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Determination of Optimal Upstream Weighting Parameter for the Finite Element Solution of Transient Transport Equation

In this study the results of a numerical experiment involving the finite element solution of the convection-dominated transport equation are presented. It is shown that, for large Peclet numbers, the standard Galerkin approach produces unacceptable oscillations. Although the upstream weighting residual method eliminates this problem for steady state problems, its application to transient flow problems has received considerable criticism, because false dispersion and/or the smearing of steep gradients are observed. The numerical experiments performed for transient problems revealed that the upstream weigting residual method can be improved considerably if the upstream weighting parameter is selected as a function of the Courant number. Based on the results of these numerical experiments, a relationship between the optimal weighting parameter and the Courant number is proposed so that oscillations are eliminated and false dispersion is reduced to an acceptable level.

In dieser Studie werden die Ergebnisse eines numerischen Experimentes vorgestellt, das die Finite-Elemente-Lösung der Transportgleichung mit vorherrschender Konvektion betraf. Es wird gezeigt, daß der Standard-Ansatz nach Galerkin für große Peclet-Zahlen unannehmbare Schwingungen erzeugt. Obgleich die Methode der stromaufwärts gewichteten Residuen (upstream weighting residual method) diese Schwierigkeit für stationäre Probleme umgeht, erfuhr deren Anwendung auf Übergangsströmungsprobleme erhebliche Kritik, da eine falsche Dispersion und/oder ein Verschmieren der steilen Gradienten beobachtet wurden. Die für Übergangsprobleme durchgeführten Experimente offenbarten, daß die Upstream-Weighting-Residual-Methode beträchtlich verbessert werden kann, falls der Upstream-Weighting-Parameter als Funktion der Courant-Zahl gewählt wird. Auf der Basis der aus diesen numerischen Experimenten erhaltenen Ergebnisse wird eine Beziehung zwischen dem optimalen Weighting-Parameter und der Courant-Zahl vorgeschlagen, durch die Schwingungen ausgeschaltet werden und die falsche Dispersion auf ein annehmbares Niveau gesenkt wird.

В данной работе представляются результаты численного эксперимента, связанного с решением методом конечных элементов уравнения переноса с преимущественной конвекцией. Показывается, что обычное приближение Галёркина при больших числах Пекле приводит к неприемлемым колебаниям. Хотя метод ориентированных против потока взвешенных элементов не приводит к трудностям при стационарных проблемах, его применение к проблемам переходных течений подвергалось критике, потому что при этом наблюдалась ошибочная дисперсия и/или размывание крутого фронта. Численные эксперименты, проведённые для переходных течений, показали, что метод ориентированных против потока взвешенных элементов может быть значительно улучшен, если его параметры выбирать как функции числа Куранта. На основе полученных из таких численных экспериментов результатов предлагается некоторое соотношение между оптимальным параметром взвешивания и числом Куранта, так что колебания исчезают, а ошибочная дисперсия сводится к приемлемому уровню.

Introduction

The finite element solution of the transport (convective-dispersive) equation presents serious difficulties when the convective term is dominant. If the Galerkin method is applied to this type of equation, an unacceptable numerical oscillation arises whenever the mesh size exceeds a certain critical value. To overcome this problem Christie et al. (1976) and Heinrich et al. (1977) developed the so-called upstream finite element method and demonstrated its efficiency for the steady-state transport equation. This scheme differs from the standard Galerkin scheme in that the spatial discretization is performed by the Petrov-Galerkin method; which employs nonsymmetric quadratic weighting functions to give the upstream weighting of the convective term in the transport equation. This scheme has received wide acceptance since its introduction and has also been applied to transient transport problems (Huyakorn and Nilkuha, 1979; Noorishad and Mehram, 1982; Huyakorn et al., 1983).

Lately, however, upstreaming has been the subject of criticism in view of the fact that false dispersion or smearing of a gradient is observed in the numerical solution (Gresho and Lee, 1980; Allen, 1984). To maintain good accuracy of the upstream finite element method by preserving the original simple weighting functions, it is necessary to choose optimal upstream weighting parameters that can efficiently eliminate the numerical oscillations and also minimize the incidental false dispersions. A series of numerical experiments was conducted to search for the optimal value of the upstream weighting parameter which is applicable to the transient transport equations, and the findings of this study are presented here.

