imply a rectangle that creates the same pressure loss a at the point E as the original upper wedge. The constant α is defined by the following relationship

$$\alpha = \frac{m}{1 + 2m}, \tag{10}$$

where $m = \cot\beta$. The width of the equivalent rectangular embankment (dashed line in Figure 1a) is defined by $S_1 = S + \alpha H$ or

$$S_1 = S + \frac{Hm}{1 + 2m}. \tag{11}$$

Note that geometric parameters $(m, l_1, l_2$ and $S_1)$ and hydraulic parameters (H and S) are interrelated via formulae

$$S = l_2 + m(l_1 - H), \qquad S_1 = l_2 + ml_1 - \frac{2Hm^2}{1 + 2m}. \tag{12}$$

Flow in the transformed rectangular domain allows application of the Dupuit approximation (Bear, 1972, p. 366). This approximation, and the hydraulic approach, are applicable wherever the length, S_1, in the direction of flow is much larger (say $> 1.5 - 2$) than the thickness of saturated layer (*ibid.*, p. 365). The hydraulic approach amounts to neglecting the seepage face NN'. Then the flow

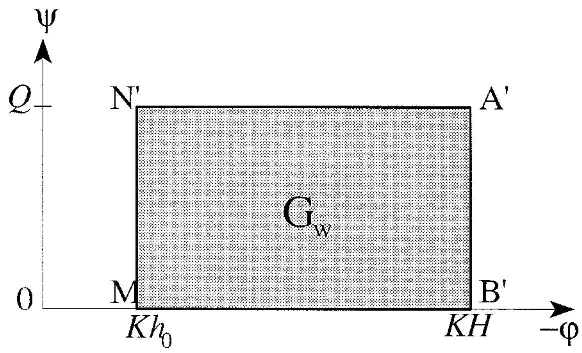

Figure 1(b). Complex potential domain.

region $G_z(B'A'N'M)$ corresponds to the rectangular G_w in the complex potential domain (Figure 1b) and (5)–(8) has the solution known as the Dupuit–Forchheimer discharge formula (*ibid.*, p. 366)

$$Q = \frac{K(H^2 - h_0^2)}{2S_1}; \qquad h^2(x) = -\frac{2Q}{K}x + H^2; \qquad V = Q/h, \tag{13}$$

where $V = \|\mathbf{V}\| = \sqrt{u^2 + v^2}$.

Written in the principal coordinates φ and ψ, the dispersion coefficient tensor **D** takes the form of a diagonal matrix whose main diagonal consists of longitudinal and transverse dispersion coefficients D_L and D_T, respectively. Then (1)–(3) can be rewritten for the complex potential domain as (Bear, 1972, p. 620)

$$\frac{\partial}{\partial\varphi}\left(D_L\frac{\partial C}{\partial\varphi}\right) + \frac{\partial}{\partial\psi}\left(D_T\frac{\partial C}{\partial\psi}\right) - \frac{\partial C}{\partial\varphi} = 0, \tag{14}$$

$$C(-KH, \psi) = C_0; \qquad C(-Kh_0, \psi) = 0, \tag{15}$$

$$\frac{\partial C}{\partial\psi}(\varphi, 0) = 0; \qquad \frac{\partial C}{\partial\psi}(\varphi, Q) = 0, \tag{16}$$

where D_L and D_T are defined as

$$D_L = D_m + \lambda_L V; \qquad D_T = D_m + \lambda_T V. \tag{17}$$

Here D_m is the coefficient of molecular diffusion, (L^2T^{-1}); and λ_L and λ_T are the longitudinal and transverse dispersivity constants, respectively, (L).

4. Analytical Solution

For the sake of simplicity let us assume molecular diffusion to be negligible compared to convective dispersion and, therefore, set $D_m = 0$ in (17). Substituting the expression for V from (13) into (14) yields

$$\lambda_L \frac{Q}{K^2} \frac{\partial}{\partial h} \left(\frac{1}{h} \frac{\partial C}{\partial h} \right) + \lambda_T \frac{Q}{h} \frac{\partial^2 C}{\partial \psi^2} + \frac{1}{K} \frac{\partial C}{\partial h} = 0. \tag{18}$$

