GRID NUMBER AND EXPANSION FACTOR FOR THE SOLUTION OF SCALAR CONVECTION-DOMINATED EQUATION: COMPARISON BETWEEN THE METHOD OF 'SHOOTING' AND THAT OF FINITE-DIFFERENCE

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ABSTRACT

There have been many researches which focus on the grid quality in computational fluid dynamics. Despite it is known that, for instance, the higher the grid number, the more accurate the results, systematic framework for the selection of grid numbers based on some flow parameters remains as an open-ended issue. This paper highlights some findings on the idea of such framework, and considers grid number and grid expansion factor as two of many factors which contribute to result accurateness. In particular, it takes scalar convection-dominated equation solution into account, in order to show that the grid number and expansion factor are predictable for a range of Peclet number of interests. Two methods are used to solve the equation. They are shooting method as well as that of finite-difference. Relationship between grid expansion factor and Peclet number, and that between grid number and Peclet number for both methods are then discussed. The results prove the predictability of the grid parameters of interest, and shed light on more general framework for the selection of grid parameters based on flow parameters.

Keywords: scalar convection-dominated equations, shooting method, finite-difference method, non-uniform grid, and grid expansion factor.

1. INTRODUCTION

The generic form of conservation equation is expressed as

$$\partial_t(\rho\varphi) + \partial_{x_j}(\rho u_j\varphi) - \partial_{x_j}\left(\epsilon\partial_{x_j}\varphi\right) = s_\varphi, \tag{1}$$

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.

If zero source or sink is assumed, then (1) is simplified as

$$D_t(\rho\varphi) - \partial_{x_j}\left(\epsilon\partial_{x_j}\varphi\right) = 0. \tag{2}$$

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

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

Substituting (3) into (2) we have

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

We can further simplify (4) into

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

by assuming that the fluids are at rest, or the velocity is small ($u_j \approx 0$), or diffusivity ϵ is large.

The steady one-dimensional scalar convection-dominated problem reduces (4) into

$$\partial_x(\rho u\varphi) - \partial_x(\epsilon\partial_x\varphi) = 0. \tag{6}$$

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, particularly in the selection of compatible grid structure over the computation domain.

We investigate the relationships between the flow parameter of interest (i.e. the Peclet number Pe) in SCDE and the minimum grid number$N$ as well asthe grid expansion factor r_e in the case of both shooting and finite difference methods. We focus on achieving accurate and/or oscillation free solution of the equation, thus unify the deduction of heuristic selections of $r_e$and $N$for solving the contaminated fluids problem that leads to less pre-computation time. Note that inappropriate choice of r_e and N for given Pe may result in over- or under-prediction and spurious oscillation, respectively. The formulation presented in this paper follows the line initiated in [2] for defining the sequence of low Peclet numbers Pe.
Note that both ρ and u are set to be equal to 1.

2. SCALAR CONVECTION-DOMINATED PROBLEMS

2.1 Finite Difference Method

There are many numerical methods for solving SCDE which are by now well formulated finite differences, finite elements, spectral procedures, and the method of lines [3]-[14]. For instance, [3] presented a comparative study between two most popular Lattice Boltzmann (LB) models for SCDE (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 [4] and [5] respectively; for the latter case, [6] proposed a finite difference LB model for nonlinear equations. In the problem where no scalar or flux jump exists, [7] introduced a numerical scheme for dealing with curved interfaces with second-order spatial accuracy in conjunction with the LB method.

Bittl *et al*. [8] summarized well-known a priori error estimates for the discontinuous Galerkin approximation which carry over to the subspace of the discontinuous piecewise-quadratic space, while [9] proposed the approximation of high order alternating evolution.

Both [10] and [11] considered compact difference scheme for solving SCDE; Zhang *et al*. [10] claimed that the fourth-order scheme requires only 15 grid points, while [11] successfully proved that it is computationally more efficient than the standard second-order central difference scheme.

Recent methods include those to solve nonlinear fractional SCDE, as homotopy analysis transform and homotopy perturbation Sumudu transform methods whose reliability and efficiency were clearly demonstrated in [12], and that based on the operational matrices of shifted Jacobi polynomials of high accuracy [13].

Martin [14] introduces a Schwarz waveform relaxation algorithm for the SCDE that converges without overlap of the subdomains.

