Some Aspects of Solving Advection Dominated Flows

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A new method for solving the fluid transport equation for advection dominated flows is introduced in this paper. A transform modifies the asymmetric fluid transport equation into a symmetric positive definite equation. Symmetry is achieved by imbedding the first order spatial derivative of the transport equation into the second order derivative term through functional transformation. A variational formulation for the finite element approximation preserves this desirable feature to generate a symmetric system of equations. For the steady state case, the proposed method has been validated against three methods: analytical solution, Galerkin finite element solution and upwind-weighted finite element solution. The results indicate that the proposed method gives the best approximation to the analytical solution. There is no constraint on the magnitude of Peclet number. For the transient case, validation shows that the proposed method is accurate but application is restricted to certain Peclet number magnitudes.

In diesem Aufsatz wird eine neue Methode zur Lösung der Dispersionsgleichung vorgestellt. Durch eine Transformation wird diese asymmetrische Stofftransportgleichung in eine symmetrische, positiv definite Gleichung umgeformt. Diese Umwandlung erfolgt durch Eingliederung der ersten räumlichen Ableitung in der zweiten mittels eine Funktionaltransformation. Hierbei ermöglicht der Variationsansatz der Methode der finiten Elemente die Generierung eines symmetrischen Gleichungssystems.
Die Validierung des neuen Ansatzes erfolgt durch den Vergleich mit drei unterschiedlichen Lösungstechniken; es sind diese: analytische Lösung, Galerkin-Verfahren und die 'upwind'-Galerkin gewichteten finite Elemente. Die Ergebnisse für den stationären Fall zeigen, daß unabhängig von dem untersuchten Peclet-Zahlbereich, die neue Methode die beste Annäherung der analytischen Lösung darstellt. Dagegen sind für die instationäre (zeitabhängige) Aufgabe gute Ergebnisse für niedrige Peclet-Zahlen erzielt worden. Für höhere Peclet-Zahlen sind die Ergebnisse weniger zufriedenstellend.

Introduction

Problems involving contaminant transport have attracted increased attention due to their importance in the field of hydrogeology, mineral, civil, and petroleum engineering, among others. Solution of the advection-diffusion equation is particularly challenging as Peclet number, indexing the ratio of advective to diffusive fluxes, increases. At high *Peclet* numbers, one is usually forced to choose between accepting the presence of nonphysical oscillations within the solution or suffering unwanted numerical dispersion. Of key importance is awareness of the changing nature of the governing equation. Where diffusion dominates, the equation is parabolic and causes no particular problem in numerical solution. Where advection dominates the behavior is analogous to a first order hyperbolic partial differential equation that exhibits a frontal character and creates annoying difficulties in numerical solution.
Considering first a simple one dimensional diffusion-advection (DA for short) equation

$$D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} = \frac{\partial c}{\partial t} \tag{1}$$

where c (x, t) is concentration with coordinate, x and time, t; D is the dispersion coefficient and v is fluid velocity.
The initial and boundary conditions may be written as

$$\begin{cases} c(x,0) = 0 \\ c(0,t) = c_0 \\ c(L,t) = 0 \end{cases} \tag{2}$$

where L is the end point in the domain, unaffected by concentration change as $x \to \infty$. An alternative boundary condition to eqn. (2) may be given as follows

$$\frac{\partial c(L,t)}{\partial x} = 0 \tag{3}$$

representing a closed system with no escape of mass.
For dimensionless representation, let

$$\begin{cases} C(X,T) = c(x,t)/c(0,t) \\ X = x/L \\ T = Dt/L^2 \\ \beta = vL/D. \end{cases} \tag{4}$$

Equation (1) is therefore transformed to

$$\frac{\partial^2 C}{\partial X^2} - \beta\frac{\partial C}{\partial X} = \frac{\partial C}{\partial T} \tag{5}$$

The initial and boundary conditions under eqns. (2) and (3) become

$$\begin{cases} C(X,0) = 0 \\ C(0,T) = 1 \\ C(L,T) = 0 \quad (for\ prescribed\ concentration) \\ \dfrac{\partial C(L,T)}{\partial X} = 0 \quad (for\ prescribed\ flux) \end{cases} \tag{6}$$

Any attempt to solve eqn. (5) for large β by any numerical technique leads to oscillatory results [1]. This numerical oscillation was first recognized by *Price* et al. [2]. To circumvent this difficulty, Guymon [3] applied a functional transformation to eqn. (5) and modified eqn. (5) into a symmetric finite element system equation, which effectively suppressed the numerical oscillation for smaller β. The most successful technique in eliminating numerical oscillations may, however, be attributed

