ELSEVIER Applied Mathematics and Computation 96 (1998) 89–100

APPLIED MATHEMATICS AND COMPUTATION

Modeling contaminant transport in groundwater: an optimized finite element method

Md. Akram Hossain [a,1], David R. Yonge [b,2]

[a] *Civil and Environmental Engineering, Washington State University – Tricities, 100 Sprout Road, Richland, WA 99352, USA*

[b] *Civil and Environmental Engineering, Washington State University, Pullman, WA 99164, USA*

Abstract

An optimized upwind Taylor–Galerkin finite element method (UTGFEM) has been developed to simulate one-dimensional contaminant transport in groundwater. The model was employed to predict the transport of contaminants from continuous, pulse, and exponentially decaying sources for a wide range of dispersion coefficients and degradation rate constants. The dispersion coefficients considered were 0.0, 1.0, and 5.0 m^2/day. The degradation rate constant was varied between 0.007 and 0.028 $(day)^{-1}$. The model was found to predict the transport dynamics for all these conditions accurately when the dispersion coefficient was greater than or equal to 0.215 m^2/day. The model would introduce some numerical dispersion if the field dispersion were smaller than this limiting value. The need for numerical dispersion can be reduced significantly by making the length of the finite elements smaller.

Keywords: Taylor-Galerkin finite element method; Groundwater transport

1. Introduction

Finite element methods (FEMs) that utilize piecewise linear basis functions (PLBFs) have been a topic of extensive research in modeling contaminant

[1] E-mail: ahossain@beta.tricity.wsu.edu.

[2] E-mail: yonge@wsu.edu.

0096-3003/98/$ – see front matter
PII: S0096-3003(97)10128-X

transport in groundwater. Consequently, a great deal of literature is available [1–5]. The FEMs can minimize solution error in a mathematically sound way and incorporate complex boundary conditions with relative ease. Additionally, the FEMs have been reported to introduce smaller numerical dispersion than finite differences [6].

Several FEMs are reported in the literature to provide stable and convergent results. However, the Galerkin FEM that utilizes asymmetric weight functions, referred to as Petrov–Galerkin FEM (PGFEM), has been reported to be the most stable one in modeling advective–dispersive transport [1,6–8]. A semi-implicit FEM based on Taylor series is also reported to be accurate for simulating advective–dispersive transport [3,9]. This method will be referred to as Taylor–Galerkin FEM (TGFEM). Hossain and Yonge [10] have shown that both TGFEM and PGFEM remain stable over a wide range of Peclet numbers from zero to infinity. However, the TGFEM was found to better predict the one-dimensional transport of contaminants with smaller numerical dispersions but with some oscillations. The PGFEM, on the other hand, provided oscillation free predictions at the expense of introducing significant numerical dispersions. Introduction of numerical dispersions results in artificially faster movement of the contaminant and underestimation of the peak concentration for pulse sources, which is undesirable because in real world application it will lead to misleading conclusions. It is, therefore, imperative to develop a model which will minimize the numerical dispersion and will accurately predict contaminant transport in groundwater.

The TGFEM, as mentioned, was found to relatively accurately predict transport of contaminants for a variety of field conditions [10]. The TGFEM predictions were, however, oscillatory. The oscillation can be avoided by introducing upwinding [6]. The objective of this paper was to develop an upwind TGFEM (UTGFEM) utilizing PLBFs and optimize the degree of upwinding so that it provides oscillation free accurate results for a wide range of field conditions with regard to dispersion and source definition.

2. Model equation

The differential equation describing one-dimensional transport of contaminants in a homogeneous and isotropic aquifer with uniform flow field can be written as follows:

$$\frac{\partial C}{\partial t} = -\frac{u}{R_d}\frac{\partial C}{\partial x} + \frac{D_L}{R_d}\frac{\partial^2 C}{\partial x^2} - \lambda C, \tag{1}$$

where C is the contaminant concentration in the groundwater (M/L^3), t the time (T), u the velocity of flow (L/T), x the distance in the direction of flow

(L), D_L the dispersion coefficient (L^2/T), R_d the retardation coefficient, and λ a decay constant (1/T). If u/R_d is replaced by v and (D_L/R_d) by D then Eq. (1) can be written as follows:

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial x} + D\frac{\partial^2 C}{\partial x^2} - \lambda C. \tag{2}$$

Eq. (2) may be solved for the following boundary and initial conditions:

$$@\ t \geqslant 0, \quad x = 0, \quad C = C_0(t), \tag{3}$$

$$@\ t \geqslant 0, \quad x = L, \quad \frac{\partial C}{\partial x} = 0, \tag{4}$$

$$@\ t = 0, \quad 0 \leqslant x \leqslant L, \quad C = C(x), \tag{5}$$

where $C_0(t)$ is the source concentration (M/L^3) as a function of time, L the length of the modeled domain (L), and $C(x)$ the spatially varying initial condition (M/L^3).

