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IJIE

Journal homepage: http://penerbit.uthm.edu.my/ojs/index.php/ijie
ISSN : 2229-838X e-ISSN : 2600-7916

The International Journal of Integrated Engineering

Non-oscillatory Spatial Solutions Criterion for Convection-Diffusion Problem

Aslam Abdullah[1*]

[1]Faculty of Mechanical & Manufacturing Engineering,
Universiti Tun Hussein Onn Malaysia, Batu Pahat, 86400, MALAYSIA

*Corresponding Author

DOI: https://doi.org/10.30880/ijie.2021.13.02.029
Received 1 January 2020; Accepted 3 December 2020; Available online 28 February 2021

Abstract: The fact that the convection-diffusion problems are essential in nature is supported by the presence of such problems in vast number of applications in both science as well as engineering. Some of these applications involve the computational domain's grid structure issues in the numerical experiment of fluid dynamics. The paper highlights the important role of convection-diffusion flow parameters in the construction of the grid structure. We propose the a priori criterion formulation to avoid non-oscillatory solutions which is based on both Peclet and grid numbers, and serves as a systematic approach in setting grid related parameters of interest. Aiming at a more efficient process in choosing grid structure for computational domain, the criterion functions as a standard which also eliminates heuristic process in the scalar concentration prediction. The test cases' calculated results verify the consistency of the criterion.

Keywords: Convection-diffusion equations, finite difference, spurious oscillation, grid number, tridiagonal matrix algorithm

1. Introduction

The generic form of conservation equation is

$$\partial_t(\rho\varphi)+\partial_{x_j}(\rho u_j\varphi)-\partial_{x_j}(\grave{o}\partial_{x_j}\varphi)=s_\varphi, \quad (1)$$

where ρ represents density, φ conserved property, u_j fluids components of velocity in with respect to spatial coordinates (x_1, x_2, x_3) at time t, $\grave{o}$ represents concentration φ diffusivity, and s_φ negative or positive sink of φ.

Note that (1) simplifies into

$$D_t(\rho\varphi)-\partial_{x_j}(\grave{o}\partial_{x_j}\varphi)=0, \quad (2)$$

if sink or source is negligible. This is convection-diffusion equation (CDE). The equation represents engineering problems arise in many models of processes from nature and technical applications. This situation will be always occur if the conserved property (dissolved or as particle, for instance) or a physical quantity as the temperature, is transported by a flow field. In mechanical engineering, CDE is important to determine, for example, the fraction of water-to-oil or the scalar concentration in petroleum pipes. The equation can be solved by means of finite-difference method. Since the

*Corresponding author: aslam@uthm.edu.my

numerical solution of CDE involves the computer programme development, there is a necessity to study the spurious oscillations which are the due to several factors. Thus the focus of this paper is to formulate the criterion to prevent such oscillations in the solution of the convection-diffusion problem. In principle, the criterion acts as a guideline for setting up the solution to ensure that the variation of the conserved property is physically accurate. This applies in the case where only limited data is known regarding the variation of such property, such as the initial and boundary conditions. By using this criterion, the variation with respect the computational domain can be visualized correctly. Further processes besides the fow field are oftenly present in real systems, like chemical reactions.

Mathematically, the substantial derivative in (2) is given by

$$D_t\left(\rho\varphi\right)=\partial_t\left(\rho\varphi\right)+\partial_{x_j}\left(\rho u_j\varphi\right). \tag{3}$$

We have, when (3) is substituted into (2),

$$\partial_t\left(\rho\varphi\right)+\partial_{x_j}\left(\rho u_j\varphi\right)-\partial_{x_j}\left(\grave{o}\partial_{x_j}\varphi\right)=0. \tag{4}$$

We can further simplify (4) into

$$\partial_t\left(\rho\varphi\right)-\partial_{x_j}\left(\grave{o}\partial_{x_j}\varphi\right)=0. \tag{5}$$

The simplified (5) is obtained when the fluids velocity is zero or negligible $\left(u_j\approx 0\right)$, or large diffusivity $\grave{o}$ is taken into account.

