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# 최적시행함수 Petrov-Galerkin 방법

## Optimal Test Function Petrov-Galerkin Method

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### Abstract

Numerical analysis of convection-dominated transport problems are challenging because of dual characteristics of the governing equation. In the finite element method, a strategy is to modify the test function to weight more in the upwind direction. This is called as the Petrov-Galerkin method. In this paper, both N+1 and N+2 Petrov-Galerkin methods are applied to transport problems at high grid Peclet number. Frequency fitting algorithm is used to obtain optimal levels of N+2 upwinding, and the results are discussed. Also, a new Petrov-Galerkin method, named as "Optimal Test Function Petrov-Galerkin Method," is proposed in this paper. The test function of this numerical method changes its shape depending upon relative strength of the convection to the diffusion. A numerical experiment is carried out to demonstrate the performance of the proposed method.

*Keywords*: transport equation, convection-diffusion equation, Petrov-Galerkin finite element method, optimal test function Petrov-Galerkin method, frequency fitting method

### 요 지

수송방정식의 양면적인 특성으로 인하여 이송항이 지배적인 흐름에 있어서 수송방정식의 수치해석은 매우 난해하다. 특히 유한요소법을 사용하여 수치해석할 때, 상류방향으로 더 많은 가중치를 두기 위하여 변화된 시행함수를 사용한다. 이러한 방법을 Petrov-Galerkin 방법이라고 한다. 본 논문에서는 N+1 과 N+2 Petrov-Galerkin 방법을 격자 Peclet 수가 큰 수송문제에 적용하였다. 주파수맞춤 기법을 사용하여 N+2 Petrov-Galerkin 방법의 적정 풍상정도를 찾아내었고, 그 결과를 토의하였다. 또한 본 논문은 새로운 Petrov-Galerkin 방법인 최적시행함수 Petrov-Galerkin 방법을 제안하였다. 이 기법의 시행함수는 이송항과 확산항의 상대적 크기에 따라 그 모양이 변화된다. 수치실험을 통하여 제시된 새로운 수치해석기법의 우수성을 설명하였다.

**핵심용어** : 수송방정식, 이송확산방정식, Petrov-Galerkin 유한요소법, 최적시행함수 Petrov-Galerkin 방법, 주파수맞춤 기법

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## 1. Introduction

Transport in the environment is described by the convection-diffusion equation (or the transport equation). The transport equation is a mixed type of partial differential equation which has both hyperbolic and parabolic characteristics. A difficulty in the numerical analysis of the transport equation lies in that the solution strategy should be chosen according to the characteristic of a given problem. That is, if the parabolic feature of the problem is stronger than the hyperbolic feature, then a numerical modeler does not have to concern numerical oscillations because the diffusion term naturally smoothes the solution. However, in a reversed case, the modeler needs to introduce a special dissipative technique for the convection term because of a possible generation of the steep gradient in the numerical solution. In the latter case, mostly, the upwinding concept should be introduced to protect the solution from the downwind contamination (Christie et al., 1976 ; Heinrich et al., 1977 ; Brooks and Hughes, 1982 ; Westerink and Shea, 1989). This may be more easily achieved, if the finite difference method is employed, by using upwind type schemes such as the backward difference scheme, MacCormack scheme, or Beam and Warming scheme.

The conventional finite element method (or Bubnov Galerkin method) shows robustness in the boundary value problem in which governing equations are self-adjoint partial differential equations. However, the Galerkin method is not so efficient for non-self-adjoint problems such as a convection-diffusion equation. This equation can be characterized by a non-dissipative convection process and a dissipative diffusion process. When the dissipative process dominate the transport phenomenon, one can get a good solution using the conventional Galerkin method. However, when the non-dissipative convection process is dominant, the partial differential equation behaves as a first-order hyperbolic partial differential equation which describes a pure wave propagation with a finite celerity. Therefore, the numerical solution may form or maintain a sharp front. When the conventional Galerkin method with linear basis functions is applied to this problem, oscillations are encountered in the numerical solution. Specifically, in the one-dimensional case, the finite element scheme can easily be shown to become centered difference finite difference scheme. Since the numerical errors arise from the symmetric treatment of the convection terms in the conventional finite element method, the test functions are modified in order to give more weight in the upwind direction as commonly done in the finite difference method. This technique is referred to as "the Petrov-Galerkin (PG) method."

The $N+k$ PG method uses the weighting functions which are $k$ polynomial degree higher than the basis functions. The N+1 PG method, having the quadratic perturbation term in the weighting functions, has been successfully applied to the steady-state convection-dominated transport problem (Christie et al., 1976 ; Heinrich et al., 1977). However, it failed to improve numerical solutions for the time-dependent problem, which necessitated introduction of the N+2 PG method. The test functions of the N+2 PG method include both asymmetric quadratic and symmetric cubic perturbation terms.

Although it is true that the N+2 PG method alleviates numerical oscillations without introducing too much dissipation, a weakness of this method lies in determining appropriate levels of upwinding. Specially, numerical experiments have shown that the symmetric cubic term rather than the asymmetric quadratic term in the weighting functions plays a major role in reducing the numerical errors due to time dependency (Dick, 1983 ; Westerink and Shea, 1989 ; Bouloutas and Celia, 1991). That is, using both quadratic and cubic terms in the N+2 PG method deteriorates numerical solutions in the time-dependent problem. Tezduyar and Ganjoo (1986) proposed perturbation functions dependent upon Courant number in the streamline upwind PG method. Westerink and Shea (1989) presented a graphical method to determine upwinding parameters for the cubic perturbation function for the pure convection problem. Miller and Cornew (1992) showed that the standard deviation of a Gaussian source affects optimal upwinding level in the N+2 PG method. Carrano and Yeh (1994) introduced a spectral weighting technique to optimize the phase error in the N+2 PG method.