3. Taylor–Galerkin formulation

The TGFEM proposed by Donea [3] and later applied to advection dominated problems by Lee et al. [11] is a semi-implicit method. It is second-order accurate in time. The method utilizes Taylor series expansion of the concentration, C^{n+1}, at any time level $n+1$, in terms of the concentration C^n at the previous time level n as shown below:

$$C^{n+1} = C^n + \Delta t\frac{\partial C^n}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 C^n}{\partial t^2} + O(\Delta t^3). \tag{6}$$

Here $O(\Delta t^3)$ is the summation of the higher-order terms and will be neglected. Therefore,

$$C^{n+1} = C^n + \Delta t\frac{\partial C^n}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial^2 C^n}{\partial t^2} \tag{7}$$

or,

$$C^{n+1} = C^n + \Delta t\frac{\partial C^n}{\partial t} + \frac{\Delta t^2}{2}\frac{\partial}{\partial t}\left(\frac{\partial C^n}{\partial t}\right) \tag{8}$$

or,

$$C^{n+1} = C^n + \Delta t\left(-v\frac{\partial C^n}{\partial x} + D\frac{\partial^2 C^n}{\partial t^2} - \lambda C^n\right) + \frac{\Delta t^2}{2}\frac{\partial}{\partial t}\left(-v\frac{\partial C^n}{\partial x} + D\frac{\partial^2 C^n}{\partial x^2} - \lambda C^n\right) \tag{9}$$

or,

$$C^{n+1} = C^n + \Delta t\left(-v\frac{\partial C^n}{\partial x} + D\frac{\partial^2 C^n}{\partial t^2} - \lambda C^n\right) - v\frac{\Delta t^2}{2}\frac{\partial}{\partial x}\left(-v\frac{\partial C^n}{\partial x} + D\frac{\partial^2 C^n}{\partial x^2} - \lambda C^n\right) + D\frac{\Delta t^2}{2}\frac{\partial^2}{\partial x^2}\left(-v\frac{\partial C^n}{\partial x} + D\frac{\partial^2 C^n}{\partial x^2} - \lambda C^n\right) - \lambda\frac{\Delta t^2}{2}\left(-v\frac{\partial C^n}{\partial x} + D\frac{\partial^2 C^n}{\partial x^2} - \lambda C^n\right) \tag{10}$$

or,

$$C^{n+1} = C^n + \Delta t\left(-v\frac{\partial C^n}{\partial x} + D\frac{\partial^2 C^n}{\partial t^2} - \lambda C^n\right) - v\frac{\Delta t^2}{2}\left(-v\frac{\partial^2 C^n}{\partial x^2} + D\frac{\partial^3 C^n}{\partial x^3} - \lambda\frac{\partial C^n}{\partial x}\right) + D\frac{\Delta t^2}{2}\left(-v\frac{\partial^3 C^n}{\partial x^3} + D\frac{\partial^4 C^n}{\partial x^4} - \lambda\frac{\partial^2 C^n}{\partial x^2}\right) - \lambda\frac{\Delta t^2}{2}\left(-v\frac{\partial C^n}{\partial x} + D\frac{\partial^2 C^n}{\partial x^2} - \lambda C^n\right) \tag{11}$$

or,

$$C^{n+1} = \left(1 - \lambda\Delta t + \lambda^2\frac{\Delta t^2}{2}\right)C^n + (-v\Delta t + v\lambda\Delta t^2)\frac{\partial C^n}{\partial x} + \left(D\Delta t + v^2\frac{\Delta t^2}{2} - D\lambda\Delta t^2\right)\frac{\partial^2 C^n}{\partial x^2} - vD\Delta t^2\frac{\partial^3 C^n}{\partial x^3} + D^2\frac{\Delta t^2}{2}\frac{\partial^4 C^n}{\partial x^4}. \tag{12}$$

