Hermitian Green element calculations of contaminant transport

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Abstract

A set of new discrete element equations or coefficients is herein derived for the transient 1-D. contaminant transport equation, and these coefficients are based on the Green element replication of the differential equation. The cubic Hermitian interpolation functions are incorporated into the numerical model to approximate the distribution of unknown quantities. The Green element method (GEM) is a novel computational method which uses the singular boundary integral theory to solve mathematical descriptions of engineering systems. Because of the unique feature of the contaminant transport problem in which steep concentration profiles are encountered for advection-dominant cases, incorporating linear interpolation functions in GEM to approximate these profiles may be inadequate. It is for that reason that we have in this paper incorporated Hermitian interpolation functions into GEM for the contaminant transport problem to assess by how much the accuracy of the solution is enhanced. The Hermitian GEM solutions are found to be superior to the linear GEM for two numerical examples presented.

Introduction

Considerable interest continues to be shown to the problem of transport of pollutants in fluid media within numerical circles and as well as in field investigations because of its ubiquitous applications to many engineering systems - pesticides and fertilizer applications on farm lands, toxic and non-toxic waste containment in underground repositories, air pollution problems, transport of pollutants in water bodies, transport of foreign bodies in animal and human blood streams, and a host of other applications, too many to mention. From the computational aspect of contaminant transport, the differential equation which governs this phenomenon exhibits intriguing features of parabolic and hyperbolic characteristics, depending on the relative values of the parameters of the equation. When diffusion or hydrodynamic dispersion is dominant, the equation behaves like a parabolic one, but when advection is dominant it behaves as a hyperbolic equation, and this poses the greater computational challenge. The relative importance of these two transport processes is indicated by the value of the dimensionless parameter known as the Peclet number.

Although a considerable number of analytic solutions to the transport equation exist in one and two dimensions, they are limited to regular geometries, and serve to evaluate field parameters and validate numerical models (Cleary and Ungs, 1978; Van Genuchten and Alves, 1982). Furthermore, a lot of work has been done in numerical circles to provide solutions to contaminant transport problems. Some of the earliest works with the finite difference method (FDM) are those of Peaceman and Rachford (1962) and Price et al. (1968), while steady research activities are continuing on the finite element method (FEM) (Anderson, 1979; Brooks and Hughes, 1982; Zienkiewicz and Taylor, 1991). Most of the various schemes of the FDM and FEM that have evolved are directed at eliminating the unpleasant features of unacceptably large spurious oscillations and induced numerical diffusion under advection-dominant transport.

The GEM is a novel approach of implementing the singular boundary integral theory concept, and has the advantage of producing a sparse banded global coefficient matrix which is easier to invert, and readily accommodates problems where the medium parameter varies with the spatial variables (heterogenous) and with the primary variable (non-linear). We have demonstrated some of these advantages in some of our earlier works (Taigbenu, 1995; 1996; Taigbenu and Onyejekwe, 1995; 1997a).

In an earlier work (Taigbenu and Onyejekwe, 1997b), we had incorporated linear functions to approximate the concentration profile in the GEM of the transport equation, but that gives significant errors for advection-dominant transport where steep gradients of the concentration profile exist. These interpolating polynomials have zero-order continuity in the sense that only the concentration is continuous, whereas its first derivative is discontinuous across elements. In this paper we attempt to incorporate the first-order cubic Hermitian interpolation functions into GEM for the contaminant transport equation to minimise numerical errors. These functions ensure that the concentration and its first derivative are continuous at the interzonal boundaries. Any improvement in the quality of the numerical solution from the use of these functions has to be at a price of higher computing cost. The marginal gains in accuracy *vis-a-vis* computational costs are evaluated. Two examples of contaminant transport in 1-D. are used for comparison of the linear and Hermitian GEMs, and the latter is found to be superior in representing the concentration front and in eliminating spurious oscillations, but at a cost of about one and a half times the computing speed of the former.