The paper reviews various PG methods for steady and unsteady transport problems. Applicability and limitation of each method are investigated. Frequency fitting is applied to finding optimal levels of upwinding in the N+2 PG method. A new PG method, the test functions of which change optimally depending upon the relative strength of convection and diffusion terms, is proposed. Numerical experiments are carried out to see the performance of the new method.

## 2. Finite Element Formulation

Consider the following one-dimensional transport equation:

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

where $t$ and $x$ denote time and distance, respectively, $c$ is the concentration, $D$ is the diffusion coefficient, and $u$ describes the velocity field. Eq. (1), a mixed type of partial differential equation, describes the transport by two different physical processes, namely, convection and diffusion. In general, we encounter numerical instabilities due to convection term when the mesh size $(\Delta x)$ exceeds a certain value. This is given by

$$Pe \equiv \frac{u\Delta x}{D} > 2 \sim 5 \tag{2}$$

which is grid Peclet number, an indicative of the relative dominance of the convection to the diffusion. The weighted residual form of Eq. (1) is written as

$$\int\left\{\left(\frac{\partial c}{\partial t}\right) + D\frac{\partial c}{\partial x}\frac{\partial w}{\partial x}\right\}dx = D\frac{\partial c}{\partial x}\Big|_{\text{boundary}} \tag{3}$$

where $w$ is a test function. After the assembly process, one can get a global system of matrix differential equation such as

$$M\frac{dc}{dt}(A^v - A^d)c = P \tag{4}$$

where $c$ is vector of nodal unknowns, $M$ is mass matrix, $A^v$ is convection stiffness matrix, $A^d$ is diffusion stiffness matrix, and $P =$ convective and diffusive boundary flux forcing vector. In the conventional Galerkin method, the basis function of the trial solution is the same as the basis function of the test function. However, the PG method employs the test function whose basis function is different from the basis function of the trial solution. The numerical oscillations encountered in the numerical analysis of the convection dominant flow come from the non-symmetry of the stiffness matrix due to $A^v$. Therefore, the PG formulation was devised to recover the symmetry of the stiffness matrix to some extent.

## 3. Steady-State Transport

### 3.1 N+1 Petrov-Galerkin Method

At steady-state, Eq. (1) can be written as

$$\frac{d^2c}{dx^2} - k\frac{dc}{dx} = 0 \qquad (5)$$

where $k = u/D$. If we denote $x \in [0,1]$ and the boundary conditions such as

$$c(x) = \begin{bmatrix} 1 & x=0 \\ 0 & x=1 \end{bmatrix} \qquad (6)$$

Then, the analytical solution of Eq. (5) is obtained as

$$c(x) = \frac{e^{kx} - e^k}{1 - e^k} \qquad (7)$$

The N+1 test functions proposed by Christie et al. (1976) are

$$w_1 = \Psi_1 - \alpha F_{QD}(\xi) \qquad (8a)$$

$$w_2 = \Psi_2 + \alpha F_{QD}(\xi) \qquad (8b)$$

where $\Psi_i$ and $F_{QD}$ denote standard linear basis functions and a quadratic perturbation function, respectively, and $\alpha$ is a parameter to control the level of upwinding by $F_{QD}$. In Eq. (8), the quadratic perturbation is defined by

$$F_{QD} = \frac{3}{4}(1 + \xi)(1 - \xi) \qquad (9)$$

Christie et al. (1976) obtained an optimal value of $\alpha$ ($\alpha_{opt}$) analytically such as

$$\alpha_{opt} = \coth\frac{Pe}{2} - \frac{2}{Pe} \qquad (10)$$

Eqs. (8)-(10) constitute test functions of the N+1 PG method, which are one polynomial degree higher than the basis functions for the trial solution.

### 3.2 Numerical Experiments

Numerical experiments are carried out to demonstrate the performance of the N+1 PG method. For the sake of comparison, two finite