When PLBFs are used, the terms higher than second-order can be neglected. The terms, higher than second-order, will not contribute to the discretized transport equation. Eq. (12) can, therefore, be written as follows:

$$C^{n+1} = \gamma_1 C^n + \gamma_2\frac{\partial C^n}{\partial x} + \gamma_3\frac{\partial^2 C^n}{\partial x^2}, \tag{13}$$

where

$$\gamma_1 = 1 - \lambda\Delta t + \lambda^2\frac{\Delta t^2}{2}, \tag{14}$$

$$\gamma_2 = -v\Delta t + v\lambda\Delta t^2, \tag{15}$$

$$\gamma_3 = v^2\frac{\Delta t^2}{2} + D\Delta t - D\lambda\Delta t^2. \tag{16}$$

4. Finite element formulation

The solution to the transport equation (13) begins with the construction of a trial solution. The trial solution is a linear combination of the basis functions φ. If $\vec{C}$ is the trial solution then it can be expressed as follows:

$$\vec{C} = \sum_{i=0}^{N} C_i(t)\varphi_i(x), \tag{17}$$

where $C_i(t)$ is the magnitude of C at any node i and is a function of time only, and N is the number of finite elements. The trial solution can be written in the following form when the boundary condition at $x = 0$ is satisfied,

$$\vec{C} = C_0(t)\varphi_0(x) + \sum_{i=1}^{N} C_i(t)\varphi_i(x). \tag{18}$$

Since $\vec{C}$ is a trial solution it may not exactly satisfy the Taylor–Galerkin equation (13). There will be residuals as shown below:

$$R^{\mathrm{T}} = \vec{C}^{n+1} - \gamma_1 \vec{C}^{n} - \gamma_2 \frac{\partial \vec{C}^{n}}{\partial \bar{x}} - \gamma_3 \frac{\partial^2 \vec{C}^{n}}{\partial \bar{x}^2}. \tag{19}$$

The TGFEM minimizes the residual R^{T} over the domain by making it orthogonal to the PLBFs, φ, as defined below,

$$\varphi_i = 0 \quad \text{if } x \leqslant x_{i-1}, \tag{20a}$$

$$\varphi_i = \frac{x - x_{i-1}}{x_i - x_{i-1}} \quad \text{if } x_{i-1} \leqslant x \leqslant x_i, \tag{20b}$$

$$\varphi_i = \frac{x_{i+1} - x}{x_{i+1} - x_i} \quad \text{if } x_i \leqslant x \leqslant x_{i+1}, \tag{20c}$$

$$\varphi_i = 0 \quad \text{if } x \geqslant x_{i+1}. \tag{20d}$$

The UTGFEM differs from TGFEM in that it utilizes two weight functions to apply the principle of orthogonality to the residual R^{T}. The weight function for the advective term in Eq. (19) is taken to be the upwind basis functions (UBFs), φ^a, given in Eqs. (21a)–(21d). The PLBFs are used as weight functions for the rest of the terms,

$$\varphi_i^a = 0 \quad \text{if } x \leqslant x_{i-1}, \tag{21a}$$

$$\varphi_i^a = \frac{x - x_{i-1}}{x_i - x_{i-1}} - 3\alpha \frac{(x - x_{i-1})(x - x_i)}{(x_i - x_{i-1})^2} \quad \text{if } x_{i-1} \leqslant x \leqslant x_i, \tag{21b}$$

$$\varphi_i^a = \frac{x_{i+1} - x}{x_{i+1} - x_i} + 3\alpha \frac{(x - x_i)(x - x_{i+1})}{(x_{i+1} - x_i)^2} \quad \text{if } x_i \leqslant x \leqslant x_{i+1}, \tag{21c}$$

$$\varphi_i^a = 0 \quad \text{if } x \geqslant x_{i+1}. \tag{21d}$$

In the above equation α is a free parameter that spans between 0 and 1. The magnitude of α determines the degree of upwinding. If α is set to zero, then the UBFs become the standard PLBFs.