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to the application of the upwinding method [4] modified from the finite difference iteration. However, despite the utility of this method in reducing spurious oscillations, excessive smearing or numerical dispersion is arbitrarily added to the solutions.
Results for higher dimensional elements in two and three dimensions where low element continuity (C^0) is maintained results in no net improvement [5]. Alternatively, higher order of elements (C^1) using cubic or bicubic Hermitian interpolating functions together with collocation finite element methods may concurrently minimize oscillation and smearing [6, 7, 8]. However, the computational costs incurred in using C^1 elements are high and formulation of the problem often turns out to be cumbersome.
It is not clear where the numerical oscillation is caused by the asymmetric feature of the first derivative term in the DA equation or if other contributing factors are equally important. Effort has been made by *Leismann* and *Frind* [9] to achieve matrix symmetry through placing the advective term at the old time level in time marching. The resulting numerical errors are minimized by introducing an artificial dispersion term and by optimal time weighting of all terms on the basis of a *Taylor* expansion of the governing equation.
In the sections that follow, some alternatives for calculating DA equations are presented. The analysis covers both steady state and transient cases. In all instances the new DA equation has been solved using the finite element technique in a variational formulation that leads implicitly to a symmetric, positive definite system matrix that can be effectively solved by a conjugate gradient method. The study shows that the new methods are promising in concurrently minimizing numerical oscillations and spurious numerical dispersion.

1. Classical Analytical Solution

An approximate analytical solution is available for eqn. (5) with initial and boundary conditions (6) for the prescribed flux [10] where the one-dimensional medium is infinite. This equation is usually expressed as

$$C = a_1 + a_2 + a_3 + a_4 \tag{7}$$

where

$$\begin{cases} a_1 = \frac{1}{2} erfc\left[\frac{x - vt}{2\sqrt{Dt}}\right] \\ a_2 = \frac{1}{2} erfc\left[\frac{x + vt}{2\sqrt{Dt}}\right] exp(\frac{vx}{D}) \\ a_3 = \frac{1}{2} erfc\left[\frac{2L - x + vt}{2\sqrt{Dt}}\right] exp(\frac{vL}{D}) \left[2 + \frac{v(2L - x)}{D} + v^2 \frac{t}{D}\right] \\ a_4 = -\sqrt{\frac{v^2 t}{\pi D}} exp\left[\frac{vL}{D} - \frac{1}{4Dt}(2L - x + vt)^2\right] \end{cases} \tag{8}$$

where erfc is the complementary error function.

2. A New Method for the Steady DA Equation

The first derivative term in eqn. (5) may be eliminated without defeaturing the DA equation. For two dimensional steady state transport, the DA equation reduces to

$$\frac{\partial^2 C}{\partial X_i^2} - \beta_i \frac{\partial C}{\partial X_i} = 0 \tag{9}$$

with identical boundary and initial conditions expounded in eqn. (6) except that X_i replaces X.
Assuming

$$\beta_i = \frac{\partial \phi}{\phi \partial X_i} \tag{10}$$

where ϕ is an arbitrary function, enables ϕ to be defined as

$$\phi = \phi_0 exp(\beta_i X_i) \tag{11}$$

where ϕ_0 is the function ϕ at its initial value.
Similarly, an analog to equation (9) may be defined as

$$\frac{\partial}{\phi \partial X_i}\left(\phi \frac{\partial \psi}{\partial X_i}\right) = \frac{1}{\phi} \frac{\partial \phi}{\partial X_i} \frac{\partial \psi}{\partial X_i} + \frac{\partial^2 \psi}{\partial X_i^2} \tag{12}$$

where ψ is another arbitrary function. From the development of eqns. (10) (11), and (12), it is apparently amenable to write from eqn. (9)

$$\frac{\partial}{\partial X_i}\left\{exp(-\beta_i X_i) \frac{\partial C}{\partial X_i}\right\} = 0 \tag{13}$$

It can be readily checked that eqn. (13) yields the exact form of eqn. (9). Analytical solution of (13) may be easily obtained (for conditions in eqn. (6) and for the one-dimensional problem only):

$$C = \frac{1}{1 - exp(-\beta)} + \frac{exp(\beta X)}{1 - exp(\beta)} \tag{14}$$

3. Finite Element Discretization

To accommodate more complex boundary conditions and arbitrary heterogeneous bodies, numerical technique such as the finite element method may be adopted. For simplicity, assume a one dimensional discretization with eqn. (9) as a governing equation. To achieve a symmetric matrix form as in eqn. (13), instead of using a *Galerkin* method, we turn to the variational formulation. The functional in eqn. (13) can be expressed as

$$J = \frac{1}{2} \int_{X_j}^{X_k} \left\{exp(-\beta X)\left(\frac{dC}{dX}\right)^2\right\} dX \tag{15}$$

