پژوهشی

# * حل دقیق معادله انتقال و انتشار جرم در آبهای زیرزمینی با استفاده از روش تلفیق پتروف و گالرکین(۱)

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**کلمات کلیدی :**

آبهای زیر زمینی ، حل تحلیلی ، حل دقیق ، حل عددی ، انتقال جرم ، عدد پکلت عدد کورانت.

**چکیده :**

به منظور حل معادلات چند بعدی انتقال و انتشار، روش تلفیق شده از پتروف و گالرکین توسط نیومن پیشنهاد گردید. از روش مذکور برای حل عددی شبکه‌های تو در تو به منظور محاسبه توابع وزنی از حل عددی استفاده می‌شود. کاربرد عددی روش مورد نظر بیانگر این نکته است که در اعداد **پکلت**(۲) کوچک بین پاسخهای تحلیلی و عددی سازگاری مناسبی وجود دارد. وقتی که عدد پکلت افزایش می‌یابد و متعاقب آن انتقال نسبت به انتشار غالب می‌شود نتایج به دست آمده بیانگر نوساناتی در نیمرخ عمودی غلظت و یا تأخیر بین پاسخ تحلیلی و پاسخ عددی می‌باشد. خود نوسانات تابعی از عدد پکلت و عدد **کورانت**(۳) هستند. پاسخهای دقیق هنگامی به دست می‌آید که برای اعداد پکلت تا ۵۰ ، عدد کورانت برابر یک باشد . برای اعداد بزرگتر از ۵۰ پاسخ عددی نسبت به پاسخ تحلیلی دارای تأخیر است. در سایر اعداد کورانت حداکثر عدد پکلت برای دستیابی به پاسخ پایدار به سرعت کاهش می‌یابد.

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** - استاد یار گروه مهندسی دانشکده محیط زیست دانشگاه تهران.

۱ - اصل مقاله به زبان انگلیسی در صفحات 2 الی 10 به چاپ رسیده است (سردبیر).

۱ - Petrov - Galerkin

۲ - Peclet

۳ - Courrant

## REFERENCES

1 - Abramowitz, M., and Stegun, I. A. 1964. Handbook of Mathematical Functions. Appl. Math. Ser., 55, National Bureau of Standards, Gaithersbug, MD. 1046 pp.

2 - Allen, M. B. and Pinder, G. F. 1983. Collocation Simulation of Multiphase Porous Medium Flow Soc. Pet. Eng. J., 23 (1): 135-142.

3 - Ardestani, K. M. 1994. Accurate and Stable Solution of Groundwater Mass Transpprt Equation using Fourier Transform and The Finite Analytical Method. Ph. D. Dissertation, Universety of Arizona.

4 - Ardestani, K. M. 1995. Solution of Advective - Dispersive Groundwater Mass Transport Equation using Fourier Transform and The Finite Analytical Method. proc. st first Regional Conference on Water Resources Management, Isfahan - Iran: 69-78.

5 - Christie, I., Griffiths, D. F. and Mitchell, A. R. 1976. Finite element method for second order differential equations with significant firstDerivatives. Int. J. Num. Method Eng., 10: 1389-1396.

6 - Hughes, T. J. R. and Brooks, A. 1982. A theoretical framework for Petov - Galerkin method with discontinuous weighting function: Application to the streamline - upwind procedure, in Finite Elements in Fluid. Vol. 4, Gallagher, et al., eds: 47-65, Wiley, N. Y.

7 - Herrera, I. 1987. The algebraic theory approach for ordinary differential equation: Highly accurate finite differencs. Numer. Meths. for Partial Differential equ. 3. (3): 199-218.

8 - Lapidus, L. and Amundson, N. R. 1952.Mathematics of adsorption in beds, VI. The effect of longitudinal diffusion in ion exchange and chromatographic column. J. Phys. Chem. 56: 984-988.

9 - Neuman, S. P. 1990. Adjoint Petrov - Galerkin Method with optimum Weight and Interpolation Functions defined on multidimensional Nested Grids. Computational Method in surface Hydrology Proc 8. International Conference Computational Methods Water Resources. Springer - Verlag, Berlin. Dept ZSW, Berlin 33, Ger: 347-356.

10 - Souissi, A. 1991. Numerical Simulation of Mass transport in Groundwater, Using Galerkin method. Ph. D. Dissrtetion, University of Arizona.

