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GRID EXPANSION FACTOR FOR THE SHOOTING METHOD SOLUTION OF CONVECTION-DIFFUSION EQUATION

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ABSTRACT

The essential nature of convection-diffusion related problems is the main reason why they are found in various science and engineering applications. This includes the computational fluid dynamics problems of grid structure for the numerical calculations. In this research, the importance of the relationships between the grid structure and the flow parameters is emphasized. A systematic technique in setting the parameter of interest is applied. In particular, we present the a posteriori formulation of low Peclet number based grid expansion factor for the numerical solution of convection-diffusion equation. The resulting function which is 'many-to-one' serves as a standard for a more efficient decision-making in the determination of the computational domain grid, and in eliminating some heuristic aspects of the scalar concentration prediction. The results confirm the effectiveness of the new approach.

Keywords: convection-diffusion equations, shooting method, non-uniform grid, grid expansion factor, and Euler's method.

1. INTRODUCTION

Conservation equation in its generic form is given by

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

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.

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

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

This is convection-diffusion equation (CDE). The substantial derivative in (2) is mathematically expressed by

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

Substituting (3) into (2) we have

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

We can further simplify (4) into

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

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 convection-diffusion problem reduces (4) into

$$\partial_x(\rho u \varphi) - \partial_x(\epsilon \partial_x \varphi) = 0 \quad (6)$$

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

We investigate the relationship between the flow parameter of interest (i.e. the Peclet number Pe) in CDE and the grid number expansion factor r_e for a minimum grid number N_{sm} in shooting method, and formulate the mathematical relationship between r_e and Pe which is necessary in achieving accurate solution of the equation, thus unify the deduction of heuristic selections of r_e for solving the contaminated fluids problem that leads to less pre-computation time. Note that inappropriate choice of r_e may result in overprediction. The formulation presented in this paper follows the line initiated in [2] for defining the sequence of low Peclet numbers Pe.

2. CONVECTION-DIFFUSION PROBLEMS

Various numerical methods for solving CDE are by now well formulated and many useful schemes can be found such as 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 CDE (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 CDE; 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 CDE, 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 CDE 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 convection-diffusion 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.

3. SHOOTING METHOD

Some variants of the shooting method 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 convection-diffusion 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, [28] 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 CDE 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.

4. SOLUTION OF THE GOVERNING EQUATION

The starting point is the CDE in differential form as given by (6);

$$\partial_x(\rho u\varphi) - \partial_x(\epsilon\partial_x\varphi) = 0$$

Assuming that the diffusivity coefficient ϵ, density ρ, and velocity u are constant such that, with some rearrangement,

$$\partial_x{}^2\varphi = {}^{\rho u}/_{\epsilon}\,\partial_x\varphi \tag{7}$$

Here we define the Peclet number Pe as

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

where L is the length of the domain. Thus, (7) becomes
$L\partial_x{}^2\varphi = Pe\partial_x\varphi$

and

$$\partial_x{}^2\varphi = Pe\partial_x\varphi \tag{8}$$

when $L = 1$.

The boundary conditions are set as

$$\left.\begin{aligned}\varphi(0) = \varphi_o = 0\\ \varphi(1) = \varphi_{N_{sm}-1} = 1\end{aligned}\right\} \tag{9}$$

The influence of the Peclet number Pe on the diffusivity coefficient ϵ can be found in [36]. A grid covers the corresponding solution domain. We define the independent variables x whose domain is discretized. The interval $x = [0, L]$ is subdivided into L/l subintervals where $l \in \mathbb{Z}$. The nodes are defined by

$$x_{k+1} = x_k + r_e\Delta x_k$$

where $0 \le k \le (N_{sm} - 2)$, $k \in \mathbb{Z}$, and r_e is the grid expansion factor. Clearly $\sum \Delta x_k = 1$, when $L = 1$. The grid is shown in Figure-1.

Figure-1. Computational molecules.

At each node, the concentration φ is calculated based on the step size Δx_i and the concentration profile slope $\partial_x\varphi$.