The form of the Equation (18) and the boundary conditions (16) indicate that the solution to the Equation (18) subject to the boundary conditions (15) and (16) depends on ψ only as a parameter and, therefore, $\partial C/\partial \psi = 0$ over the whole region G_w. Then, change of the variable $z = h^2$ such that

$$\frac{\partial C}{\partial h} = \frac{\partial C}{\partial z} \frac{\partial z}{\partial h} = 2h \frac{\partial C}{\partial z}, \tag{19}$$

transforms (18) into an ordinary differential equation

$$\frac{\mathrm{d}^2 C}{\mathrm{d}z^2} + \frac{K}{2Q\lambda_L} \frac{\mathrm{d}C}{\mathrm{d}z} = 0, \tag{20}$$

subject to the boundary conditions

$$C/C_0 = 1, \quad z = H^2; \qquad C/C_0 = 0, \quad z = h_0^2. \tag{21}$$

The solution to the problem (20)–(21) is given by (Nikolaevskij, 1990, p. 438)

$$\frac{C}{C_0} = \frac{\exp\left(-\frac{Kh^2}{2Q\lambda_L}\right) - \exp\left(-\frac{Kh_0^2}{2Q\lambda_L}\right)}{\exp\left(-\frac{KH^2}{2Q\lambda_L}\right) - \exp\left(-\frac{Kh_o^2}{2Q\lambda_L}\right)}, \tag{22}$$

and describes 1-D distribution of a conservative contaminant as a function of piezometric head h in the domain transformed by the Dupuit approximation.

As noted by Bear (1972, p. 366), ‘the discrepancy between the flow curves predicted by the exact theory of the phreatic surface boundary and by the Dupuit approximation is negligible except in the vicinity of the outflow boundary’. The same must hold for the concentration curves.

For most practical purposes, a detailed analysis of the concentration field is not always required and it may be enough to evaluate only major integral characteristics such as the total flux of contaminant through the embankment. It follows from (4) that the amount of contaminant seeping per unit time and width into the downstream reservoir can be calculated as

$$\begin{aligned} Q_c &= -\int_0^Q D_L \frac{\partial C(\varphi = -Kh_0, \psi)}{\partial \varphi} \, \mathrm{d}\psi \\ &= -Q\lambda_L V \frac{\partial C(\varphi = -Kh_0, \psi)}{\partial \varphi}. \end{aligned} \tag{23}$$

Substitution of (22) into (23) yields

$$Q_c = C_0 V h_0 \left[1 - \exp\left(-K \frac{H^2 - h_0^2}{2Q\lambda_L} \right) \right]^{-1}, \tag{24}$$

or, taking into account (13)

$$Q_c = \frac{K(H^2 - h_0^2)C_0}{2S_1(1 - \mathrm{e}^{-S_1/\lambda_L})} = \frac{C_0 Q}{1 - \mathrm{e}^{-S_1/\lambda_L}}. \tag{25}$$

Expression (25) relates the total flux of contaminant with the total water flux through an embankment. In particular, for purely advective transport $(\lambda_L = 0)$ it leads to the well-known result $Q_c = C_0 Q$. Impact of the dispersion phenomena is manifested through the exponential term in (25). It follows from (25) that dispersion $(\lambda_L > 0)$ enhances transport process, i.e. it increases the contaminant flux. In many practical situation, this impact may be negligibly small considering the magnitude of the ratio S_1/λ_L. Rewriting (25) in terms of the dimensionless quantities

$$H^* = \frac{H}{S}; \qquad h_0^* = \frac{h_0}{S}; \qquad \lambda_L^* = \frac{\lambda_L}{S}; \qquad Q_c^* = \frac{Q_c}{C_0 K S}, \tag{26}$$

yields, considering (11)

$$Q_c^* = \frac{(H^{*2} - h_0^{*2})}{2\left(1 + \frac{H^* m}{1+2m}\right)} \left[1 - \exp\left(-\frac{1 + \frac{H^* m}{1+2m}}{\lambda_L^*}\right)\right]^{-1}. \tag{27}$$

Figures 2(a) and 2(b) show how dimensionless contaminant flux Q_c^* through rectangle $(m = 0)$, and trapezoid $(m = 1)$, vary with dimensionless water level in the upstream pond H^*, for $h_0^* = 0$, and $\lambda_L^* = 0.0, 0.1, 0.3, 0.5$. It can be seen that, when dimensionless longitudinal dispersivity $\lambda_L^* \leqslant 0.1$, total dimensionless contaminant flux Q_c^* can be modeled by pure advection only. For larger λ_L^*, dispersion manifests itself by increasing Q_c^*. Comparing Figures 2(a) and 2(b) shows that dispersion is more significant in rectangular embankment than in trapezoidal embankment.