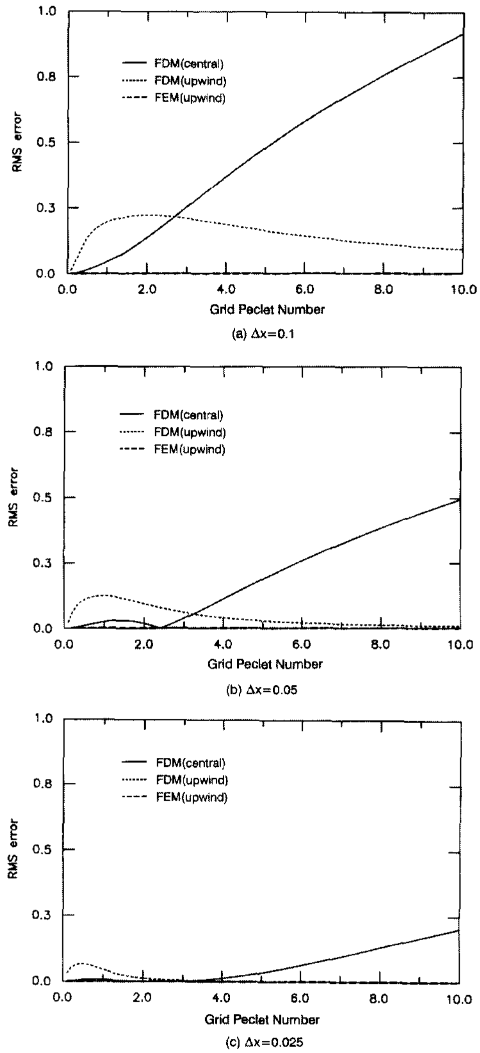



**Fig. 1. Grid Peclet Number versus RMS Error**

difference methods (centered and backward difference schemes) are also used for numerical analysis. The root mean square (RMS) error versus grid Peclet number is plotted in Fig. 1, where the RMS error is estimated by comparing the numerical solution with the analytical solution by Eq. (7) at all computational nodes. Computations with various grid Peclet numbers are performed by changing the convection velocity with a fixed grid size. It is seen that the N+1 PG method works perfectly in all cases. Whereas the RMS error from the backward difference scheme has a maximum value for problems at low Peclet numbers such as $0 < Pe < 2$, but the error tends to decrease as $Pe$ increases further. The centered difference scheme is good for problems at low Peclet numbers such as $Pe < 2$. However, as $Pe$ increases, the error increases monotonically. The current numerical experiments indicate that one way to eliminate the numerical instability with conventional methods of non-upwinding type is to severely refine the mesh such that convection is no longer dominant in the element level. However, this would require too much computational costs.

## 4. Time-Dependent Transport

### 4.1 N+2 Petrov-Galerkin Method

In the time-dependent transport problem, $\alpha_{opt}$ derived for the steady-state problem is no longer valid due the truncation error from time discretization. Therefore, both spatial and temporal discretization should be taken into account in determining the upwind level. The temporal discretization is important especially when the velocity field is not uniform.

The test functions of the N+2 PG method are given by

$$w_1 = \Psi_1 - \alpha F_{QD}(\xi) - \beta F_{CU}(\xi) \quad (11a)$$

$$w_2 = \Psi_2 + \alpha F_{QD}(\xi) + \beta F_{CU}(\xi) \quad (11b)$$

where $F_{CU}$ is a cubic perturbation function and $\beta$ is a parameter to control the level of cubic upwinding. The cubic perturbation function in Eq. (11) is defined as

$$F_{CU}(\xi) = \frac{5}{8}\xi(1+\xi)(1-\xi) \quad (12)$$

In Eq. (11), the cubic function $F_{CU}$ provides test functions with symmetric modification while $F_{QD}$ makes asymmetric modification. Simple integration of the above test functions leads to the following matrices given by Eq. (4) for a single element (Westerink and Shea, 1989):

$$M^{(e)} = \frac{\Delta x}{6}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} + \alpha\frac{\Delta x}{4}\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} + \beta\frac{\Delta x}{24}\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \quad (13a)$$

$$A^{v(e)} = \frac{u}{2}\begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} + \alpha\frac{u}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \quad (13b)$$

$$A^{d(e)} = \frac{D}{\Delta x}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \quad (13c)$$

Through truncation error analysis, Westerink and Shea (1989) showed that, for pure convection problems, the N+2 PG method with the choice of $\beta = 2Cr^2$ works well by reducing the error up to $O(h^3)$ with $\alpha$ and $O(h^4)$ without $\alpha$. For combined convection and diffusion problems, Westerink and Shea (1989) also showed that the N+1 upwinding does not offer an effective mechanism for time dependent problems. While the N+2 PG method with $\beta = 2Cr^2$ significantly improves the numerical solution especially for the problem at high Peclet number and Courant number close to unity.

### 4.2 Numerical Experiments

A convection-dominated transport problem with $u$ = 0.05 m/day, $D = 2.5 \times 10^{-5}$ m$^2$/day is solved by using the N+2 PG method. An initial condition of $c(x, t=0) = 0$ is used, and such boundary conditions as

$$\left(uc - D\frac{\partial c}{\partial x}\right)_{x=0} = uc_{\text{feed}} \quad (14a)$$

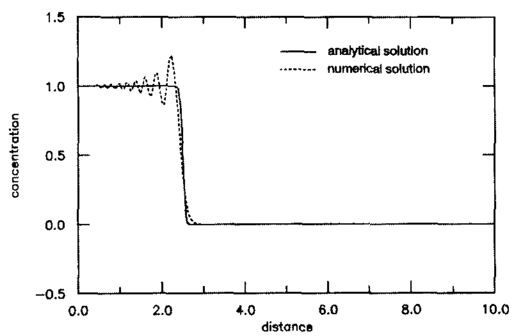
$$c(x \to \infty, t) = 0 \quad (14b)$$

are used at the upstream and the downstream boundaries, respectively. Values of $c_{feed} = 1.0$, $\Delta t = 1.0$ day, and $\Delta x = 0.05$ m are used in the computation, resulting $Cr = 1$ and $Pe =$ 100. The value of grid Peclet number is large enough to cause oscillations in the numerical solutions.

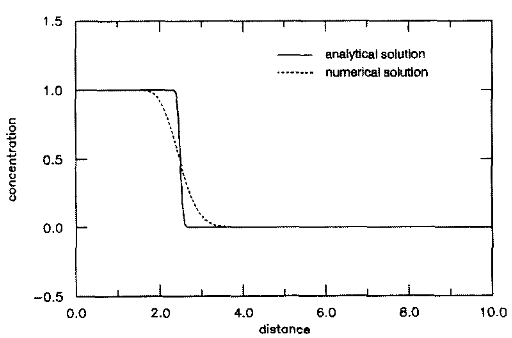
Fig. 2 shows the computed results by the standard Galerkin method. One can see numerical oscillations from phase error in Fig. 2(a) when Crank-Nicolson time integration is employed. Numerical dissipations from amplitude error are seen in Fig. 2(b) when fully-implicit time integration scheme is used. The results in Fig. 2(a) and (b) conform to Fourier analysis in Pinder and Gray (1977).

