EXPLICIT FINITE DIFFERENCE SOLUTION FOR CONTAMINANT TRANSPORT PROBLEMS WITH CONSTANT AND OSCILLATING BOUNDARY CONDITIONS

by

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For constant and oscillating boundary conditions, the 1-D advection-diffusion equation with constant coefficients, which describes a contaminant flow, is solved by the explicit finite difference method in a semi-infinite medium. It is shown how far the periodicity of the oscillating boundary carries on until diminishing to below appreciable levels a specified distance away, which depends on the oscillation characteristics of the source. Results are tested against an analytical solution reported for a special case. The explicit finite difference method is shown to be effective for solving the advection-diffusion equation with constant coefficients in semi-infinite media with constant and oscillating boundary conditions.

Key words: *advection-diffusion equation, contaminant flow, finite difference method, oscillating boundary conditions*

Introduction

Water-pollution can often be regarded as a hydraulic mixing process with attenuating pollutant concentrations along the downstream transport of the waste. Such concentrations, in space and time, are described by the advection-diffusion equation: a PDE of the parabolic-type that was derived from the Fick's diffusion laws and mass conservation principle. The advection-diffusion equation could be used, for example, to assess concentration of toxic pollutants downstream of mining operations and plan the remedial management of the aquatic flora and fauna [1]. The same advection-diffusion equation can similarly describe transport phenomena in a variety of other disciplines such as chemical and petroleum engineering, biophysics, or soil-physics [1].

Various numerical and analytical methods are used for solving advection-diffusion equation, such as finite difference methods (FDM), finite element methods (FEM), and finite volume methods (FVM) – naturally, all three discretize governing equations and initial and boundary conditions. Even in 1-D, this equation has been solved only for cases with special initial and boundary conditions [1-6]. These are unlikely to match most engineering problems in practice [7-10]. While the numerical methods employ various discretization schemes [11-14], it is generally accepted that FEM may be better suited for complex 3-D geometries whereas 1-D problems are more easily solved by FDM.

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Time varying boundary concentrations are clearly of interest for realistic applications [15]. For example, the intensity of the pollution source (at $x = 0$) may be a periodic function of time. An analytical solution of the advection-diffusion eq. (2) does not exist for such pulsating pollution sources, necessitating a numerical solution. In this paper, the 1-D advection-diffusion equation with constant coefficients is solved by the explicit FDM (EFDM). The solution is given for the solute transport in a semi-infinite medium that is solute free initially and with: constant boundary conditions and oscillating (periodic in time) concentration at one of the two boundaries. To the best of authors knowledge for the first time, we propose in this paper an effective, accurate and most simple explicit finite difference scheme for solving advection-diffusion equation for a contaminant transport with oscillating concentration at one of the two boundaries.

The governing equation

For the downstream transport of the solute particles in the longitudinal direction x ($0 \le x < \infty$), the governing advection-diffusion partial differential equation is 1-D [16]:

$$\frac{\partial C(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[D(x,t)\frac{\partial C(x,t)}{\partial x} - u(x,t)C(x,t) \right] \tag{1}$$

In eq. (1), the solute concentration is denoted by $C(x,t)$. It is a function of time, t, and position x along the longitudinal direction of dispersion. Mathematically, the PDE (1) has dual nature: hyperbolic for advection-dominated problems and parabolic for dispersion dominated ones. For the latter, the constant D represents a dispersion coefficient; a fixed u indicates that the flow velocity is uniform.

For constant D and u, eq. (1) reduces to:

$$\frac{\partial C(x,t)}{\partial t} = D\frac{\partial C^2(x,t)}{\partial x^2} - u\frac{\partial C(x,t)}{\partial x} \tag{2}$$

The domain is semi-infinite and solute free initially, meaning that the initial condition is:

$$C(x,t) = 0 \;\; x \ge 0, \quad t = 0 \tag{3}$$

Two kinds of boundary conditions are analyzed: constant and periodically fluctuating. For the former case (constant boundary condition), it is:

$$C(x,t) = C_0, \quad x = 0, \quad t \ge 0 \tag{4}$$

$$C(x,t) = 0, \quad x \to \infty, \quad t \ge 0 \tag{5}$$

Equation (2) has been solved analytically for such constant boundary conditions [17]:

$$C(x,t) = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{x-ut}{2\sqrt{Dt}} \right) + \exp\left(\frac{ux}{D} \right)\operatorname{erfc}\left(\frac{x+ut}{2\sqrt{Dt}} \right) \right] \tag{6}$$

In the case of a periodic fluctuation of concentration at the boundary $x = 0$, the expression (4) can take the following form:

$$C(x,t) = C_0[1 + \varepsilon \sin(\omega t)], \quad x = 0, \quad t \ge 0 \tag{7}$$

where ε is the magnitude and ω is the frequency of the concentration oscillations. The boundary condition at $x \to \infty$ remains the same as in eq. (5). For such oscillatory boundary condition (7) (with $\varepsilon \neq 0$), the advection-diffusion eq. (2) must be solved numerically because an analytical solution has not been reported.

