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PREDICTION OF SPURIOUS OSCILLATION IN THE SOLUTION OF UNSTEADY SCALAR CONVECTION-DOMINATED PROBLEM

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ABSTRACT

The convection-dominated problems, mainly due to their essentiality in nature, are found in numerous science and engineering applications. Such problems include those concerning the computational fluid dynamics issues of spurious oscillations in the numerical solutions. In this research, the importance of the relationship between the numerical solution stability and the unsteady scalar convection-dominated flow parameters is emphasized. A systematic technique in setting the parameters under consideration is applied. Specifically, we present the a priori formulation of criterion to avoid non-physical oscillatory solutions. The criterion serves as a standard for a more efficient decision-making in the determination of the flow parameters, and in eliminating some heuristic aspects of the scalar concentration prediction. The test case results are consistent with the criterion.

Keywords: unsteady scalar convection-dominated equations, finite difference method, Crank-Nicolson method, spatial error growth model.

1. INTRODUCTION

The principle of property conservation is mathematically expressed in its generic form as

$$\frac{\partial}{\partial t}(\rho\varphi)+\frac{\partial}{\partial x_j}(\rho u_j\varphi)-\frac{\partial}{\partial x_j}\left(\epsilon\frac{\partial}{\partial x_j}\varphi\right)=s_\varphi, \quad (1)$$

where ρ is the density, φ is the conserved property, u_j are velocity components of the fluid in the axes directions at the point (x_1, x_2, x_3) at time t, ϵ is the diffusivity of φ, and s_φ is the source or sink of φ.

In the case there is neither source nor sink, (1) becomes simpler as

$$\frac{D}{Dt}(\rho\varphi)-\frac{\partial}{\partial x_j}\left(\varepsilon\frac{\partial}{\partial x_j}\varphi\right)=0. \quad (2)$$

This is unsteady scalar convection-dominated equation (UCDE). The substantial derivative in (2) is mathematically expressed by

$$\frac{D}{Dt}(\rho\varphi)=\frac{\partial}{\partial t}(\rho\varphi)+\frac{\partial}{\partial x_j}(\rho u_j\varphi). \quad (3)$$

Substituting (3) into (2) one has

$$\frac{\partial}{\partial t}(\rho\varphi)+\frac{\partial}{\partial x_j}(\rho u_j\varphi)-\frac{\partial}{\partial x_j}\left(\varepsilon\frac{\partial}{\partial x_j}\varphi\right)=0. \quad (4)$$

One can further simplify (4) into

$$\frac{\partial}{\partial t}(\rho\varphi)-\frac{\partial}{\partial x_j}\left(\varepsilon\frac{\partial}{\partial x_j}\varphi\right)=0 \quad (5)$$

if one is to assume that the fluids are at rest, or the velocity is negligibly small ($u_j \approx 0$), or diffusivity ϵ is large. If one is to assume that the flow is steady and occurs in only one-dimension, then convection-dominated problem reduces (4) into

$$\frac{\partial}{\partial x}(\rho u\varphi)-\frac{\partial}{\partial x}\left(\varepsilon\frac{\partial}{\partial x}\varphi\right)=0 \quad (6)$$

involving the scalar whose concentration is denoted by φ For more details on these equations, see [1]. The abrupt growth of φ provides a severe test for computational methods, for instance in the study of spurious oscillation in the solution of UCDE, and the selection of compatible grid structure over the computation domain.

We give focus on a specific spatial error growth model which results from the discretization of UCDE, and describe some aspects of spurious oscillation that hinders physically accurate solution of the equation to presence. This focus sheds light on good practice in numerically solving UCDE. Note that inappropriate pair of Peclet number Pe and grid number N would result in such numerical oscillation [2]. The work presented in this paper follows the line initiated in [2] and [3] for defining the sequence of low Peclet numbers Pe.