Let

$$\varphi_o = 0$$

$$\begin{aligned}\varphi_1 &= \varphi_o + \Delta x_o(\partial_x\varphi)_o\\ \varphi_2 &= \varphi_1 + \Delta x_1(\partial_x\varphi)_1\\ &\vdots\\ \varphi_{N_{sm}-1} &= \varphi_{N_{sm}-2} + \Delta x_{N_{sm}-2}(\partial_x\varphi)_{N_{sm}-2}\end{aligned} \quad (10)$$

and

$$\begin{aligned}(\partial_x\varphi)_o &= \begin{cases}-0.1 \text{ for the first 'shot'}\\ 0.1 \text{ for the second 'shot'}\end{cases}\\ (\partial_x\varphi)_1 &= (\partial_x\varphi)_o + \Delta x_o\left(\partial_x{}^2\varphi\right)_o\\ (\partial_x\varphi)_2 &= (\partial_x\varphi)_1 + \Delta x_1\left(\partial_x{}^2\varphi\right)_1\\ &\vdots\\ (\partial_x\varphi)_{N_{sm}-1} &= (\partial_x\varphi)_{N_{sm}-2} + \Delta x_{N_{sm}-2}\left(\partial_x{}^2\varphi\right)_{N_{sm}-2}\end{aligned} \quad (11)$$

where, from (8),

$$\left(\partial_x{}^2\varphi\right)_i = Pe(\partial_x\varphi)_i$$

The minimum two initial results of $\varphi_{N_{sm}-1}$ which are based on guessed values of the derivatives $(\partial_x\varphi)_o$ are required in order to predict the correct value by interpolation. The values of $(\partial_x\varphi)_o$ and the resulting $\varphi_{N_{sm}-1}$ are listed in Table-1.

Table-1. The guessed values and the initial results of $(\partial_x\varphi)_o$ and $\varphi_{N_{sm}-1}$, respectively.

$(\partial_x\varphi)_o$	$\varphi_{N_{sm}-1}$
-0.1	φ_a
0.1	φ_c

The interpolated derivative $(\partial_x\varphi)_o = (\partial_x\varphi)_b$ can then be calculated as

$$(\partial_x\varphi)_b = -0.1 + 0.2\frac{(1-\varphi_a)}{(\varphi_c-\varphi_a)} \quad (12)$$

Substituting (12) into (10) and (11) would give the expected scalar concentration profile φ that fulfils the boundary conditions (9).
We set

$$\rho = 1.0, u = 1.0, N_{sm} = 41 \quad (13)$$

throughout the calculations in (10)-(12). The grid number N_{sm} in (13) is obtained by the equation [37]

$$N_{sm} = 12.820Pe + 0.496$$

provided that the boundary conditions and other parameter settings for CDE (i.e. equation in (6)) are as in (13). In [37], it is shown that $r_e = 1.0$ for $Pe = 3.125$. The corresponding plot for the concentration φ is given in Figure-2.

Note that the incompatibility of certain grid expansion factor r_e might lead to inaccurate profile, where the solution overestimates the scalar concentration as depicted in Figure-3.

5. SEQUENCES OF THE PECLET NUMBERS AND THE 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

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

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

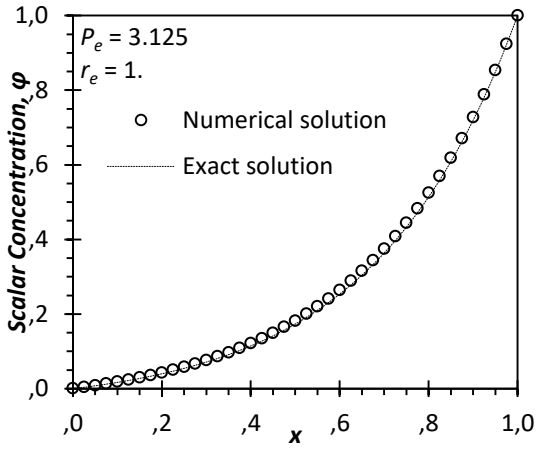

Figure-2. Concentration profile at $Pe = 3.125$ and $r_e = 1.0$[37].

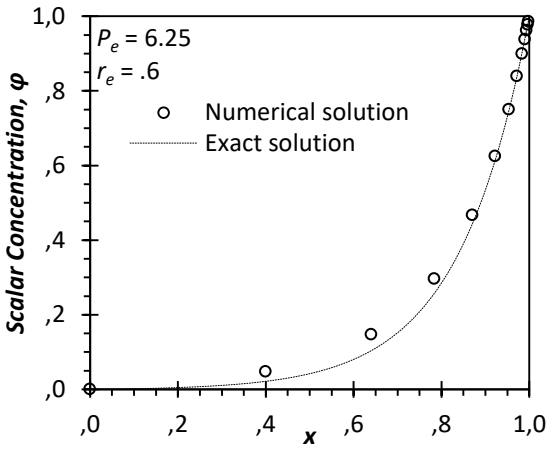

Figure-3. Inaccurate behavior of scalar concentration profile φ due to an incompatible grid expansion factor r_e in computational domain.