The N+2 PG method is now applied to the same problem. In order to get optimal values of $\alpha$ and $\beta$, only $\beta$ should be altered at first with $\alpha = 0$. By comparing the RMS error, an optimal value of upwinding parameter $\beta$ which produces minimum error, can be sought. Then, an optimal value of $\alpha$ with a fixed value of $\beta$ can be obtained by the same procedure. This procedure is based on the fact that $\alpha$ does not vary significantly compared to $\beta$.

In the present example, such values of upwinding parameters as $\alpha = 0.3$ and $\beta = 1.9$ are obtained by numerical experiments. Time integration by Crank-Nicolson scheme is used therein. Concentration profiles computed after 50 days and 100 days are presented in Fig. 3(a) and (b), respectively. A significant improvement due to the N+2 upwinding is observed in the computed solution compared with the solutions in Fig. 3. The optimal upwinding parameter $\beta$ = 1.9 is found to be very close to the value from $\beta = 2Cr^2$ suggested by Westerink and

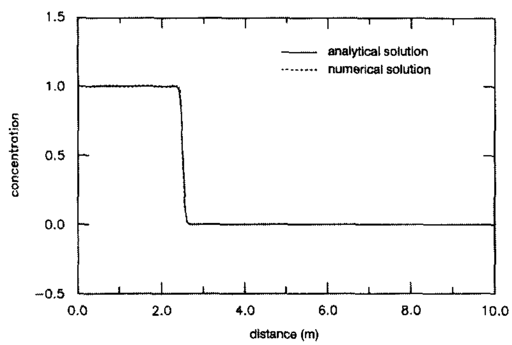


(a) Crank-Nicolson Time Integration

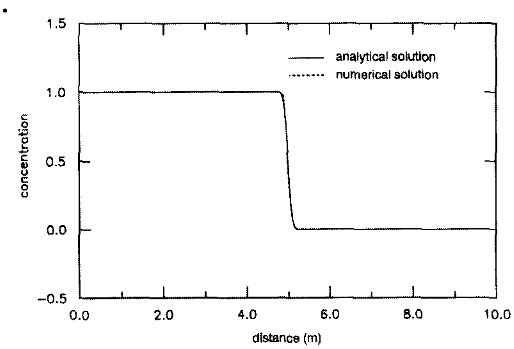


(b) Fully-implicit Time Integration

Fig. 2. Comparison of Numerical Solution by Galerkin Method and Analytical Solution



(a) Concentration after 50 days ($\alpha$=0.3, $\beta$=1.9)



(b) Concentration after 100 days ($\alpha$=0.3, $\beta$=1.9)

Fig. 3. Numerical Solution by N+2 PG Method

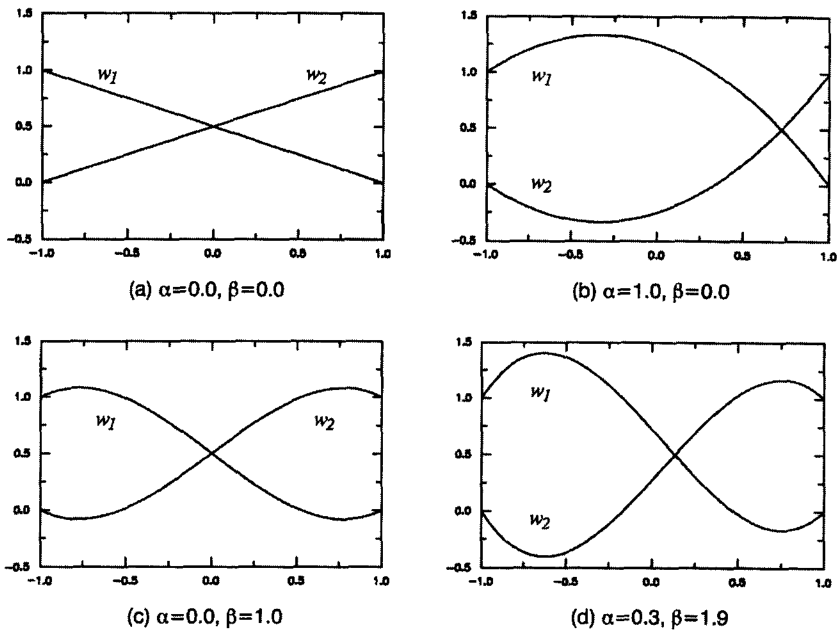



**Fig. 4. Test Functions of N+2 Petrov-Galerkin Method**

Shea (1989). Also, it can be noted that the role of quadratic perturbation function is not so important compared to that of cubic perturbation function.

Fig. 4 shows test functions of the N+2 PG method, the shape of which varies depending upon upwinding parameters $\alpha$ and $\beta$. When both $\alpha$ and $\beta$ are zero, the resulting test functions become linear basis functions as depicted in Fig. 4(a). The role of the quadratic perturbation function by $\alpha$ appears to make the test functions asymmetric over the length of element while the role of the cubic function by $\beta$ is to make the weight function symmetric, which is seen in Fig. 4(b) and (c), respectively. Fig. 4(d) shows optimal test functions for the previous example, which are obtained after many runs of numerical experiments.