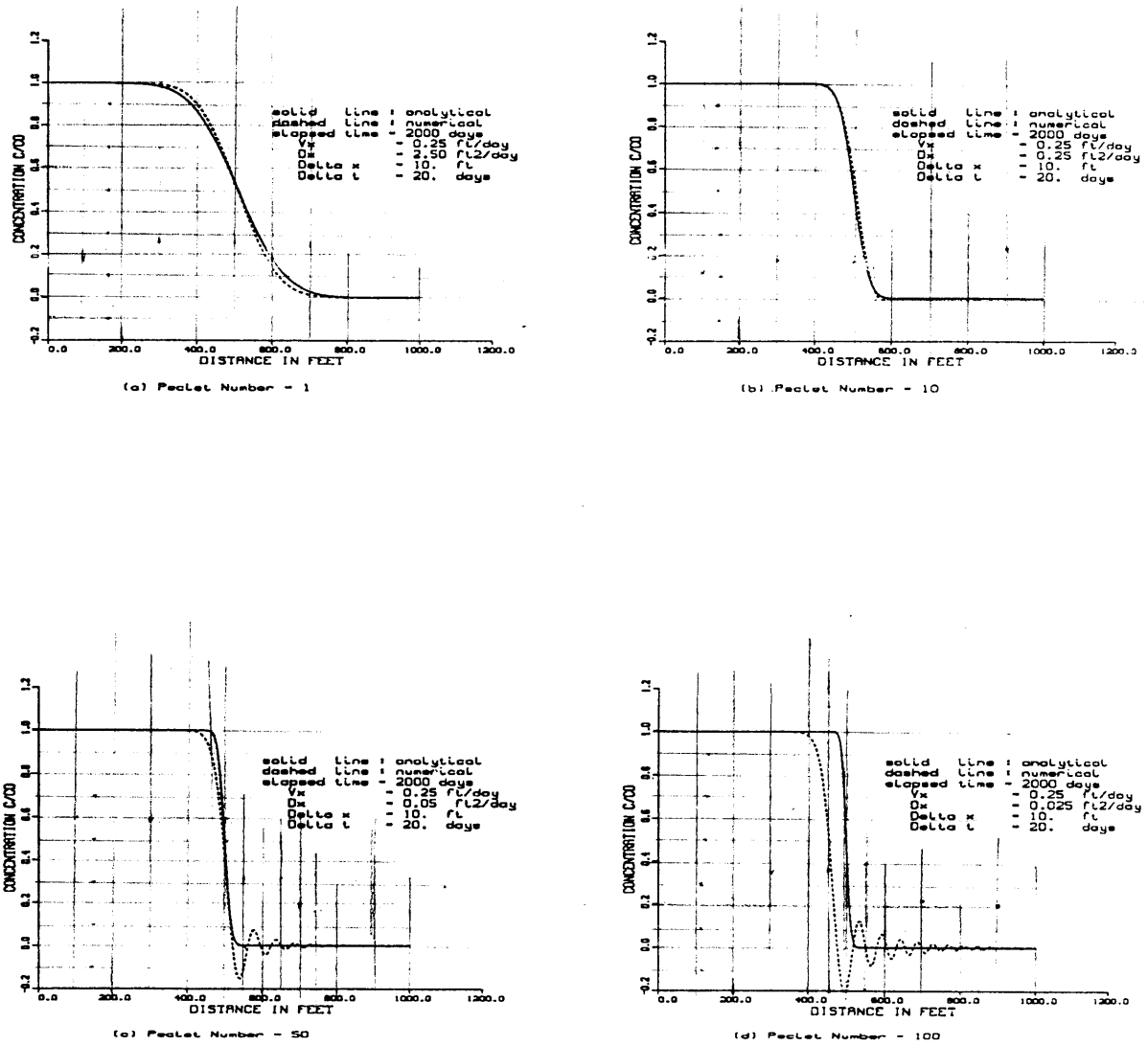


Figure 4. Comparison of analytical and numerical solutions. Incomplete cubic hermitian basis Function