Expression (4) reduces to

$$\partial_x\left(\rho u\varphi\right)-\partial_x\left(\grave{o}\partial_x\varphi\right)=0 \tag{6}$$

in the case of 1-dimensional steady convection-diffusion problem, involving the concentration represented in the form of scalar φ. More details on these equations can be found in [1]. Interestingly, when zero sink or source is assumed as in (6), and the computational domain is of unit length, the boundary condition $\varphi(0)=0$ and $\varphi(1)=0$ will result in $\varphi=0$ throughout the whole domain.

Despite the fact that the problem is that of one-dimension, it is widely accepted that the main difficulties arise already. Since the analysis for one-dimensional problems is comparably simple, one can construct for the problems numerical methods which produce, in a certain sense, perfect numerical solutions. Furthermore, the nature of growth of φ becomes a challenge in computational methods; φ sudden growth is a heavy test, in particular in choosing of the structure of computational grid with the ability to capture the growth over space and time.

We establish a criteria that links interested flow parameter in CDE as the Peclet number Pe to the compatible number of grid N. The formulation of the criteria is therefore important to predict the equation solution which is physically accurate. Numerical oscillation could happen if Pe and N are inappropriately paired [2]. Thus the formulation unifies the heuristic choices deduction in determination of N in the solution of CDE for contaminated fluids problem which results in reduced time in pre-computation activity. The work in the paper is presented following the approach developed in [2] and [3] to define both Peclet numbers Pe and grid numbers N sequence. In general, we consider linear two-point boundary value problem, and apply boundary condition of first kind or Dirichlet boundary condition in the solution of the CDE.

2. Methods and Materials

2.1 Convection-diffusion Problems

Bast there are many well formulated numerical methods such as lines method, spectral procedures, finite elements as well as finite differences [4] - [15] which serve as practical schemes to solve CDE. For example, [4] comparatively studied 2-dimensional Lattice Boltzmann models (LB) with two variants which are generally considered as the most popular; those with five discrete lattice and nine discrete lattice velocities.

The aspects of accuracy and practicability of LB model have been thoroughly considered in [5] and [6]. In particular, [5] focused on LB model of multiple-relaxation-time for the diffusion process that is axisymmetric, while [6] investigated the model for isotropic and anisotropic diffusion process. These two models are other variants of standard LB model. For the case in [6], [7], in solving nonlinear governing equations, is a proponent of LB model of finite-difference. When scalar or flux jump is negligible, [8] dealt with curvy interfaces by, in conjunction with the Lattice Boltzmann method, introducing a second-order spatial accuracy numerical scheme.

Galerkin estimate carries over to the subspace of the intermittent piecewise-quadratic space. A well-known a priori error approximation for such numerical scheme is systematically summarized in [9], while the high order alternating evolution estimate for the scheme is proposed by [10].

Zhang et al. proposed that the higher order compact difference scheme (i.e. that of fourth-order) just needs 15 grid or meshing points [11] in order to solve CDE. Moreover, the scheme is successfully proven to be relatively computationally efficient in comparison to typical central difference scheme of the second-order [12].

It has become a trend to apply both the Sumudu transformation of homotopy perturbation and the transform of homotopy analysis as methods for solving CDE involving nonlinear fractions [13],[14]. The methods are based on high accuracy shifted Jacobi polynomials as operational matrices [14].The efficiency and reliability of them were proven in depth in [13].

One problem faced by much algorithms for the solution of CDE is the that they converge yet with subdomains overlap. It was a Schwarz waveform relaxation algorithm which succeeds in eliminating such problem [15].

At the initial stage of a numerical model development, particularly in the case of convection-diffusion analysis, it is crucial to ensure that computational mesh or grid for the purpose of discretizing the governing partial differential equations by using any of compact scheme, expansion of Taylor series, and polynomial fitting (i.e. the schemes for obtaining estimates of variables derivative in space and time coordinates) is appropriate [4]-[19]. Interpolation also is an aspect which is worthy of noting, which allows the variable values at undefined grid or mesh nodes to be determined in order to ensure the 'smoothness' of the solutions. In general, there are direct method [20]-[22] and iterative one [23]-[26] which can be used in the determination of the solutions, both of which are crucial in solving discretized algebraic equations.