2. CONVECTION-DOMINATED PROBLEMS

Many useful and well formulated schemes such as finite differences, finite elements, spectral procedures, and the method of lines [4]-[15] can be found for solving UCDE. For instance, [15] presented a comparative study between two most popular Lattice Boltzmann (LB) models for UCDE (i.e. those in two dimensions with five and nine discrete lattice velocities, respectively). Other variants include multiple-relaxation-time LB model for the axisymmetric, as well as isotropic and anisotropic diffusion processes whose both applicability and accuracies have been investigated by [14] and [13] respectively; for the latter case, [12] proposed a finite-difference LB model for nonlinear equations. In the

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problem where no scalar or flux jump exists, [11] introduced a numerical scheme for dealing with curved interfaces with second-order spatial accuracy in conjunction with the LB method.

While Liu and Pollack [9] proposed the approximation of high order alternating evolution, [10] summarized well-known a priori error estimates for the discontinuous Galerkin approximation which carry over to the subspace of the discontinuous piecewise-quadratic space.

Both [8] and [7] considered compact difference scheme for solving UCDE; while [8] claimed that the fourth-order scheme requires only 15 grid points, [7] successfully proved that it is computationally more efficient than the standard second-order central difference scheme.

Recent methods include those to solve nonlinear fractional UCDE, as homotopy analysis transform and homotopy perturbation Sumudu transform methods whose reliability and efficiency were clearly demonstrated in [6], and that based on the operational matrices of shifted Jacobi polynomials of high accuracy [5].

In dealing with UCDE that converges without overlap of the subdomains, Martin [4] introduces a Schwarz waveform relaxation algorithm for the equations.

At the onset of numerical modelling of the convection-dominated problems as in [4]-[19], it is necessary to choose suitable computational grid to discretize the governing partial differential equations (e.g. by means of polynomial fitting, Taylor series expansion and compact scheme to obtain approximations to the derivatives of the variables with respect to the coordinates). It is worth to note here that the variable values at locations other than the defined grid nodes can also be determined by interpolation. Another important aspect is the method to solve the discretized algebraic equations. The solution is obtained via either direct [20]-[22] or iterative [23]-[26] methods.

Another important method for determining convection-dominated flow properties is called the shooting method. Its variants are those of Goodman and Lance [27], parallel shooting method [28], Green's function and Gaussian quadrature based methods, Ritz's method [29], and Euler shooting method. In relatively complex problems, the method deals with non-linear property of the differential equations. A remark on this was given by [30], while [31] and [32] illustrated the relevant application in solving beam equation, and predicting convection-dominated flow, respectively. The method's advantages include the ability to prove the presence of kinks of, for instance, the extended Fischer-Kolmogorov equation [33] and the existence of multiple solutions in an indefinite Neumann problem [34]. Moreover, the method yields, in some cases, better results than those obtainable via fixed-point techniques [35], [36]. The formulation of low Peclet number based grid expansion factor for the shooting method solution of scalar convection-dominated equation was given by [37].

Despite of the advantages, [29] highlighted general limitations of the shooting method.

The discretization of UCDE on uniform grids where the expansion factor$r_e = 1$takes place in the following section. A Fourier series is utilized to model the spatial error resulting from insufficient grid number. The criterion for predictingφ profile without non-physical oscillation is then formulated.

3. DISCRETIZATION AND SOLUTION OF THE GOVERNING EQUATION

We begin with the UCDE in differential form as given by simplified version of (4) for one-dimensional case;

$$\frac{\partial}{\partial t}(\rho\varphi) + \frac{\partial}{\partial x}(\rho u\varphi) - \frac{\partial}{\partial x}\left(\varepsilon\frac{\partial}{\partial x}\varphi\right) = 0. \quad (7)$$

Defining the boundary conditions at any time$t$as

$$\varphi(0) = 0,$$
$$\varphi(1) = 1. \quad (8)$$

Here we define Pe as

$$Pe = \frac{\rho u L}{\epsilon}.$$

The influence of Pe on the diffusivity coefficient ϵ can be found in [24]. The profiles for different times are illustrated in Figure-1.