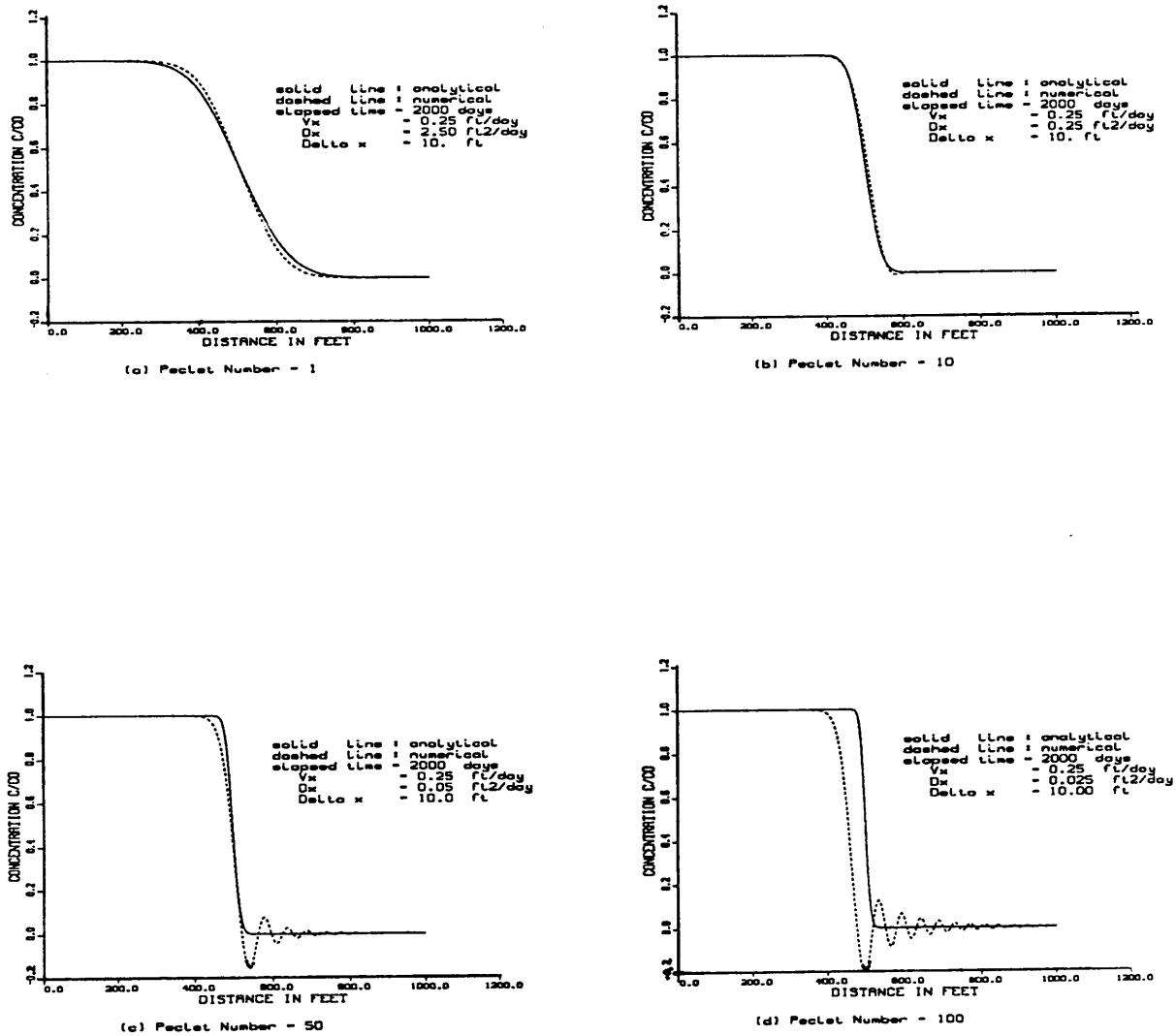


Figure 3. Comparison of analytical and numerical solutions. Linear basis function

