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# A ZOOMABLE AND ADAPTABLE HIDDEN FINE-MESH APPROACH TO SOLVING ADVECTION-DISPERSION EQUATIONS

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## ABSTRACT

A zoomable and adaptable hidden fine-mesh approach (ZAHFMA), that can be used with either finite element or finite difference methods, is proposed to solve the advection-dispersion equation. The approach is based on automatic adaptation of zooming a hidden fine-mesh in the place where the sharp front locates. Preliminary results indicate that ZAHFMA used with finite element methods can handle the advection-dispersion problems with Peclet number ranging from 0 to ∞.

## INTRODUCTION

Contaminant transport in the subsurface is often modeled with advection-dispersion equations. Many numerical methods have been employed to solve the advection-dispersion equations. Most conventional numerical methods can be classified into two major categories: Eulerian and Lagrangian approaches. In the Eulerian approach, the equation is discretized by a finite difference or a finite element grid system fixed in space. In the Lagrangian approach, either a deforming grid or a fixed grid in deforming coordinate can be used.

Experiments have shown that the Eulerian approach using conventional finite element methods (FEMs) or finite difference methods (FDMs) has performed well for dispersion dominant transport problems. For advection dominant transport problems, oscillation solutions may result when the Eulerian approach is used in conjunction with conventional FEMs or FDMs. The Lagrangian method can also be used to circumvent the problem of oscillations but it is not always easily adapted to deal with complex subsurface media (Neuman[1]).

A third approach which is a mix of the Lagrangian-Eulerian method has been gaining popularity in the past decade (Neuman[1],

Konikow and Bredehoeft[2], Molz et al.[3]). In this mixed method, one adopts a Lagrangian viewpoint when dealing with the advection terms and an Eulerian viewpoint when dealing with all other terms in the transport equations. In the Lagrangian step, either continuous forward particle tracking -- CFPT (Konikow and Bredehoeft[2]), single-step reverse particle tracking -- SRPT (Molz et al.[3]), or the combination of both (Neuman[1]) has been used. The SRPT could introduce a significant amount of numerical dispersion (Yeh and Tripathi[4]). Futhermore, if continuous multi-sources are present in interior nodes, the SRPT would give incorrect solution unless the Courant number is less than or equal to 1. For the CFPT, the treatment of complex boundary conditions and nonlinearities is not straightforward and the constant handling of numerous particles is troublesome and time consuming. The combined SRPT and CFPT approach eliminate some of these deficiencies but still leaves many questions unanswered (Neuman[1]). For example, how the solution quality depends the number of particles and the density of particles around sharp front.

From the above discussions, it is clear that the Eulerian approach is still the simplest and most straightforward way to solve advection-dispersion equations provided numerical oscillations can be eliminated. The easiest way of eliminating numerical oscillations can be achieved by restricting the spatial grid size such that the mesh Peclet number is less than certain critical number, which depends on the numerical scheme used (Jensen and Finlayson[5]). However, it is not always practical to reduce the grid size; and it is certainly impossible to achieve the elimination of oscillations by reducing grid size for the case of pure advection. The alternative is to use upstream FDMs or FEMS that are able to eliminate oscillations for mesh Peclet number ranging from 0 to $\infty$. However, upstream methods introduce a large numerical dispersion coefficient. Numerical dispersion can be reduced by using a fine-grid system or by using higher-order approximations in space, time, or both. Using higher-order finite element techniques may re-introduce oscillations. Hence, higher-order approximations have not proven capable of entirely and efficiently eliminating both numerical oscillation and numerical dispersion. On the other hand, using an extremely fine grid throughout the whole region to reduce the numerical dispersion coefficient may not be practical for many problems.

Since numerical dispersion depends on both the numerical dispersion coefficient and the gradient of concentration, there is no need to reduce numerical dispersion coefficient at the region where the gradient of concentration is very small. Therefore, we propose a zoomable and adaptable hidden fine-mesh approach (ZAHFMA) to solving the advection-dispersion equations. ZAHFMA coupled with upstream methods would entirely eliminate the numerical oscillation and sufficiently reduce the

ZOOMABLE AND ADAPTABLE HIDDEN FINE-MESH APPROACH (ZAHFMA)

Let us use a simple linear line finite element (Fig. 1) to illustrate how the ZAHFMA is implemented. First, we discretize the region with M elements (for example M = 3) and N nodes (for example N = 4) in the region (Fig. 1a). Second, we embed a predetermined number of nodes L and elements K (for example L = 3, K = 4) in each element (Fig. 1a). Third, we apply the spatial finite element and temporal finite difference to an advection-dispersion equation for each element to yield an element matrix equation

$$[A^e]\{C^e\} = \{R^e\} \tag{1}$$

where $[A^e]$ is the element coefficient matrix, $\{C^e\}$ is the unknown vector of the concentration, and $\{R^e\}$ is the element load vector. Fourth, we loop over all elements to determine if steep concentration gradient exists within an element. If the element is not a sharp-front element, regular finite element integration is used to obtain $[A^e]$ and $\{R^e\}$. Then $[A^e]$ and $\{R^e\}$ are assembled into the global coefficient matrix and global load vector, respectively.