The introduction of upwinding and the application of Galerkin principle to the residual R^T, as discussed in Section 3, lead to the following system of ODEs,

$$\int_0^L R^T \varphi_j \, dx = \int_0^L \left[\vec{C}^{n+1} \varphi_j - \gamma_1 \vec{C}^n \varphi_j - \gamma_2 \frac{\partial \vec{C}^n}{\partial \bar{x}} \varphi_j^a - \gamma_3 \frac{\partial^2 \vec{C}^n}{\partial \bar{x}^2} \varphi_j \right] dx \quad \text{for } j = 1, 2, \ldots, N. \tag{22}$$

Appropriate mathematical manipulation transforms the above equation to the following:

$$[A]\{C\}^{n+1} = \gamma_1 [A]\{C\}^n + \gamma_2 [A^a]\{C\}^n - \gamma_3 [A^d]\{C\}^n + \{D\}, \tag{23}$$

where

$$a_{ij} = \int_0^L \varphi_i(x) \varphi_j(x) \, dx \quad i, j = 1, 2, 3, \ldots, N, \tag{24}$$

$$a_{i,j}^a = \int_0^L \frac{d\varphi_i(x)}{dx} \varphi_j^a(x) \, dx \quad i, j = 1, 2, 3, \ldots, N, \tag{25}$$

$$a_{i,j}^d = \int_0^L \frac{d\varphi_i(x)}{dx} \frac{d\varphi_j(x)}{dx} \, dx \quad i, j = 1, 2, 3, \ldots, N, \tag{26}$$

$$d_i = -\frac{\Delta x}{6} C_0^{n+1} + \gamma_1 \frac{\Delta x}{6} C_0^n - \frac{\gamma_2 (1 + \alpha)}{2} + \frac{\gamma_3}{\Delta x} \quad \text{for } i = 1, \tag{27}$$

$$d_i = 0 \quad \text{for } i \neq 1, \tag{28}$$

where C_0^{n+1} and C_0^n are the source concentrations at $n + 1$ and n time levels, respectively.

5. Solution technique

The UTGFEM is semi-implicit in nature. The matrix equation given in the UTGFEM formulation can be written in the following form:

$$[A]\{C\}^{n+1} = \{R\}, \tag{29}$$

where $\{R\} = \gamma_1 [A]\{C\}^n + \gamma_2 [A^a]\{C\}^n - \gamma_3 [A^d]\{C\}^n + \{D\}$.

The matrix $[A]$ was decomposed into lower and upper triangular matrices by employing the principle of lower and upper (LU) decomposition. Details of LU decomposition can be found elsewhere [12]. At each time step the decomposed system of equations were solved for concentrations at the nodes by forward and backward substitution. Burden and Faires [12] provide a good treatment of forward and backward substitution.

6. On TGFEM

The breakthrough profile presented in Fig. 1 is for unretarded advective transport of a contaminant in a uniform flow field of length of 100 m. A continuous source of 1 mg/L was considered for this simulation. The flow velocity was 2 m/day. The advective transport was considered because it is the most important transport mechanism from stability considerations. Further, stability for advective transport is an assurance of stability for advective–dispersive transport with or without degradation.

It is reported by Peraire et al. [9] that TGFEM for advective–dispersive transport should remain stable if the following condition is satisfied.

$$\mathrm{Cr} \leqslant \sqrt{\left[\frac{1}{\mathrm{Pe}^2} + \frac{1}{3}\right]} - \frac{1}{\mathrm{Pe}} \tag{30}$$

Here $\mathrm{Cr} = v\Delta t/\Delta x$, and is the mesh Courant number. Pe is the Peclet number and is equal to $v\Delta x/D$. The stability of pure advective transport is, therefore, assured when $\mathrm{Cr} \leqslant 1/\sqrt{3} = 0.577$. The model was found to remain stable as long as Cr was less than or equal to 0.577. The breakthrough profile in Fig. 1 is for a Courant number of 0.001 corresponding to $\Delta t = 5 \times 10^{-5}$ days. The model prediction is in good agreement with the analytical results. The correlation coefficient was computed to be 0.999. However, the prediction is oscillatory and the model also predicted negative concentrations at the early part of the breakthrough curve. Negative concentration is a physical impossibility and is a numerical phenomenon. The oscillation is also a numerical phenomenon. Both oscillation and negative concentrations are, therefore, undesirable and should be avoided for the model to be accurate and predictive.