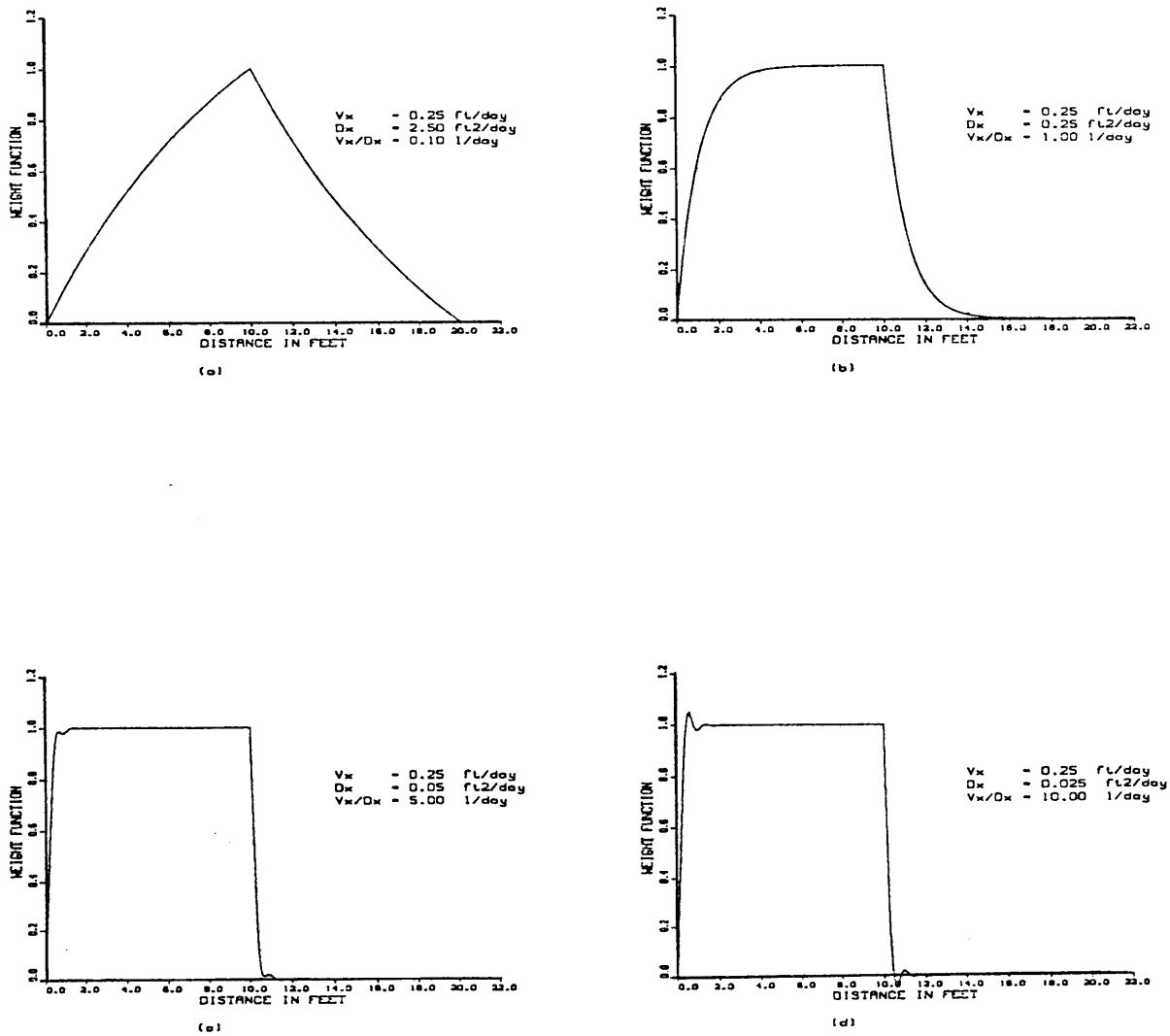


Figure 2. Weight function calculated from solution of the adjoint equation for different values of Vx/Dx

## NUMERICAL RESULTS

The program was applied to a one - dimensional aquifer of length l. At time t=0, the concentration of a pollutant is zero everywhere in the aquifer. For t>0, the concentration at x=0 is maintained at unity. The length of the aquifer is chosen so that the concentration at x=1 will be zero and will not influence the concentration within the aquifer.

The initial and boundary condition are summarized as:

