

Nodal domain integration model of one-dimensional advection-diffusion

T. V. HROMADKA II and G. L. GUYMON

Department of Civil Engineering, School of Engineering, University of California, Irvine, Ca 92717, USA

The nodal domain integration method is applied to a one-dimensional advection-diffusion mathematical model without a source term. Comparison of the resulting numerical model to the well known Galerkin finite element, subdomain, and finite difference domain models indicates that a single numerical statement can be developed which includes the Galerkin finite element, subdomain, and finite difference models as special cases.

INTRODUCTION

The determination of an optimum numerical method to model problems analogous to soil-moisture transport in a one-dimensional domain has received some recent attention. The primary numerical modelling (domain) approaches has generally been either the Galerkin finite element or finite difference methods. Pinder and Gray¹⁰ present a comparison of these two modelling approaches for a linear, one-dimensional advection-diffusion problem where the advection component is large; the finite element method is concluded as superior. Hayhoe⁴ demonstrated that a finite difference analog produced better numerical accuracy than a finite element model for a non-linear soil-water diffusion model problem in which a highly sensitive soil-water diffusivity parameter caused a sharp wetting front, making a numerical modelling effort difficult. Hromadka and Guymon⁵ re-examined the sharp wetting front problem with a finite element numerical model using a quasi-constant element soil-water diffusivity computation scheme; the numerical model results were found to be comparable to Hayhoe's finite difference analog results, but gave a better prediction of the wetting front penetration. In a more detailed study, Hromadka and Guymon⁸ integrated the soil-water diffusivity parameter with respect to time and determined another modelling approach (nodal domain integration) to the sharp wetting front problem. In this later study, other comparable numerical methods (finite difference, Galerkin finite element, subdomain integration) were rewritten into a single matrix system modelling statement of nodal point values and equation parameters similar to the element matrix system generated by the Galerkin finite element method. This resulting element matrix formulation is strictly a function of the element capacitance (time derivative) matrix diagonal entry as determined for a linear polynomial trial function approximation between nodal points. Consequently, numerical 'efficiency'^{1-3,7,10} in modelling a one-dimensional diffusivity model of soil-water transport could be viewed as a function of a single element matrix system parameter. In order to better estimate the soil-water content function spatially, Hromadka and Guymon⁸, examined two methods of approximating a

higher order or more complex family of trial functions between nodal points by a linear polynomial trial function approximation. This technique would incorporate some of the benefits provided by a higher order state variable approximation between nodal points and yet retain the symmetry and smaller matrix bandwidths resulting from a linear trial function approximation. Both approaches resulted in the combined matrix system statement identified above but with the element capacitance matrix diagonal component variable with respect to time and space.

The purpose of this paper is twofold. First, the advection-diffusion equation is analysed to determine an appropriate element matrix modelling statement which incorporates the finite element, finite difference, and subdomain integration modelling approaches. The second objective is to model a higher order spatial trial function approximation between nodal points with a linear trial function approximation in a diffusion dominated process. This linear approximation effort is based upon determining a higher order trial function approximation of the state variable between nodal points using information provided by the spatial distribution of the time derivative of the state variable. For numerical model development, a Fickian dispersion process of a conservative dissolved species with solute concentration C within pure water is considered as a case study.

NODAL DOMAIN INTEGRATION MODEL DEVELOPMENT

The one-dimensional form of the advection-diffusion equation for non-reactive dissolved constituents in saturated, homogeneous, isotropic materials under steady-state uniform flow is:

$$\left. \begin{aligned} \frac{\partial}{\partial x} \left[D \frac{\partial C}{\partial x} \right] - \frac{\partial}{\partial x} [UC] = \frac{\partial C}{\partial t}; x \in \Omega \\ \Omega \equiv \{x|0 \leq x \leq L\} \end{aligned} \right\} \quad (1)$$

where x is the spatial coordinate taken along the flowline direction in spatial domain Ω ; U is the mean linear flow

velocity; D is the coefficient of hydrodynamic dispersion in the x -direction; and C is the solute concentration. Chemical, biological and radioactive effects are neglected. In equation (1), the parameters D and U are left within the spatial gradient terms in order to provide a more general numerical model development.

The domain Ω can be discretized by n nodal points C_j ($j = 1, 2, \dots, n$) into n disjoint subdomains:

$$\begin{aligned} \Omega_1 &\equiv \{x | 0 \leq x \leq (x_1 + x_2)/2\} \\ \Omega_2 &\equiv \{x | (x_1 + x_2)/2 < x \leq (x_2 + x_3)/2\} \\ &\vdots \\ \Omega_n &\equiv \{x | (x_{n-1} + x_n)/2 < x \leq x_n = L\} \end{aligned} \quad (2)$$

where x_j is the spatial coordinate associated to nodal point value C_j , and

$$\Omega = \bigcup_{i=1}^n \Omega_i \quad (3)$$

Equation (1) must be satisfied on each Ω_j . Therefore, n equations are generated by solving:

$$\frac{\partial}{\partial x} \left[D \frac{\partial C}{\partial x} \right] = \frac{\partial C}{\partial t} + \frac{\partial}{\partial x} [UC]; \quad x \in \Omega_j, \forall j \quad (4)$$

where it is assumed

$$\begin{cases} D = D(C) \\ C = C(x, t) \end{cases} \quad (5)$$

Integrating equation (4) with respect to space gives the subdomain model:

$$\left\{ D \frac{\partial C}{\partial x} \right\} \Big|_{\Gamma_j} = \frac{\partial}{\partial t} \int_{\Omega_j} C \, dx + \{UC\} \Big|_{\Gamma_j}; \quad x \in \Omega_j, \forall j \quad (6)$$