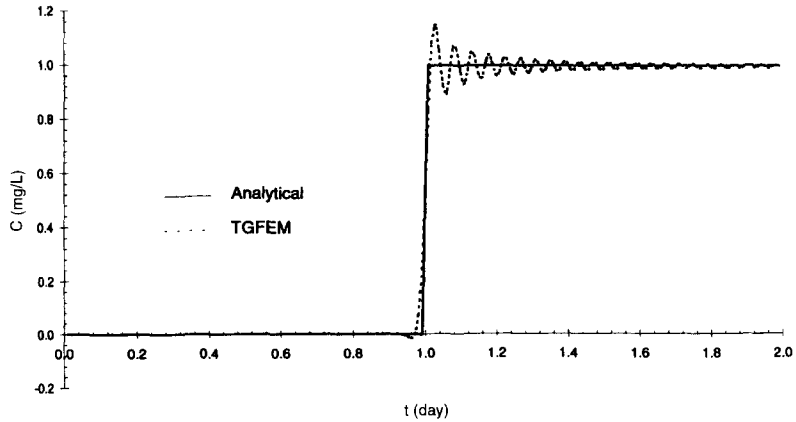

Fig. 1. TGFEM prediction versus analytical solution of advective transport for a continuous source.

7. Optimization of UTGFEM

The oscillation and the numerical phenomenon of negative concentrations are usually controlled by the introduction of upwinding as discussed earlier. The magnitude of upwinding is defined by the parameter α in Eq. (21). Higher value of α results in higher numerical dispersions. Therefore, α is to be determined in a way that it eliminates numerical oscillation leading to avoidance of negative concentrations and, at the same time, minimizes numerical dispersions.

A numerical experiment was performed to obtain the optimum value of α which is sufficient to eliminate oscillations and to avoid negative concentrations in the model prediction by UTGFEM. The experiment was conducted for a wide range of Peclet and Courant numbers. The flow field simulated was 30 m long. The flow velocity was 0.60 m/day. The dispersion coefficient was varied from 0.0 to 5 m^2/day. Therefore, the Peclet number was varied from 0.40 to infinity. The Courant number was varied from 0.005 to 0.1. A functional relationship was then developed to express optimum α as a function of Peclet and Courant numbers as shown in Eq. (31),

$$\alpha_{\text{optimum}} = \left[0.214474 - \frac{2.038077}{\text{Pe}}\right] + \left[1.232398 - \frac{0.072569}{\text{Pe}}\right]\text{Cr} \qquad (31)$$

This expression for the optimum value of upwinding, as mentioned, was developed by considering a constant source boundary condition. It was found that it also holds for a pulse input or an exponentially decaying boundary condition.

8. Model predictions versus analytical results

The accuracy of the optimized model was verified by comparing its predictions with analytical results reported by van Genuchten [13]. The simulated flow field was 100 m long and was divided into 100 finite elements. Therefore Δx was equal to 1 m. The velocity of flow was 2 m/day. The dispersion coefficient was varied between 0 and 5 m^2/day and Δt was equal to 5.0×10^{-4} day.

Fig. 2 presents the predicted breakthrough profiles for dispersion coefficients of 0.0, 1.0, and 5.0 m^2/day. The model predictions are in excellent agreement with the analytical results for the larger dispersion coefficients. The computed correlation coefficients were 0.999. The agreement is not quite as good for pure advective transport i.e., when the dispersion coefficient is zero and it was reflected in the poor correlation coefficient of 0.955. Similar results were obtained for advective–dispersive transport with degradation. Fig. 3 presents model predictions for a widely ranging degradation rate constant of 0.007– 0.028 d^{-1} and for a dispersion coefficient of 1.0 m^2/day. The excellent agreement between the model predictions and the analytical results yielded a high correlation coefficient of 0.999.

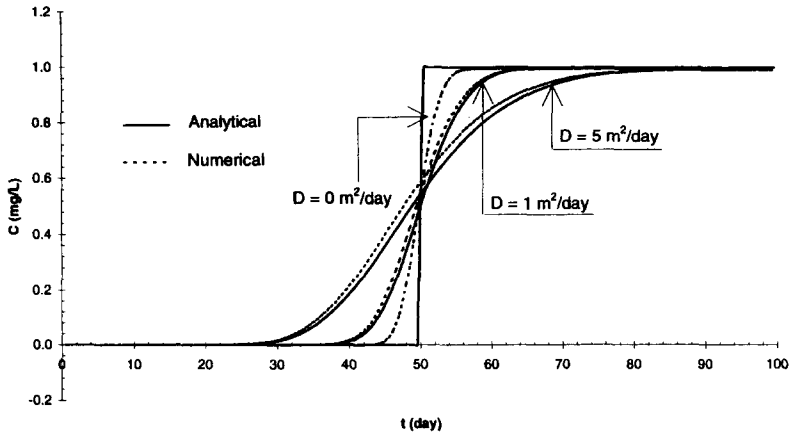

Fig. 2. UTGFEM predictions versus analytical solution of advective–dispersive transport for a continuous source.