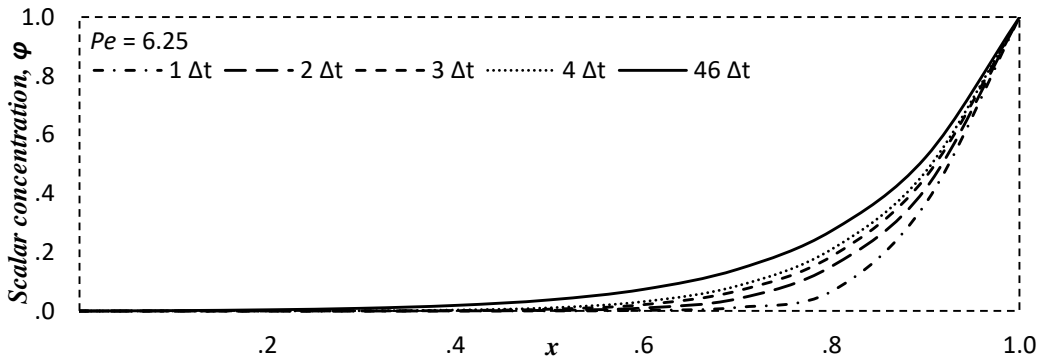

Figure-1. Boundary conditions and solution profiles as a function of time at Pe = 6.26.

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We define the independent variables$x$whose domain is discretized and covered by computational molecules in grid arrangement. The interval $x = [0,1]$ is subdivided into $(N-1)/h$ where N and h are odd and even integers, respectively. Defining the molecules;

$$x_{i+1} = x_i + r_e \Delta x_i,$$

where $1 \le i \le (N-2)$, $i \in \mathbb{Z}$, and r_e is the grid expansion factor. Clearly $\sum \Delta x_i = 1$. The grid is shown in Figure-2.

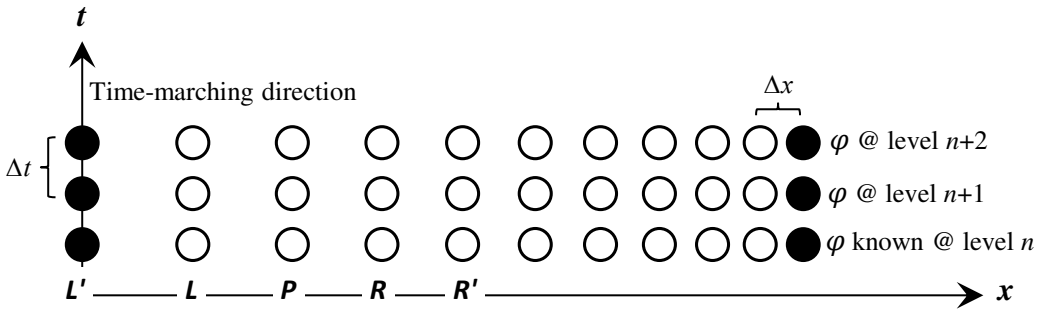

Figure-2. Computational molecules. Concentration of the scalars φknown at level n are used to calculate those at level $n + 1$. Then, those calculated at level $n + 1$ are used for the calculation at level $n + 2$ until the solution is converged.