Another feature of the solution (27) is that the Dupuit approximation, when applied to the given mass transport problem, eliminates the dependance of total mass flux (and concentration distribution field) on the transverse component of dispersion. That is, however, due to particularly specified boundary conditions and does not necessarily hold true for other situations.

5. Numerical Simulations

Variable substitution which we used to derive the analytical solution reduces partial differential Equation (18) into ordinary differential Equation (20). It should enable one to look at stability of the idealized solution and the impact of numerical dispersion and grid orientation on the numerical approximation by employing the analysis of Fanchi (1983). While recognizing the importance of such analysis, we

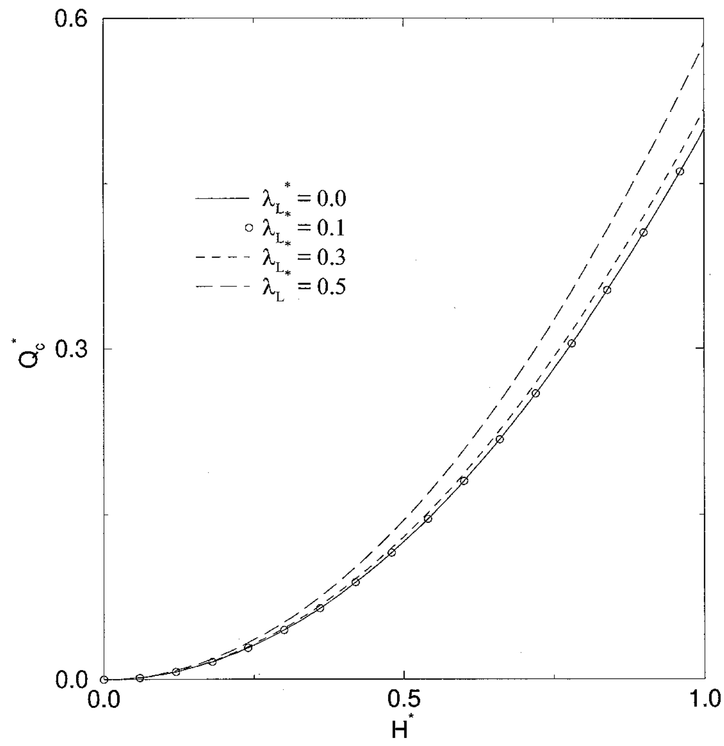

Figure 2(a). Dimensionless contaminant flux, Q_c^*, through rectangular embankment $(m = 0)$ as a function of dimensionless upstream head, H^*, for $h_0^* = 0$ and different values of λ_L^*.

leave it out of the scope of the present investigation. Instead, we concentrate on analyzing the simplifying assumptions which lead to our solution: (i) applying the hydraulic approach (neglecting the seepage face); and (ii) replacing the real trapezoidal domain with hydraulically equivalent rectangle.

Answers to these questions provide limits of applicability of our solution in terms of mass flux, *i.e.* limits of the hydraulic gradient and/or ratio λ_T/λ_L within which the Dupuit approximation is applicable to mass transport phenomena. To obtain these answers, we solve numerically 2-D convection-dispersion equation in the original domain, considering, when not negligible, the presence of a seepage face.

The code FREESURF I (Neuman and Witherspoon, 1970; Neuman, 1976) is used to solve the flow problem. FREESURF I is designed to solve problems of steady seepage in the presence of free surfaces through discretization of the domain in movable, linear quadrilateral finite elements. Here, it is used to construct the flow net and to calculate water fluxes in each element. In all simulation runs, the grid was made progressively finer until no difference in downstream seepage face was observed.