where Γ_j is the spatial boundary of region Ω_j . Integrating equation (6) with respect to time gives:

$$\int_{k\Delta t}^{(k+1)\Delta t} \left\{ D \frac{\partial C}{\partial x} \right\} \Big|_{\Gamma_j} dt = \int_{\Omega_j} \{C\} \Big|_{\Gamma_j} dx + \int_{k\Delta t}^{(k+1)\Delta t} \{UC\} \Big|_{\Gamma_j} dt \quad (7)$$

where Γ_j is the limits of temporal integration between timesteps $k\Delta t$ and $(k+1)\Delta t$. Equation (7) can be rewritten by using the linear transformation:

$$\begin{cases} t = k\Delta t + \varepsilon \\ 0 \leq \varepsilon \leq \Delta t \end{cases} \quad (8)$$

Thus,

$$\begin{aligned} \int_0^{\Delta t} \left\{ D(k\Delta t + \varepsilon) \frac{\partial C(k\Delta t + \varepsilon)}{\partial x} \right\} \Big|_{\Gamma_j} d\varepsilon &= \int_{\Omega_j} \{C\} \Big|_{\Gamma_j} dx + \\ &\int_0^{\Delta t} \{U(k\Delta t + \varepsilon)C(k\Delta t + \varepsilon)\} \Big|_{\Gamma_j} d\varepsilon \end{aligned} \quad (9)$$

The diffusivity and advection parameters can be expressed with respect to time by the Taylor series:

$$\xi(x = x_0, k\Delta t + \varepsilon) = \sum_{i=0}^{\infty} \frac{\xi^{(i)}(x = x_0, k\Delta t) \varepsilon^i}{i!}; \quad \xi = U, D \quad (10)$$

where (i) is the i th order temporal partial differential operator; and x_0 is a specified spatial coordinate. Combining equations (9) and (10) gives:

$$\begin{aligned} \int_0^{\Delta t} \left\{ \left(\sum_{i=0}^{\infty} \frac{D^{(i)}(k\Delta t) \varepsilon^i}{i!} \right) \frac{\partial C(k\Delta t + \varepsilon)}{\partial x} \right\} \Big|_{\Gamma_j} d\varepsilon &= \int_{\Omega_j} \{C\} \Big|_{\Gamma_j} dx + \\ \int_0^{\Delta t} \left\{ \left(\sum_{i=0}^{\infty} \frac{U^{(i)}(k\Delta t) \varepsilon^i}{i!} \right) C(k\Delta t + \varepsilon) \right\} \Big|_{\Gamma_j} d\varepsilon \end{aligned} \quad (11)$$

For a spatial local coordinate system defined by:

$$\begin{cases} y \equiv \{y | 0 \leq y \leq l_j, x \in \Omega_j\} \\ dy = dx \\ l_j = |\Omega_j| \end{cases} \quad (12)$$

Equation (11) can be expanded as:

$$\begin{aligned} \sum_{i=0}^{\infty} \frac{D^{(i)}(y=l_j, k\Delta t)}{i!} \int_0^{\Delta t} \varepsilon^i \left\{ \frac{\partial C(k\Delta t + \varepsilon)}{\partial y} \right\} \Big|_{y=l_j} d\varepsilon - \\ \sum_{i=0}^{\infty} \frac{D^{(i)}(y=0, k\Delta t)}{i!} \int_0^{\Delta t} \varepsilon^i \left\{ \frac{\partial C(k\Delta t + \varepsilon)}{\partial y} \right\} \Big|_{y=0} d\varepsilon \\ = \int_{\Omega_j} \{C\} \Big|_{\Gamma_j} dy + \sum_{i=0}^{\infty} \frac{U^{(i)}(y=l_j, k\Delta t)}{i!} \int_0^{\Delta t} \varepsilon^i \{C(k\Delta t + \varepsilon)\} \Big|_{y=l_j} d\varepsilon - \\ \sum_{i=0}^{\infty} \frac{U^{(i)}(y=0, k\Delta t)}{i!} \int_0^{\Delta t} \varepsilon^i \{C(k\Delta t + \varepsilon)\} \Big|_{y=0} d\varepsilon \end{aligned} \quad (13)$$

To this point, equation (13) is an exact statement of equation (1), and to proceed to a solvable numerical algorithm the following inexact approximation is made:

$$\begin{cases} C \simeq \hat{C} \\ \hat{C} = \sum_{r=1}^n N_r \left(\sum_{m=0}^{k+1} M_m C_r^m \right) \end{cases} \quad (14)$$

where the solute-concentration function is approximated spatially and temporally and where N_r and M_m are the linearly independent spatial and temporal shape functions, and

$$C_r^m = \hat{C}(x = x_r, t = m \Delta t) \quad (15)$$

where the C_r^m are known values for timesteps m

= {0, 1, ..., k}, and x_r is the spatial coordinate of node r . The spatial gradient of the soil-water content function is approximated by:

$$\frac{\partial C}{\partial x} \approx \frac{\partial \hat{C}}{\partial x} = \sum_{r=1}^n \frac{\partial N_r}{\partial x} \left(\sum_{m=0}^{k+1} M_m C_r^m \right) \quad (16)$$