If the element is a sharp-front element, we zoom the element and renumber the hidden nodes and the global nodes on the boundary of the element consecutively (Fig. 1b). We then obtain $[A^e]$ and $\{R^e\}$ by assembling the fine-mesh element matrix

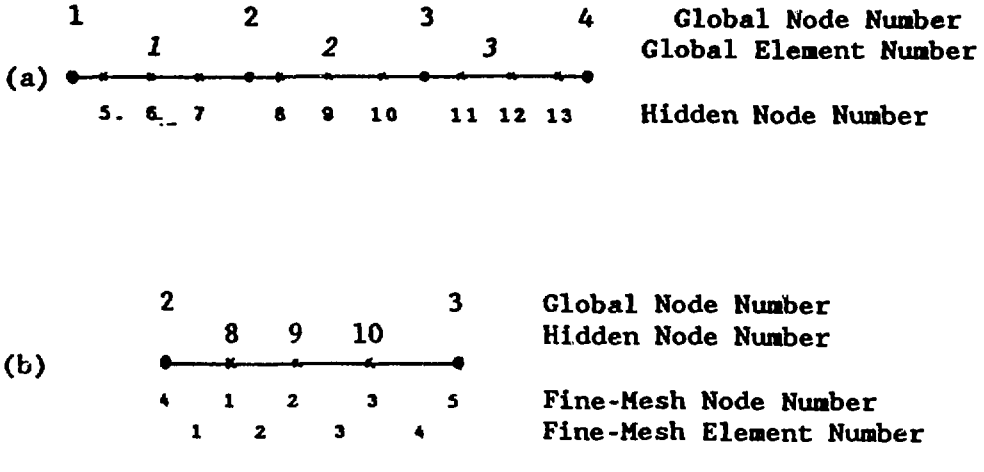


Fig. 1 Example schematic layout of ZAHFMA: N = 4, M = 3, L = 3, K = 4.

and fine-mesh element load vector (both of which are obtained by finite element integration) over K fine-mesh elements. Since $\{C^e\}$ can be subdivided into parts associated with hidden fine- mesh nodes, $\{C_f^e\}$, and others associated with global nodes, $\{C_g^e\}$, we make Gaussian reduction of Eq. (1) up to the L-th equation to yield

$$[U^e]\{C_f^e\} + [V^e]\{C_g^e\} = \{R_f^{*e}\} \tag{2}$$

$$[A^{*e}]\{C_g^e\} = \{R_g^{*e}\} \tag{3}$$

where $[U^e]$ is the upper triangular element coefficient matrix, $[V^e]$ and $[A^{*e}]$ are the reduced element coefficient matrices, and $\{R_f^{*e}\}$ and $\{R_g^{*e}\}$ are the reduced $\{R_f^e\}$ and $\{R_g^e\}$, respectively, after Gaussian reduction. $[A^{*e}]$ and $\{R_g^{*e}\}$ represent the element coefficient matrix and element load vector, respectively, of the zoomed element. Therefore, after the Gaussian reduction, $[A^{*e}]$ and $\{R_g^{*e}\}$ are assembled into the global coefficient matrix and global load vector, respectively.

Fifth, we solve the assembled global matrix equation to yield the concentrations at all global nodes. Finally, we compute the concentrations at all hidden nodes. If the hidden nodes are not in a sharp-front element, we compute the concentrations using a consistent finite element interpolation formula. If the hidden nodes are in a sharp-front element, we can easily solve the concentrations with Eq. (2) because $[U^e]$, $[V^e]$, $\{C_g^e\}$, and $\{R_f^{*e}\}$ are already known. The procedure outlined above completes a one-time step computation.

The remaining task is to develop an adaptive mechanism to determine if an element is a sharp-front element. Our current answer to this question is empirical. We use the following formula

$$(\max C_n - \min C_n) \leq \text{ADPARM} \times \max C_n \tag{4}$$

where max $C_n$ and min $C_n$ are the maximum and minimum values, respectively, of all nodes in an element, and ADPARM is an empirical adaptation parameter. If Eq. (4) is satisfied, we say the element is not a sharp-front element. If Eq. (4) is violated, we say the element is a sharp-front element.

## APPLICATION

To test the performance of the ZAHFMA, we consider a one-dimensional transient transport from an upstream concentration. Initially, the concentration over the region $0 \leq x \leq 2$ is assumed zero everywhere. Boundary conditions are given as $C = 1$ at $x = 0$ and $C = 0$ at $x = 2$. For ZAHFMA simulation, the region is discretized with 8 elements with element length equal to 0.25. A time step size of 0.1 is used for simulation. The

adaptation parameter used is ADPARM = 0.1. Two examples are used for illustration. In the first example, we use a velocity of zero and a dispersion coefficient of 0.01. Thus, the first example represents pure dispersion with Peclet number equal to 0. In the second example, we use a velocity of 0.25 and a dispersion coefficient of zero, which represents a pure advection with Peclet equal to ∞. Figure 2a shows the concentration profile at time equal to 10 and Figure 2b depicts the concentration profile at time equal to 4. It is seen that, for the first example, ZAHFMA yields very close results to the analytical solution whether the hidden nodes are 0, 1, or 3. On the other hand, for the second example, numerical dispersion is greatly reduced with 9 hidden nodes per element. Thus, the number of hidden nodes per element required to reduce numerical dispersion to an acceptable level depends on the nature of problems.