Next, defining a sequence of r_e by

$$\begin{aligned} &re_j, \\ &re_{j+1} = re_j + q, \\ &re_{j+2} = re_{j+1} + q, \\ &re_{j+3} = re_{j+2} + q, \\ &\vdots \\ &re_m = re_{m-1} + q, \end{aligned} \quad (15)$$

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

Let W and Y be the domain and the target of h, respectively, where the function$h$ from W to Y is a collection of ordered pairs of the form (Pe, r_e). Note that Pe and r_e are in W and Y, respectively. The collection implies and is implied by the following conditions;

Condition a For each Pe in W, there is an element $\mathrm{r_e}$ in Y such that $(\mathrm{Pe}, \mathrm{r_e})$ is one of the ordered pairs. In other words, each element Pe in the domain of h has a value h(Pe) under h.

Condition b If $(\mathrm{Pe}, \mathrm{r_e})$ and $(\mathrm{Pe}, \mathrm{r_e'})$ are both among the ordered pairs that make up the function, then $\mathrm{r_e} = \mathrm{r_e'}$. This means that every element of the domain has at most one value under h. The function h is therefore a mechanism that assigns to each element Pe of the domain a unique element h(Pe)of the target.

We write

$$r_e = h(Pe)$$

indicating that the ordered pair (Pe, r_e) is in the collection of ordered pairs which define the function h. Thus the set $\{h(Pe): Pe$ is a real number in W$\}$ of values of h is theimage of h.

Let

$$\begin{aligned} &i = j = 1, n = 6, m = 2, Pe_1 = 100, re_1 = 0.9, p = 2, \\ &q = 0.1, \end{aligned} \quad (16)$$

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

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

and

$$0.9, 1.0;$$

respectively.

Proposition a The sequences' elements in (14) and (15), whose boundary values and independent variables are given in (16), form the ordered pairs $(\mathrm{Pe}, \mathrm{r_e})$ which satisfy Condition a and b such that;

$$\begin{aligned} &\{(Pe_1, re_1), (Pe_2, re_1), (Pe_3, re_1), \ldots\ldots, (Pe_6, re_2)\} \\ &= \{(100, 0.9), (50, 0.9), (25, 0.9), (12.5, 0.9), \\ &(6.25, 0.9), (3.125, 1.0)\}. \end{aligned}$$

Proposition b *If* $0 \leq Pe \leq 3.125$, then the ordered pair $(\mathrm{Pe}, \mathrm{r_e}) = (\mathrm{Pe}, 1)$.

6. RESULTS OF CALCULATIONS

The concentration φ profiles which are numerically calculated for $Pe = 6.25, 12.5, 25, 50, 100$ are plotted in Figure-4 and Figure-5. For the sake of space, only profiles involving $r_e = 1.0, 0.9, 0.8$ have been included. 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 $r_e = 1.0, 0.8, 0.7, \ldots, 0.1$). This proves *Proposition a*. 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.

Note that since $r_e = 1.0$ 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. *Proposition b* is thus proven.

Theorem Let $0 \leq Pe \leq 100$, the grid expansion factor $\mathrm{r_e}$ for solving the convection-diffusion equation in (6), with the flow conditions in (9) and (13), is expressed as;

$$r_e = A$$

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

$$r_e = B$$

for $0 \leq Pe \leq 3.125$, *where* A, B *constants, and* $A \neq B$.

7. CONCLUSIONS

A new technique in the determination of grid expansion factor r_e which represents a quantitative guideline for the shooting method solution of the convection-diffusion equations is proposed. The understanding on the influence of the Peclet number Pe on the grid expansion factor r_e formes a basis for a more effective approach in the selection of grid type for the computational procedure.

The key aspect in this research is the formulation of the special function as a collection of ordered pairs of the form $\left(Pe_i, r_{e_j}\right), i = 1,2, \ldots, n; j = 1,2, \ldots, m$ for the given CDE. This sheds light on the possibility of a more general framework for the selection of grid type in computational fluid dynamics, the relationship between the flow parameter/s and the grid quality in the shooting method solution, as well as the influence of Pe (e.g. low, transition, high) on the numerical error pattern.