Another popular method is called the shooting method. Its usefulness in predicting convection-diffusion properties is reflected by its various variants proposed by numerous reserchers [27]-[36]. For instance, Euler shooting method, Ritz method, Green function and Gaussian's quadrature based methods [29], parallel shooting-method [28], and Goodman and Lance method [27]. This method is also capable of predicting non-linear property in the differential equations in highly complex problems. The details on this can be found in [30]. Examples of the complex problems are accessible via [31] and [32] concerning convection-diffusion as well as beam equations, respectively. Other advantages of the shooting method include the visualization of the existence of multiple solutions in an indefinite Neumann problem [34], and the presence of kinks in the property profile in the solution of extended Fischer-Kolmogorov equation [33], for instance. At some extent, the method proves to produce outputs better than those produced via fixed-point techniques [35], [36]. The shortcomings were extensively discussed in [29], in spite of the shooting method's robustness.

In the following section, the CDE is discretized on uniform grids, where the expansion factor $r_e = 1.$ A Fourier series is utilized to model the spatial error resulting from insufficient grid number. The criterion for predicting φ profile without non-physical oscillation is then formulated.

2.2 Discretization and Solution of the Governing Equation

We begin with the differential form of CDE as expressed in (6);

$$\partial_x \left(\rho u \varphi\right) - \partial_x \left(\grave{o} \partial_x \varphi\right) = 0 .$$

The boundary conditions are defined by

$$\begin{aligned} \varphi(0) &= 0, \\ \varphi(1) &= 1. \end{aligned} \quad (7)$$

The Peclet number Pe is defined by

$$Pe = \frac{\rho u L}{\grave{o}}.$$

The Peclet number Pe influence on the coefficient of diffusivity $\grave{o}$ was described in [24]. The concentration profiles are shown in Figure 1 for different Pe range.

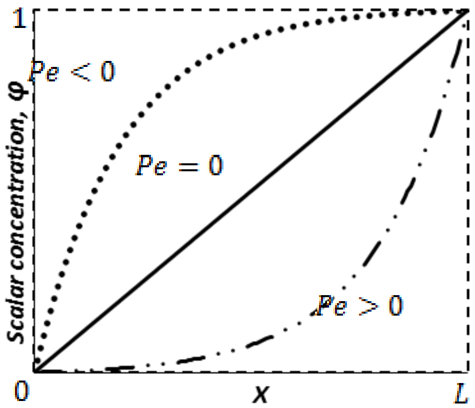

Fig. 1 - Concentration profiles as a function of the Peclet number at different boundary conditions

A grid covers the corresponding discretized solution domain in which x being independent variables. The subintervals is defined as $(N-1)/h$. The full interval is $x=[0,1]$. Both N and h are integers. The definition of nodes is given by

$$x_{i+1} = x_i + r_e x_i$$

where $1 \le i \le (N-1)$, $i \in \mathrm{Z}$, and r_e is the grid or mesh expansion factor. Obviously $\sum x_{i+1} = 1$. The grid is shown in Figure 2.

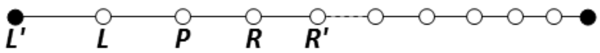

Fig. 2 - Computational molecules

At each node, the governing equation is approximated by replacing the partial derivatives with nodal values. The result is an algebraic CDE per node, in which the variables at that and immediate nodes appear as unknowns. The system of equations is expressed by

$$C_P \varphi_P + \sum_m C_m \varphi_m = Q_p, \tag{8}$$

where the equations are assigned at the grid nodes which are signified by *P*, and m index runs over the neighboring nodes. Non-zero terms in the corresponding matrix C in (8) are on its main diagonal, and the immediate diagonals above and below it (represented by C_{ii}, and C_R for the upper and C_L for the lower diagonal terms, respectively). By applying three-point computational molecules, we have an expanded version of (8) as

$$C_P \varphi_P + C_R \varphi_{i+1} + C_L \varphi_{i-1} = Q_P. \tag{9}$$

Three $n \times n$ array is the form in which the matrix elements in the equation are stored. The numerical solution of (9) does not need to be linearized due to linearity of convection-diffusion differential equation (i.e. only linear terms appear in the approximation by algebraic equation).