Substituting equations (14) and (16) into equation (13) gives the numerical approximation:

$$\begin{aligned} & \sum_{i=0}^{\infty} \frac{D^{(i)}(y=l_j, k\Delta t)}{i!} \int_0^{\Delta t} \varepsilon^i \left\{ \sum_{r=1}^n \frac{\partial N_r}{\partial x} \left(\sum_{m=0}^{k+1} M_m C_r^m \right) \right\} \Big|_{y=l_j} d\varepsilon - \\ & \sum_{i=0}^{\infty} \frac{D^{(i)}(y=0, k\Delta t)}{i!} \int_0^{\Delta t} \varepsilon^i \left\{ \sum_{r=1}^n \frac{\partial N_r}{\partial x} \left(\sum_{m=0}^{k+1} M_m C_r^m \right) \right\} \Big|_{y=0} d\varepsilon \\ & = \int_0^{l_j} \left\{ \sum_{r=1}^n N_r \left(\sum_{m=0}^{k+1} M_m C_r^m \right) \right\} \Big|_{\Gamma_j} dy + \end{aligned} \quad (17)$$

$$\begin{aligned} & \sum_{i=0}^{\infty} \frac{U^{(i)}(y=l_j, k\Delta t)}{i!} \int_0^{\Delta t} \varepsilon^i \left\{ \sum_{r=1}^n N_r \left(\sum_{m=0}^{k+1} M_m C_r^m \right) \right\} \Big|_{y=l_j} d\varepsilon - \\ & \sum_{i=0}^{\infty} \frac{U^{(i)}(y=0, k\Delta t)}{i!} \int_0^{\Delta t} \varepsilon^i \left\{ \sum_{r=1}^n N_r \left(\sum_{m=0}^{k+1} M_m C_r^m \right) \right\} \Big|_{y=0} d\varepsilon \end{aligned}$$

The unknown values of nodal points C_r^{k+1} can be solved by:

$$\sum_{i=0}^{\infty} \frac{D^{(i)}(y=l_j, k\Delta t)}{i!} \int_0^{\Delta t} \varepsilon^i \left\{ \sum_{r=1}^n \frac{\partial N_r}{\partial x} M_{k+1} C_r^{k+1} \right\} \Big|_{y=l_j} d\varepsilon -$$

$$\sum_{i=0}^{\infty} \frac{D^{(i)}(y=0, k\Delta t)}{i!} \int_0^{\Delta t} \varepsilon^i \left\{ \sum_{r=1}^n \frac{\partial N_r}{\partial x} M_{k+1} C_r^{k+1} \right\} \Big|_{y=0} d\varepsilon$$

$$\begin{aligned} & = \int_0^{l_j} \sum_{r=1}^n N_r C_r^{k+1} dx + \sum_{i=0}^{\infty} \frac{U^{(i)}(y=0, k\Delta t)}{i!} \times \\ & \int_0^{\Delta t} \varepsilon^i \left\{ \sum_{r=1}^n N_r M_{k+1} C_r^{k+1} \right\} \Big|_{y=0} d\varepsilon - \end{aligned}$$

$$\begin{aligned} & \sum_{i=0}^{\infty} \frac{U^{(i)}(y=l_j, k\Delta t)}{i!} \int_0^{\Delta t} \varepsilon^i \left\{ \sum_{r=1}^n N_r M_{k+1} C_r^{k+1} \right\} \Big|_{y=l_j} d\varepsilon \\ & = \sum_{i=0}^{\infty} \frac{D^{(i)}(y=0, k\Delta t)}{i!} \int_0^{\Delta t} \varepsilon^i \left\{ \sum_{r=1}^n \frac{\partial N_r}{\partial x} \left(\sum_{m=0}^k M_m C_r^m \right) \right\} \Big|_{y=0} d\varepsilon - \end{aligned}$$

$$\sum_{i=0}^{\infty} \frac{D^{(i)}(y=l_j, k\Delta t)}{i!} \int_0^{\Delta t} \varepsilon^i \left\{ \sum_{r=1}^n \frac{\partial N_r}{\partial x} \left(\sum_{m=0}^k M_m C_r^m \right) \right\} \Big|_{y=l_j} d\varepsilon -$$

$$\begin{aligned} & \int_0^{l_j} \sum_{r=1}^n N_r C_r^k dx + \sum_{i=0}^{\infty} \frac{U^{(i)}(y=l_j, k\Delta t)}{i!} \times \\ & \int_0^{\Delta t} \varepsilon^i \left\{ \sum_{r=1}^n N_r \left(\sum_{m=0}^k M_m C_r^m \right) \right\} \Big|_{y=l_j} d\varepsilon - \end{aligned} \quad (18)$$

DISCRETIZED DOMAIN NUMERICAL MODEL

The space-time surface approximated by equation (14) can be simplified by assuming that the functional surfaces $C(x,t)$ can be described by sets of piecewise continuous functions. For a first order polynomial spatial trial function approximation \hat{C} for C between nodal points (C_{j-1}, C_j, C_{j+1})

$$\left. \begin{aligned} \frac{\partial \hat{C}}{\partial x} \Big|_{y=l} &= (C_{j+1} - C_j)/l \\ \frac{\partial \hat{C}}{\partial x} \Big|_{y=0} &= (C_j - C_{j-1})/l \\ \int_0^l \hat{C} dy &= \frac{l}{8} [C_{j-1} + 6C_j + C_{j+1}] \\ \{\hat{C}\} \Big|_{\Gamma_j} &= \frac{1}{2} (C_{j+1} - C_{j-1}) \end{aligned} \right\} \quad (19)$$

where for discussion purposes it is assumed that $l_j = l$.