At every molecule, molecule values replace partial derivatives to approximate the governing equation. The result is an algebraic UCDE per molecule, in which the variables at that and immediate molecules appear as unknowns. The system of equations is expressed by, after discretizing both the diffusion and convection terms by using central difference scheme (CDS) and the time derivative by using that of forward difference (FDS),

$$C_p \varphi_p^{n+1} + \sum_m C_m \varphi_m^{n+1} = Q_p^n \tag{9}$$

where P signifies the molecules at which the equations are assigned and m index runs over the immediate molecules. The corresponding matrix C in (9), which is also called tridiagonal matrix, has non-zero terms only on its main diagonal (represented by C_{ii}) and the diagonals immediately above and below it (represented by C_R and C_L, respectively). The matrix elements are stored as three $n \times n$ array. Applying the three-point computational molecules, (9) becomes

$$C_p \varphi_p^{n+1} + C_R \varphi_{i+1}^{n+1} + C_L \varphi_{i-1}^{n+1} = Q_p^n, \tag{10}$$

where

$$C_R = \frac{\rho u}{4\Delta x} - \frac{\epsilon}{2(\Delta x)^2},$$
$$C_L = -\frac{\rho u}{4\Delta x} - \frac{\epsilon}{2(\Delta x)^2},$$
$$C_p = \frac{\rho}{\Delta t} - (C_R + C_L),$$
$$Q_p^n = \left(C_R + C_L + \frac{\rho}{\Delta t}\right)\varphi_i^n - C_R \varphi_{i+1}^n - C_L \varphi_{i-1}^n.$$

Since the unsteady scalar convection-dominated differential equation is linear, then the approximation contains only linear terms, and the numerical solution will not require linearization. Tridiagonal matrix algorithm, which is also known as Thomas' algorithm, is applied for solving linear system of the algebraic equation (10). We set

$$\rho = 1.0, u = 1.0, r_e = 1. \tag{11}$$

Note that the spatial instability might lead to spurious oscillation, where the solution is nonphysical as depicted in Figure-3.

4. SEQUENCES OF THE PECLET NUMBERS AND TIMES BASED NUMERICAL RESULTS

The range of low Peclet numbers Pe of interests is $[0,100]$. The mathematical relationship between Pe and time t is represented by a set of ordered pairs $(Pe_l, t_l), l = 1,2, \dots, n$. We define a sequence of Pe by

$$\begin{aligned} &Pe_i, \\ &Pe_{i+1} = Pe_i/p, \\ &Pe_{i+2} = Pe_{i+1}/p, \\ &Pe_{i+3} = Pe_{i+2}/p, \\ &\cdot \\ &\cdot \\ &\cdot \\ &Pe_n = Pe_{n-1}/p, \end{aligned} \tag{12}$$

where the constants $i, p \in \mathbb{Z}^+$.
Next, defining a sequence of normalized time t by

$$\begin{aligned} &t_i, \\ &t_{i+1} = i\frac{k}{2p}t_i, \\ &t_{i+2} = (i+1)\frac{k}{2p}t_i, \\ &\mathrm{t_{i+3}} = (\mathrm{i}+2)\frac{\mathrm{k}}{2\mathrm{p}}\mathrm{t_i}, \end{aligned} \tag{13}$$

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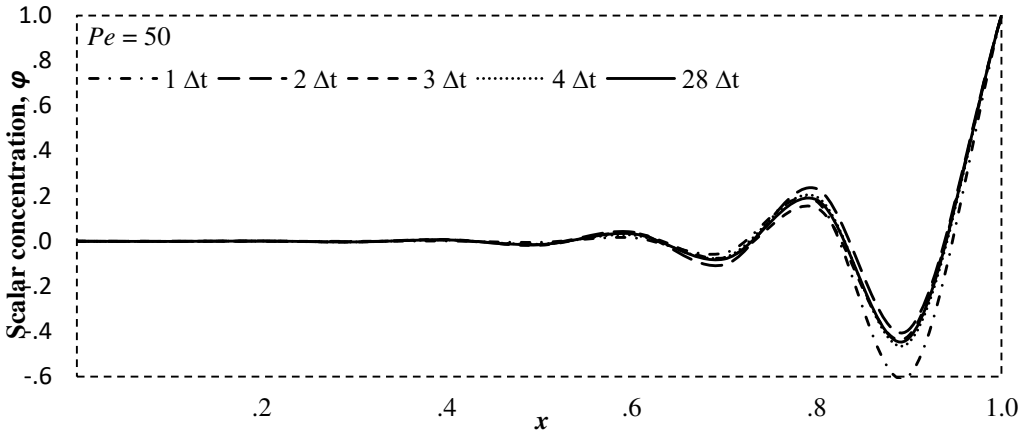

Figure-3. Nonphysical behavior of scalar concentration profile φ due to the spatial instability.