Transport equation

The partial differential equation that describes one-dimensional transport with first-order decay in a homogeneous medium is given by:

$$D\frac{\partial^2 c(x,t)}{\partial x^2} - U\frac{\partial c(x,t)}{\partial x} - \frac{\partial c(x,t)}{\partial t} - \mu c = f(x,t), \qquad on\ x_0 \le x \le x_L \tag{1}$$

where:

c = c(x,t) is the solution concentration
D is the hydrodynamic dispersion coefficient [L^2/T]
U is the ambient flow velocity in the x-direction [L/T]

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x and t are, respectively, the spatial and temporal independent variables

μ is the rate constant of first-order decay for a non-conservative pollutant [T^{-1}]

L = $x_L - x_0$ is considered the length of the flow domain.

The enormous interest generated by the solution of Eq. (1) stems from its extensive applications in the areas of agriculture, chemical, environmental, and water resources engineering. The solution of Eq. (1) requires information on the boundary conditions at x_0 and x_L, and the data on c(x,t) at the initial time t_0. The first-type or Dirichlet condition specifies the concentration at the end points:

$$c(x_0,t) = g_0(t), \quad c(x_L,t) = g_L(t) \tag{2a}$$

and the second-type or flux-type or Neumann condition specifies the flux of the substance being transported:

$$D\frac{\partial c(x_0,t)}{\partial x} = f_0(t), \qquad D\frac{\partial c(x_L,t)}{\partial x} = f_L(t) \tag{2b}$$

or an appropriate linear combination of both boundary conditions can be specified. The initial data specify the concentration at the initial time t_0:

$$c(x,t_0) = c_0(x), \quad x_0 \le x \le x_L \tag{2c}$$

Hermitian Green element model

A complementary differential equation is proposed to Eq. (1) of the form:

$$\frac{d^2G}{dx^2} = \delta(x-x_i), \qquad -\infty \le x \le \infty \tag{3}$$

where δ is the Dirac delta function. The solution to Eq. (2), referred to as the free-space Green's function, is:

$$G(x,x_i) = \frac{1}{2}(|x-x_i| + k) \tag{4}$$

where k is an arbitrary constant. As in our previous works (Taigbenu, 1996) k is set to the longest spatial element $\tilde{l}$ used in discretising the solution domain. Within an element denoted as $[x_1, x_2]$, Green's second identity, which is given by:

$$\int_{x_1}^{x_2}\left[c\frac{d^2G}{dx^2} - G\frac{\partial^2 c}{\partial x^2}\right]dx = \left[c\frac{dG}{dx} - G\frac{\partial c}{\partial x}\right]_{x=x_1}^{x=x_2} \tag{5}$$

is applied to Eqs. (1) and (3) to give the integral equation

$$D\left\{-\lambda c(x_i,t) + \left[c\frac{\partial G}{\partial x}\right]_{x=x_1}^{x=x_2} - \left[G\frac{\partial c}{\partial x}\right]_{x=x_1}^{x=x_2}\right\} + \int_{x_1}^{x_2} G\left[U\frac{\partial c}{\partial x} + \frac{\partial c}{\partial t} + \mu c + f(x,t)\right]dx = 0 \tag{6}$$

Eq. (6) can also be expressed as:

$$D\left[-\lambda c(x_i,t) + G^*(x_2,x_i)c(x_2,t) - G^*(x_1,x_i)c(x_1,t) - G(x_2,x_i)\phi(x_2,t) + G(x_1,x_i)\phi(x_1,t)\right] + \int_{x_1}^{x_2} G(x,x_i)\left[U\phi(x,t) + \frac{\partial c(x,t)}{\partial t} + \mu c(x,t) + f(x,t)\right]dx = 0; \qquad i=1,2 \tag{7}$$

in which $\phi(x,t) = \partial c(x,t)/\partial x$, and

$$G^*(x,x_i) = \frac{dG(x,x_i)}{dx} = \frac{H(x-x_i) - H(x_i-x)}{2} \tag{8a}$$

$$\lambda = \int_{-\infty}^{x_i}\delta(x-x_i)dx + \int_{x_i}^{\infty}\delta(x-x_i)dx = \int_{x_i-\epsilon}^{x_i}\delta(x-x_i)dx + \int_{x_i}^{x_i+\epsilon}\delta(x-x_i)dx \tag{8b}$$

where:

ε is any small positive quantity and

H is the Heaviside function.