The choice of 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) is necessary at the onset of numerical modelling of the scalar convection-dominated problems as in [3]-[18]. 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 [19]-[21] or iterative [22]-[25] methods.

2.2 Shooting Method

The shooting method has variances. Some of them are those of Goodman and Lance [26], parallel shooting method [27], Green's function and Gaussian quadrature based methods, Ritz's method [28], 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 [29], while [30] and [31] illustrated the relevant application in solving beam equation, and predicting scalar 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 [32] and the existence of multiple solutions in an indefinite Neumann problem [33]. Moreover, the method yields, in some cases, better results than those obtainable via fixed-point techniques [34], [35]. Despite of the advantages, [36] highlighted general limitations of the shooting method.

The Euler shooting method is the focus of the next section of this paper. Then, the resulting general solution of the SCDE will be taken as a basis to obtain the grid expansion factor r_e that permits agreement between numerical and exact solutions for a given Peclet number.

All the finite-difference method solutions given in this paper follow the conditions set in [1] and [2], while those of the shooting method follow the conditions set in [37] and [38].

3. LOW PECLET NUMBER BASED GRID EXPANSION FACTOR

3.1 Sequences of Peclet Numbers and Grid Expansion Factors

The range of low Peclet numbers Pe of interests is $[0,100]$. The mathematical relationship between Pe and grid expansion factors r_e is represented by a set of ordered pairs $\left(Pe_i, r_{e_j}\right), i = 1,2,\dots,n; j = 1,2,\dots,m$.

We define, as in [1], a sequence of Pe by

$$
\begin{aligned}
&Pe_i,\\
&Pe_{i+1} = Pe_i/p,\\
&Pe_{i+2} = Pe_{i+1}/p,\\
&Pe_{i+3} = Pe_{i+2}/p,\\
&\vdots\\
&Pe_n = Pe_{n-1}/p,
\end{aligned}
\tag{7}
$$

where the constants $i, p \in \mathbb{Z}^+$.

Next, defining a sequence of r_e by

$$
\begin{aligned}
&re_j,\\
&re_{j+1} = re_j + q,\\
&re_{j+2} = re_{j+1} + q,\\
&re_{j+3} = re_{j+2} + q,\\
&\vdots\\
&re_m = re_{m-1} + q,
\end{aligned}
\tag{8}
$$

where the constants $j \in \mathbb{Z}^+, q \in \mathbb{R}^+$.

Let

$$
i = j = 1, n = 6, m = 10, Pe_1 = 100, re_1 = 0.1, p = 2,\\
q = 0.1, \tag{9}
$$

such that the sequence in (15) and (16) become

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

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and

0.1,0.2,0.3,…,1.0;

respectively. All 60 possible pairs have been considered to determine those which give accurate φ profiles.In this case, the grid number N is set to be 11.

3.2 The Profiles

The concentration φ profiles which are numerically calculated are plotted in Figure-1(a) and Figure-1(b) in the case of shooting method and in Figure-2 in the case of finite difference method. The results 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.

3.2.1 Shooting Method

For the sake of space, only profiles involving $r_e = 1.0, 0.9, 0.8$ have been included in Figure-1(a) and Figure-1(b). The profiles which are numerically calculated show good agreement with the exact solutions when $r_e = 0.9$, but are over- or underestimated when $r_e \neq 0.9$ (i.e. when $r_e = 1.0, 0.8, 0.7, \dots, 0.1$).

Theorem (shooting method) Let$0 \leq Pe \leq 100$, the grid expansion factor r_e for solving the scalar convection-dominated equation in (6) is expressed as;

$$r_e = A$$

for$3.125 < Pe \leq 100$, and;

$$r_e = B$$

for$0 \leq Pe \leq 3.125$, whereA, Bconstants, and$A \neq B$. [38]

3.2.2 Finite-Difference Method

The concentration φ profiles in Figure-2 show good agreement with the exact solutions. It is found that the expansion factor r_e is inversely proportional to the logarithm of Pe.

Theorem (finite-difference method) Let $0 \leq Pe \leq 100$, the grid expansion factor r_e for solving the scalar convection-dominated equation in (6) is expressed as a linear function of $lg\ Pe$;

$$r_e = m \lg Pe + b,$$

for $3.125 \leq Pe \leq 100$, and as a constant;

$$r_e = 1,$$

for $0 \leq Pe \leq 3.125$, where m and b are curve slope and a constant, respectively. [1]

3.2.3 Remarks

Note that in both cases (i.e. that of shooting method and finite-difference method), $r_e = 1.0$ matches $Pe = 3.125$. Then $r_e = 1.0$ is appropriate for $0 \leq Pe \leq 3.125$ where φ profile is close to linearity with respect to x. The uniform grid is therefore sufficient for the correct prediction of Pe within the range.