Background

The general procedure of the upstream finite element formulation will be described by considering, as an example, the one-dimensional transient transport equation with constant dispersivity and velocity:

$$D\frac{\partial^2 C}{\partial X^2} - V\frac{\partial C}{\partial X} = \frac{\partial C}{\partial t}. \tag{1}$$

The initial and boundary conditions are

$$C(X, 0) = 0\,, \qquad C(\infty, t) = 0\,, \qquad C(0, t) = \hat{C} \qquad \text{(2a), (2b), (2c)}$$

in which the dependent variable, C, denotes the concentration of the solute. To discretize (1) by the upstream weighted residual finite element scheme, the spatial (convective and dispersive) terms and the temporal term are weighted by use of nonsymmetric weighting functions, W_I, and standard basis functions, N_I, respectively, to give

$$\int_R W_I \frac{\partial}{\partial X}\left(D \frac{\partial C}{\partial X} - VC\right) \mathrm{d}R - \int_R N_I \frac{\partial C}{\partial t} \mathrm{d}R = 0\,, \qquad I = 1, 2, \dots, n\,. \tag{3}$$

Application of Green's theorem to the second derivative (dispersive) term of Eq. (3) yields

$$\int_R W_I \frac{\partial}{\partial X}\left(D \frac{\partial C}{\partial X}\right) \mathrm{d}R = \int_S W_I D \frac{\partial C}{\partial X} n_x \,\mathrm{d}s - \int_R \frac{\partial W_I}{\partial X} D \frac{\partial C}{\partial X} \mathrm{d}R \tag{4}$$

in which the surface integral term represents the dispersive flux on the boundary (this term is assumed to be zero in this study because the convective-dominated case is considered). Next, the trial function is introduced in the following form:

$$C(X, t) = N_J(X)\, C_J(t)\,, \qquad J = 1, 2, \dots, n \tag{5}$$

in which N_J are the common linear basis functions. Substitution of Eq. (4) into Eq. (3) and application of Eq. (5) yields

$$H_{IJ} \frac{\mathrm{d}C_J}{\mathrm{d}t} + M_{IJ} \varepsilon_J = 0 \tag{6}$$

where

$$H_{IJ} = \sum_e \int_{R^e} N_I N_J \,\mathrm{d}R\,, \tag{7a}$$

$$M_{IJ} = \sum_e \int_{R^e} D \frac{\mathrm{d}W_I}{\mathrm{d}X} \frac{\mathrm{d}N_J}{\mathrm{d}X} \mathrm{d}R + \sum_e \int_{R^e} V W_I \frac{\mathrm{d}N_J}{\mathrm{d}X} \mathrm{d}R\,. \tag{7b}$$

Time integration of Eq. (6) by use of a time-centered (Crank-Nicolson) finite difference scheme gives

$$A_{IJ} C_J^{K+1} = B_{IJ} C_J^K \tag{8}$$

where

$$A_{IJ} = \frac{H_{IJ}}{\Delta t} + \frac{M_{IJ}}{2}\,, \tag{9a}$$

$$B_{IJ} = \frac{H_{IJ}}{\Delta t} - \frac{M_{IJ}}{2} \tag{9b}$$

in which K and Δt represent the time step and time increment, respectively. The weighting functions, W_I, in Eq. (7b) are given by the following quadratic functions (Heinrich et al., 1977) expressed in terms of local coordinates:

$$W_1 = 1 - (1 + 3\alpha) \frac{X}{L} + \frac{3\alpha X^2}{L^2}\,, \tag{10a}$$

$$W_2 = (1 + 3\alpha) \frac{X}{L} - \frac{3\alpha X^2}{L^2} \tag{10b}$$

where L is the element length and α is the weighting

$$H_{IJ} = \frac{L}{6}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}, \tag{11a}$$

$$M_{IJ} = \frac{D}{L}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} + \frac{V}{2}\begin{bmatrix} -1 + \alpha & 1 - \alpha \\ -1 - \alpha & 1 + \alpha \end{bmatrix}. \tag{11b}$$

According to Heinrich et al. (1977), for stable and oscillatory free conditions the upstream weighting parameter, α, should have the value of

$$\alpha = 0 \quad \text{for} \quad P_e < 2 \tag{12a}$$

and

$$\alpha \geqq 1 - \frac{2}{P_e} \quad \text{for} \quad P_e \geqq 2 \tag{12b}$$

where P_e is the mesh Peclet number, defined as

$$P_e = \frac{|V| \Delta X}{D} \tag{13}$$

where ΔX denotes the mesh size. By analyzing the finite element assembled equation system for a node, Christie et al. (1976) showed that the error in the difference equations becomes zero when

$$\alpha = \left(\coth \frac{P_e}{2}\right) - \frac{2}{P_e} \tag{14}$$

if steady state conditions are assumed. The α values given by criteria (12) and (14) are called the critical and the optimal upstream weighting parameters, respectively, and they have been commonly employed in the upstream finite element solution of convective-dispersive equations.