Using the property of the Dirac delta function, λ takes the value of unity when x_i is within the element $x_1 < x < x_2$, and $\lambda = 0.5$ when x_i is at the nodes of the element. To evaluate the line integral in Eq. (7) over a typical element, there is the need to prescribe a distribution of c and ϕ over each element. Earlier we had used interpolation functions of zero-order continuity, that is interpolation functions which provide only for the continuity of the quantity being interpolated; its spatial derivative is discontinuous across elements (Taigbenu and Onyejekwe, 1997b). Here we focus on a special class of interpolation functions which are based on the Hermitian polynomials. They allow not only for the continuity of the interpolated quantity, but also its first spatial derivative. For a two-nodal one-dimensional element these conditions are satisfied by first-order continuous cubic Hermitian interpolation polynomials which give the following representation for c(x,t):

$$c(x,t) \approx \Omega_j(\zeta)c_j(t) + \hat{\Omega}_j(\zeta)\frac{\partial c_j(t)}{\partial x} = \Omega_j(\zeta)c_j(t) + \hat{\Omega}_j\phi_j(t) \tag{9}$$

where $\Omega_j(\zeta)$ and $\hat{\Omega}_j(\zeta)$ are the Hermitian basis functions which, in terms of the local co-ordinate $\zeta = (x - x_1)/l$, are given by:

$$\Omega_1 = 1 - 3\zeta^2 + 2\zeta^3 \tag{10a}$$

$$\Omega_2 = 3\zeta^2 - 2\zeta^3 \tag{10b}$$

$$\hat{\Omega}_1 = l\zeta(1-\zeta)^2 \tag{10c}$$

$$\hat{\Omega}_2 = l\zeta^2(\zeta - 1) \tag{10d}$$

in which $l = x_2 - x_1$. Since the Hermitian polynomials allow for the continuity of the spatial derivative of c(x,t), the quantity $\phi(x,t)$ is approximated by the relation:

$$\phi(x,t) \approx \frac{d\Omega_j}{dx}c_j(t) + \frac{d\hat{\Omega}_j}{dx}\phi_j(t) \tag{11}$$

When the relationships provided by the interpolation for c, ϕ and f are substituted into the integral Eq. (7), it simplifies to:

$$D\left[-\lambda c(x_i,t) + G^*(x_2,x_i)c(x_2,t) - G^*(x_1,x_i)c(x_1,t) - G(x_2,x_i)\phi(x_2,t) + G(x_1,x_i)\phi(x_1,t)\right] + \int_{x_1}^{x_2} G(x,x_i)\left\{U\left(\frac{d\Omega_j}{dx}c_j + \frac{d\hat{\Omega}_j}{dx}\phi_j\right) + \Omega_j\left(\frac{dc_j}{dt} + \mu c_j + f_j\right) + \hat{\Omega}_j\left(\frac{d\phi_j}{dt} + \mu\phi_j + \frac{\partial f_j}{\partial x}\right)\right\}dx = 0; \qquad i,j=1,2 \tag{12}$$

The line integral in Eq. (12) is evaluated using the expressions for the Hermitian functions, and the result is a system of discretised equations (element equations) which apply to a typical element $[x_1, x_2]$:

$$D[R_{ij}c_j + L_{ij}\phi_j] + [US_{ij} + \mu T_{ij}]c_j + T_{ij}\left(\frac{dc_j}{dt} + f_j\right) + [U\hat{S}_{ij} + \mu\hat{T}_{ij}]\phi_j + \hat{T}_{ij}\left(\frac{d\phi_j}{dt} + \frac{\partial f_j}{\partial x}\right) = 0; \quad i,j=1,2 \tag{13}$$

in which the element matrices R_{ij} and L_{ij} come from evaluating G* and G at the nodes of the element, and they have the expressions:

$$R_{ij} = \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} = (-1)^{i+j-1}; \quad i,j=1,2 \tag{14a}$$

$$L_{ij} = \begin{bmatrix} \tilde{l} & -(l+\tilde{l}) \\ l+\tilde{l} & -\tilde{l} \end{bmatrix}; \quad i,j=1,2 \tag{14b}$$