$C(x, 0)=0$ for $0 \le x \le 1$

$C(x, t)=1$ for $t>0$

$C(l, t)=0$ for $t>0$

The parameter values used to construct the different curves are: node spacing ($\Delta x$)=10 ft, apparent groundwater velocity (VXE)=0.075 ft/day, porosity (n)=0.3, groundwater seepage velocity (VXEP)=0.25 ft/day, time step ($\Delta t$)=20 days, simulation time (t)=2000 days, retardation factor (**R**)=1, decay coefficient $\lambda$=0. The first node was treated as a constant concentration node with a relative concentration of 1. The dispersivity ($\alpha_L$) was varied so that the Peclet number ($P_e = \frac{V_x \Delta x}{D_x}$) of 1, 10, 50 and 100 were obtained. The Courant number ($C_u = \frac{V_x \Delta t}{D_x}$) was held constant for all four runs at 0.5. The exact concentration distrbution versus distance can be obtained form the analytical solution of [8] as

$$\frac{C}{C_0} = \frac{1}{2}\left[\text{erfc}\left(\frac{x - V_l t}{2\sqrt{D_l t}}\right) + \exp\left(\frac{V_l x}{D_l}\right)\text{erfc}\left(\frac{x + V_l t}{2\sqrt{D_l t}}\right)\right] \quad (22)$$

where erfc (u)=1 - erf (u) is the complementary error function [1].

The solution of equation (18) for concentration C was obtained using the appropriate weighting function $\omega$ and a linear interpolation function. The results of this method for different Peclet numbers are given in figures 3 (a) - 3 (d). The method was repeated using the incomplete cubic Hremitian function as the interpolation function. The results of these runs are shown in figure 4(a) - 4(d). The dashed line represents the numerical solution and the solid line represnts the analytical solution.

For low Peclet numbers less than 10, satisfactory results are obtained. The match between the analytical and numerical solution is quite good. When the Peclet number increases, advection becomes dominant and oscillations appear at downstream of the concentration front. For a Peclet number of 100, the oscillations increase in magnitude and the numerical solution lags behind the analytical solution.

## CONCLUSION

This numerical example clearly demonstrate the close interaction between the spatial and temporal derivatives in the mass transport equation. Inappropriate derivative approximations either in space or time (eq. 18) can degrade the accuracy of the overal solution regardless of how accurately the other approximations are obtained [4].

The solution of the adjoint equation results in weighting function that are similer to the upstream weighting technique. Use of the these weighting functions and an interpolation function in the Petrov - Galerkin method results in a variable technique for solving mass transport problems in groundwater. Oscillation - free solution are obtained for right combination of Peclet and Courant numbers.

involving only diffusion across grid lines. **B** is a non symmetric $\mathbf{I}_x\mathbf{I}$ matrix.

$$\mathbf{B}_{ik} = \sum_n \int_{\Omega n} \mathbf{R}\omega_i \frac{d\phi_k}{dt} d\Omega \quad (12)$$

defined over cell interiors which vanishes if $\phi_k$ are independent of time, C is an I - dimensional vector of nodal concentration values. **F**is a symmetric $\mathbf{I}_x\mathbf{I}$ matrix.

$$\mathbf{F}_{ik} = \sum_n \int_{\Omega n} \mathbf{R}\omega_i \phi_k d\Omega \quad (13)$$

and **Q** is an I - dimensional vector.

$$\mathbf{Q}=\mathbf{G}+\mathbf{H} \quad (14)$$

consisting of interior source terms.

$$\mathbf{G}_i = \sum_n \int_{\Omega n} S\omega_i d\Omega \quad (15)$$

and boundary flux terms

$$\mathbf{H}_i = - \sum_n \int_{\Gamma n} q.\nu\omega_i d\Gamma \quad (16)$$

The differential equations are free of advective terms and terms involving diffusion and decay in the interior of the grid cells; the corresponding information is carried entirely by the weight functions. Hence the accuracy of the terms in equation (10) to (16) depends not on the refinement of the original grid but on the accuracy with which $\omega_i(x, t)$ and $\phi_i(x, t)$ are evaluated over each neighborhood $\tilde{\Omega}_i$.

If $\omega_i$ is independent of time, the matrix [B] is equal to zero and equation (10) becomes

$$[\mathbf{A}]\{C\} + \{\mathbf{F}\}\left\{\frac{\partial C}{\partial t}\right\} = [\mathbf{Q}] \quad (17)$$

Equation (17) is a system of ordinary differential equations, the solution of which provides values of {C} and $\left\{\frac{\partial C}{\partial t}\right\}$ at each node in the finite element mesh at each time. This equation can be solved using a finite difference approximation for $\left\{\frac{\partial C}{\partial t}\right\}$.

$$\left\{\frac{\partial C}{\partial t}\right\} = \frac{1}{\Delta t}(\{C\}_{t+\Delta t} - \{C\}_t) \quad (18)$$

where the subscript denotes the time level and $\Delta t$ is the length of the tims step.