Numerical method

Analytical solutions of advection-diffusion equations have been reported for specific initial and boundary conditions. This restriction, compounded with their complexity, limits their applicability. Numerical methods, on the other hand, are generally applicable with arbitrary initial and boundary conditions [18-20]. In the 1970's and 1980's, implicit FDM (IFDM) were generally preferred over explicit ones (EFDM). This trend has been changing with the advancement of computers, shifting the emphasis to EFDM. Being often unconditionally stable, the IFDM allows larger step lengths. Nevertheless, this does not translate into IFDM's higher computational efficiency because extremely large matrices must be manipulated at each calculation step. We find that the EFDM is also simpler in addition to being computationally more efficient [19, 21].

For $\varepsilon = 0$ in eq. (7), the analytical solution of the advection-diffusion eq. (2) is given in eq. (6). In the case of $\varepsilon \neq 0$, the analytical solution of the advection-diffusion eq. (2) is not known. In order to test our numerical method (EFDM), we first solve the advection-diffusion eq. (2) with constant boundary conditions (4) and (5). The central difference scheme is used to represent the term $[\partial^2 C(x,t)/\partial x^2]$ and $[\partial C(x,t)/\partial x]$ and a forward difference scheme for the derivative term $[\partial C(x,t)/\partial t]$ [21]. With these substitutions, eq. (2) transforms into:

$$C_{i,j+1} = \left(\frac{D\Delta t}{\Delta x^2} + \frac{u\Delta t}{2\Delta x}\right) C_{i-1,j} + \left(1 - 2\frac{D\Delta t}{\Delta x^2}\right) C_{i,j} + \left(\frac{D\Delta t}{\Delta x^2} - \frac{u\Delta t}{2\Delta x}\right) C_{i+1,j} \tag{8}$$

where $C_{i,j} \equiv C(x_i, t_j)$, indexes i and j refer to the discrete step lengths Δx and Δt for the co-ordinate x and time t, respectively, such that $x_i = i\Delta x$ and $t_j = j\Delta t$. Equation (8) represents a formula for $C_{i,j+1}$ at the $(i, j + 1)^{\text{th}}$ mesh point in terms of known values along the j^{th} time row. The truncation error for the difference eq. (5) is $O(\Delta t,\ \Delta x^2)$. Using a small-enough value of Δt and Δx, the truncation error can be reduced until the accuracy achieved is within the error tolerance [21].

The initial condition (3) for eq. (2) can be expressed in the finite difference form:

$$C_{i,0} = 0, \quad x \geq 0, \quad t = 0 \tag{9}$$

Boundary conditions (4) and (5), rewritten in the finite difference form:

$$C_{0,j} = C_0, \quad x = 0, \quad t \geq 0 \tag{10}$$

$$C_{N,j} = 0, \ x \to x_\infty, \quad t \geq 0 \tag{11}$$

where $N = x_\infty/\Delta x$ is the grid dimension in the x direction and x_∞ is the distance in the direction x at which $\partial C(x,t) = 0$, x_∞ replaces $x \to \infty$ in eq. (6). In the case of periodic boundary condition (7), it can be rewritten in the finite difference form:

$$C_{0,j} = C_0[1 + \varepsilon \sin(\omega t_j)], \quad x = 0, \quad t \geq 0 \tag{12}$$

In this manner, solute concentration can be determined at different times. A typical solution run takes up to 7 seconds on the Intel (R) Core (TM) i3 CPU 540 at 3.07 GHz personal computer for the longest time analyzed (50 day).

Results

Figures 1-3 show EFDM solutions of the advection-diffusion eq. (2) with constant boundary condition (4) at $x = 0$. The flow velocity used is $u = 1$ m per day and the dimensionless source concentration was $C_0 = 10$. Solute transport problems for $D = 0.1$, 2.5 and 10 m^2 per day were considered [17]. In the case of constant boundary condition (5), the concentrations at time t equal to 5, 10, 20, 30, 40, and 50 days are computed by EFDM and analytically (6). The EFDM numerical results shown in figs. 1-3 agree well with the analytical solutions, both for the advection-dominated cases, figs. 1 and 2, and the high-dispersion case, fig. 3.