4. RELATIONSHIP BETWEEN GRID AND LOW PECLET NUMBERS

4.1 Sequences of Peclet and Grid Numbers

The range of low Peclet numbers Pe of interests is $[0,100]$. The mathematical relationship between Pe and grid numbers N is represented by a set of ordered pairs $(Pe_i, N_i), i = 1,2,\dots,$ n.
We define a sequence of Pe by

$$\begin{aligned} Pe_{i+0} &= Pe_i/p^0, \\ Pe_{i+1} &= Pe_i/p^1, \\ Pe_{i+2} &= Pe_i/p^2, \\ Pe_{i+3} &= Pe_i/p^3, \\ &\vdots \\ Pe_n &= Pe_i/p^{n-1}, \end{aligned} \tag{10}$$

where the constants $i, p \in \mathbb{Z}^+$.

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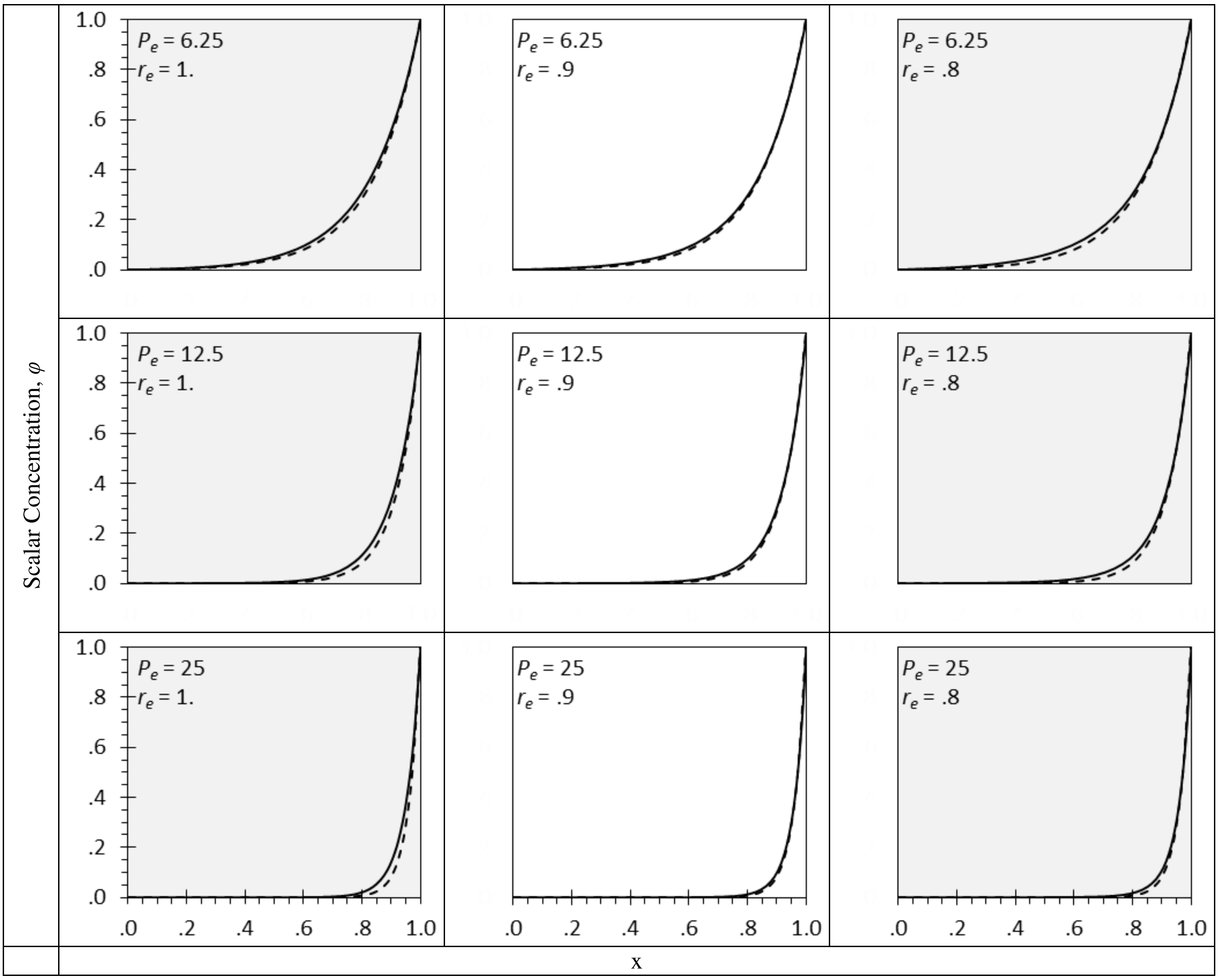