The choice of time, between t and $t+\Delta t$, at which {C} is evaluated, is controlled by the time relaxation factor $\beta$.

$$\{C\}=(1-\beta)\{C\}_t+\beta\{C\}_{t+\Delta t} \quad (19)$$

Substitution of these two equations into equation (17), result in.

$$([\mathbf{F}]+\beta\Delta t[\mathbf{A}])\{C\}_{t+\Delta t} = ([\mathbf{F}]-(1-\beta)\Delta t[\mathbf{A}])\{C\}_{t+\Delta t} ((1-\beta)\{\mathbf{Q}\}_t+\beta\{\mathbf{Q}\}_{t+\Delta t}) \quad (20)$$

The solution procedure begins by specifying the initial values of {C} as $\{C_{t0}\}$, then we solve the system of linear equations to obtain values of {C} at the end of the first tims step, $\{C\}_{t0+\Delta t}$ we then set.

$$\{C\}_t=\{C\}_{t0+\Delta t} \quad (21)$$

in equation (18) and repeat the solution process for the next time step, and so on.

## WEIGHT FUNCTION

The adjoint equation (4) is solved for $\omega$ using the Galerkin finite element method. To evaluate the coefficients of the matrix [**A**] one has to obtion the weight function $\omega$ and its spatial derivative $\frac{d\omega}{dx}$ at each node of the fine grid. A cubic Hermitian interpolation function was used in the solution of the weight function $\omega$. The distribution of $\omega$ over two adjacent elements for different values of (V/D) are shown in figures 2(a) - 2(d). Examination of the these figures shows that when V/D is small, diffusion dominates and the weight functions approach piecewise linear. When advection becomes progressively dominant, the weight functions become increasingly skewed in the upstream direction. For large values of V/D, numerical oscillations appear in the distributions. Despite the oscillations, it seems more rational to use these weight functions rather than using arbitrary upstream weight factors.

The weak form of equation (1) is

$$\int_{\Omega}(\Gamma C)\omega(\underline{x})d\Omega=\int_{\Omega}(-\nabla.\mathbf{q}-\lambda\mathbf{R}C+S-\mathbf{R}\frac{\partial C}{\partial t})\omega(\underline{x})d\Omega \quad (2)$$

The application of Green's first identity to equation (2) twice gives.

$$\int_{\Omega}(\Gamma C)\omega(\underline{x})d\Omega=\int_{\Omega}[V.\nabla\omega+\nabla.(D\nabla\omega)-\lambda\mathbf{R}\omega]CdS\Omega$$

$$+\int_{\Omega}\left[S-\mathbf{R}\frac{\partial C}{\partial t}\right]\omega d\Omega-\int_{\int}(S.v\omega+D\nabla\omega.vC)\,d\int=0 \quad (3)$$

where $\int$ is boundary of $\Omega$ and $v$ a unit vector normal to $\int$ pointing outward.

To evaluate the weight functions $\omega_i$ (x, t), one has superimpose a relatively fine local grid $E^1$ on $\tilde{\Omega}^{ij}$ ($\Omega^{ij}\cup\int^{ij}$) and evaluate $\omega_i$ (x, t), numerically at the nodes of this new grid. This will be done by the standard finite element method. $\omega_i$ (x, t), have to satisfy the formal adjoint of $\Gamma C$ which is:

$$\Gamma^*\omega_i=V.\nabla\omega_i+\nabla\cdot(D\nabla\omega_i)-\lambda\mathbf{R}\omega_i=0 \text{ on each } \Omega_n\in\Omega^i \quad (4)$$

subject to the local boundary conditions:

$$\omega_i(\underline{x}, t)=0 \quad \text{at} \quad \underline{x}\in\int^i \text{ such that } \underline{x}\notin\int \quad (5)$$

$$D\nabla\omega_i\cdot v=0 \quad \text{at} \quad \underline{x}\in\int^i \text{ such that } \underline{x}\in\int \quad (6)$$

$\Omega^i$=the union of $\Omega^{ij}$

$\int^i$ are the boundaries of $\Omega^i$

In addition, $\omega_i$ ($\underline{x}$, t), satisfies

$\omega_i(\underline{x}, t)=\delta_{ik}$ for all k=1, 2, ..., I

$\omega_i(\underline{x}, t)=0$ for all $\underline{x}\notin\tilde{\Omega}^{ij}$

$\omega_i$ ($\underline{x}$, t) is continuous everywhere in $\tilde{\Omega}^i$ but the normal component $D\nabla\omega_i$ exhibits discontinuity across all grid lines associated with $\tilde{\Omega}^i$, including the grid lines $\gamma^{ij}$ in the interior of $\tilde{\Omega}^i$.$\tilde{\Omega}^i=\int^i\cup\Omega^i$.