### 4.3 Frequency Fitting of N+2 Petrov-Galerkin Method

By using the Fourier series expansion, the analytical solution of the transport equation can be expressed as

$$c(x, t) = \sum_m C_m \exp(i\sigma_m x + i\beta_m t) \qquad (15)$$

where $\sigma_m$ and $\beta_m$ are space and time frequencies of the m-th component, respectively. Then the analytical enlargement factor $\lambda\ [= c(x, t+\Delta t)/c(x, t)]$ becomes

$$\lambda_n = \exp(i\beta_n \Delta t) \qquad (16)$$

for the n-th component. We can express the time frequency in terms of the space frequency by substituting the solution, Eq. (15), into Eq. (1). That is, we have

$$\beta_n = i\, D\sigma_n^2 - u\sigma_n \qquad (17)$$

With the help of Eq. (17), the analytical enlargement factor can be rewritten as

$$\lambda = \exp(-i\ Cr \cdot y - Cr \cdot y^2/Pe) \qquad (18)$$

where $Cr = u\Delta t/\Delta x$ and $y = \sigma\Delta x$. Expanding Eq. (18) in a series form leads to

$$\lambda = 1 + A_1 y + A_2 y^2 + A_3 y^3 + A_4 y^4 + O(y^5) \quad (19)$$

where the coefficients $A_i$ are

$$A_1 = -i\ Cr$$
$$A_2 = Cr/Pe - Cr^2/2$$
$$A_3 = i(Cr^2/Pe + Cr^3/6)$$
$$A_4 = Cr^2/2Pe^2 + Cr^3/2Pe + Cr^4/24$$

Similarly, the numerical enlargement factor $l$ of the N+2 PG method is obtained. That is,

$$l = \frac{1-(1/3+\beta/12+\omega' Cr\alpha+2\omega' Cr/Pe)(1-\cos y)-i(\alpha/2+\omega' Cr)\sin y}{1-(1/3+\beta/12-\omega Cr\alpha-2\omega Cr/Pe)(1-\cos y)-i(\alpha/2-\omega Cr)\sin y} \quad (20)$$

where $\omega' = 1-\omega$. If the Crank-Nicolson time integration scheme is used ($\omega$ = 0.5), then Eq. (20) can be expressed in a series form such as

$$l = 1 + a_1 y + a_2 y^2 + a_3 y^3 + a_4 y^4 + O(y^5) \quad (21)$$

where the coefficients $a_i$ are

$$a_1 = -i\ Cr$$
$$a_2 = -Cr/Pe - Cr^2/2$$
$$a_3 = -i\frac{Cr}{24Pe}(12\alpha - 24Cr + \beta Pe - 6Cr^2 Pe)$$
$$a_4 = \frac{Cr}{48Pe^2}(24Cr - 4Pe + 12\alpha^2 Pe - 2\beta Pe - 24\alpha Cr Pe + 36Cr^2 Pe - 2\alpha Pe^2 + \alpha\beta Pe^2 - 2\beta Cr Pe^2 + 6Cr^3 Pe^2)$$

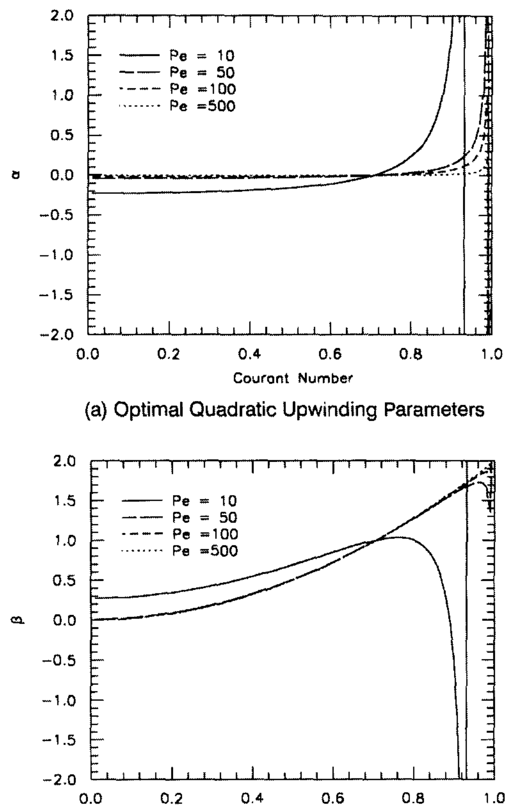
It is seen that the standard Galerkin method without any upwinding is second-order accurate when the Crank-Nicolson time stepping is used. For the N+2 PG method to have fourth-order accuracy, the third- and fourth-order terms in Eq. (19) should be the same as the terms for the numerical enlargement factor given by Eq. (21). This leads to the solution of two simultaneous equations with unknowns $\alpha$ and $\beta$, which are obtained as

$$\alpha = \frac{2Pe(1-2Cr^2)}{12 - Pe^2 + Cr^2 Pe^2} \quad (22)$$

$$\beta = \frac{2(-12 + 36Cr^2 - Cr^2Pe^2 + Cr^4Pe^2)}{12 - Pe^2 + Cr^2 Pe^2} \quad (23)$$

When the fully-implicit time integration is used ($\omega = 1$), the coefficients of the numerical enlargement factor become

$$a_1 = -i\ Cr \qquad a_2 = -Cr/Pe - Cr^2$$
$$a_3 = -i\frac{Cr}{24Pe}(12\alpha - 48Cr + \beta Pe - 24Cr^2 Pe)$$
$$a_4 = \frac{Cr}{48Pe^2}(48Cr - 4Pe + 12\alpha^2 Pe - 2\beta Pe - 48\alpha Cr Pe + 144Cr^2 Pe - 2\alpha Pe^2 + \alpha\beta Pe^2 - 4\beta Cr Pe^2 + 48Cr^3 Pe^2)$$



(b) Optimal Cubic Upwinding Parameters

Fig. 5. Optimal Upwind Parameters for N+2 PG Method

Comparison of the above coefficients with the coefficients of the analytical factor indicates that the standard Galerkin method with fully-implicit time integration is first-order accurate, and the upwinding affects only third- and fourth-order error terms.