Figure-1(a). Concentration profile at $Pe = 25, 12.5, 6.25$. - - - - - and ——— indicate the exact and numerical calculations, respectively.The concentration was calculated by using shooting method. The shaded plots indicate either underestimate or overestimate φ profiles which are numerically calculated.

Next, defining a sequence of N by

$$N_i\,,$$
$$N_{i+1} = floor\left(\frac{N_i + 1}{q}\right),$$
$$N_{i+2} = floor\left(\frac{N_{i+1} + 1}{q}\right),$$
$$N_{i+3} = floor\left(\frac{N_{i+2} + 1}{q}\right), \quad (11)$$
$$\vdots$$
$$N_m = floor\left(\frac{N_{m-1} + 1}{q}\right),$$

where the constants $i, q \in \mathbb{Z}^+$.
Let

$i = 1, m = 8, n = 10, Pe_1 = 100, N_i = 321,$

and

$$p = q = 2 \quad (12)$$

such that the sequence in (10) and (11) become

$100, 100/2, 100/4, 100/8, 100/16, 100/32, 100/64, 100/128, 100/256, 100/512$

and $321, 161, 81, 41, 21, 11, 6, 3,$

respectively.

All 80 possible pairs have been considered to determine those which give accurate or non-oscillating φ profiles. In this case, the grid expansion factor $r_e = 1$ is set to be 1.

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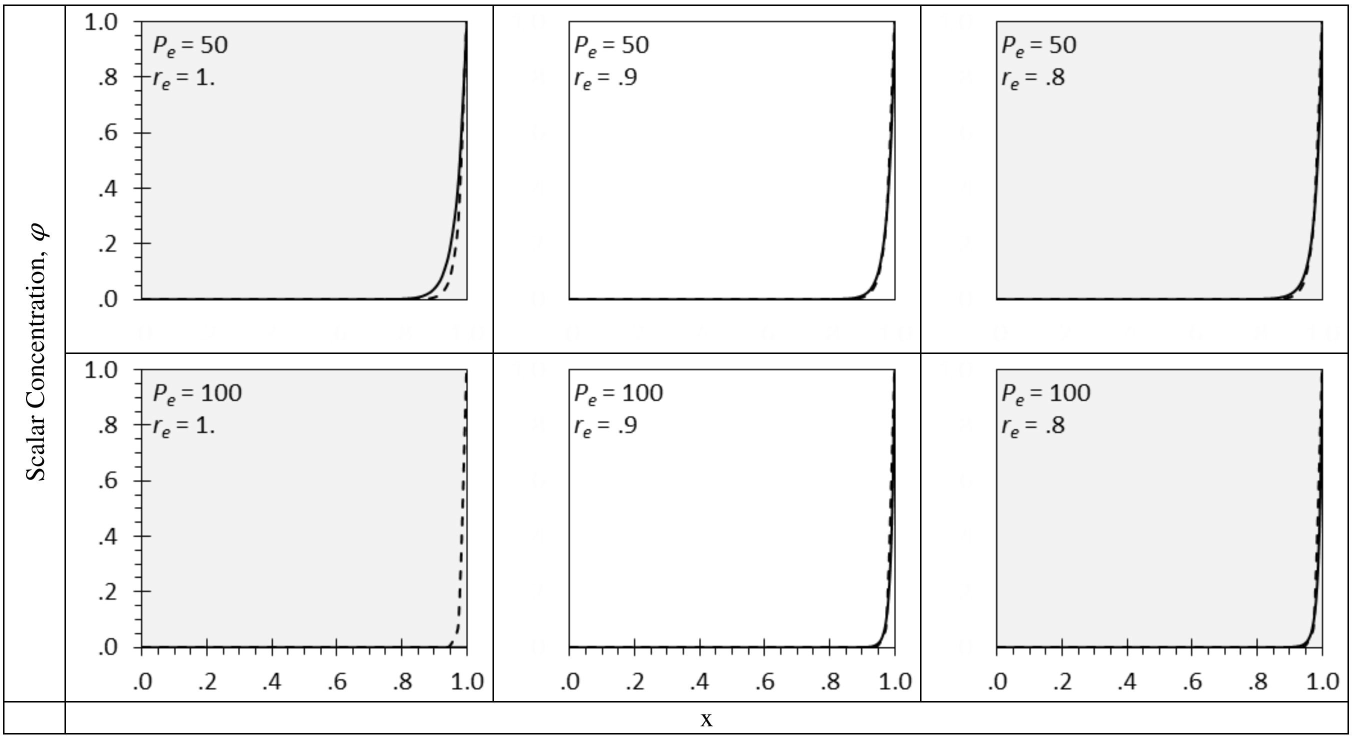