For Δt timesteps of equation (18) small, a linear polynomial function approximation may be used for the time curves between timesteps ($k, k+1$) where ($k+1$) is the timestep to be evaluated, thus

$$\left. \begin{aligned} C_j(k\Delta t + \varepsilon) &= (C_j^{k\Delta t}) \left(\frac{\Delta t - \varepsilon}{\Delta t} \right) + (C_j^{(k+1)\Delta t}) \frac{\varepsilon}{\Delta t} \\ k\Delta t \leq t \leq (k+1)\Delta t \\ d\varepsilon &= dt \end{aligned} \right\} \quad (20)$$

Combining equations (19) and (20), the spatial gradient approximation during the time-step Δt as a function of time is:

$$\left. \begin{aligned} \frac{\partial \hat{C}}{\partial x} \Big|_{y=l} &= (C_{j+1}^2 - C_{j+1}^1 - C_j^2 + C_j^1)\varepsilon/l\Delta t + (C_{j+1}^1 - C_j^1)/l \\ \frac{\partial \hat{C}}{\partial x} \Big|_{y=0} &= (C_j^2 - C_j^1 - C_{j-1}^2 + C_{j-1}^1)\varepsilon/l\Delta t + (C_j^1 - C_{j-1}^1)/l \\ 0 \leq \varepsilon \leq \Delta t \end{aligned} \right\} \quad (21)$$

where superscripts 1 and 2 refer to timesteps $k\Delta t$ and $(k+1)\Delta t$, respectively. Combining equations (18), (19), (20) and (21) gives a type of subdomain integration model incorporating the expansion of the non-linear terms $D(C)$ and $U(C)$ over the timestep Δt :

$$\begin{aligned} & \sum_{i=0}^{\infty} \frac{D^{(i)}(y=l)}{i!} \int_0^{\Delta t} \left\{ (C_{j+1}^2 - C_{j+1}^1 - C_j^2 - C_j^1) \frac{\varepsilon^{i+1}}{l\Delta t} + \right. \\ & \left. (C_{j+1}^1 - C_j^1) \frac{\varepsilon^i}{l} \right\} d\varepsilon - \sum_{i=0}^{\infty} \frac{D^{(i)}(y=0)}{i!} \times \\ & \int_0^{\Delta t} \left\{ (C_j^2 - C_j^1 - C_{j+1}^2 + C_{j+1}^1) \frac{\varepsilon^{i+1}}{l\Delta t} + (C_j^1 - C_{j-1}^1) \frac{\varepsilon^i}{l} \right\} d\varepsilon \\ & = \frac{l}{8} [C_{j-1}^2 + 6C_j^2 + C_{j+1}^2] - \frac{l}{8} [C_{j-1}^1 + 6C_j^1 + C_{j+1}^1] + \\ & \sum_{i=0}^{\infty} \frac{U^{(i)}(y=l)}{i!} \int_0^{\Delta t} \frac{1}{2} \left\{ C_{j+1}^1 \varepsilon^i + (C_{j+1}^2 - C_{j+1}^1) \frac{\varepsilon^{i+1}}{\Delta t} \right\} d\varepsilon - \\ & \sum_{i=0}^{\infty} \frac{U^{(i)}(y=0)}{i!} \int_0^{\Delta t} \frac{1}{2} \left\{ C_{j-1}^1 \varepsilon^i + (C_{j-1}^2 - C_{j-1}^1) \frac{\varepsilon^{i+1}}{\Delta t} \right\} d\varepsilon \quad (22) \end{aligned}$$

Carrying out the indicated integration in equation (22) gives:

$$\begin{aligned} & [C_{j+1}^2 - C_j^2] \sum_{i=0}^{\infty} \frac{D^{(i)}(y=l)(\Delta t)^{i+1}}{i! (i+2)} - \\ & [C_j^2 - C_{j-1}^2] \sum_{i=0}^{\infty} \frac{D^{(i)}(y=0)(\Delta t)^{i+1}}{i! (i+2)} + \\ & [C_{j+1}^1 - C_j^1] \sum_{i=0}^{\infty} \frac{D^{(i)}(y=l)(\Delta t)^{i+1}}{i! (i+1)(i+2)} - \\ & [C_j^1 - C_{j-1}^1] \sum_{i=0}^{\infty} \frac{D^{(i)}(y=0)(\Delta t)^{i+1}}{i! (i+1)(i+2)} \quad (23) \\ & = \frac{l}{8} [C_{j-1}^2 + 6C_j^2 + C_{j+1}^2] - \frac{l}{8} [C_{j-1}^1 + 6C_j^1 + C_{j+1}^1] + \\ & \frac{1}{2} C_{j+1}^2 \sum_{i=0}^{\infty} \frac{U^{(i)}(y=l)(\Delta t)^{i+1}}{i!(i+2)} + \frac{1}{2} C_{j+1}^1 \sum_{i=0}^{\infty} \frac{U^{(i)}(y=l)(\Delta t)^{i+1}}{(i+2)!} - \\ & \frac{1}{2} C_{j-1}^2 \sum_{i=0}^{\infty} \frac{U^{(i)}(y=0)(\Delta t)^{i+1}}{i!(i+2)} - \frac{1}{2} C_{j-1}^1 \sum_{i=0}^{\infty} \frac{U^{(i)}(y=0)(\Delta t)^{i+1}}{(i+2)!} \end{aligned}$$