Fig. 5(a) presents a plot of the quadratic upwinding parameter $\alpha$ versus $Cr$ for different values of $Pe$. It is seen that $\alpha$ from Eq. (22) is approximately zero except for a value of $Cr$ close to unity, and that $\alpha$ is not sensitive to $Pe$ once it exceeds 10. That is, the asymmetric quadratic perturbation function in the N+2 PG method does not play a significant role in upwinding for problems at large $Pe$. A plot of cubic upwinding parameter $\beta$ versus $Cr$ for different values of $Pe$ is given in Fig. 5(b). The value of $\beta$ from Eq. (23) is seen to increase from 0 to 2 as $Cr$ increases from 0 to 1 when $Pe$ is greater than 10. Also, $\beta$ is found to be insensitive to $Pe$ unless $Pe$ is significantly small. It is also seen that both $\alpha$ and $\beta$ blow up when $Cr$ is very close to unity.

The foregoing results coincide with the results in Bouloutas and Celia (1991), where they showed that the cubic PG method with $\beta = 2Cr^2$ is third- or fourth-order accurate when $Pe$ is extremely large (Herein, the cubic PG method means the N+2 PG method with $\alpha$ =0). Notice also that the N+2 PG method or the cubic PG method with $\beta = 2Cr^2$ becomes the standard Galerkin method when $Cr$ is small and $Pe$ is large.

## 5. Optimal Test Function Petrov-Galerkin Method

### 5.1 Optimal Test Function Method

Before introducing the OTFPG method, it may be worth to mention Optimal Test Function (OTF) method by Celia et al. (1989). Consider an operator form of the one-dimensional transport equation such as

$$Lc \equiv D\frac{\partial^2 c}{\partial x^2} - u\frac{\partial c}{\partial x} = \frac{\partial c}{\partial t} - f(x), \quad 0 \le x \le l \tag{24}$$

with the following boundary conditions:

$$c(0) = g_o \text{ and } c(l) = g_l \tag{25}$$

The weighted residual form of Eq. (24) is

$$\int_0^l (Lc)\, w(x) dx = \int_0^l \left( \frac{\partial c}{\partial t} - f(x,t) \right) w(x)\, dx \tag{26}$$

where $w(x)$ is a test function. If we discretize the domain into $E$ sub-intervals with $E+1$ nodal points, then Eq. (26) can be written as

$$\int_0^l (Lc)\, w(x) dx = \sum_{j=0}^{E-1} \int_{x_j}^{x_{j+1}} (Lc)\, w(x)\, dx \tag{27}$$

Since the optimal test function method is based on a weak form of the governing equation, integration by parts of the RHS of Eq. (26) after applying Eq. (24) leads to

$$\int_0^l (Lc)\, w(x) dx = \sum_{j=0}^{E-1}\left\{ \left[ Dw\frac{dc}{dx} - uwc \right]_{x_j}^{x_{j+1}} - \int_{x_j}^{x_{j+1}} \left( D\frac{dc}{dx} - uc \right) \frac{dw}{dx}\, dx \right\} \tag{28}$$

Another integration by parts of the second term of the RHS of Eq. (28) yields

$$\int_0^l (Lc)\, w(x) dx = \sum_{j=0}^{E-1}\left\{ \left[ Dw\frac{dc}{dx} - D\frac{dw}{dx}c - uwc \right]_{x_j}^{x_{j-1}} + \int_{x_j}^{x_{j+1}} (L^* w) c(x) dx \right\} \tag{29}$$

where $L^*$ is the formal adjoint of $L$. If one takes a test function which satisfies $L^* w = 0$ within each element, the following relationship should be hold:

$$\int_0^l (Lc)\, w(x)dx = \sum_{j=0}^{E-1}\left\{\left[Dw\frac{dc}{dx} - Dw\frac{dc}{dx} - uwc\right]_{x_j}^{x_{j+1}}\right. \tag{30}$$

Then, we have the following final form of equation from the OTF method:

$$\int_0^l (Lc)\, w(x)dx = \sum_{j=0}^{E-1}\left\{\left[Dw\frac{dc}{dx} + uw\right]_{x_j} c_j - [Dw]_{x_j}\frac{dc_j}{dx}\right\} + \left[(-D\frac{dw}{dx} - uw)c + (Dw)\frac{dc}{dx}\right]_0^l \tag{31}$$

where [ ] is a jump operator defined as

$$[\cdot]_{x_j} = [\cdot]_{x_j^+} - [\cdot]_{x_j^-} \tag{32}$$

If explicit forms of $w(x)$ can be derived, Eq. (31) leads to $(2E+2)\times(2E+2)$ algebraic equations, a 5 bandwidth matrix. The unknowns are essentially nodal values of function $c_j$ and their derivatives, i.e., $[c_j, dc_j/dx]_{j=1}^E$. Notice that no approximation has been introduced in the formulation so far. However, the homogeneous adjoint equation exhibits non-constant coefficients and cannot be solved exactly, in general.