Figure-1(b). Concentration profile at$Pe = 100{,}50$. - - - - - and ——— indicate the exact and numerical calculations, respectively. The concentration was calculated by using shooting method. The shaded plots indicate either underestimate or overestimateφ profiles which are numerically calculated.

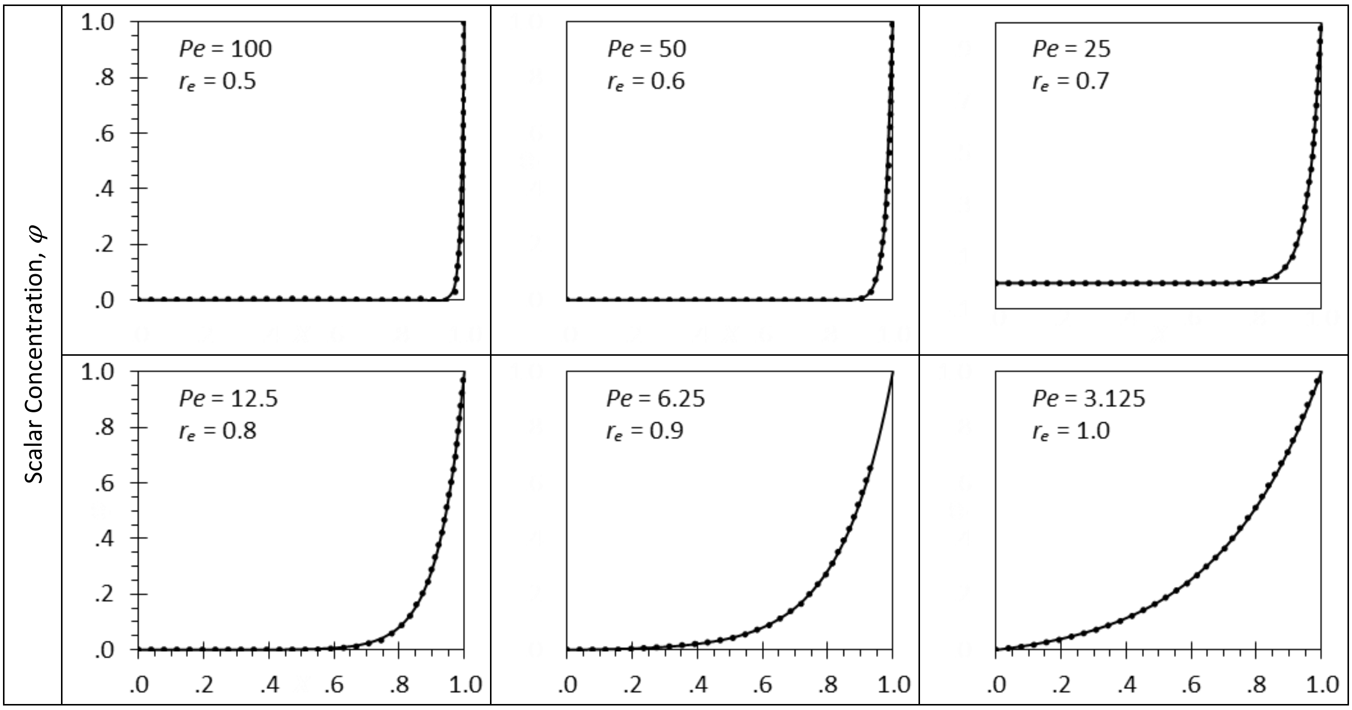

Figure-2. Concentration profile at $Pe = 3.125{,}6.25{,}12.5{,}25{,}50{,}100$. —— and .... indicate the exact and numerical calculations, respectively. The concentration was calculated by using finite difference method.