while the other element matrices in Eq. (13) have the following expressions:

$$S_{ij} = \int_{x_1}^{x_2} \frac{d\Omega_j}{dx} G(x,x_i)\,dx = \frac{1}{2}\begin{bmatrix} -(2\tilde{l}+l) & 2\tilde{l}+l \\ -(2\tilde{l}+l) & 2\tilde{l}+l \end{bmatrix} \tag{14c}$$

$$\hat{S}_{ij} = \int_{x_1}^{x_2} \frac{d\hat{\Omega}_j}{dx} G(x,x_i)\,dx = \frac{l^2}{12}R_{ij} = \frac{l^2}{12}(-1)^{i+j-1} \tag{14d}$$

$$T_{ij} = \int_{x_1}^{x_2} \Omega_j G(x,x_i)\,dx = \frac{l}{20}\begin{bmatrix} 10\tilde{l}+3l & 10\tilde{l}+7l \\ 10\tilde{l}+7l & 10\tilde{l}+3l \end{bmatrix} \tag{14e}$$

$$\hat{T}_{ij} = \int_{x_1}^{x_2} \hat{\Omega}_{ij} G(x,x_i)\,dx = \frac{l^2}{60}\begin{bmatrix} 5\tilde{l}+2l & -(5\tilde{l}+3l) \\ 5\tilde{l}+3l & -(5\tilde{l}+2l) \end{bmatrix} \tag{14f}$$

Eq. (13) is a system of first-order discrete equations in time. There are a number of avenues available to us for simplifying the temporal derivatives Since Eq. (13) is a system of initial-value differential equations, Euler and Runge-Kutta methods could be applied to the system of equations. However, we elect to use a difference approximation for the temporal derivative

$$\left.\frac{dc_j}{dt}\right|_{t=t_m+\alpha\Delta t} \approx \frac{c_j(t_m+\Delta t) - c_j(t_m)}{\Delta t} = \frac{c_j^{(m+1)} - c_j^{(m)}}{\Delta t}; \quad 0 \le \alpha \le 1 \tag{15}$$

Eq. (15) indicates that the temporal derivative is evaluated at a time $t_m + \alpha\,\Delta t$, where t_m is the previous time level, $\Delta t = t_{m+1} - t_m$ is the time step or temporal element size, and t_{m+1} is the current time level at which numerical solutions are desired, and α is a difference weighting factor whose value varies between 0 and 1. The value of α positions the time level at which the temporal derivative is evaluated. Using familiar nomenclature in finite difference and finite element circles, a scheme with $\alpha = 0$ is said to be the fully explicit scheme, that with $\alpha = 0.5$ is the Crank-Nicholson scheme, while that with $\alpha = 1.0$ is usually referred to as the fully implicit scheme. Since the temporal derivative has been evaluated at $t_m + \alpha\Delta t$, it is reasonable to evaluate the other terms of Eq. (13) at that time level using a weighted average of the form:

$$\left[\alpha(DR_{ij} + US_{ij} + \mu T_{ij}) + \frac{T_{ij}}{\Delta t}\right]c_j^{(m+1)} + \left[\alpha(DL_{ij} + U\hat{S}_{ij} + \mu\hat{T}_{ij}) + \frac{\hat{T}_{ij}}{\Delta T}\right]\phi_j^{(m+1)} + \left[(1-\alpha)(DR_{ij} + US_{ij} + \mu T_{ij}) - \frac{T_{ij}}{\Delta t}\right]c_j^{(m)} + \left[(1-\alpha)(DL_{ij} + U\hat{S}_{ij} + \mu T_{ij}) - \frac{\hat{T}_{ij}}{\Delta t}\right]\phi_j^{(m)} + \alpha[T_{ij}f_j^{(m+1)} + \hat{T}_{ij}\frac{\partial f_j^{(m+1)}}{\partial x}] + (1-\alpha)[T_{ij}f_j^{(m)} + \hat{T}_{ij}\frac{\partial f_j^{(m)}}{\partial x}] = 0 \tag{16}$$