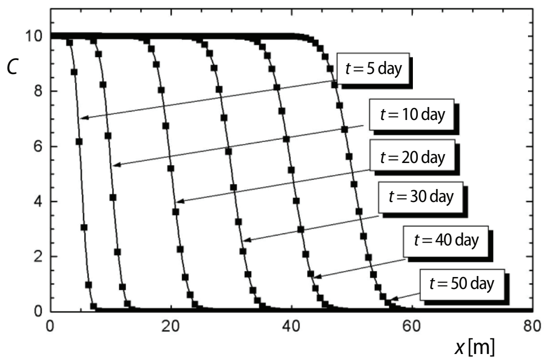

Figure 1. Numerically calculated concentration distributions at different times (solid lines) for $D = 0.1$ m^2/day and $u = 1$ m/day shown in comparison to analytical results (solid squares)

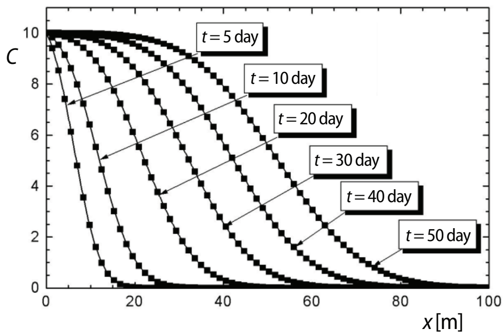

Figure 2. Numerically calculated concentration distributions at different times (solid lines) for $D = 2.5$ m^2/day, $u = 1$ m/day shown in comparison to analytical results (solid squares)

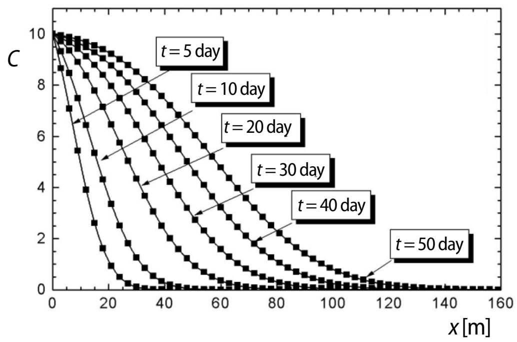

Figure 3. Numerically calculated concentration distributions at different times (solid lines) for $D = 10$ m^2/day, $u = 1$ m/day shown in comparison to analytical results (solid squares)

The concentration values are shown in these figures as functions of the longitudinal direction x at different times. We used $x_\infty = 200$ m in eq. (6) (for both cases) to represent the distance wherefrom there is no further change in the concentration $C(x,t)$. Larger values for x_∞ do not affect the solution appreciably while unnecessarily enlarging the size of the grid and increasing the computation time. Since the stability conditions of the finite difference scheme (8) are $0 \leq D\Delta t/\Delta x^2 \leq \leq 0.5$ and $0 \leq u\Delta t/\Delta x \leq 2(1 - D\Delta t/\Delta x^2)$, the step lengths were $\Delta x = 0.1$ m and $\Delta t = 0.001$ day for $D = 0.1$, 2.5 m^2 per day, and $\Delta x = = 0.1$ m and $\Delta t = 0.0005$ day for $D = 10$ m^2 per day. The analytical solution (6) of the advection-diffusion eq. (2) is represented by filled squares in figs. 1-3. As the dispersion coefficient increases from 0.1 in fig. 1 to 2.5 in fig. 2, and 10 in fig. 3 m^2 per day, the solute distribution narrows among these figures and tails-off at greater distance along the x-axis for the dispersion dominated case in fig. 3 relative to the advection dominated processes in figs. 1 and 2.

While the numerical and analytical results match closely, a measure of this match is evaluated by the mean square error defined as:

$$\text{error} = \frac{1}{N}\sum_{i=1}^{N}\left(C_i^{\text{num}} - C^{\text{analyt}}\right)^2 \tag{13}$$

where N is the total number of observation points. Errors in solute concentration shown in fig. 3 (for D = 10 m^2 per day and u = 1 m/s) and calculated by (13) are given in tab. 1 at t = 10 to 50 days (the longest time analyzed). The error values increase with time, so the maximum deviation between the results obtained between analytical and numerical solutions over a 50-day period is ≈ 0.002%.

For the periodic boundary condition (7), solute transport problems for D = 10 m^2 per day is considered for two oscillation amplitudes ε = 0.15 and 0.5 and frequency $\omega = \pi/2$. Figures 4 and 5 show concentrations at time t equal to 5, 10, 20, 30, 40, and 50 days, computed by EFDM for ε = 0.15 and 0.50, respectively. Figure 6 shows concentration at distance x equal to 1, 10, and 15 m for ε = 0.15 and fig. 7 shows concentration at distance x equal to 1, 10, and 20 m for ε = 0.50. The solute concentration near the boundary x = 0 (small x) is clearly affected by the periodicity of the