### 5.2 Optimal Test Function Petrov-Galerkin Method

The main idea of the OTFPG method originates from applying the test function of the OTF method to the PG method. That is, instead of solving Eq. (31), one can use the test function satisfying $L^*\omega = 0$ from Eq. (30) in the PG formulation. In order to obtain the test function, the following equation should be solved:

$$L^*w = D\frac{d^2w}{dx^2} + u\frac{dw}{dx} = 0 \tag{33}$$

which is a second-order homogeneous linear ordinary differential equation. We, thus, have two fundamental solutions which are linearly independent, i.e.,

$$w_1(x) = 1 \tag{34a}$$

$$w_2(x) = \exp[-(u/D)x] \tag{34b}$$

Any linear combination of these solutions can be a solution of Eq. (33). However, we have the following two restrictions for $w_i$ to be test functions:

$$w_1(0) = 1, \qquad w_1(\Delta x) = 0 \tag{35a}$$

$$w_2(0) = 0, \qquad w_2(\Delta x) = 1 \tag{35b}$$

After applying the fundamental solutions of Eq. (34) into Eq. (35), we have two particular solutions such as

$$w_1(x) = \frac{\exp(-ux/D) - \exp(-u\Delta x/D)}{1-\exp(-u\Delta x/D)}, 0 \le x \le \Delta x \tag{36a}$$

$$w_2(x) = \frac{1-\exp(-ux/D)}{1-\exp(-u\Delta x/D)}, 0 \le x \le \Delta x \tag{36b}$$

Fig. 6 shows test functions from Eq. (36), which have various shapes depending upon the relative strength of convection term to the dispersion term. When $u/D = 0.1\,\text{m}^{-1}$, the test functions in Fig. 6(a) are nearly the same as linear shape functions, and when $u/D$ is increased up to 2000.0 $\text{m}^{-1}$, the test functions in Fig. 6(d) have a shape like a step function.

A steady-state transport problem with $u$ = 0.05 m/day and $D = 2.5\times10^{-5}\ \text{m}^2/\text{day}$ is solved by the OTFPG method. The resulting grid Peclet number is 100. Fig. 7 shows both numerical solution and analytical solution given by Eq. (7). Perfect agreement between two solutions is seen in the figure, which illustrates that $Pe$-dependent weighting in the PG method is sufficient for the steady-state transport

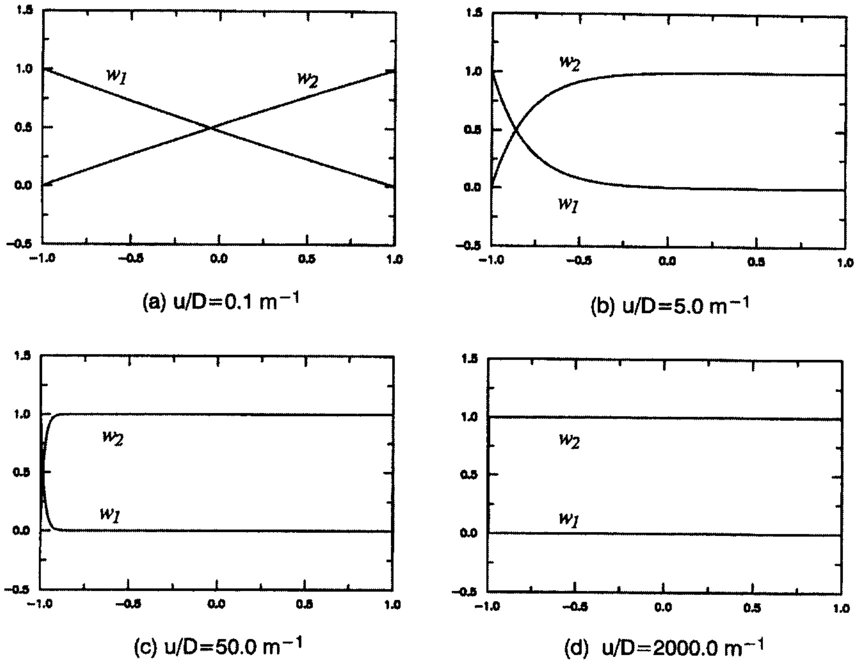



Fig. 6. Optimal Test Functions of OTFPG Method

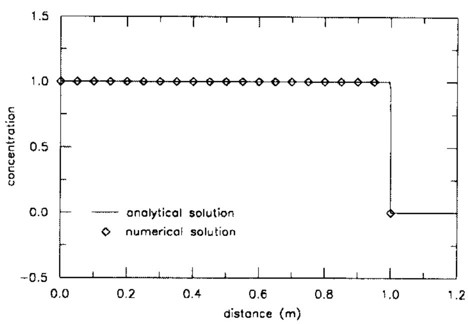



Fig. 7. Solution of Steady-State Transport Problem by OTFPG Method

problem.