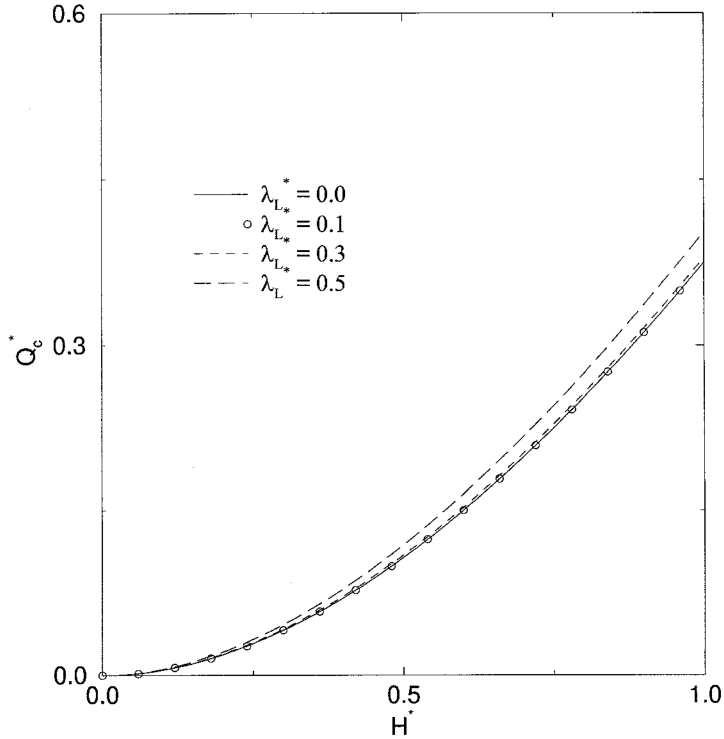

Figure 2(b). Dimensionless contaminant flux, Q_c^*, through trapezoidal embankment $(m = 1)$ as a function of dimensionless upstream head, H^*, for $h_0^* = 0$ and different values of λ_L^*.

The flow results are subsequently used as an input file to the finite element transport code ST1 (Istok, 1989, p. 283) to evaluate the actual concentration field and the total mass flux. ST1 offers a choice of element types; we adopt the linear, quadrilateral ones. The code is allowed to run until steady-state conditions are attained. A no-flow boundary condition, $\partial c/\partial x = 0$, is assumed along the seepage face; in all cases, an upstream constant concentration $c_0 = 1\,\mathrm{kg/m^3}$ is assumed.

We perform several numerical experiments in order to isolate the impact of each of the approximations mentioned above. In our first set of simulations, we consider a rectangular domain $(l_1 = 4$ m$, l_2 = 6$ m$, m = 0)$, thereby eliminating the need for constructing the equivalent rectangle. Repeated runs of FREESURF I allow us to determine the parameters for which the downstream seepage face was practically negligible. The latter case corresponds, for example, to water levels $H = 2$ m$, h_0 = 1$ m, implying an average hydraulic gradient equal to 0.1667. Such a choice of parameters eliminates the potential impact of the seepage face on transport, allowing us to isolate the effect of transverse dispersivity. Figure 3(a) shows how dimensionless contaminant flux Q_c^* varies with dimensionless longitudinal dispersivity λ_L^*, for $H^* = 0.5, h_0^* = 0.25$, and $m = 0$. It can be seen from

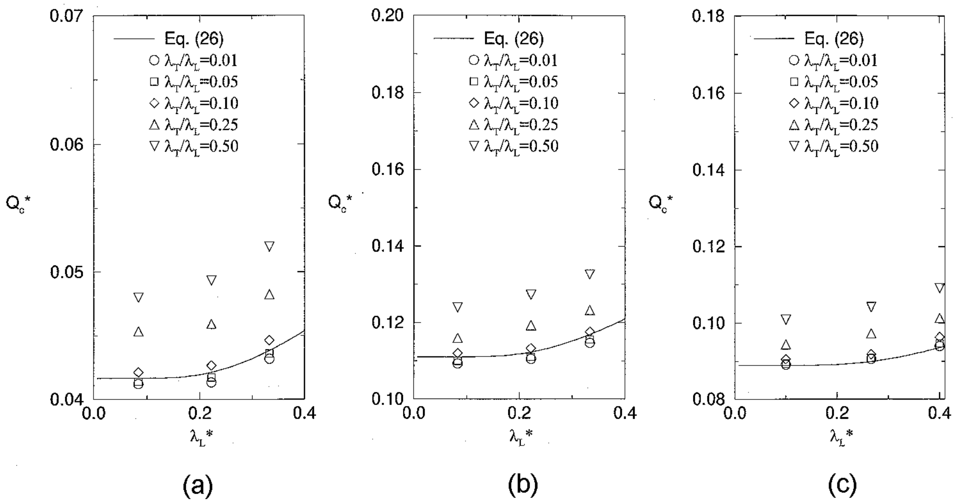

Figure 3. Dimensionless contaminant flux from numerical simulations for (a) rectangular domain without seepage face $(H^* = 0.5, h_0^* = 0.25, m = 0)$.

Figure 3(a) that when $\lambda_T/\lambda_L \leqslant 0.1$, the analytical solution is in good agreement with numerical results; for greater values of λ_T/λ_L, the analytical solution introduces a slight underestimation of mass flux.