To discretize the domain with k elements, we write

$$J = \sum_{e=1}^{k} J^{(e)} = \sum_{e=1}^{k} \frac{1}{2} \int_{X_j}^{X_k} \left\{exp(-\beta X)\left(\frac{dC^{(e)}}{dX}\right)^2\right\} dX \tag{16}$$

or

$$J^{(e)} = \frac{1}{2} \int_{X_j}^{X_k} \left\{exp(-\beta X)\left((N_j' \; N_k')\begin{pmatrix} C_j \\ C_k \end{pmatrix}\right)^2\right\} dX \tag{17}$$

Where N is the shape function for the element e. Minimizing the functional, J, with respect to nodal values C_i, (i = 1, 2, ..., k) yields the following system equations in matrix form

$$\sum_{e=1}^{k} A^{(e)} C^{(e)} = 0 \tag{18}$$

where

$$A^{(e)} = \int_{X_j}^{X_k} exp(-\beta X) \begin{pmatrix} N_j' & N_j' & N_j' & N_k' \\ N_k' & N_j' & N_k' & N_k' \end{pmatrix} dX \qquad (19)$$

$$C^{(e)} = (C_i\ C_{i+1})^T \qquad (20)$$

where T represents the vector transpose.
Assuming linear interpolation functions $N^{(e)}$ in each element, and also assuming that the function exp ($-\beta X$) is constant over each element yields the symmetric matrix

$$A^{(e)} = \frac{exp(-\beta X^{(e)})}{l} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \qquad (21)$$

where l is element length.

4. Validation of Proposed Method

To validate the proposed method, four alternative methods are selected for comparison. These are analytical solution (14), the *Galerkin* finite element method, the *Galerkin* method with upwind weighting and eqn. (18) referred henceforth as the proposed method.
For the parametric analysis, local element Peclet numbers in the numeric methods are chosen between 0.01 and 10.
Among the four methods, numerical oscillations are observed only in the Galerkin method when the Peclet number is equal to 10 (*Fig. 1*). Both the *Galerkin* method with upwind weighting using an optimal weighting coefficient and the proposed method using eqn. (18) exhibit oscillation free behavior even for the highest *Peclet* number of 10. The proposed method gives the best approximation to the analytical solution as illustrated in *Table I* and *Fig. 2* for a Peclet number of 1 and *Fig. 3* for a Peclet number of 10. In both cases, unwanted numerical dispersion is less severe for the proposed method than for the upwind weighted method.

Table I: Concentration versus distance (a)

Distance	Analytical	Proposed	Upwind
0.0	1.0000	1.0000	1.0000
0.1	0.9999	0.9893	0.9889
0.2	0.9997	0.9786	0.9727
0.3	0.9991	0.9676	0.9492
0.4	0.9976	0.9560	0.9151
0.5	0.9933	0.9421	0.8657
0.6	0.9817	0.9220	0.7939
0.7	0.9503	0.8845	0.6897
0.8	0.8647	0.7989	0.5384
0.9	0.6322	0.5811	0.3188
1.0	0.0000	0.0000	0.0000

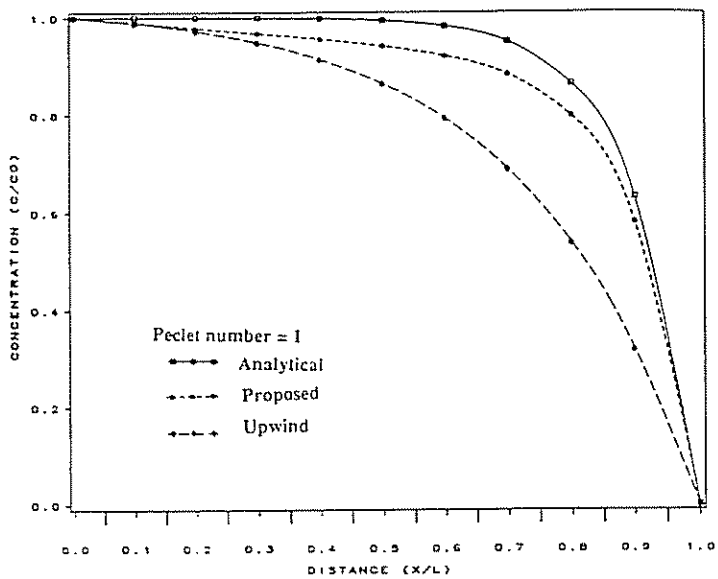

Fig. 2: Steady State Fluid Transport by Various Methods (a)