The superscripts *m+1* and *m* denote the current and previous time levels. Eq. (16) is assembled for all elements that are employed to discretise the computational domain to obtain the global coefficient matrix equation:

$$A_{ij}u_j^{(m+1)} = B_i \tag{17}$$

where A_{ij} is the global coefficient matrix which has a half bandwidth of 2, $u_j^{(m+1)} = \{c_j^{(m+1)}, \phi_j^{(m+1)}\}^T$ is the mixed vector of nodal unknowns, and B_i is the right-hand-side vector which receives contribution from boundary and initial data, and from externally imposed contaminant load. Eq. (17) is solved at each time level to obtain the nodal solutions $c_j^{(m+1)}$ and $\phi_j^{(m+1)}$.

Numerical examples

Two numerical examples of transient contaminant transport in 1-D. spatial dimension are used to evaluate the level of enhancement of accuracy achieved by the Hermitian Green element model described in the foregoing section. Our evaluation is based on comparison of the current model with that of the earlier model which incorporates linear interpolation functions to approximate the distribution of the concentration. The two examples used have exact solutions which serve as bench-marks for the assessment of accuracy. Since one of the unique features of the solution to the transport problem is that the initial concentration profile is maintained with time when advection is dominant (large value of Peclet number), the examples have been so designed that the initial concentration profile is steep, and transport takes place when advection is dominant. The Hermitian and linear Green element calculations of the two examples are carried out with the Crank-Nicholson scheme ($\alpha = 0.5$) which had earlier been found to give optimal results from the linear model (Taigbenu and Onyejekwe, 1997b).

Example 1

This first example is the classical 1-D. transport problem which has been used by many investigators in evaluating the performance of their numerical models. The problem is governed by Eq. (1) with $\mu = 0$ and $f(x,t) = 0$. The boundary and initial conditions are:

$$c(0, t) = 1, \quad \frac{\partial c(x=\infty,t)}{\partial x} = 0, \text{ and } c(x, t = 0) = 0 \tag{23}$$

The solution to this transport problem with the above conditions is well-known (Ogata and Banks, 1976). The element Peclet number, which is a dimensionless parameter, is defined as:

$$Pe = \frac{Ul}{D} \tag{24}$$

and it is indicative of the relative magnitude of dispersion or diffusion with respect to advection in the transport process. Since the case when advection dominates the transport provides the most severe test for any numerical scheme in eliminating such

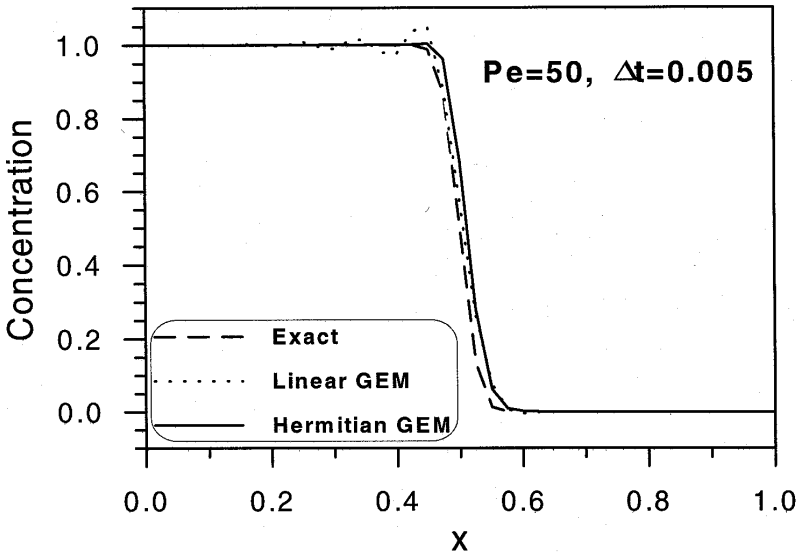

Figure 1
Linear and Hermitian GEM solutions of contaminant transport (Example 1)