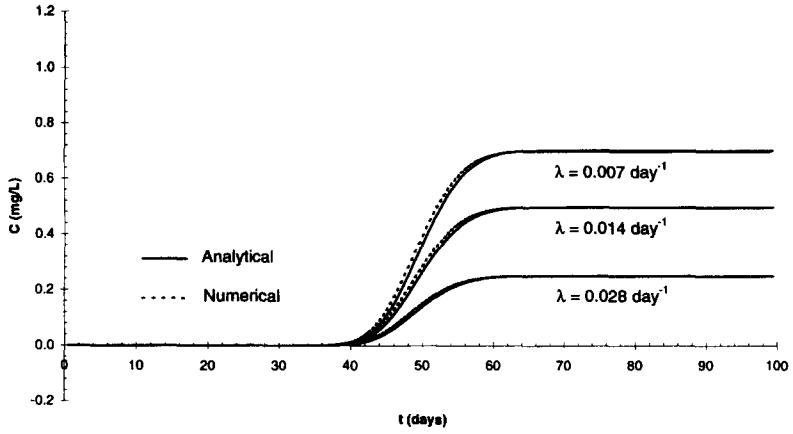

Fig. 3. UTGFEM predictions versus analytical solution of advective–dispersive transport with degradations for a continuous source.

Fig. 4 contains the model predictions for a pulse source of duration 5 days and for a dispersion coefficient of 1.0 m^2/day. The computed correlation coefficient was 0.999 indicating the excellent agreement between the model prediction and the analytical solution. Similar agreement was observed for a dispersion coefficient of 5.0 m^2/day too.

An exponentially decaying source was also considered. The boundary condition given in Eq. (3) can be written as follows:

$$C_0(t) = C_0 e^{-\kappa t}. \tag{32}$$

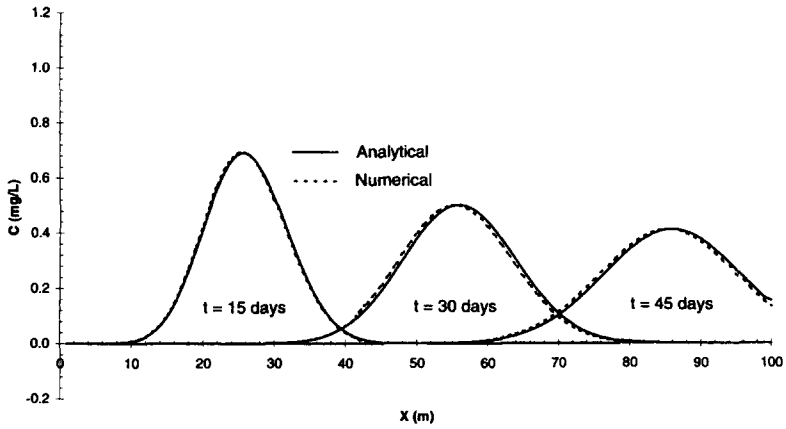

Fig. 4. UTGFEM predictions versus analytical solution of advective–dispersive transport for a pulse source.

The model predictions for this boundary condition are presented in Fig. 5. The source decay constants, κ, utilized were 0.01, 0.03, and 0.05 $(\text{day})^{-1}$. The dispersion coefficients for these predictions were 1.0 m^2/day. The model predictions are again in excellent agreement with the analytical solution. The correlation coefficient was 0.999. The agreement was also excellent for the dispersion coefficient of 5.0 m^2/day.