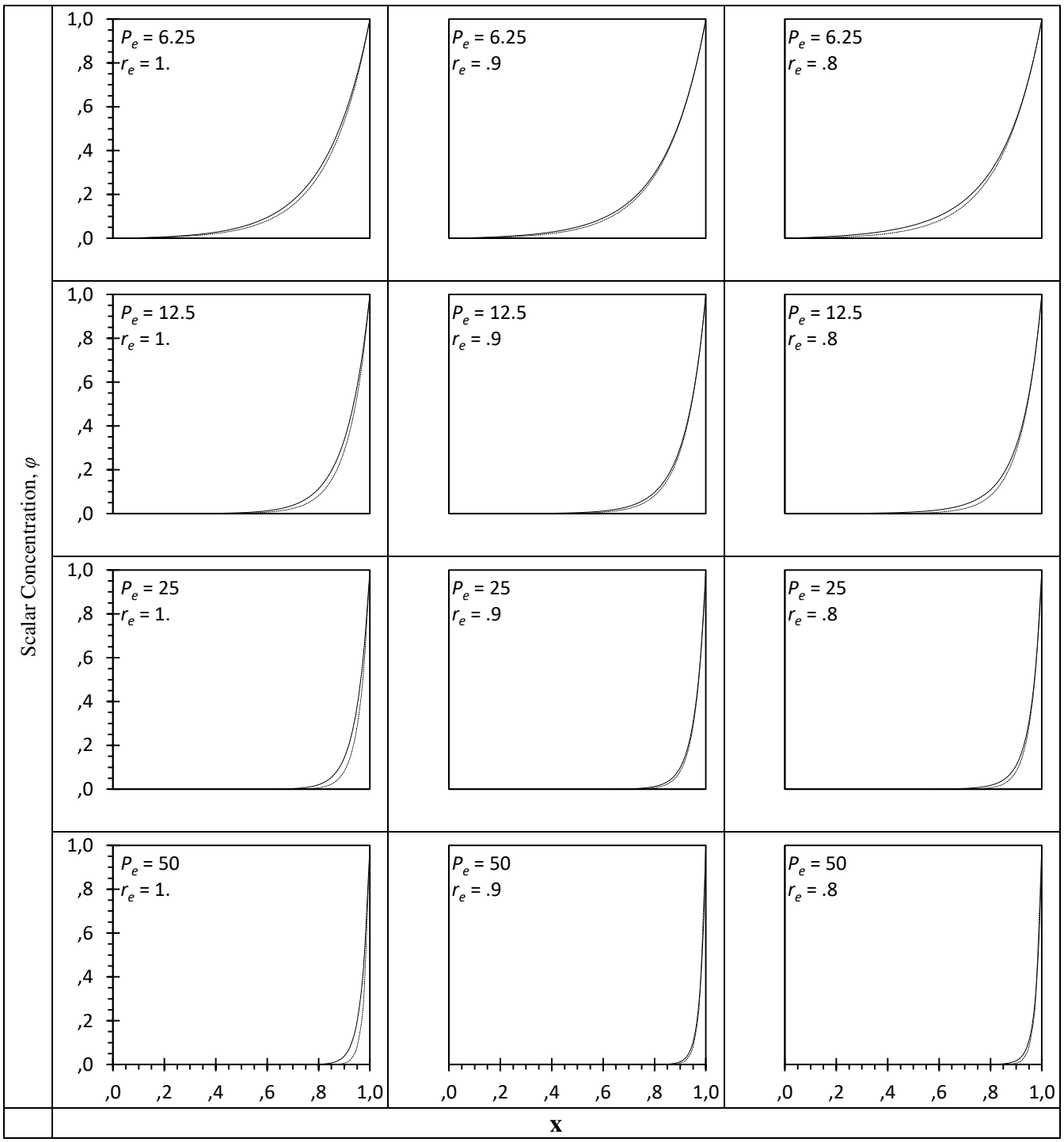

Figure-4. Concentration profile at $Pe = 50, 25, 12.5, 6.25$. - - - - - and ——— indicate the exact and numerical calculations, respectively.