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4.2 The Profiles

4.2.1 Shooting Method

The concentration φ profiles as plotted in Figure-3 show perfect agreement between numerical and exact solutions for Pe within the range of $[100/512, 100/4]$. When Pe is greater than 25, N greater than 312 is necessary to produce accurate results. Such N is beyond the scope of this research.

Note that since $N = 3$ matches $Pe = 100/512$,then $N = 3$ is appropriate for $0 \leq Pe \leq 100/512$ where φ profile is close to linearity with respect to x. The grid number $N = 3$ is therefore sufficient for the φ profile to agree with the exact solution.

Theorem (shooting method) Let $0 \leq Pe \leq 25$, the minimum grid number $N_{min}$for solving the SCDE in (6) is expressed as a linear function of$Pe;$

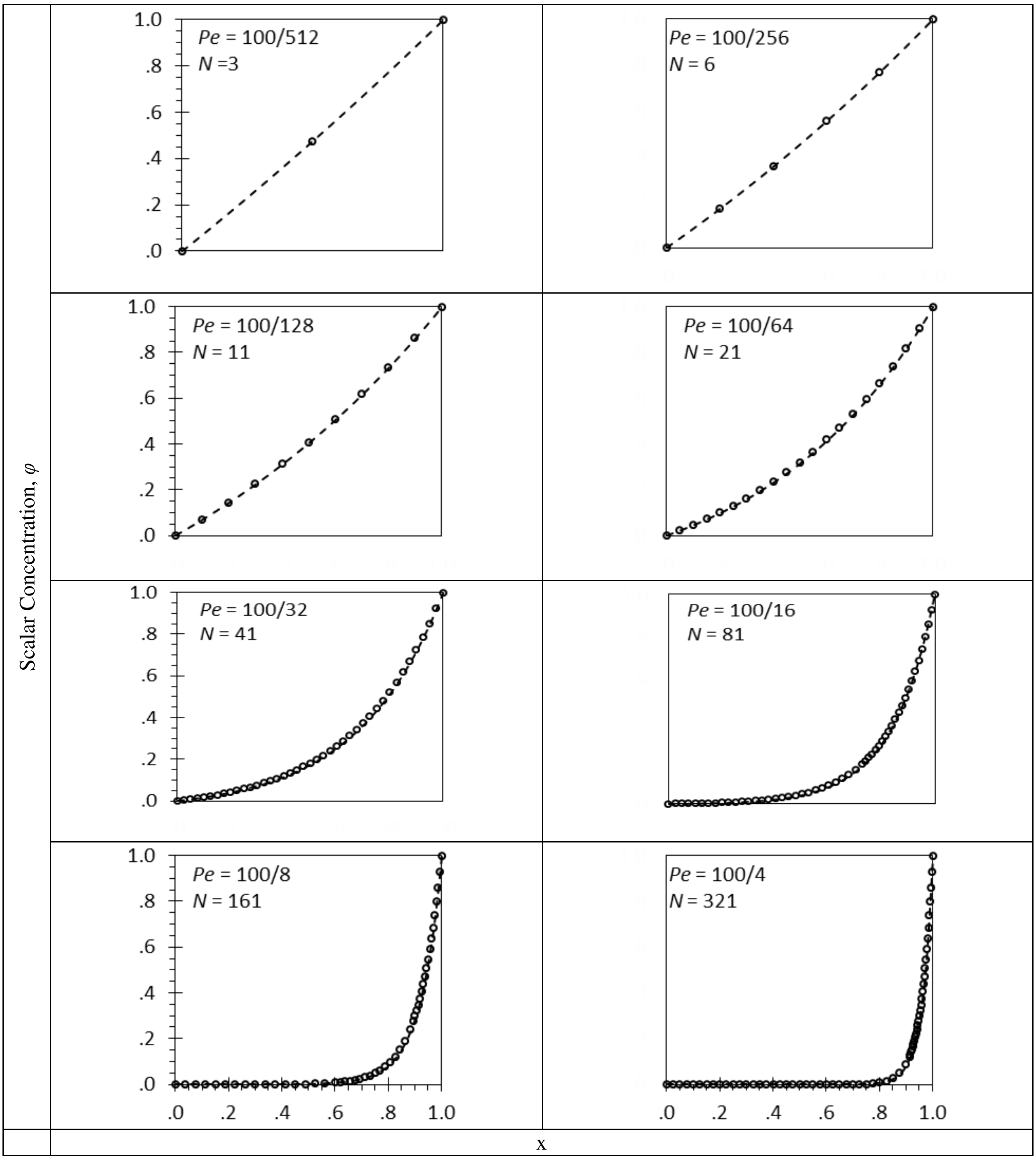

Figure-3. Concentration profile at low $Pe = \frac{100}{512}, \frac{100}{256}, \frac{100}{128}, \ldots, \frac{100}{24}$. o and - - - represent the numerical and exact solutions, respectively. Shooting method is used for the solutions.

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$N_{min} = mPe + c$
for $100/512 \leq Pe \leq 25$, and as a constant;

$N_{min} = 3$

for $0 \leq Pe \leq 100/512$, where m and c are curve slope and a constant, respectively. [37]