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$$t_{n-1} = (n-2)\frac{k}{2p}t_i,$$

where $j, q \in \mathbb{Z}^+$ and k is the the number of time step Δt when the solution of (10) converges.
Let

$$i = 1, n = 6, m = 5, Pe_1 = 3.125, t_i = \Delta t, p = 2,$$

such that the sequence in (12) and (13) become
$3.125, 6.25, 12.5, 25, 50, 100$

and

$$\Delta t, .25k\,\Delta t, 0.5k\,\Delta t, 0.75k\,\Delta t, k\,\Delta t$$

respectively. All 30 possible pairs (Pe, t) based on the elements in these sequences are considered as test cases, following the line used in [2] and [3]. The numerical solutions for such cases are presented in Figure-4.

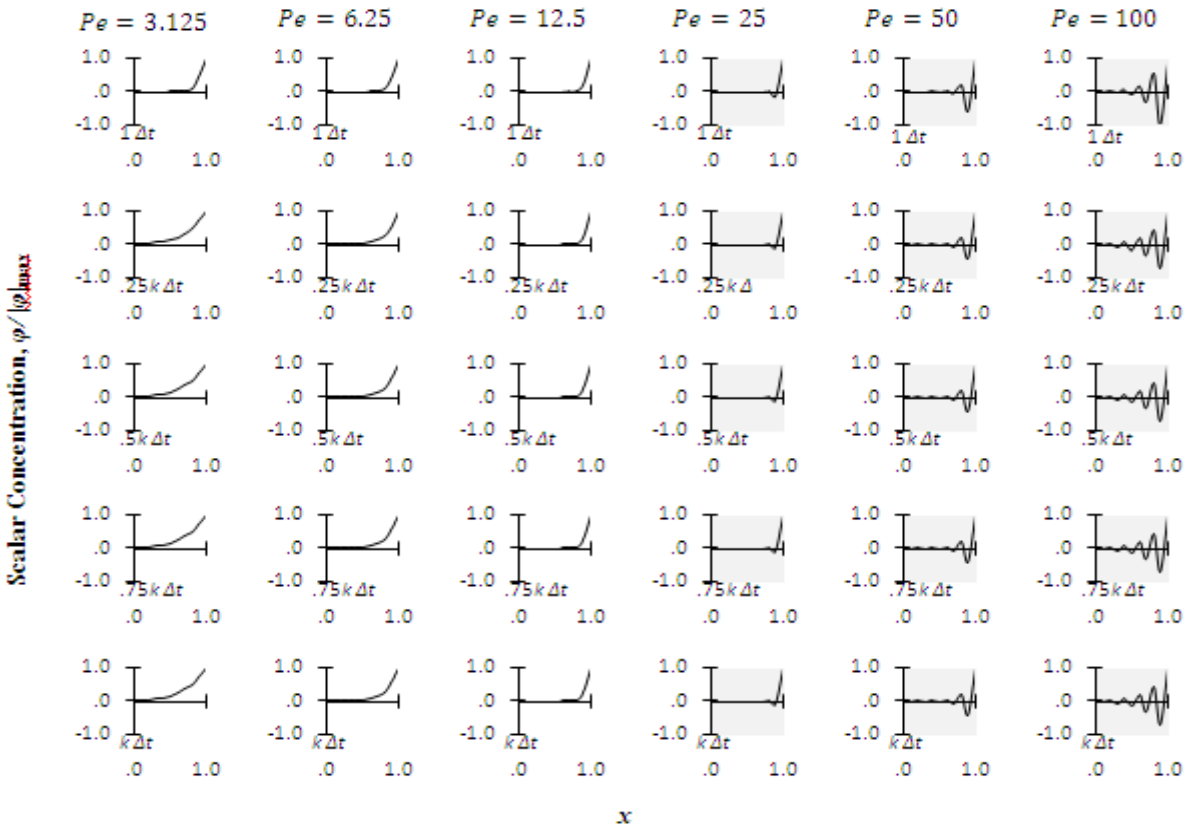

Figure-4. Concentration profile $\varphi/|\varphi|_{max}$ at Pe as in sequence (12) and $t$in sequence (13). The shaded plots indicate cases where the spurious oscillations appear.

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It is obvious that, as depicted in Figure-4, spurious oscillations occurat certain Pe, irrespective of time *t*. In other words, such oscillations are only a function of Pe. Furthermore, the amplitudes grow with respect to$x$. This will be further confirmed mathematically in the next two sections.

Note that the profiles in the unshaded plots (i.e. those not involving oscillations) vary exponentially in *x*-direction, and the area under the curve represented by the integral

$$\int_0^1 \varphi(x)\,dx$$

is inversely proportional toPe.

5. INSTABILITY MODEL

Discretizing (7) by applying Crank-Nicolson method;

$$\frac{\varphi_i^{n+1}-\varphi_i^n}{\Delta t} = A + B, \qquad (14)$$

where

$$A = -\frac{1}{2\Delta x}\left(\frac{\varphi_{i+1}^{n+1}+\varphi_{i+1}^n}{2} - \frac{\varphi_{i-1}^{n+1}+\varphi_{i-1}^n}{2}\right),$$