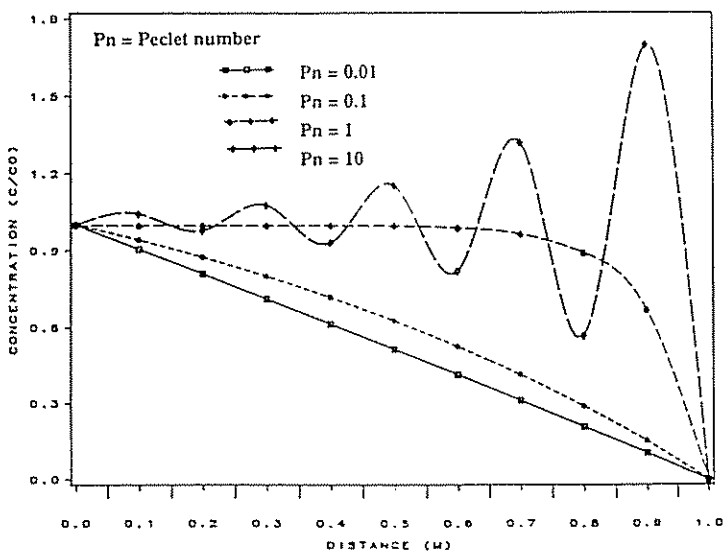

Fig. 1: Steady State Fluid Transport by Galerkin Method

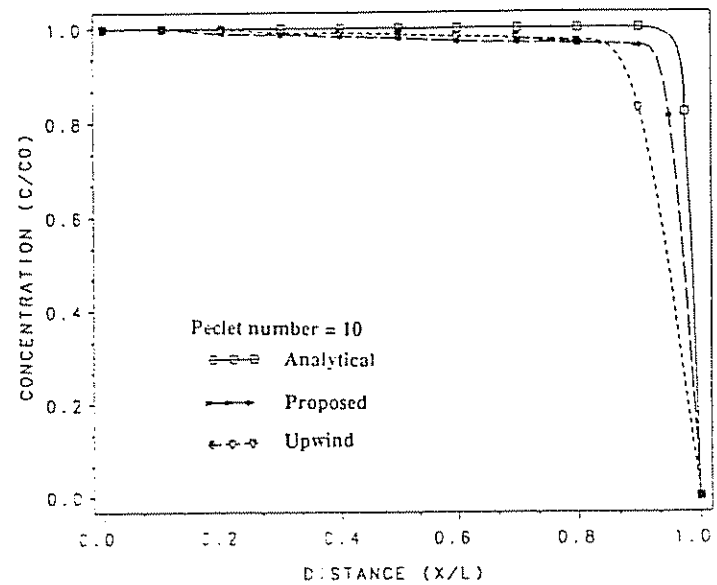

Fig. 3: Steady State Fluid Transport by Various Methods (b)

Upwind weighting techniques are developed to minimize numerical oscillation, as quoted by *Fletcher* [11], and all fully upwind schemes are oscillation free. Upwind weighting is specially designed to compensate for the asymmetric feature resulting from the presence of the first order spatial derivative in the governing equation. It therefore appears that if system matrix generated by the DA equation can be modified into a symmetric form, the numerical oscillation can, in most cases (not in all cases), be eliminated.

5. Error Analysis

In terms of accuracy, *Table II* indicates the maximum error between the analytical solution and solution by the proposed method in which the element spacing has been progressively reduced. In the unit length system, 5, 10 and 20 elements are used, respectively. The order of accuracy, r, can be estimated by the equation.

$$r = log_2\left(\frac{e_l}{e_{\frac{l}{2}}}\right) \tag{22}$$

where e_l represents the error for the element with length l, and $e_{(\frac{l}{2})}$ is the error for the element with length $\frac{l}{2}$.

Table II: Error between analytical and proposed methods

Scheme	5 elements	10 elements	20 elements
Max. error	0.0792	0.0658	0.0622

The improvement in the order of accuracy between 5 element and 10 element models is 0.267, while between 10 element and 20 element models it is 0.081. It may be inferred from this trend that increasing the number of elements results in a diminishing improvement on solution accuracy.
Similarly, the order of accuracy for the upwind weighting method may be obtained as shown in *Table III*. The improvement in the order of accuracy between 5 element and 10 element models is 0.376, while between 10 element and 20 element models it is 0.179. It may be noted that the absolute errors are substantially larger than those in the proposed method shown in *Table II*.

Table III: Error between analytical and upwind methods

Scheme	5 elements	10 elements	20 elements
Max. error	0.5041	0.3884	0.3430

The *Galerkin method, on the other hand, although subject to numerical oscillation, is sensitive to the spatial discretization. It can be seen in Table IV* that a dramatic reduction in error results as the number of elements increase from 10 to 20. The improvement in the order of accuracy between 5 element and 10 element models is 0.462, while between 10 element and 20 element models is 2.215 calculated by eqn. (22).

Table IV: Error between analytical and Galerkin methods

Scheme	5 elements	10 elements	20 elements
Max. error	0.3647	0.2647	0.0607

The above phenomena imply that numerical oscillations and computational accuracy are paradoxically linked. Consequently, partial influence of these characteristics may require to be tolerated.