In a different notation, equation (23) can be rewritten as:

$$\begin{aligned} & \bar{D}_l [C_{j+1}^2 - C_j^2] - \bar{D}_0 [C_j^2 - C_{j-1}^2] - \frac{1}{2} \bar{U}_l C_{j+1}^2 + \frac{1}{2} \bar{U}_0 C_{j-1}^2 - \\ & \frac{l}{8} [C_{j-1}^2 + 6C_j^2 + C_{j+1}^2] = -\frac{l}{8} [C_{j-1}^1 + 6C_j^1 + C_{j+1}^1] - \end{aligned}$$

$$\bar{D}_l [C_{j+1}^1 - C_j^1] + \bar{D}_0 [C_j^1 - C_{j-1}^1] + \frac{1}{2} \bar{U}_l C_{j+1}^1 - \frac{1}{2} \bar{U}_0 C_{j-1}^1 \quad (24)$$

where

$$\left. \begin{aligned} \bar{D}_\lambda &= \sum_{i=0}^{\infty} \frac{D^{(i)}(y=\lambda)(\Delta t)^{i+1}}{i!(i+2)!}; \lambda=0, l \\ \bar{D}_\lambda &= \sum_{i=0}^{\infty} \frac{D^{(i)}(y=\lambda)(\Delta t)^{i+1}}{(i+2)!}; \lambda=0, l \\ \bar{U}_\lambda &= \sum_{i=0}^{\infty} \frac{U^{(i)}(y=\lambda)(\Delta t)^{i+1}}{i!(i+2)!}; \lambda=0, l \\ \bar{U}_\lambda &= \sum_{i=0}^{\infty} \frac{U^{(i)}(y=\lambda)(\Delta t)^{i+1}}{(i+2)!}; \lambda=0, l \end{aligned} \right\} \quad (25)$$

For the advective and diffusivity parameters constant in Ω , and for a linear polynomial trial function approximation of solute concentration between nodal points with respect to both space and time, equation (24) reduces to:

$$\begin{aligned} & \frac{D_0}{2l} [C_{j+1}^2 - 2C_j^2 + C_{j-1}^2 + C_{j+1}^1 - 2C_j^1 + C_{j-1}^1] - \\ & \frac{U_0}{2} [(C_{j+1}^2 - C_{j-1}^2)/2 + (C_{j+1}^1 - C_{j-1}^1)/2] \quad (26) \end{aligned}$$

$$= \frac{l}{\Delta t} [(C_{j-1}^2 + 6C_j^2 + C_{j+1}^2)/8 - (C_{j-1}^1 + 6C_j^1 + C_{j+1}^1)/8]$$

Pinder and Gray¹⁰ develop a finite difference and Galerkin finite element numerical analog for equation (1) in order to compare relative numerical efficiency between these two common modelling approaches. The finite element, finite difference, and subdomain integration formulation of equation (26) can be represented by a single modelling statement for a Crank-Nicolson time advancement approximation:

$$\begin{aligned} & \frac{D_0}{2l} [C_{j+1}^2 - 2C_j^2 + C_{j-1}^2 + C_{j+1}^1 - 2C_j^1 + C_{j-1}^1] - \\ & \frac{U_0}{2} [(C_{j+1}^2 - C_{j-1}^2)/2 + (C_{j+1}^1 - C_{j-1}^1)/2] \quad (27) \end{aligned}$$

$$= \frac{l}{2\Delta t(\eta+1)} [(C_{j-1}^2 + 2\eta C_j^2 + C_{j+1}^2) - (C_{j-1}^1 + 2\eta C_j^1 + C_{j+1}^1)]$$

where in equation (27) the finite element, subdomain integration, and finite difference methods are determined by $\eta = (2, 3, \infty)$ respectively. Equation (27) can be written in an element matrix system:

$$\begin{aligned} & -\frac{D_0}{l} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{Bmatrix} C_i \\ C_{i+1} \end{Bmatrix} + \frac{U_0}{2} \begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix} \begin{Bmatrix} C_i \\ C_{i+1} \end{Bmatrix} \\ & = \frac{l}{2(\eta+1)} \begin{bmatrix} \eta & 1 \\ 1 & \eta \end{bmatrix} \begin{Bmatrix} \partial C_i / \partial t \\ \partial C_{i+1} / \partial t \end{Bmatrix} \quad (28) \end{aligned}$$

where the so-called capacitance matrix (time derivative component) contains all η -term information similar to the soil-water diffusivity model matrix system determined in Hromadka and Guymon⁵. For a Crank-Nicolson time advancement approximation equation (28) may be written as:

$$\left(\mathbf{P} + \frac{\Delta t}{2}\mathbf{S}\right)\{\mathbf{C}^2\} = \left(\mathbf{P} - \frac{\Delta t}{2}\mathbf{S}\right)\{\mathbf{C}^1\} \quad (29)$$

where $\{\mathbf{C}^k\}$ are the element nodal points at timestep k , and

$$\mathbf{S} = \frac{D_0}{l} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} - \frac{U_0}{2} \begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix} \quad (30)$$

$$\mathbf{P} = \frac{l}{2(\eta + 1)} \begin{bmatrix} \eta & 1 \\ 1 & \eta \end{bmatrix} \quad (31)$$

LINEAR MODEL OF HIGHER ORDER SHAPE FUNCTION (NODAL DOMAIN INTEGRATION MODEL)

Hromadka and Guymon⁶ examined two methods of approximating a higher order or more complex family of trial functions by a linear polynomial trial function approximation. One method used the Alternation theorem in order to determine an 'optimum' linear polynomial estimate of a higher order approximator. A second approach was the definition of an element matrix system that approximated the integration and gradients of a higher order approximator \hat{C} of C within each nodal domain, Ω_j . This second approach is reviewed in the following, and another technique of determining η as a function of time examined in a following section. A constant diffusivity diffusion process (without advection) is used for model development purposes.