The discretization of diffusion term for both its outer and inner derivatives as well as convection terms uses central difference scheme (CDS) such that

$$-\left[\partial_x\left(\grave{o}\partial_x\varphi\right)\right]_i \approx \frac{\left(\grave{o}\partial_x\varphi\right)_{i+\frac{1}{2}}-\left(\grave{o}\partial_x\varphi\right)_{i-\frac{1}{2}}}{\frac{1}{2}\left(x_{i-1}-x_{i+1}\right)} \tag{10}$$

and

$$\left.\begin{aligned} \left(\grave{o}\partial_x\varphi\right)_{i+\frac{1}{2}} &\approx \grave{o}\,\frac{\varphi_{i+1}-\varphi_i}{x_{i+1}-x_i} \\ -\left(\grave{o}\partial_x\varphi\right)_{i-\frac{1}{2}} &\approx \grave{o}\,\frac{\varphi_i-\varphi_{i-1}}{x_{i-1}-x_i} \end{aligned}\right\} \tag{11}$$

(i.e. the discretization of diffusion term) as well as

$$-\left[\partial_x\left(\rho u\varphi\right)\right]_i \approx \rho u\,\frac{\varphi_{i+1}-\varphi_{i-1}}{x_{i-1}-x_{i+1}}. \tag{12}$$

(i.e. the discretization of convection terms). The convection and diffusion terms contribute to the algebraic equation (8) coefficients in such a way that;

$$\begin{aligned} C_R &= C_R^{conv}+C_R^{diff} \\ &= \frac{\rho u}{x_{i+1}-x_{i-1}}-\frac{2\grave{o}}{\left(x_{i+1}-x_{i-1}\right)\left(x_{i+1}-x_i\right)}; \\ C_L &= C_L^{conv}+C_L^{diff} \\ &= -\frac{\rho u}{x_{i+1}-x_{i-1}}-\frac{2\grave{o}}{\left(x_{i+1}-x_{i-1}\right)\left(x_i-x_{i-1}\right)}; \\ C_P &= C_P^{conv}+C_P^{diff} \\ &= -\left(C_R^{diff}+C_L^{diff}\right). \end{aligned}$$

In order to solve linear system of the algebraic equation (9), tridiagonal matrix in particular Thomas algorithm is applied. We choose that

$$\rho = 1.0,\ u = 1.0,\ r_e = 1. \tag{13}$$

It is worthy of noting that numerical oscillation might occur if the grid number is minimized. The solution is therefore nonphysical (see illustration in Figure 3).

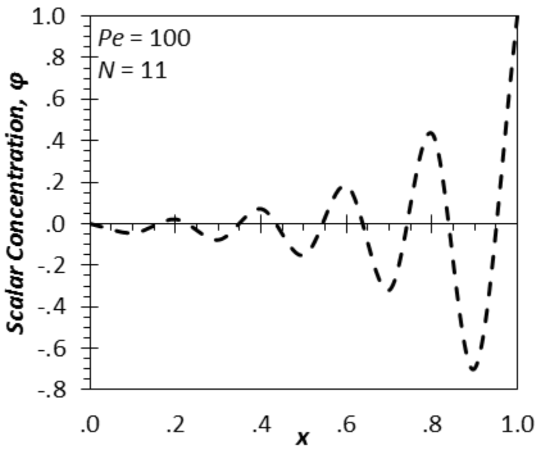

Fig. 3 - Insufficient computational domain's grid number that leads to nonphysical oscillatory behaviour of concentration of scalar profile φ

2.3 Peclet and grid numbers sequences

We set the low Peclet number Pe range of interest as $[0,100]$, and a set of pairs representing the mathematical relationship between Pe and grid number N as (Pe_i, N_j).

A sequence of Pe_i is defined by

$$\begin{aligned} &Pe_i, \\ &Pe_{i+1} = Pe_i(p), \\ &Pe_{i+2} = Pe_{i+1}(p), \\ &Pe_{i+3} = Pe_{i+2}(p), \\ &. \\ &. \\ &. \\ &. \\ &Pe_n = Pe_{n-1}(p), \end{aligned} \tag{14}$$

with the constants $i, p \in \mathrm{Z}^+$.