6. Efficient Solution of the Transient DA Equation

In fluid transport problems the steady state is generally of limited relevance; therefore interest is focused on transient behavior in this section. Problems of numerical dispersion and oscillation are of equal importance to the steady state case but additional problems related to time stepping, must be concurrently addressed. Thus, correct and adequate time discretization is critical in many circumstances and is controlled by the *Courant* number. The Courant number, $C_r = V\Delta t/l$, represents the ratio of front propagate distance within a time step increment ($V\Delta t$) to element length, l.

6.1 Modified Guymon's method for transient fluid transport

An alternative to solving eqn. (5) can be referred to *Guymon's* work [3]. In the following, however, some modifications to *Guymon's* method are proposed to accommodate boundary conditions (6) in a transient analysis (referred in the following as MTA).
If we assume in eqn. (5) that

$$\eta = Cexp(-\beta\frac{X}{2}) \tag{23}$$

Taking a first differentiation with respect to X

$$\frac{\partial\eta}{\partial X} = exp\left(-\beta\frac{X}{2}\right)\left(\frac{\partial C}{\partial X} - \frac{\beta}{2}C\right) \tag{24}$$

It follows directly that the second order derivative is

$$\frac{\partial^2\eta}{\partial X^2} = exp\left(-\beta\frac{X}{2}\right)\left(-\beta\frac{\partial C}{\partial X} + \frac{\beta^2}{4}C + \frac{\partial^2 C}{\partial X^2}\right) \tag{25}$$

Substituting eqns. (23) and (25) into

$$\frac{\partial^2\eta}{\partial X^2} - \frac{\beta^2}{4}\eta = \frac{\partial\eta}{\partial T} \tag{26}$$

enables eqn. (5) to be directly recovered.
It is particalarly significant that no first order spatial derivative terms are present in eqn. (26). Corresponding to eqn. (6), recalling eqn. (23), the initial and boundary conditions must be transformed as

$$\begin{cases} \eta(X,0) = 0 \\ \eta(0,T) = C_0 = 1 \\ \eta(L,T) = C_1 exp(-\frac{\beta}{2}) = 0 \end{cases} \tag{27}$$

If boundary condition is the prescribed flux in eqn. (6) then the following requirement must also be accommodated:

$$\left(\frac{\partial\eta}{\partial X} + \frac{\beta}{2}\eta\right)_{X=1} = 0 \tag{28}$$

The functional for eqn. (26) and the associated conditions of eqn. (27) can be written as

$$J = \frac{1}{2}\sum_{e=1}^{k}\int_{X_1}^{X_k}\left\{\frac{\partial\eta^{(e)}}{\partial X} + \frac{\beta^2}{4}\eta^{(e)^2} + \frac{\partial\eta^{(e)}}{\partial T}\eta^{(e)}\right\}dX \tag{29}$$

where at local coordinate system, $\beta = Vl/D$. Minimizing the functional J with respect to η generates a system of equation such that

$$\sum_{e=1}^{k}\left[E^{(e)}\eta^{(e)} + G^{(e)}\dot{\eta}^{(e)}\right] = 0 \tag{30}$$

where the individual matrices are

$$E^{(e)} = \begin{pmatrix} e_{11} & e_{21} \\ e_{12} & e_{22} \end{pmatrix} \tag{31}$$

$$\begin{cases} e_{11} = e_{22} = \dfrac{D}{l} + \dfrac{v^2 l}{12D} \\ e_{12} = e_{21} = -\dfrac{D}{l} - \dfrac{v^2 l}{24D} \end{cases} \tag{32}$$

$$G^{(e)} = \frac{L'}{6} \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \tag{33}$$

$$\eta^{(e)} = [\eta_i \ \eta_{j+1}]^T \tag{34}$$

$$\eta^{(e)} = \left\{ \frac{\partial \eta_i}{\partial t} \ \frac{\partial \eta_{i+1}}{\partial t} \right\}^T \tag{35}$$

In this particular formulation eqn. (30) is both symmetric and positive definite. After obtaining the solution for η_i, the following equation has to be used to retransform η_i to obtain nodal concentration C_i as

$$C_i = \eta_i exp(\beta \frac{X}{2}) \tag{36}$$

This transformation may cause problems if the *Peclet* number becomes larger. However, this may be remedied by reducing the element length, l, although this manipulation may be counter productive.

6.2 Validation of modified Guymon's method

The behavior of this modified method may be examined. *Fig. 4* shows a comparison of concentration versus distance from the source using three methods: analytical solution, the *Galerking* method and the MTA method for the case of a Peclet number of 0.01 and T = 1. Unfortunately, both *Galerkin* and MTA methods exhibit numerical instability when X < 0.3. However, MTA yields a marginally closer approximation to the analytical solution than the *Galerkin* method. For T = 5, again a slightly better fit to the analytical solution is achieved by MTA over the *Galerkin* method as illustrated in *Fig. 5*.