Now, the same transport problem but transient case is solved to demonstrate the applicability of the proposed OTFPG method. Time step of $\Delta t = 1$ day is used to satisfy $Cr = 1$. Computed results are presented in Fig. 8(a) and (b), which show excellent agreement between the analytical and numerical solutions. This illustrates the capability of the numerical

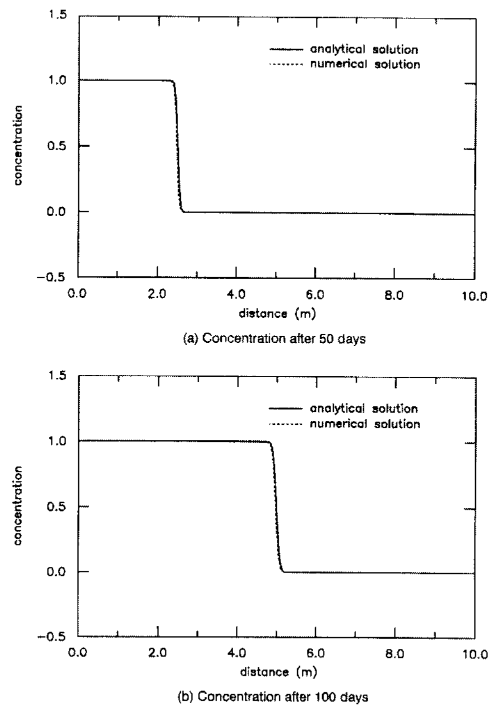



Fig. 8. Numerical Solution by OTFPG Method

method which removes fictitious oscillations around the high-gradient region in the solution while maintaining a quite steep front.

### 5.3 Courant Number Restriction

Courant number restriction of $Cr = 1$ plays an important role in the numerical analysis of the time-dependent, convection-dominated, transport problem. As discussed, the transport equation behaves as the linear convection equation (transport equation without the diffusion term) if the convection dominates the transport process. Satisfying the Courant number restriction becomes significant in the numerical analysis of the linear convection equation. It is well known that the simple backward difference scheme applied to the linear convection equation, yields the exact solution when Courant number is unity (Anderson et al., 1984).

The example in the previous section showed the applicability of the OTFPG method when Courant number is unity. Concentration profiles computed when Courant number is not unity are given in Fig. 9. When Courant number is greater than unity, overshooting in the numerical solution is observed while undershooting is seen when Courant number is less than unity. Thus, it should be emphasized that Courant number restriction should be satisfied when grid $Pe$-dependent test functions are used in the PG method.

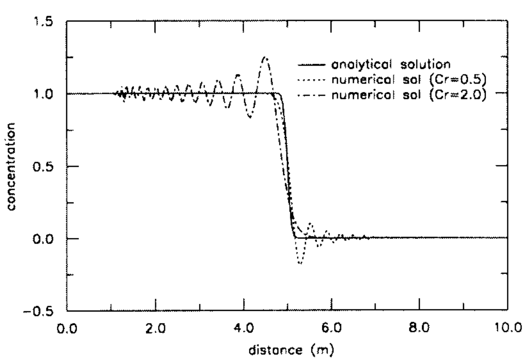



**Fig. 9. Impact of Courant Number in OTFPG Method**

## 6. Conclusions

The paper reviewed various PG methods for steady-state and time-dependent convection-dominated transport problems. The N+1 PG method produced accurate results for the steady-state problem due to the optimal upwinding level obtained analytically. However, in the time-dependent problem, the time discretization error necessitates the introduction of the N+2 PG method. Although the N+2 PG method provides much better numerical algorithm than the N+1 PG method, a significant drawback of this method lies in finding appropriate levels of upwinding. The frequency fitting algorithm was applied to the N+2 PG method, which showed that only cubic upwinding term played an important role in the time dependent problem. This coincides with the results from numerical experiments (Dick, 1983 ; Westerink and Shea, 1989 ; Bouloutas and Celia, 1991).

A new PG method, termed as optimal test function Petrov-Galerkin method, is also introduced in this paper. The test functions of the new method are functions of grid Peclet number so that they change their shapes according to the characteristic of the transport problem. The new method was applied to a convection-dominated transport problem, and was found to yield excellent agreement between the analytical and the numerical solutions. The present study explicitly indicated that the test functions of the PG method should be dependent on grid Peclet number in the convection-dominated transport problem once the Courant restriction is satisfied. The numerical modeler, who is to select either numerical oscillations or numerical dissipations, has to worry in order to satisfy the Courant number restriction when the

Pe-dependent weighting is made in the new Petrov-Galerkin method.

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## Appendix

For the OTFPG method, components of the matrices in Eq. (4) for a single element are given as follows:

$$m_{11} = \frac{2 - 2e^{be} + 2Pe\, e^{Pe} - Pe^2}{2\, Pe\, (u/D)\, (-1 + e^{Pe})}$$

$$m_{12} = \frac{-2 + 2e^{Pe} - 2Pe - Pe^2}{2\, Pe\, (u/D)\, (-1 + e^{Pe})}$$

$$m_{21} = \frac{-2 + 2e^{Pe} - 2\,Pe\,e^{Pe} - Pe^2}{2\,Pe\,(u/D)\,(-1+e^{Pe})}$$

$$m_{22} = \frac{2 - 2e^{Pe} + 2Pe + Pe^2\,e^{Pe}}{2\,Pe\,(u/D)\,(-1 + e^{Pe})}$$

$$a_{11} = \frac{1 - e^{Pe} + Pe}{Pe\,(e^{Pe} - 1)}$$

$$a_{12} = \frac{-1 + e^{Pe} - Pe}{Pe\,(e^{Pe} - 1)}$$

$$a_{21} = \frac{-1 + e^{Pe} - Pe\,e^{Pe}}{Pe\,(e^{Pe} - 1)}$$

$$a_{22} = \frac{1 - e^{Pe} + Pe\,e^{Pe}}{Pe\,(e^{Pe} - 1)}$$

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