Table 1. Errors in solute concentration shown in fig. 3 at *t* = 10 to *t* = 50 days (the longest time analyzed)

t [day]	*error*
1	0.00000012
5	0.00000067
10	0.00000257
20	0.00000559
30	0.00000775
40	0.00000909
50	0.00002041
60	0.00003055
70	0.00004045

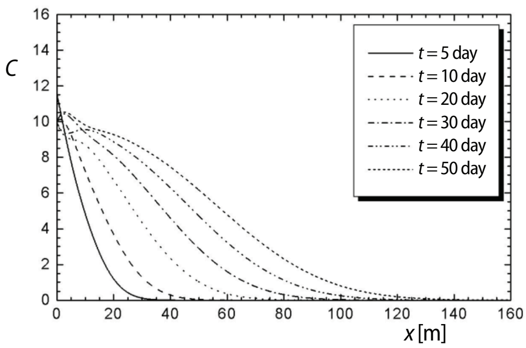

Figure 4. Numerically calculated concentration distributions at different times for *D* = 10 m^2/day, *u* = 1 m/day, ε = 0.15 and $\omega = \pi/2$

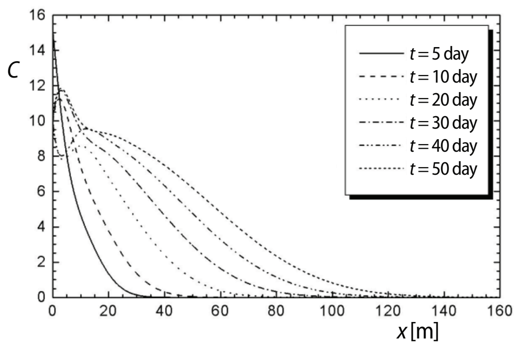

Figure 5. Numerically calculated concentration distributions at different times for *D* = 10 m^2/day, *u* = 1 m/day, ε = 0.5 and $\omega = \pi/2$

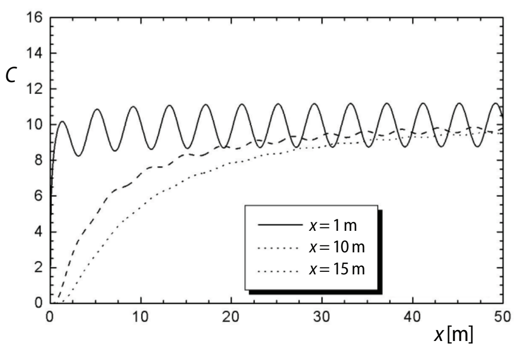

Figure 6. Numerically calculated concentration distributions at different positions for *D* = 10 m^2/day, *u* = 1 m/day, ε = 0.15 and $\omega = \pi/2$

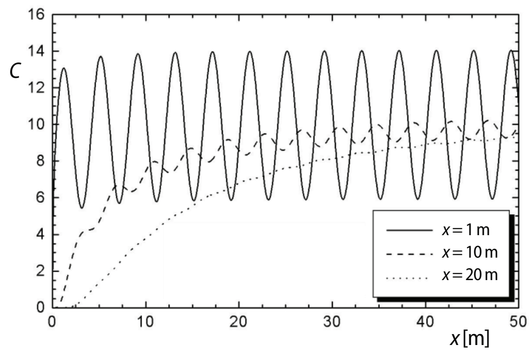

Figure 7. Numerically calculated concentration distributions at different positions for *D* = 10 m^2/day, *u* = 1 m/day, ε = 0.5 and $\omega = \pi/2$

forcing function (12). Such periodicity diminishes with distance away from the $x = 0$ boundary and is practically unnoticeable at $x = 15$ m for the case shown in fig. 6 or at 20 m for the case shown in fig. 7. The distance range within which the oscillating boundary effects the time-evolution of the solute concentration is assessable in figs. 4 and 5. The effect is more pronounced for larger oscillation amplitudes when these oscillations at boundary $x = 0$ are detectable at greater distances.

Conclusion

We report on the finite difference solution of the 1-D advection-diffusion equation with constant coefficients in semi-infinite media for solute transport with constant and periodic boundary conditions. High accuracy of the method is apparent from the comparison of numerical results with those obtained with analytical solutions that are available for special cases. Furthermore, the EFDM presented in this work for solving advection-diffusion equation is the simplest among other commonly used numerical methods. It is shown that, for given oscillation frequency, the periodically oscillating boundary concentration (at $x = 0$) significantly influences the time-evolution of the concentration distribution near this boundary. This influence is more pronounced for larger amplitude of the oscillating boundary concentration. We have shown that explicit finite difference method is effective and accurate for solving 1-D advection-diffusion equation with constant coefficients in semi-infinite media, which is especially important when arbitrary initial and boundary conditions are required. Similarly, in our previous work, we have also shown that explicit finite difference method is effective and accurate for solving two-dimensional solute transport problems [22].

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