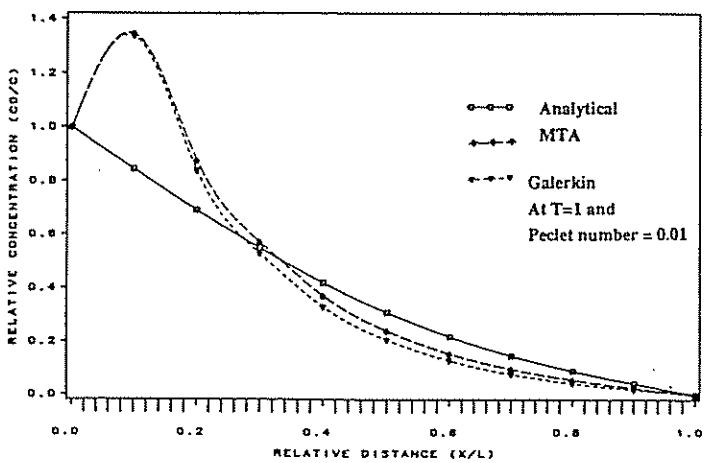

Fig. 4: Comparison of Fluid Transport by Three Methods (a)

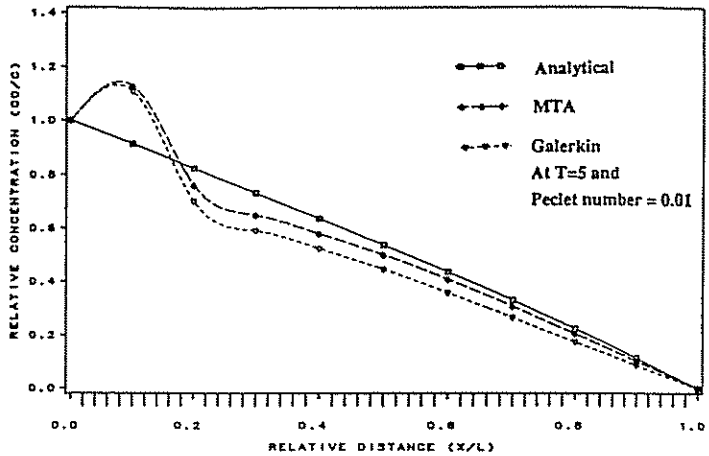

Fig. 5: Comparison of Fluid Transport by Three Methods (b)

The dominance of the first order spatial derivative term in the DA equation may not be the only source of the numerical oscillation. To define the relative importance of sources, a higher order time stepping scheme such as the *Crank Nicolson* method together with conjugate gradient method as a system equation solver, is applied to a similar problem with a higher Peclet number of 0.1. The result is giver in *Fig. 6*, where the MTA method yields a considerable improvement over the Galerkin method and is largely free from oscillation. The importance of accurate time discretization is clearly apparent in this example.

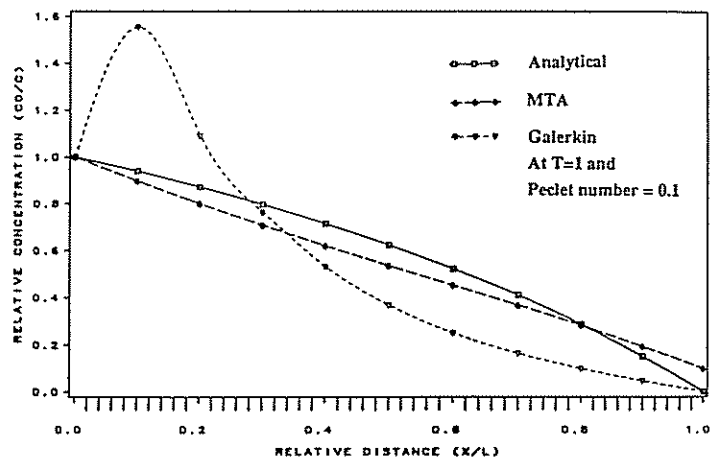

Fig. 6: Comparison of Fluid Transport by Three Methods (c)

6.3 Proposed method for solution of the DA equation

The MTA method works, however, subject to the following limitations:

a. The tranformation of eqn. (23) is the result of a function product [since C = C(X, T)]. The variational formulation has to be modified if the boundary or initial conditions are changed.

b. In the formulation, β is restricted to constant values, only. However, these restrictions can be removed if a proposed method is used (referred to MTB method).