$$B = \frac{\epsilon}{(\Delta x)^2}(C + D + E),$$

$$C = \frac{\varphi_{i+1}^{n+1}+\varphi_{i+1}^n}{2},$$

$$D = -\frac{2\varphi_i^{n+1}+2\varphi_i^n}{2},$$

$$E = \frac{(\varphi_{i-1}^{n+1}+\varphi_{i-1}^n)}{2}.$$

Since Crank-Nicolson method is unconditionally time-stable, then the averaged φat two different times may be suppressedand the change of $\varphi$with respect to time may be ignored, in modeling the instability such that

$$A = -\frac{1}{2\Delta x}(\varphi_{i+1}^n - \varphi_{i-1}^n),$$

$$B = \frac{\epsilon}{(\Delta x)^2}(\varphi_{i+1}^n - 2\varphi_i^n + \varphi_{i-1}^n),$$

$$C = \varphi_{i+1}^n,$$

$$D = -2\varphi_i^n,$$

$$E = \varphi_{i-1}^n.$$

Thus (14) becomes

$$0 = \left(-\frac{\varphi_{i+1}^n - \varphi_{i-1}^n}{2\Delta x}\right) + \left(\epsilon\frac{\varphi_{i+1}^n - 2\varphi_i^n + \varphi_{i-1}^n}{(\Delta x)^2}\right).$$

For simplicity, we rewrite the last equation as

$$0 = \left(-\frac{\varphi_{i+1} - \varphi_{i-1}}{2\Delta x}\right) + \left(\epsilon\frac{\varphi_{i+1} - 2\varphi_i + \varphi_{i-1}}{(\Delta x)^2}\right). \qquad (15)$$

The spatial error is defined as

$$\gamma = \mathcal{N} - E, \qquad (16)$$

where $\mathcal{N}$ and E are finite accuracy numerical solution from a real computer and exact solution of difference equation, respectively. Note that the numerical solution $\mathcal{N}$ satisfies the difference equation (15). A Fourier series model can be used to analytically represent the random variation of γ with respect to space;

$$\gamma(x) = \sum_l e^{\alpha x} e^{ik_l x}, l = 1,2,3 \ldots, \qquad (17)$$

where$e^{\alpha x}$ is the amplification factor, $k_l$is the wave number, and α is a constant.