The solution corresponding to any $\tilde{\Omega}^{ij}$ is indepenpent of that over $\tilde{\Omega}^{kl}$, k≠j and/or l≠j and hence these can in principle be evaluated simultaneously on parallel processors. The dependent variable C will be approximated by.

$$\hat{C}(x, t)=\sum_{k=1}^{I}C(x_k, t)\,\phi(x, t) \quad (7)$$

The solution of the adjoint equation or any Lagrangian interpolation function can be used as $\phi$(x, t). With weight functions thus defined, equation (3) can be written as:

$$\int_{\Omega}\Gamma C\omega_i\,d\Omega=\sum_{n=1}^{N}\int_{\Omega n}[V.\nabla\omega_i+\nabla.(D\nabla\omega_i)-\lambda\,\mathbf{R}\omega_i]\,CdS\Omega$$

$$+\sum_{n=1}^{N}\int_{\Omega n}\left[S-\mathbf{R}\frac{\partial C}{\partial t}\right]\omega_i\,d\Omega-\sum_{n=1}^{N}\int_{\int n}(\mathbf{q}.v\omega_i$$

$$+D\nabla\omega_i.vC)\,d\int-\sum_{n=1}^{N}\sum_{m=1}^{N}\int_{\int nm}(\mathbf{q}.v\omega_i$$

$$+D\nabla\omega_i.vC)\,d\int=0 \quad (8)$$

The integrals over $\int_{nm}$ are evaluated by approaching this intercell boundary (or grid line) from within $\Omega_n$. In such integrals $v$ is a unit normal to $\int_{nm}$ directed away from $\Omega_n$. The double sum of integrals involving $\mathbf{q}.v\omega_i$ vanishes due to the continuity of the solute mass and $\omega_i$(x, t) in $\Omega$. The integrals of [ ] C over $\Omega_n$ are zero by virtue of equation (4), and equation (8) simplifies to:

$$\sum_{n}\left[\int_{\int n}D\nabla\omega_i.vCd\int+\sum_{m}\int_{\int nm}D\nabla\omega_i.Cd\int\right]$$

$$+\sum_{n}\int_{\Omega n}\mathbf{R}\frac{\partial C}{\partial t}\omega_i\,d\Omega=\sum_{n}\int_{\Omega n}S\omega_i\,d\Omega-\sum_{n}\int_{\int n}\mathbf{q}.v\omega_i d\int \quad (9)$$

The substitution of equation (7) into equation (9) yield a system of ordinary differential equation.

$$(\mathbf{A}+\mathbf{B})\{C\}+[\mathbf{F}]\left\{\frac{\partial C}{\partial t}\right\}=[\mathbf{Q}] \quad (10)$$

where **A** is a non symmetric $\mathbf{I}_x\mathbf{I}$ matrix.

$$\mathbf{A}_{ik}=\sum_{n}\left[\int_{\int n}D\nabla\omega_i\cdot v\phi_k d\int+\sum_{m}\int_{\int nm}D\nabla\omega_i\cdot v\phi_k d\int\right] \quad (11)$$

## INTRODUCTION

The simulation of contaminant transport in both surface and subsurface hydrology requires solution of the advective - dispersive equation which have great importance in many fields of engineering and science. This equation, in its compact form, can be written as:

$$\Gamma C = -\nabla.\mathbf{q} - \lambda RC + S - \mathbf{R}\frac{\partial C}{\partial t} = 0 \qquad (1)$$