Let \bar{C} be an approximation function of a higher order approximation \hat{C} of C , where the spatial gradients of \bar{C} on Γ_j are defined by:

$$\left\{ \frac{\partial \bar{C}}{\partial x} \right\}_{\Gamma_j} = \frac{(C_{j+1} - C_j)}{l} - \frac{(C_j - C_{j-1})}{l} \quad (32)$$

A spatial gradient adjustment function $e(x,t)$ is defined by:

$$e(x,t) = \begin{cases} \frac{\partial \hat{C}}{\partial x} / \frac{\partial \bar{C}}{\partial x}; & 0 < e < \infty \\ 1; & \text{otherwise} \end{cases} \quad (33)$$

Therefore, it is assumed that:

$$D \frac{\partial \hat{C}}{\partial x} = e D \frac{\partial \bar{C}}{\partial x} \quad (34)$$

where

$$\left\{ D \frac{\partial \hat{C}}{\partial x} \right\}_{\Gamma_j} = \left\{ e D \frac{\partial \bar{C}}{\partial x} \right\}_{\Gamma_j} \quad (35)$$

On Γ_j , define

$$eD = A(t); \quad k\Delta t \leq t \leq (k+1)\Delta t \quad (36)$$

such that:

$$A(k\Delta t + \varepsilon) = \sum_{i=0}^{\infty} A^{(i)}(k\Delta t) \frac{\varepsilon^i}{i!}; \quad 0 \leq \varepsilon \leq \Delta t \quad (37)$$

where (i) represents the ith order temporal partial differential operator. Then

$$\left\{ D \frac{\partial \hat{C}}{\partial x} \right\}_{\Gamma_j} = \left\{ \sum_{i=0}^{\infty} A^{(i)}(k\Delta t) \frac{\varepsilon^i \partial \bar{C}}{i! \partial x} \right\}_{\Gamma_j} \quad (38)$$

A function $\eta(t)$ is defined by

$$\int_{\Omega_j} \hat{C} dx = \frac{l}{2[\eta(t)+1]} [C_{j-1} + 2C_j\eta(t) + C_{j+1}] \quad (39)$$

where

$$\eta(t) \neq -1 \quad (40)$$

The value of 3 in equation (40) corresponds to a first order polynomial \hat{C} function subdomain approximation for C , whereas $\eta(t) = 2$ corresponds to a Galerkin finite element model, and $\eta(t) = \infty$ determines a finite difference model.

The \bar{C} approximator is also defined to have the property:

$$\int_{\Omega_j} \bar{C} dx \equiv \int_{\Omega_j} \hat{C} dx, \quad \eta(t) \neq -1 \quad (41)$$

For a diffusion process without advection, $U_0 = 0$ in equation (1). Therefore, substituting equations (38) and (41) into equation (18) gives the modelling statement (for $U_0 = 0$):

$$\int_{\Delta t} \left\{ \sum_{i=0}^{\infty} A^{(i)}(k\Delta t) \frac{\varepsilon^i \partial \bar{C}}{i! \partial x} \right\}_{\Gamma_j} d\varepsilon = \frac{l[C_{j-1} + 2C_j\eta(k\Delta t + \Delta t) + C_{j+1}]}{2[\eta(k\Delta t + \Delta t) + 1]} - \frac{l[C_{j-1} + 2C_j\eta(k\Delta t) + C_{j+1}]}{2[\eta(k\Delta t) + 1]} \quad (42)$$

where

$$\eta(k\Delta t + \varepsilon) = \sum_{i=0}^{\infty} \eta^{(i)}(k\Delta t) \frac{\varepsilon^i}{i!}; \quad 0 \leq \varepsilon \leq \Delta t \quad (43)$$

Analogous to the development leading to equations (24) and (25):

$$\left. \begin{aligned} \bar{A}(\lambda) &= \frac{1}{l} \sum_{i=0}^{\infty} \frac{A_i(\xi)(\Delta t)^{i+1}}{i!(i+2)} \\ \bar{A}(\lambda) &= \frac{1}{l} \sum_{i=0}^{\infty} \frac{A_i(\xi)(\Delta t)^{i+1}}{(i+2)!} \end{aligned} \right\} \lambda = (0, l) \quad (44)$$

The nodal domain integration element matrix system similar to equation (29) is written as:

$$\left(\bar{\mathbf{p}} + \frac{\Delta t}{2}\bar{\mathbf{s}}\right)\{C^2\} = \left\{\bar{\mathbf{p}} - \frac{\Delta t}{2}\bar{\mathbf{s}}\right\}\{C^1\} \quad (45)$$

where,

$$\left. \begin{aligned} \bar{\mathbf{s}} &= \bar{\mathbf{A}} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \\ \bar{\mathbf{s}} &= \bar{\mathbf{A}} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \\ \bar{\mathbf{p}} &= \frac{l}{2(\bar{\eta} + 1)} \begin{bmatrix} \bar{\eta} & 1 \\ 1 & \bar{\eta} \end{bmatrix} \\ \bar{\mathbf{p}} &= \frac{l}{2(\bar{\eta} + 1)} \begin{bmatrix} \bar{\eta} & 1 \\ 1 & \bar{\eta} \end{bmatrix} \end{aligned} \right\} \quad (46)$$

where $\bar{\eta} = \eta(k\Delta t + \Delta t)$, $\bar{\eta} = \eta(k\Delta t)$.