4.2.2 Finite Difference Method

The concentration φ profiles which are numerically calculated for $Pe = [3.125,100]$ are plotted in Figure-4, and show correct physical behaviours.

We use similar argument as that in the case of shooting method; since$N = 3$ matches $Pe = 3.125$, then $N = 3$ is appropriate for $0 \leq Pe \leq 3.125$ where φ profile is close to linearity with respect to x. The grid number $N = 3$ is therefore sufficient for the φprofile to behave physically correctly inthe prediction of Pe within the range of [0,3.125].

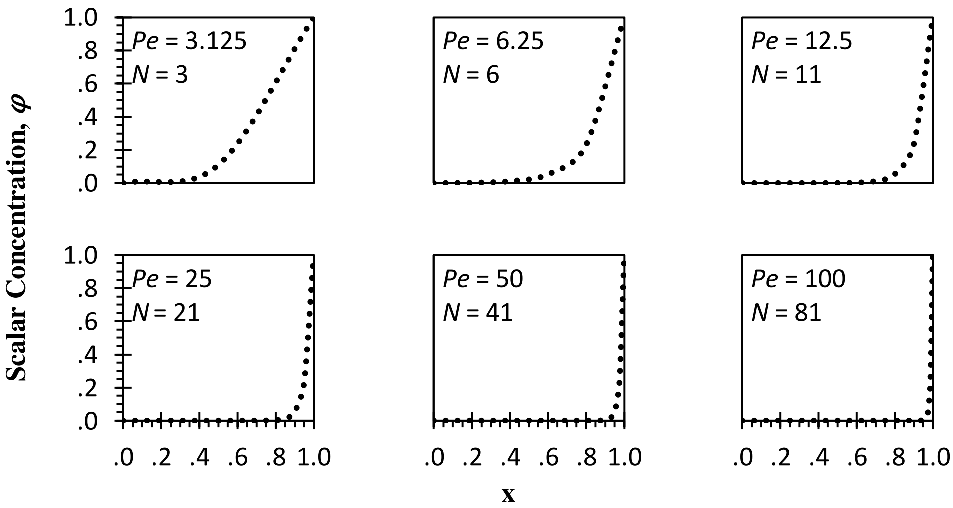

Figure-4. Concentration profile at low Pe, numerically calculated.Finite difference method is used for the solutions.

Theorem (finite-difference method) Let $0 \leq Pe \leq 100$, the minimum grid number N_{min} for solving SCDE in (6) is expressed as a linear function of Pe;

$N_{min} = m\,Pe + b$,

for $3.125 \leq Pe \leq 100$, and as a constant;

$N_{min} = 3$,

for $0 \leq Pe \leq 3.125$, where m and b are curve slope and a constant, respectively [2].

5. SUMMARY

The findings are summarized in Table-1 and Table-2 regarding $r_e - Pe$and $N - Pe$ relations, respectively.

5.1 $r_e - Pe$ relation

Table-1. Comparisons between shooting and finite-difference methods.