A general two dimensional DA equation may be written as

$$\frac{\partial^2 C}{\partial X_i^2} - \beta_i \frac{\partial C}{\partial X_i} = \frac{\partial C}{\partial T} \tag{37}$$

Following a similar derivation to that in steady state case, we obtain from eqn. (37)

$$\frac{\partial}{\partial X_i}\left\{exp(-\beta_i X_i)\frac{\partial C}{\partial X_i}\right\} = exp(-\beta_i X_i)\frac{\partial C}{\partial T} \tag{38}$$

For a variational formulation, the functional J can be given for eqn. (38) as

$$J = \frac{1}{2}\int_{X_i}^{X_k}\left\{exp(-\beta_i X_i)\left(\frac{dC}{dX_i}\right)^2 - exp(-\beta_i X_i)\left(\frac{dC}{dt}\right)^2\right\}dX \tag{39}$$

To minimize the functional, then $\frac{\partial J}{\partial C} = 0$, resulting in

$$\frac{\partial J}{\partial C} = \sum_{e=1}^{k}(A^{(e)}C^{(e)} - B^{(e)}\dot{C}^{(e)}) = 0 \tag{40}$$

where

$$A^{(e)} = \int_{X_j}^{X_k} exp(-\beta X)\begin{pmatrix} N_j' & N_j' & N_j' & N_k' \\ N_k' & N_j' & N_k' & N_k' \end{pmatrix} dX \tag{41}$$

$$B^{(e)} = \int_{X_j}^{X_k} exp(-\beta X)\begin{pmatrix} N_j & N_j & N_j & N_k \\ N_k & N_j & N_k & N_k \end{pmatrix} dX \tag{42}$$

$$C^{(e)} = (C_j\ C_{j+1})^T \tag{43}$$

$$\dot{C}^{(e)} = \left[\frac{\partial C_j}{\partial T}\ \frac{\partial C_{j+1}}{\partial T}\right]^T \tag{44}$$

Again, assuming a piecewise linear interpolation function together with a constant value for exp ($-\beta$X) over each element, eqns. (41) and (42) reduce to

$$A^{(e)} = \frac{exp(-\beta X^{(e)})}{l}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \tag{45}$$

$$B^{(e)} = \frac{l}{6}exp(-\beta X^{(e)})\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \tag{46}$$

where l is element length. It is apparent that eqn. (45) is identical to eqn. (21). Also, the system of eqn. (40) is symmetric and positive definite. By further observation of eqns. (45) and (46), it is clear that the term exp ($-\beta$X) is essentially a weighting function. Recalling that $\beta = Vl/D$, then as β increases, a stronger influence is imposed from the weighting function. The other observation is that β cannot be a too large unless the element length l is sufficiently small to keep the solution stable.

6.4 Validation of the proposed method

The problem is investigated at a specific time (T = 1) with changing magnitudes of *Peclet* number. Analytical solutions are obtained by the method described previously. Excellent agreement is achieved between the analytical solution and the proposed method for a *Peclet* number of 0.1, illustrated in *Fig. 7* and *Table V*. The maximum error is estimated to be 0.023.

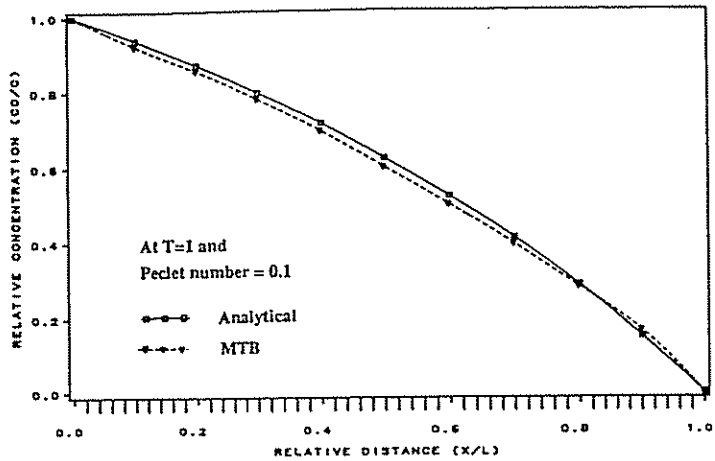

Fig. 7: Transient Fluid Transport by Analytical Solution and MTB (a)

Table V: Concentration versus distance (b)

Distance	Analytical	MTB
0.0	1.0000	1.0000
0.1	0.9388	0.9226
0.2	0.8712	0.8550
0.3	0.7964	0.7782
0.4	0.7138	0.6928
0.5	0.6225	0.5995
0.6	0.5216	0.4992
0.7	0.4101	0.3929
0.8	0.2868	0.2815
0.9	0.1506	0.1662
1.0	0.0000	0.0000

Further comparison of the MTB method with the analytical solution is completed for Peclet numbers of 0.01, 0.05 and 0.5, respectively. These results are illustrated in Fig. 8 and are rather scattered. Slight overshoot occurs in the MTB for a Peclet number 0.5. This situation would be further complicated for greater β magnitudes.