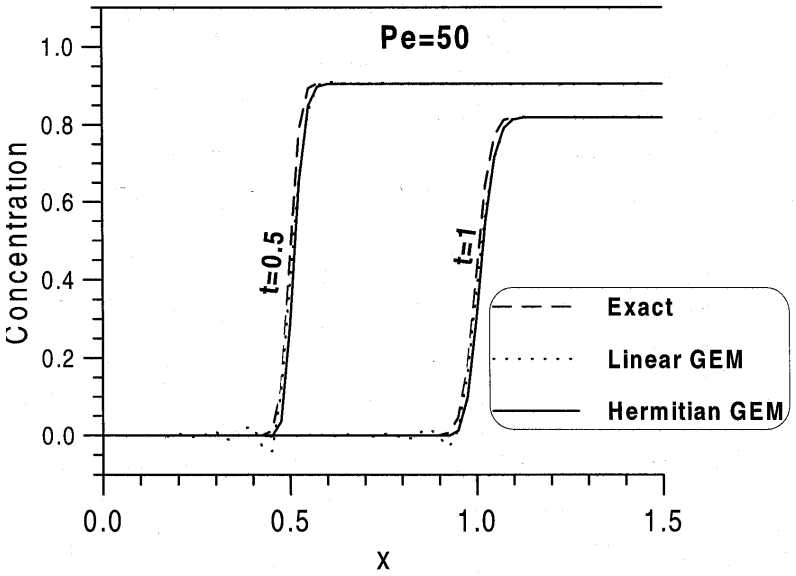

Figure 2
Linear and Hermitian GEM solutions of contaminant transport (Example 2)

undesirable features of numerical diffusion and spurious oscillations, a value of 50 is used for the element Peclet number in the numerical calculations. The simulations are done with a uniform ambient velocity $U = 1$, spatial size of each element $l = 0.025$, a uniform time step of 0.005, and the solution of the concentration front is presented at $t = 0.5$. The exact solution and those of the linear and Hermitian GEM are presented in Fig. 1. The results indicate that the Hermitian model reproduced the concentration front better than the linear one, and it does so without any oscillation.

Example 2

The second example is that of contaminant transport in a polluted stream which undergoes decontamination by mechanical means of advection from a source of freshwater and a biological/chemical process which induces first-order decay of the pollutant. The initial and boundary conditions are:

$$c(x,t=0) = 1,\ c(x=0,t>0), \text{ and } \frac{\partial c(x=\infty,t>0)}{\partial x} = 0 \quad (25)$$

The exact solution is given by Van Genuchten and Alves (1968).

$$c(x,t) = \exp(-\mu t)\left\{1 - \frac{1}{2}erfc\left[\frac{x-Ut}{2\sqrt{Dt}}\right] - \frac{1}{2}\exp\left(\frac{Ux}{D}\right)erfc\left[\frac{x+Ut}{2\sqrt{Dt}}\right]\right\} \quad (26)$$

The following parameter values are incorporated in the numerical calculations: U = 1, D = 0.0005, Pe = 50, and μ = 0.2. The Crank-Nicholson scheme and a uniform time step of 0.025 are used in both the linear and Hermitian GEMs. The numerical and exact solutions, obtained at times of 0.5 and 1.0, are presented in Fig. 2. While both models did equally well in approximating the concentration front, the results of the Hermitian model are free of the oscillations which are observed in the linear model.

Conclusion

A new set of discrete element equations has been obtained for the transient 1-D. contaminant transport equation by a GEM which incorporates the Hermitian interpolation functions for the approximation of unknown quantities. The model uses the free-space Green's function of the 1-D. Laplace operator in the derivation of its integral equation, and approximates the temporal

derivative by a weighted difference expression which yields a time marching scheme. For transport processes where advection is dominant and the gradients of the concentration profile are large, the use of linear interpolation functions for the representation of the profile is fraught with computational errors which manifest as spurious oscillations and a smeared concentration front. For such situations, the use of higher-order interpolation functions like Hermitian basis functions, becomes necessary. Although, incorporating Hermitian interpolation functions into GEM results in a more cumbersome formulation which takes longer computer runs, it nonetheless enhances the accuracy of the solution. Two numerical examples of contaminant transport were used in this paper to demonstrate this fact. The stability characteristics of this Hermitian model have earlier been carried out and presented in Taigbenu (1998), and it exhibits better stability characteristics than the linear model.

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