Numerical experiments

To clarify the controversial issues involved in the upstreaming scheme, (1) was solved by the standard Galerkin method and by UWRM (upstream weighted residual method) for the simple linear model. It has 20 equal-length elements ($\Delta X = L = 0.5$) with constant velocity ($V = 0.5$). The longitudinal dispersivity, D, was selected as 0.25, 0.025, and 0.0025, corresponding to the mesh Peclet number, P_e of 1, 10, and 100, respectively. The exact analytical solution for this simple case is available and can be expressed as (Ogata et al., 1961)

$$\frac{c}{\hat{c}} = \frac{1}{2}\left[\operatorname{erfc}\left\{\frac{X - Vt}{2\sqrt{Dt}}\right\} + \exp\left(\frac{VX}{D}\right)\operatorname{erfc}\left\{\frac{X + Vt}{2\sqrt{Dt}}\right\}\right] \tag{15}$$

where $c/\hat{c}$ denotes the dimensionless concentration and erfc is the complementary error function.

The results of the analysis reveal that, for $P_e = 1$ and 10, the standard Galerkin method produces fairly accurate solutions: hence, upstream weighting (nonzero α) is unnecessary. This conclusion is consistent with the findings of Pinder and Grey (1977). For $P_e = 100$, however, the standard Galerkin method exhibits significant oscillations, especially near the concentration front. Although the UWRM successfully eliminates numerical oscillations for all values of the Peclet number, smearing of the concentration front (false dispersion) develops as P_e increases. Accordingly, it is logical to expect that the value of the upstream weighting parameter may be reduced to a point at which the numerical oscillations are sufficiently eliminated while the false dispersions are simultaneously minimized. Since criterion (14) is applicable to a steady-state condition, it is necessary to evaluate the influence of the time size associated with the time integration of the transient transport equation. To quantify the effect of the time step size, the Courant number defined by the following ratio is introduced (Huyakorn and Nilkuha, 1979):

$$C_r = \frac{|V|\,\Delta t}{\Delta X}. \tag{16}$$

It should be mentioned that the Courant number is commonly used in the discrete perturbation stability analysis for the transient transport equations in finite difference schemes (Roache, 1972).

A series of numerical experiments was then conducted to search for the optimal values of α (defined as values which eliminate numerical oscillations and also minimize false dispersions by applying different Peclet numbers and different Courant numbers for the solution of the transient transport equation). The Peclet number was controlled by choosing different dispersivities in Eq. (13), and the Courant number was changed by using different time step sizes in Eq. (16). A similar attempt was made by Huyakorn and Nilkuha (1979) for the same differential equation, Eq. (1), and using the same numerical model.

These numerical experiments led to the conclusion that the optimal value of the upstream weighting parameter, α_{opt}, is related to the Courant number. The relationship between α_{opt} and C_r for the case where $P_e = \infty$ (pure convection) is presented in Fig. 1 and may be expressed as

$$\alpha_{\text{opt}} = 0.11 \exp(1.1 C_r)\,. \tag{17}$$

If the Peclet number is different from $P_e = \infty$, the optimal α's line up slightly below the indicated curve, but the numerical oscillations and dispersions remain within acceptable limits. If the Courant number, C_r, lies in the range

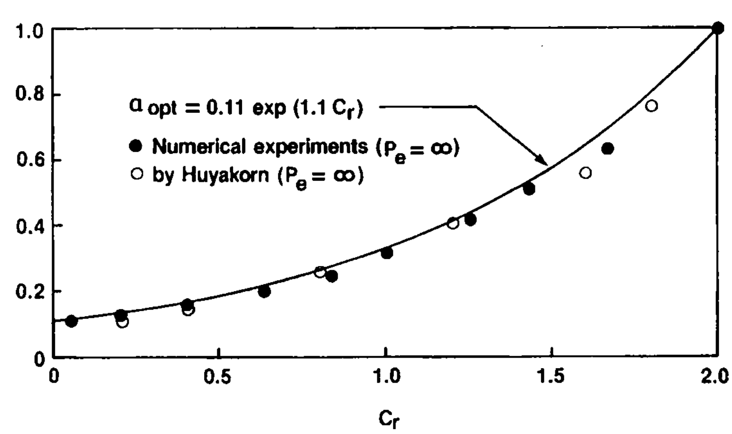

Fig. 1. Relationship between optimal upstream weighting factor and Courant number, $P_e = \infty$