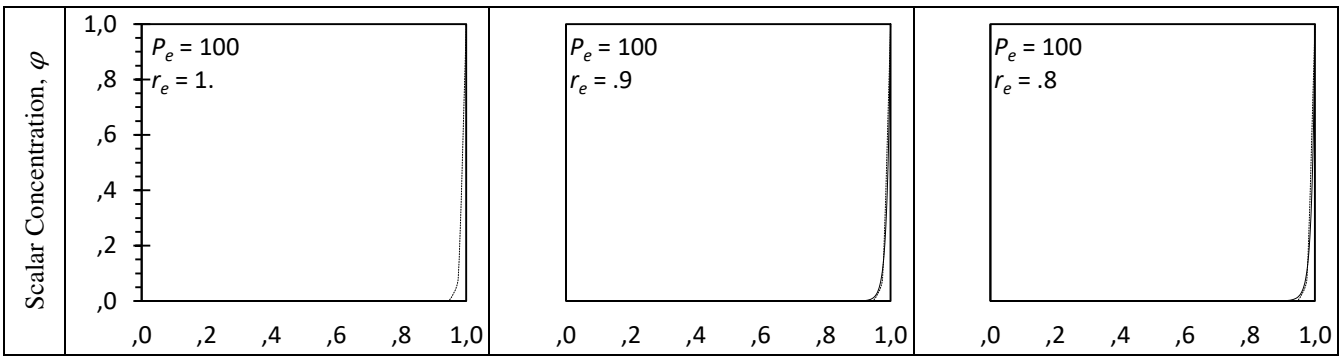

Figure-5. Concentration profile at$Pe = 100.$ - - - - - and ——— indicate the exact and numerical calculations, respectively. Note that the profile is underestimated at $r_e = 1.0$.

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REFERENCES

[1] Abdullah A. 2018. Formulation of low Peclet number based grid expansion factor for the solution of convection-diffusion equation. Eng. Technol. Appl. Sci. Res. 8: 2680-2684.

[2] Abdullah A. 2018. Mathematical relationship between grid and low Peclet numbers for the solution of convection-diffusion equation. ARPN J. Eng. Appl. Sci. 13(9): 3182-3187.

[3] Li L., Mei R. and Klausner J. F. 2017. Lattice Boltzmann models for the convection-diffusion equation: D2Q5 vs D2Q9. Int. J. Heat Mass Transf. 108: 41-62.

[4] Li L., Mei R. and Klausner J. F. 2013. Multiple-relaxation-time lattice Boltzmann model for the axisymmetric convection diffusion equation. Int. J. Heat Mass Transf.67: 338–351.

[5] Hu Y., Li D., Shu S. and Niu X. 2016. Lattice Boltzmann flux scheme for the convection-diffusion equation and its applications. Comput. Math. with Appl. 72(1): 48-63.

[6] Wang H., Shi B., Liang H. and Chai Z.2017. Finite-difference lattice Boltzmann model for nonlinear convection-diffusion equations. Appl. Math. Comput. 309: 334-349.

[7] Hu Z. X., Huang J., Huang W. X. and Cui G. X. 2017. Second-order curved interface treatments of the lattice Boltzmann method for convection-diffusion equations with conjugate interfacial conditions. Comput. Fluids. 144: 60-73.

[8] Bittl M., Kuzmin D. and Becker R. 2014. The CG1-DG2 method for convection-diffusion equations in 2D. J. Comput. Appl. Math. 270: 21-31.

[9] Liu H. and Pollack M. 2016. Alternating evolution discontinuous Galerkin methods for convection-diffusion equations. J. Comput. Phys. 307: 574-592.

[10] Zhang J., Ge L. and Kouatchou J. 2000. A two colorable fourth-order compact difference scheme and parallel iterative solution of the 3D convection diffusion equation. Math. Comput. Simul. 54(1-3): 65-80.

[11] Sun H., Kang N., Zhang J. and Carlson E. S. 2003. A fourth-order compact difference scheme on face centered cubic grids with multigrid method for solving 2D convection diffusion equation. Math. Comput. Simul. 63(6): 651-661.

[12] Singh J., Swroop R. and Kumar D. 2016. A computational approach for fractional convection-diffusion equation via integral transforms. Ain Shams Eng. J. 1-10.

[13] Behroozifar M. and Sazmand A. 2017. An approximate solution based on Jacobi polynomials for time-fractional convection-diffusion equation. Appl. Math. Comput. 296: 1-17.