In a second set of simulations, we allow for the presence of a visible seepage face, by setting, for the same domain, $H = 3\,\text{m}, h_0 = 1\,\text{m}$ (i.e., an average hydraulic gradient of 0.3333). Under these conditions, FREESURF I yields a seepage face with $a_0 = 0.20$ m (Figure 1(a)). Running a second set of transport simulations for different values of longitudinal and transverse dispersivity produces the results illustrated in Figure 3(b). Comparison with Figure 3(a) shows that considering or neglecting the seepage face has no significant impact on results for contaminant flux; the effect of an increasing transverse dispersivity is still evident, as in the previous case.

In a third set of simulations, we consider a trapezoidal domain with $l_1 = 4\,\text{m}, l_2 = 4\,\text{m}, m = 1\ (\beta = 45°)$, and boundary conditions identical to the previous set of simulations $(H = 3\,\text{m}, h_0 = 1\,\text{m})$. In this case, FREESURF I yields a seepage face with $a_0 = 0.12$ m (Figure 1(a)). These geometric parameters give, by means of (12), $S_1 = 6$ m. Thus the equivalent rectangle for this trapezoidal domain is identical to the rectangle considered in the first two sets of simulations, allowing a meaningful comparison between them. Results of the transport simulations in terms of contaminant flux are shown in Figure 3(c). They are slightly larger than their counterparts in the second set of simulations, indicating that the influence of the trapezoidal shape is not entirely negligible in this case. This effect, however, is due to the particular choice of values for the geometric parameters in this case, i.e., $l_2 = l_1$. In a more elongated domain with $l_2 = 2l_1$ or larger, the influence of the tranformation from trapezoidal shape to rectangular is negligible.

We conclude this section with a brief discussion on the accuracy of numerical simulations. It is well known that numerical solutions of the advection-dispersion equation are affected by numerical dispersion: for the one-dimensional problem, the ST1 transport code adopted by us compares favorably with an analytical solution (Istok, 1989, p. 292). Accuracy analysis in multi-dimensional problems is less standard since multi-dimensional numerical dispersion can also induce grid orientation errors, as shown by Fanchi (1983) for various finite difference techniques. Fanchi presents explicit expressions for the components of the numerical dispersion tensor, as growing functions of the magnitude of velocity components, time step and, for some solution techniques, grid size. Likewise, his analysis shows how the rotation of the principal flow axes induced by multi-dimensional numerical dispersion depends crucially on discretization in time. In general, both effects can be minimized by suitably reducing the time step.

We followed this criterion in designing and conducting our numerical simulations, although no exact counterpart to Fanchi's results is available for finite element schemes. Furthermore, the grid Péclet number was kept smaller than two in both directions for all simulations and elements, thereby extending the well-known one-dimensional constraint (Fletcher, 1988). Results of a mass balance calculation for different simulation domains indicated a maximum mass balance error inferior to 2 percent.

6. Conclusions

We consider 2-D steady-state contaminant transport in a variable velocity field. The latter and presence of a free surface greatly complicate a solution to the problem, as well as numerical simulations. We use a domain transformation and the hydraulic approach, to derive a compact, closed form expression relating mass flux of contaminant with the total water flux and the dispersive properties of media. Numerical simulations performed allow us to establish criteria for validity of this expression. The magnitude of the transverse dispersivity has the greatest impact on results: the ratio of transverse to longitudinal dispersivity has to be less than or equal to 0.1 for the numerical results to reliably reproduce the analytical solution. For larger ratios, our expression moderately underestimates the mass flux. The latter constraint is somewhat analogous to the condition of applicability of the Dupuit–Forchheimer theory to flow problems, i.e., $j^2 \ll 1$, where j is the slope of the phreatic surface in isotropic porous media (Bear, 1972, p. 363). For the transport problem, on the contrary, the presence of the seepage face has little impact on the value of resulting contaminant flux; the effect of an increasing transverse dispersivity is still evident, as in the previous case. For a trapezoidal embankment, the impact of the domain tranformation to an equivalent rectangle is visible only when the ratio between the longitudinal dimension and the transversal one is close to one. In this case, our analytical formula slightly underestimates the contaminant flux. For larger values of this ratio, the approximation introduced by the domain transformation is negligible.

Finally, we note that, although our solution was derived to describe the mass transport through an embankment, it is clearly applicable to a transport phenomena in any domain bounded by a pair of streamlines and a couple of equipotentials, e.g. contaminant transport between two wells, as modeled by Fry *et al*. (1993).

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