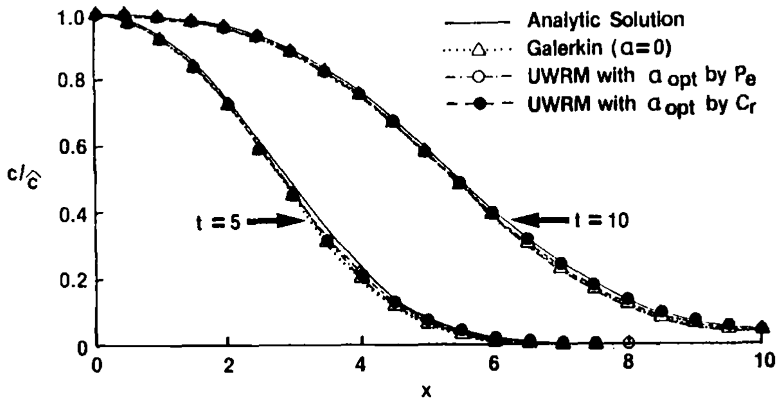

Fig. 2. Comparison of analytical and numerical results for $P_e = 1$

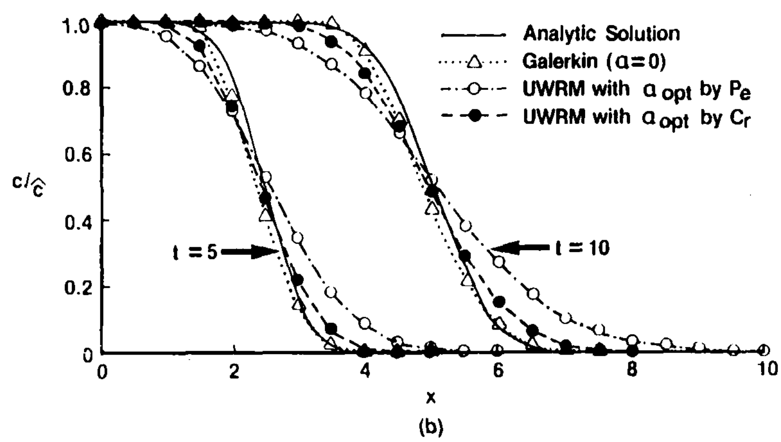

Fig. 3. Comparison of analytical and numerical results for $P_e = 10$

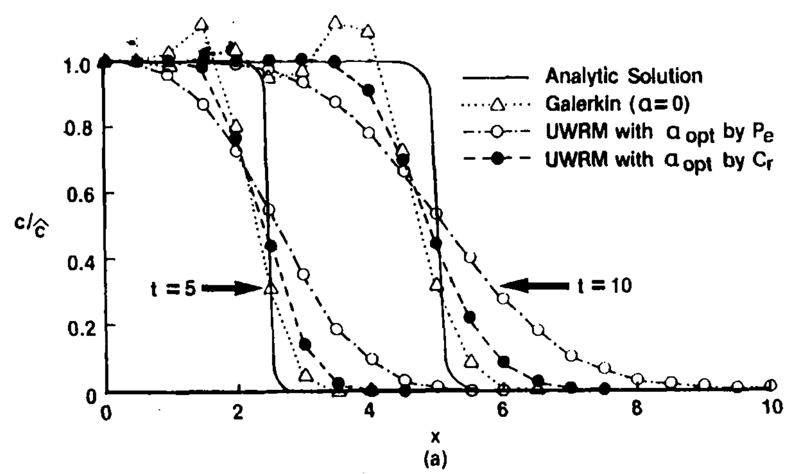

Fig. 4. Comparison of analytical and numerical results for $P_e = 100$

of $1 \leqq C_r \leqq 2$, slight oscillations are observed in the first few time steps, but these oscillations diminish rapidly. When $C_r < 1$, no numerical oscillation can be noticed if α is chosen according to Eq. (17).

Finally, the adequacy of criterion (17) for the upstream finite element solution of the transient transport equation was tested for the one-dimensional model. The time step size was chosen as $\Delta t = 0.5$ for each case, corresponding to a constant Courant number of 0.5. Figures 2 to 4 illustrate the comparison between the numerical solutions obtained by the standard Galerkin method ($\alpha = 0$), UWRM with α_{opt} based on the mesh Peclet number (criterion (14)), UWRM with α_{opt} based on the Courant number (criterion (17)), and the exact analytical solutions for different convection/dispersion rates. It is evident from these figures that the C_r-based UWRM is capable of not only eliminating numerical oscillations but also minimizing incidental false dispersions in every case. Although slight false dispersions still exist, the C_r-based UWRM gives a better solution with respect to the divergence from the exact solutions.

It should also be added that the proposed optimal weighting parameter has been used and gave excellent results in multidimensional problems.

Conclusions

The proposed approach appears to be effective in eliminating numerical oscillations while minimizing false dispersions in the analysis of convection-dominated transient transport problems. It is concluded, therefore, that the optimal upstream weighting parameter, α_{opt}, in the upstream finite element method can be fully controlled only if it is selected in terms of the Courant number, C_r. The lack of an analytical solution dictated that an appropriate criterion be determined by numerical experiments. Within the limits of this study, the α_{opt} values calculated thus determined guarantee oscillation free results with minimum false dispersion. If the size of the element mesh is restricted or fixed, the size of time step selected for the numerical analysis should correspond to $C_r \leqq 1$.

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