APPLICATION OF LINEAR MODEL

The approach to be used for determining a higher order approximation \hat{C} of C in Ω is to determine C as a function of $\partial C/\partial t$ spatially distributed within each Ω_j . The problem of a one-dimensional diffusion process with constant parameters where the solute concentration is initially C_0 and the concentration is decreased in stepwise fashion to C_1 at both ends of the one-dimensional domain Ω is used in order to compare previous modelling results⁸ to the proposed approach. The diffusion problem can be normalized as:

$$\frac{\partial^2 C}{\partial x^2} = \frac{\partial C}{\partial t}, \quad x \in \Omega \quad (47)$$

where

$$\begin{aligned} \Omega &\equiv \{x|0 \leq x \leq 1\} \\ C(x,t=0) &= 1, \quad x \in \Omega \\ C(x=0,1;t > 0) &= 0 \end{aligned} \quad (48)$$

The problem domain Ω is assumed discretized into two finite elements ($\bar{\Omega}_1, \bar{\Omega}_2$) of equal length by three nodal points (C_1, C_2, C_3) where $(x_1, x_2, x_3) = (0, 0.5, 1)$. Owing to the boundary conditions of equation (48), the resulting system of modelled linear equations reduces to a single equation of one unknown, C_2 . In order to evaluate the effectiveness of the proposed numerical approach to modelling equations (47) and (48), the Galerkin finite element, finite difference, subdomain, and nodal domain integration solutions will also be presented for comparison purposes.

For the study problem of equations (47) and (48), the considered domain numerical solutions result in the expression⁸:

$$\lim_{\Delta t \rightarrow 0} C_2(t) = \exp\left[-8\left(\frac{\eta+1}{\eta}\right)t\right], \quad t \geq 0 \quad (49)$$

where η is the entry in the capacitance matrix $\mathbf{P}(\eta)$ of equation (31).

Within Ω_2 , an approximation \hat{C} of C can be determined from equation (47) by integrating twice (with respect to x)

the time derivative of C . Thus, for some instant in time t_0 , it may be assumed in Ω_2 :

$$\frac{\partial C}{\partial t}(x,t=t_0) \approx \dot{C}_2 = \frac{\partial^2 \hat{C}}{\partial x^2} \quad (50)$$

where \dot{C}_2 is a finite difference estimate of the time derivative of C at the variable nodal point. Integrating equation (50) with respect to space gives for Ω_2 :

$$\frac{\partial \hat{C}}{\partial x}(x,t=t_0) \approx \dot{C}_2 x + \alpha \quad (51)$$

A finite difference estimate of $\partial C/\partial x$ at node 2 determines the value α . Integrating a second time,

$$\hat{C}(x,t=t_0) = \frac{1}{2}\dot{C}_2 x^2 - \frac{1}{2}\dot{C}_2 x + \beta \quad (52)$$

Evaluating equation (52) for C_2 gives in Ω_2 :

$$\hat{C}(x,t=t_0) = \frac{1}{2}\dot{C}_2 \left(x^2 - x + \frac{1}{4}\right) + C_2 \quad (53)$$

For the approximation \hat{C} of C in Ω_2 given in equation (53),

$$\int_{\Omega_2} \hat{C} \, dx = \frac{\dot{C}_2}{192} + \frac{C_2}{2} \quad (54)$$

From equations (45) and (46), for $e=1$, the modelling statement similar to equation (49) is:

$$\left. \begin{aligned} \frac{\partial}{\partial t} \left[\frac{\dot{C}_2}{192} + \frac{C_2}{2} \right] &= -4C_2 \\ C_2(t) &= (-0.11237)e^{-87.1918t} + (1.11237)e^{-8.8082t}; \quad t > 0 \end{aligned} \right\} \quad (55)$$

Table 1 gives a comparison of the analytical solution to equations (47) and (48) to the considered domain solutions of 49 (for $\eta=2,3,\infty$) and the proposed model of equation (55). From Table 1, a significant increase in accuracy is provided by the proposed modelling

Table 1. Numerical solution of normalized diffusion problem (one variable nodal point)

Time	$\eta=2^*$	$\eta=3^\dagger$	$\eta=\infty^\ddagger$	Linear model**	Analytic solution
0.01	0.887	0.889	0.923	0.972	0.999
0.02	0.787	0.808	0.852	0.913	0.975
0.03	0.698	0.726	0.787	0.846	0.918
0.04	0.619	0.653	0.726	0.779	0.846
0.05	0.549	0.587	0.670	0.715	0.772
0.10	0.301	0.344	0.449	0.461	0.474
0.15	0.165	0.202	0.301	0.297	0.290
0.20	0.091	0.118	0.202	0.191	0.171
0.25	0.050	0.069	0.135	0.123	0.108
0.30	0.027	0.041	0.091	0.080	0.066

* Galerkin finite element method
 † Subdomain model
 ‡ Finite difference model
 ** Nodal domain integration model

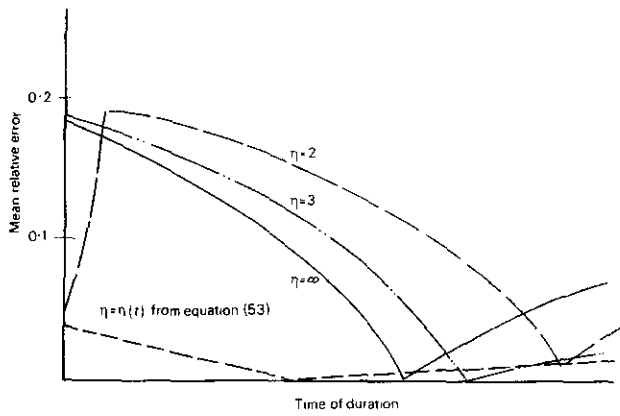


Figure 1. Typical mean relative error from numerical model of diffusion-dominated process ($D_0 = 1.0$; $U_0 = 0.05$)

approach. As another example, a second order polynomial estimate of $\hat{C}_2(x, t = t_0)$ is possible using the information provided at all three nodes. Thus in Ω_2 ,

$$\hat{C}_2(x, t = t_0) = \frac{\partial^2 \hat{C}_2}{\partial x^2} = -4x^2 \hat{C}_2 + 4x \hat{C}_2 \quad (56)$$

Similar to equations (50)-(55), for $x \in \Omega_2$

$$\hat{C}(x, t = t_0) = \left(-\frac{1}{3} \hat{C}_2 \right) \left[x^4 - 2x^3 + x - \frac{5}{16} \right] + C_2 \quad (57)$$

giving

$$C_2 = (-0.1086)e^{-89.678t} + (1.1086)e^{-8.7836t}; t \geq 0 \quad (58)$$

Comparison of equations (55) and (58) shows that little advantage is gained by the extra computational effort in a higher order estimate of \hat{C} in Ω_2 by the proposed technique.