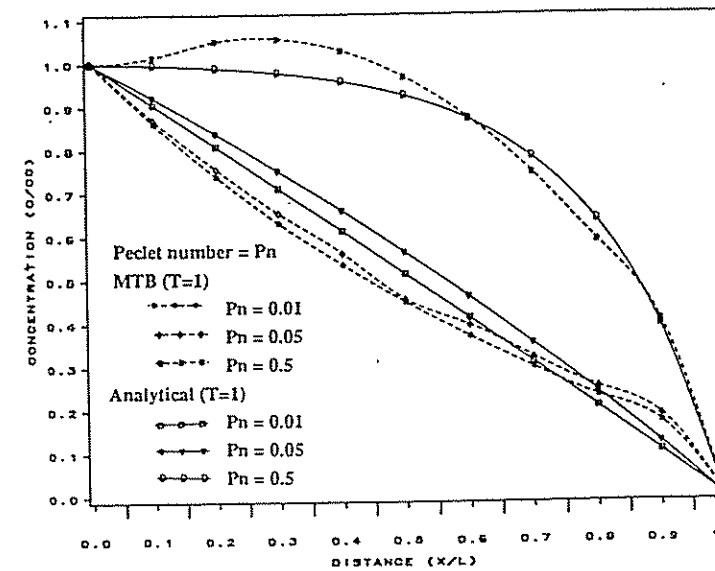

Fig. 8: Transient Fluid Transport by Analytical Solution and MTB (b)

Conclusions

This paper discusses some classical problems of solving the diffusion advection equation (DA equation) and presents spe-

cific methods used to concurrently damp oscillations and minimize numerical dispersion. The significant conclusions are as follows.

(a) A method solving the steady state DA equation is introduced that modifies the asymmetric DA equation into a symmetric positive definite one. Symmetry is achieved by imbedding the first order spatial derivative of the equation into the second order derivative term. The variational formulation is used to preserve symmetry in the resulting system of equations. An efficient conjugate gradient method is applied to solve the symmetric system and can be readily extended to higher dimensional problems.

(b) For the steady state case, the proposed method is validated against three other methods: analytical solution, a *Galerkin* finite element method and an upwind weighted *Galerkin* method. The results show that the proposed method remains oscillation free and exhibits minimal numerical diffusion for a variety of *Peclet* numbers up to at least 10. Retaining symmetry in the equation minimizes numerical oscillations.

(c) In terms of computational accuracy, the analyses presented in the preceding illustrate that increasing the element density may not significantly improve the accuracy of the estimation, excluding the *Galerkin* method.

(d) The proposed method is further extended to solve the transient DA equation. Validation indicates that the proposed method performs well but remains restricted to certain magnitudes of *Peclet* numbers.

(e) A method based on a modification of *Guymon's* method [3] is also introduced for solving the transient DA equation. The method is shown to offer improved accuracy over the traditional Galerkin method. Accuracy is further improved by using a higher order time stepping scheme such as the central difference or *Crank-Nicolson* method.

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Coal Specifications

The IEA Coal Research, London, has published a report (IEACR/52) titled "Coal specifications – impact on power station performance". As most of the coal used to generate electricity is consumed as pulverised fuel, the focus of the report is on performance in pulverised fuel (PF) power station units. The properties that are currently employed as specifications for coal selection are reviewed together with their influence on power station performance. Major coal-related items in a power station are considered in relation to those properties which affect their performance. There is a review of 'tools' being used for coal selection and prediction of station performance which includes an overview of the types of computer models that are available and those that are being developed.

The principal coal properties that were found to cause greatest concern to operators included the ash, sulphur, moisture and volatile matter contents, heating value and grindability. Little has changed over the years in the way that coal is assessed and selected for combustion. Operators continue to use tests as specifications that were mostly developed for coal uses other than combustion. Because the procurement specifications are based on tests which do not relate well to actual practice, there is still a need for expensive large scale test burns to confirm suitability. With the advances that have been made in computer technology, there is a growing number of utilities that are adopting 'expert' unit or integrated models that aid in the planning and operation of generating units. Others have shown scepticism over the capability of devising a truly representative model of a coal combustion plant using the coal data produced from current testing procedures.

Specific requirements that have been identified include the need to develop internationally acceptable methods of defining coal characteristics so that combustion plant performance can be predicted more effectively. There is also a need to establish economic parameters which can serve to measure the effects of coals on plant performance and hence on the cost of electricity.

Major coalfields of the world

At least 90% of world hard coal output will be produced from fewer than 20 major coalfields during the next two decades. The IEA Coal Research publication (IEACR/51) analyses these coalfields from both a geological and economic perspective. Introductory chapters provide an overview of the economic and geological history of world hard coal. The changing pattern of output and demand over the past century, including the growth in international coal trade is described briefly. Next considered are the formation of coal deposits at various stages in geological history and the resultant differences in coal type, grade and rank. Each major coalfield is analysed against this background. The geology, structure and stratigraphy, rank and quality, resources and areas of interest of each coalfield are discussed. Industry structure and performance over the recent past are then considered, together with the transport infrastructure, production costs and market potential associated with each coalfield.