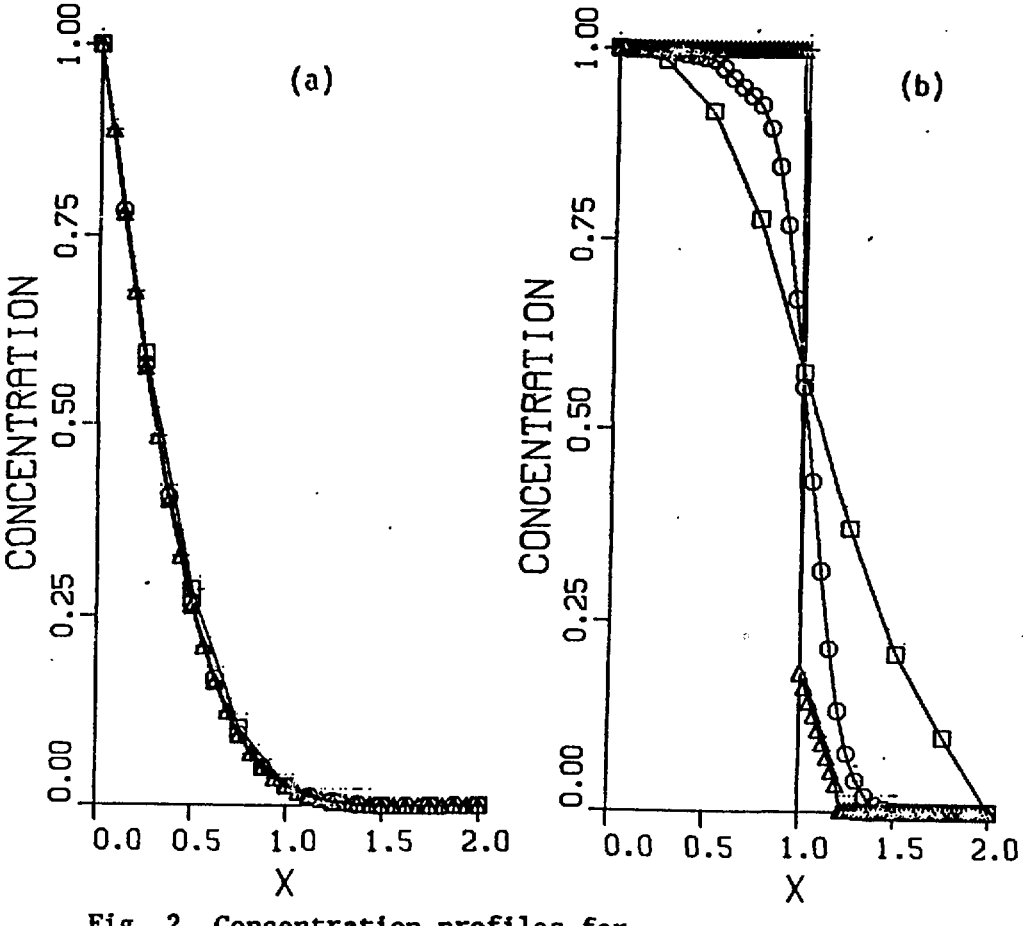


Fig. 2 Concentration profiles for
(a) pure dispersion -
□ = 0 hidden node, o = 1 hidden node, and
Δ = 3 hidden nodes, and + = analytical
(b) pure advection -
□ = 0 hidden node, o = 4 hidden nodes,
Δ = 9 hidden nodes, and + = analytical.

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REFERENCES

1. Neuman, S. P. (1983), Computer Prediction of Subsurface Radionuclide Transport -- An Adaptive Numerical Method., NUREG/CR-3076, Dept. of Hydrology and Water Resources, University of Arizona, Tucson, Arizona.

2. Konikow, L. F. and Bredehoeft, J. D. (1978), Computer Model of Two-Dimensional Solute Transport and Dispersion in Groundwater, Techniques of Water-Resources Investigation of the United States Geological Survey, Chapter C2, Book 7, USGS, Reston, Virginia.

3. Molz, F. J. M., Widdowson, M. A., and Benefield, L. D. (1986), Simulation of microbial growth dynamics coupled to nutrient and oxygen transport in porous media, Water Resour. Res., Vol.22, pp. 1207-1216.

4. Yeh, G. T. and Tripathi, V. S. (1987), A Lagrangian-Eulerian approach to modeling hydrogeochemical transport of multi-component systems, in Proc. International Conference on Groundwater Contaminant: Use of Models in Decision-Making in the European Year of Environment, Amsterdam, The Netherlands, October 26-29, 1987.

5. Jensen, O. K. and Finlayson, B. A. (1980), Oscillation limits for weighted residual methods applied to convective diffusion equations, International Journal for Numerical Methods in Engineering, Vol. 15, pp. 1681-1689.