APPLICATION TO ADVECTIVE-DIFFUSION PROBLEM

The advection-diffusion element matrix system statement of equation (29) is a function of the element capacitance matrix diagonal entry, η . For constant parameters, the following problem was analysed in order to evaluate the sensitivity of equation (29) to variations of η :

$$D_0 \frac{\partial^2 C}{\partial x^2} - U_0 \frac{\partial C}{\partial x} = \frac{\partial C}{\partial t}; x \in \Omega \quad (59)$$

with initial and boundary conditions

$$\left. \begin{aligned} C(x, t = 0) &= 0; x \in \Omega \\ C(1, t > 0) &= 1 \\ C(\infty, t \geq 0) &= 0 \\ \Omega: \{x | x \geq 0\} \end{aligned} \right\} \quad (60)$$

For a linear trial function approximation of the state variable C with respect to time, the numerical analog reduces to the Crank-Nicolson time advancement

approximation. Diffusivity (D_0) was set to 1.0 whereas the parameter U_0 was varied from 0.0 to 10.0. More than 200 separate simulations were made in order to evaluate η as a function of uniform element size Δx , timestep size Δt , and advective parameter U_0 . Results of this sensitivity study indicates that with respect to relative error, the use of a constant η value throughout the simulation (e.g. $\eta = 2, 3, \infty$) provides varying qualities of accuracy (Fig. 1). That is, for each assumed constant η -value, the resulting numerical analog produced good results depending where in time and space the model solution is examined for error. It was noted, however, that for the smaller U_0 values tested, better results were obtained for small η values ($\eta = 2, 3$); whereas for large U_0 values, large η values ($\eta = \infty$) produced better results. Additionally, it is noted that these determinations are based on a specific advection-diffusion problem; another class of problems may produce different conclusions of modelling trends such as found in Hromadka and Guymon⁵ where η was found to be somewhat dependent on the spatial gradient of the problem's solution profile. From the above, varying η as a function of time (and between elements) is suggested. Two methods of determining values of $\eta(t)$ are given in Hromadka and Guymon⁸ where the approach used is to determine a linear polynomial trial function approximation of a higher order or more complex family of state variable approximation functions. A third approach in determining $\eta(t)$ is given in the previous section where a strict diffusion process is modelled.

CONCLUSIONS

A method of modelling a higher order trial function approximation of advection-diffusion by an improved linear trial function approximation set has been developed. This method retains the smaller symmetric matrix system associated to numerical models of advection-diffusion based on a linear polynomial trial function, but increase the numerical accuracy of the model by incorporating some of the benefits of a higher order approximation.

Since similarities between the various considered numerical methods (finite difference, Galerkin finite element, subdomain integration) are used in the proposed model, it is concluded that the proposed numerical approach may lead to a generalized modelling method for many classes of advection-diffusion problems. The computer code used for each simulation is identical except for a variation in the capacitance diagonal entry, η . Therefore, a comparison of numerical efficiency between the finite difference, Galerkin finite element, subdomain integration, and the proposed variable η term (nodal domain integration) approach is provided by the results obtained herein.

ACKNOWLEDGEMENT

This research was supported by the US Army Research Office (Grant No. DAAG29-79-C-0080).

REFERENCES

- 1 Desai, C. S. *Elementary Finite Element Methods*, Prentice-Hall, Englewood Cliffs, 1979
- 2 Cheney, E. W. *Introduction to Approximation Theory*, McGraw-Hill, New York, 1966
- 3 Guymon, G. L. and Luthin, J. N. A coupled heat and moisture

- transport model for arctic soils, *Water Resour. Res.* 1974, **10**, (5), 995
- 4 Hayhoe, H. N. Study of relative efficiency of finite difference and Galerkin techniques for modeling soil-water transfer, *Water Resour. Res.* 1978, **14**(1), 97
 - 5 Hromadka II, T. V. and Guymon, G. L. Some effects of linearizing the unsaturated soil-moisture transfer diffusion model, *Water Resour. Res.* 1980, **16**, 643
 - 6 Hromadka II, T. V. and Guymon, G. L. Numerical mass balance for soil-moisture transfer problems, *Adv. Water Resour.* 1980, **3**, 107
 - 7 Hromadka II, T. V. and Guymon, G. L. A note on time integration of unsaturated soil moisture transport, *Adv. Water Resour.* 1980, **3**, 181
 - 8 Hromadka II, T. V. and Guymon, G. L. Improved linear shape function model of soil moisture transport, *Water Resour. Res.* 1981, **17**, 504
 - 9 Philip, J. R. and Knight, J. H. On solving the unsaturated flow equation: 3, New quasi-analytic technique, *Soil Sci.* 1974, **117**, 1
 - 10 Pinder, G. F. and Gray, W. G. *Finite Element Simulation in Surface and Subsurface Hydrology*, Academic Press, New York, 1977