where

$\Gamma$ = differential operator

C = concentration

$\nabla$ = gradient with respect to the space coordinates

$\mathbf{q}$ = solute mass flux $\mathbf{q}=VC-D\nabla C$

V = seepage velocity

D = dispersion tensor

$\lambda$ = exponential decay coefficient

$\mathbf{R}$ = rearsation coefficient

S = source term

a considerable interest in finding accurate numerical solution to equation (1) exists because these solutions characteristically exhibit oscillations "over shoot" and/or excessive numerical dispersion [3]. Considerable work has been expended in developing formulate to overcome this kind of problem ([2], [5], [6], [10]). Most methods to eliminate the oscillations have focused on upstream weighting techniques [10]. A fundamental criticism of these methods is the essentially ad-hoc nature of their development. This is manifested through the use of an arbitrary parameter, the magnitude of which has to be selected by the analyst. An alternate and very promising approach has been introduced by Herrera [7]. In this approach, Herrera chooses the weight function to be a solution of the homogeneous adjoint differential equation associated with the original governing differential operator. When the homogenous adjoint differential equation has constant coefficients, it can be solved exactly. It cannot be solved exactly if the coefficients are not constants. Neuman [9] presented a method to approximate the solution to $\Gamma^*\omega=0$ thereby providing good estimates for the weight functions. where $\Gamma^*$ is the adjoint opertor. Neuman superimposed a relatively fine local grid over a coarser one and used a finite element method to solve the weight functions. Once the weight functions are obtained they are used to compute the field variable over the coarser grid.

## DEVELOPMENT OF THE METHOD

The method is described in detail by Neuman [9] it is presented below in summary form. The domain $E^0$ is divided into subdomains $\Omega_n$ (n=1, 2,3, ...,n), forming four sided areas. The boundary segments of $\Omega_n$ are designated by $\int_n$, if they coincide with the global domain boundary $\int$ and by $\int_{nm}$ if they are contiguous on another subdomain $\Omega_m$, $m\neq n$. The intersections of these segments form nodal points, i=1,2,3,..., I (I=20 in Figure 1), and pairs of contiguous nodes $i\neq j$ from grid lines $\gamma^{ij}$ which coincide with the boundaries $\int_n$ and/or $\Gamma_{nm}$ of contiguous subdomains $\Omega_n$. Associated with each $\gamma^{ij}$ is a subdomain $\Omega^{ij}$, defined as $\Omega^{ij}=\Omega_n\cup\Omega_m$, $m\neq n$ which forms the union $\cup$ of the two contiguous subdomains $\Omega_n$ and $\Omega_m$ on the two opposite sides of $\gamma^{ij}$ (Figure 1).

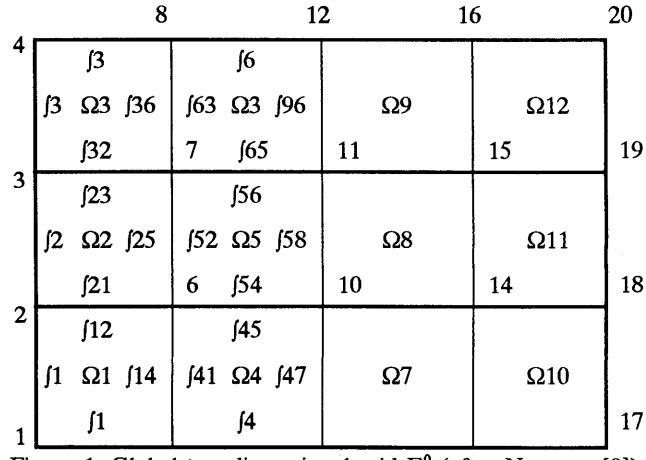

Figure 1. Global two-dimensional grid $E^0$ (after Neuman [9]).

# Accurate solution of groundwater mass transport equation using the adjoint Petrov - Galerkin method

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## Abstract :

An adjoint Petrov - Galerkin method was proposed by Neuman [1] to solve multidimensional advection - dispersion equation. The method uses a numerical solution of the adjoint state equation on a sequence of nested grids to compute the weight functions. A numerical application of the method shows that at low Peclet numbers, the application of method results in a satisfactory match between the analytical and the numerical solutions. When the Peclet number increases and advection become dominant, the results obtained show oscillations of the concentration profile and a lag between the analytical and the numerical solution. The oscillations are a function of the Peclet and Courant numbers. Accurate solutions are obtained when the Courant number is equal to one, for Peclet number up to 50. For Peclet number greater than 50, the numerical solution lags behind the analytical solution. At other Courant numbers, the maximum Peclet number for stable solution drops off rapidly.

**Key words :**

Groundwater, Analytical Solution, Accurate Solution, Numerical Solution, Mass Transport, Peclet Number, Courant Number.

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