Method	Similarity	Difference	Remarks
Shooting method	r_e is predictable in both cases.	Relatively simpler; involving only 2 r_e for all Pe of interests in order to obtain accuracy. (advantage)	(i) The relationship $r_e - Pe$ proves to be applicable in both mehods. (ii) Prediction of r_e for a given Pe is less complicated in the case of shooting method due to only constant value of r_e involved for each sub-case.
Finite-difference method		Linear log relation to obtain accuracy, shows that r_e is predictable for a given Pe. See Figure-5. (advantage)	

5.2 $N - Pe$ relation

Method	Similarity	Difference	Remarks
Shooting method	N as a linear function of Pe. See Figure-6 and Figure-7.	(i) Range is relatively smaller, i.e. $Pe = [0.25]$. (disadvantage) (ii) Requires much more number of grids. (disadvantage)	(i) The relationship $N - Pe$ proves to be applicable in both methods. (ii) Unless accuracy is a concern, prediction of N for a given Pe is more effective in the case of finite-difference method since only small grid number is required for the whole range of Pe of interest to produce non-oscillatory solutions.
Finite-difference method		(i) Solutions are physically correct in the sense that they do not spuriously oscillate. (advantage) (ii) Further effort is required to achieve the accuracy where the numerical and exact solutions are in good agreement. (disadvantage)	

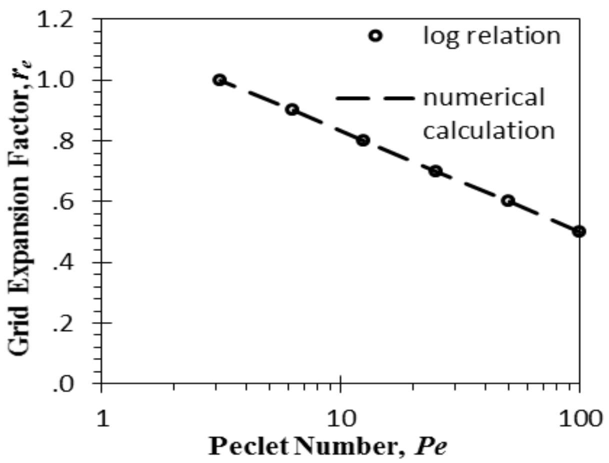

Figure-5. Grid expansion factor r_e as a function of logarithm of the Peclet number Pe, for the calculation of concentration by using finite difference method.

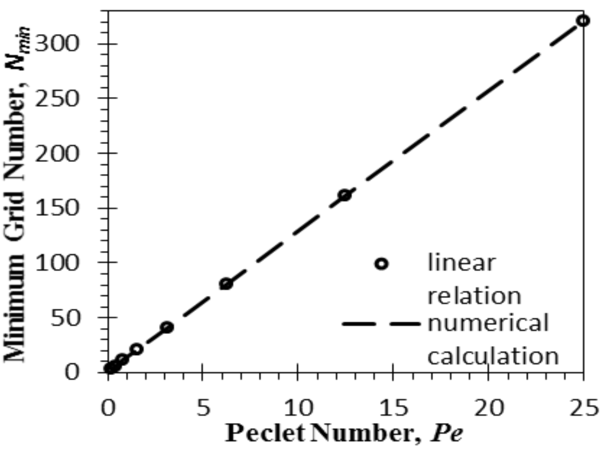

Figure-6. Linear function of the Peclet number Pe, for the calculation of concentration by using shooting method.

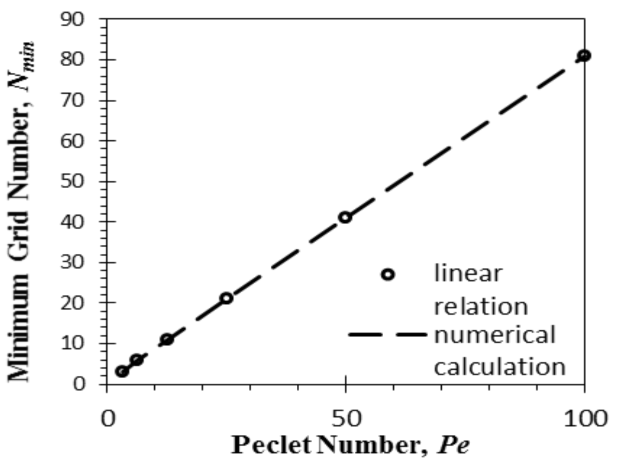

Figure-7. Minimum grid number N_{min} as a linear function of the Peclet number Pe, for the calculation of concentration by using finite-difference method.

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