Lets $e^{\alpha x}$ in (17) be proportional to$x$when numerical oscillation occurs as represented in Figure-3. Thus it is sufficient to consider only the growth of$e^{\alpha x}$. Direct substitution of$e^{\alpha x}$ into the finite difference equation (15) gives

$$\frac{e^{\alpha(x+\Delta x)} - e^{\alpha(x-\Delta x)}}{2\epsilon} = \frac{e^{\alpha(x+\Delta x)} - 2e^{\alpha x} + e^{\alpha(x-\Delta x)}}{\Delta x}. \qquad (18)$$

Divide (18) by $e^{\alpha x}$, we have

$$\frac{e^{\alpha\Delta x} - e^{-\alpha\Delta x}}{2\epsilon} = \frac{e^{\alpha\Delta x} - 2 + e^{-\alpha\Delta x}}{\Delta x}$$

which, after some rearrangement, becomes

$$e^{\alpha\Delta x} = \frac{e^{-\alpha\Delta x}(\Delta x + 2\epsilon) - 4\epsilon}{\Delta x - 2\epsilon}.$$

If$e^{\alpha x}$presumably grows with respect to x, then

$$\frac{e^{\alpha(x+\Delta x)}}{e^{\alpha x}} > 1,$$

or simply

$$e^{\alpha\Delta x} > 1.$$

Therefore, in order to have non-growing error amplification, the criterion

$$\frac{e^{-\alpha\Delta x}(\Delta x + 2\epsilon) - 4\epsilon}{\Delta x - 2\epsilon} \le 1 \qquad (19)$$

must be fulfilled.

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6. RESULTS OF CALCULATIONS

Rewriting (19) in terms of $Pe$and N;

$$\frac{e^{-\frac{\alpha}{N-1}}\left(\frac{1}{N-1}+\frac{2}{Pe}\right)-\frac{4}{Pe}}{\frac{1}{N-1}-\frac{2}{Pe}} \leq 1. \quad (20)$$

Substituting$N = 11$ into (20);

$$\frac{e^{-\frac{\alpha}{10}}\left(\frac{1}{10}+\frac{2}{Pe}\right)-\frac{4}{Pe}}{\frac{1}{10}-\frac{2}{Pe}} \leq 1. \quad (21)$$

We define

$$G = \frac{e^{-\frac{\alpha}{10}}\left(\frac{1}{10}+\frac{2}{Pe}\right)-\frac{4}{Pe}}{\frac{1}{10}-\frac{2}{Pe}}$$

Thus (21) becomes

$$G \leq 1. \quad (22)$$

The criterion in (22) is clearly a function of single variablePe. The values in sequence (12) and their corresponding G are listed in Table-1.

Table-1. Peclet numbers Pe, and G as incriterion (22) where$\alpha = -0.1$. The shaded cells indicate cases where the spurious oscillations appear.

Pe	G
3.125	.99
6.25	.98
12.5	.96
25	1.09
50	1.02
100	1.02

Data in Table-1 confirm the numerical results in Figure-4, where physically accurate non-oscillatory solutions are achieved for the smallest three Peclet numbers of interest (i.e. when $G \leq 1$).

6. CONCLUSIONS

A technique in predicting spurious oscillationsin the solutions of UCDE is highlighted. The understanding on the influence of Peclet number,Pe, rather than time,t, on the physically accurate results forms a basis for a more effective approach in solving UCDE.

The key aspect in this research is the modelling of spatial error growth which result from the discretization technique. This opens the possibility of a more general framework for the selection of numerical scheme in computational fluid dynamics, and the relationship between the flow parameter/s and the solution quality in finite difference method.

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