Therefore, it can be concluded that the model predictions are in excellent agreement with the analytical solution for advective–dispersive transport. The model appears to introduce some numerical dispersion when the dispersion is zero. The numerical dispersion introduced is the minimum needed to

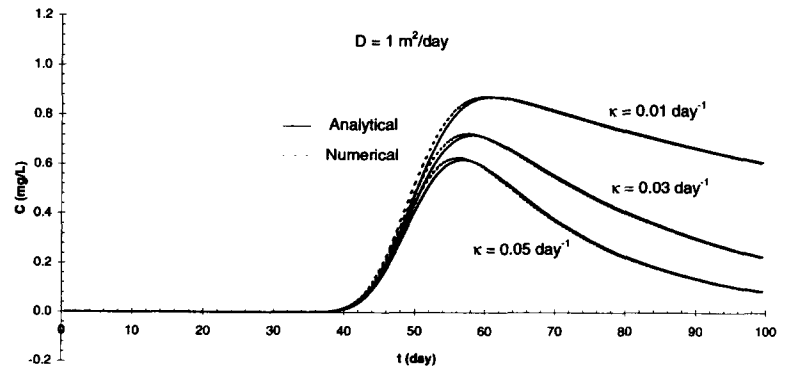

Fig. 5. UTGFEM predictions versus analytical solution of advective–dispersive transport for an exponentially decaying source.

eliminate oscillation and avoid negative concentrations and was equal to $(\alpha_{\text{optimum}} v\Delta x/2) = 0.215$ m^2/day. The model was found to provide excellent agreement between its prediction and the analytical solution when the dispersion coefficient was greater than or equal to 0.215 m^2/day. If a smaller numerical dispersion is desired then it can be achieved by making Δx smaller because the numerical dispersion is proportional to it.

9. Conclusions

The optimized UTGFEM was employed to simulate contaminant transport in groundwater for continuous, pulse, and exponentially decaying sources. The model was found to provide accurate predictions for dispersion coefficients greater than or equal to a limiting value 0.215 m^2/day. If the dispersion coefficient is smaller than 0.215 m^2/day then some numerical dispersions need to be introduced to obtain oscillation free results and to avoid physically impossible negative concentrations. The magnitude of the numerical dispersion introduced is 0.215 m^2/day minus the field dispersion. The magnitude of the numerical dispersion to be introduced can, further, be reduced by making Δx smaller.

References

[1] I. Christie, A.R. Mitchell, Upwinding of high order Galerkin methods in conduction–convection problems, Int. J. Num. Meth. Eng. 14 (1978) 1764–1771.
[2] E. Dick, Accurate Petrov–Galerkin methods for transient convective diffusion equation, Int. J. Num. Meth. Eng. 19 (1983) 1425–1433.
[3] J. Donea, A Taylor–Galerkin method for convective transport problems, Int. J. Num. Meth. Eng. 20 (1984) 101–119.
[4] R. Ganesan, N.J. Salamon, Solution of the one-dimensional convection diffusion equation by a multilevel Petrov–Galerkin method, Int. J. Num. Meth. Eng. 39 (1996) 2095–2109.
[5] S.R. Idelsohn, J.C. Heinrich, E. Onate, Petrov–Galerkin methods for the transient advective–diffusive equation with sharp gradients, Int. J. Num. Meth. Eng. 39 (1996) 1455–1473.
[6] P.S. Huyakorn, Solution of steady state convective transport equation using an upwind finite element scheme, Appl. Math. Modeling 1 (1977) 187–195.
[7] J.C. Heinrich, P.S. Huyakorn, O.C. Zienkiewicz, A.R. Mitchell, An upwind finite element scheme for two-dimensional convective transport equation, Int. J. Num. Meth. Eng. 11 (1977) 131–143.
[8] P.S. Huyakorn, K. Nilkuha, Solution of transient transport equation using an upstream finite element scheme, Appl. Math. Modelling 3 (1979) 7–17.
[9] J. Peraire, O.C. Zienkiewicz, K. Morgan, Shallow water problems: A general explicit formulation, Int. J. Num. Meth. Eng. 22 (1986) 547–574.
[10] M.A. Hossain, D.R. Yonge, Linear finite element modeling of contaminant transport in groundwater, submitted for publication in J. Envir. Eng., ASCE.

[11] J.H.W. Lee, J. Peraire, O.C. Zienkiewicz, The characteristic-Galerkin method for advection-dominated problem – an assessment, Comput. Meth. Appl. Mech. Eng. 61 (1987) 359–369.
[12] R.L. Burden, J.D. Faires, Numerical Analysis, PWS-KENT Publishing Company, Boston, MA, 1995, p. 323.
[13] M.Th. Genuchten, Analytical solutions for chemical transport with simultaneous adsorption, zero-order production and first-order decay, J. Hydrology 49 (1981) 213–233.