We define a sequence of N by

$$\begin{aligned} &N_j\ , \\ &N_{j+1} = floor\left(\frac{N_j + 1}{q}\right), \\ &N_{j+2} = floor\left(\frac{N_{j+1} + 1}{q}\right), \\ &N_{j+3} = floor\left(\frac{N_{j+2} + 1}{q}\right), \\ &. \\ &. \\ &. \end{aligned} \tag{15}$$

$$N_m = floor\left(\frac{N_{m-1}+1}{q}\right),$$

where the constants $j, q \in \mathrm{Z}^+$.
Let

$$i = j = 1, n = m = 6, Pe_1 = 3.125, N_1 = 81, \qquad p = q = 2,$$
(16)

such that the sequence in (14) and (15) become

$$3.125, 6.25, 12.5, 25, 50, 100$$

and

$$81, 41, 21, 11, 6, 3$$

respectively. All 36 possible pairs (Pe, N) based on the elements in these sequences are considered as test cases, following the line used in [2] and [3].

2.4 Spatial Error Growth Model

Substituting (10), (11), and (12) into (6);

$$\frac{\varphi_{i+1}-\varphi_{i+1}}{2\varepsilon} = \frac{\varphi_{i+1}-2\varphi_i+\varphi_{i-1}}{\Delta x}. \quad (17)$$

The spatial error is defined as

$$\gamma = N - E, \quad (18)$$

where N and E are finite accuracy numerical solution from a real computer and exact solution of difference equation, respectively. Note that the numerical solution N satisfies the difference equation (17). A Fourier series model can be used to analytically represent the random variation of γ with respect to space;

$$\gamma(x) = \sum_l e^{\alpha x} e^{ik_l x}, \quad l = 1, 2, 3..., \quad (19)$$

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

Lets $e^{\alpha x}$ in (19) 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 (17) gives

$$\frac{e^{\alpha(x+\Delta x)}-e^{\alpha(x-\Delta x)}}{2\grave{o}} = \frac{e^{\alpha(x+\Delta x)}-2e^{\alpha x}+e^{\alpha(x-\Delta x)}}{\Delta x}. \quad (20)$$

Divide (20) by $e^{\alpha x}$, we have

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

which, after some rearrangement, becomes

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

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 a non-growing error amplification, the criterion

$$\frac{e^{-\alpha\Delta x}\left(\Delta x+2\varepsilon\right)-4\varepsilon}{\Delta x-2\varepsilon}\le 1 \quad (21)$$

must be fulfilled.

3. Results and Discussion

Rewriting (21) in terms of Pe and N;

$$\frac{e^{-\frac{\alpha}{N-1}}\left(\frac{1}{N-1}+\frac{2}{Pe}\right)-\frac{4}{Pe}}{\frac{1}{N-1}-\frac{2}{Pe}}\le 1 . \quad (22)$$

We define

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

Thus (22) becomes

$$G\le 1. \quad (23)$$

The criterion in (23) was checked against all 36 possible pairs $\left(Pe_i,N_j\right)$ based on sequences (14) and (15). The output is given in Table 1. For $Pe=3.125$, all grid numbers in sequence (15) are appropriate in achieving physically accurate non-oscillatory solutions. This is indicated by G being less than or equal to 1. The appropriate range of N shrinks by one element each time the next Pe in sequence (14) is considered.

The values of G tabulated in Table 1 were verified by plotting the concentration φ which are numerically calculated for Pe against N as shown in Figure 4. It is confirmed now that in any case where $G>1,$ the numerical oscillations appear, and the amplitudes grow with respect to x. Note that in cases where $G\le 1$, φ profiles exponentially change with respect to *x*. The cases are represented by shaded plots where the integral

$$\int_0^1 \varphi\left(\mathrm{x}\right)d\mathrm{x}$$

gives the area under the curve which is inversely proportional to Pe.

$Pe = 3.125$		$Pe = 6.25$		$Pe = 12.5$		$Pe = 25$		$Pe = 50$		$Pe = 100$	
	G		G		G		G		G		G
			>1								
					>1						
							>1				
1		1		1		1		1	>1	1	>1
1	≤ 1	1	$\leq$	1	$\leq$	1		1		1	
1		1		1		1	$\leq$	1	$\leq$	1	
1		1		1		1		1		1	≤ 1

Table 1. Range of grid numbers N that fulfils to the criterion in (23) where $\alpha = -0.1$

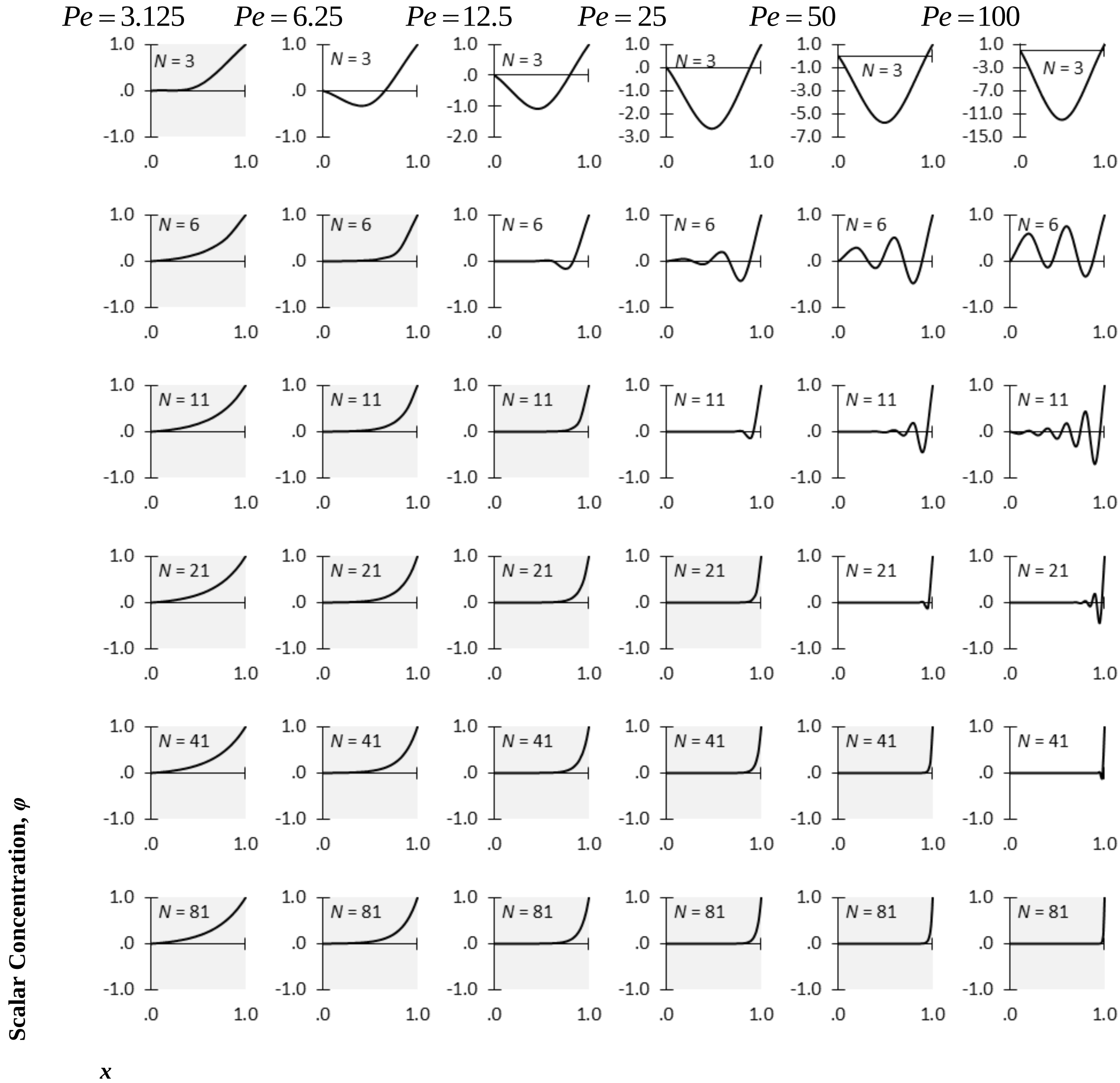

Fig. 4 - Concentration profile φ at Pe as in sequence (14)

4. Final Remarks

We devised a criterion to avoid numerical oscillation in the prediction of concentration profile the criterion improves the way we understand contribution towards oscillation, and thus serves as a qualitative guideline for the convection-diffusion solutions. The criterion also gives the minimum values of below which non-physical solutions occur. It opens the possibilities of choosing type of grid structure in computational fluid dynamics, obtaining ‘flow parameters-grid quality’ relationship, as well as investigating the influence of on other numerical error patterns, via a more general framework.

Acknowledgement

The author would like to thank Ministry of Education of Malaysia (MoE) and Universiti Tun Hussein Onn Malaysia (UTHM) for facilitating the research.

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