[14] Martin V. 2005. An optimized Schwarz waveform relaxation method for the unsteady convection diffusion equation in two dimensions. Appl. Numer. Math. 52(4): 401-428.

[15] Tian Z. F. and Yu P. X. 2011. A high-order exponential scheme for solving 1D unsteady

convection-diffusion equations. J. Comput. Appl. Math. 235(8): 2477-2491.

[16] Mittal R. C. and Jain R. K. 2012. Redefined cubic B-splines collocation method for solving convection-diffusion equations. Appl. Math. Model. 36(11): 5555-5573.

[17] Cao H. H., Liu L. B., Zhang Y. and Fu S. M. 2011. A fourth-order method of the convection-diffusion equations with Neumann boundary conditions. Appl. Math. Comput. 217(22): 9133-9141.

[18] Shukla H. S. and Tamsir M. 2017. An exponential cubic B-spline algorithm for multi-dimensional convection-diffusion equations. Alexandria Eng. J. 1-8.

[19] Biringen S. 1981. A note on the numerical stability of the convection-diffusion equation. J. Comput. Appl. Math. 7(1): 17-20.

[20] Zhai S., Feng X. and He Y. 2014. An unconditionally stable compact ADI method for three-dimensional time-fractional convection-diffusion equation. J. Comput. Phys. 269: 138-155.

[21] Zhou Z. and Liang D.2017. The mass-preserving and modified-upwind splitting DDM scheme for time-dependent convection-diffusion equations. J. Comput. Appl. Math. 317: 247-273.

[22] Ge L. and Zhang J. 2001. High accuracy iterative solution of convection-diffusion equation with boundary layers on nonuniform grids. J. Comput. Phys. 171(2): 560-578.

[23] Ma Y. and Ge Y. 2010. A high order finite difference method with Richardson extrapolation for 3D convection-diffusion equation. Appl. Math. Comput. 215(9): 3408-3417.

[24] Mohamed S. A., Mohamed N. A., Gawad A. F. A. and Matbuly M. S. 2013. A modified diffusion coefficient technique for the convection diffusion equation. Appl. Math. Comput. 219(17): 9317-9330.

[25] Boret S. E. B. and Jimnez O. J. 2017. Integrated framework for solving the convection-diffusion equation on 2D Quad mesh relying on internal boundaries. Comput. Math. with Appl. 74(1): 218-228.

[26] Roberts S. M. and Shipman J. S. 1967. Continuation in shooting methods for two-point boundary value problems. J. Math. Anal. Appl. 18: 45-58.

[27] Marzulli P. 1991. Global error estimates for the standard parallel shooting method. J. Comput. Appl. Math. 34(2): 233-241.

[28] Ha S. N. 2001. A nonlinear shooting method for two-point boundary value problems. Comput. Math. with Appl. 42(10–11): 1411-1420.

[29] Hieu N. 2003. Remarks on the shooting method for nonlinear two-point boundary-value problems. VNU J. Sci. 3: 18-25.

[30] Amster P. and Alzate P. P. C. 2008. A shooting method for a nonlinear beam equation. Nonlinear Anal. Theory, Methods Appl. 68(7): 2072-2078.

[31] Rehman K. U. and Malik M. Y. 2017. Application of shooting method on MHD thermally stratified mixed convection flow of non-Newtonian fluid over an inclined stretching cylinder. IOP Conf. Ser. J. Phys. 822: 1-12.

[32] Peletier L. A. and Troy W. C.1996. A Topological shooting method and the existence of kinks of the extended Fischer-Kolmogorov equation. Topl. Methods Nonlinear Anal. 6: 331-355.

[33] Feltrin G. and Sovrano E. 2018. Three positive solutions to an indefinite Neumann problem: a shooting method. Nonlinear Anal. Theory, Methods Appl. 166: 87-101.

[34] Kwong M. K. 2006. The shooting method and multiple solutions of two/multi-point BVPs of second-order ODE. Electron. J. Qual. Theory Differ. Equations. 6: 1-14.

[35] Demir H. and Baltürk Y. 2017. On numerical solution of fractional order boundary value problem with shooting method. ITM Web of Conferences. 13: 01032.

[36] Han R. G., Bhakta J. N. W. and Carbonell. 1985. Longitudinal and lateral dispersion in packed beds: effect of column length and particle size distribution. AIChE J. 31: 277-288.

[37] Abdullah A.2018. Obtaining grid number for the shooting method solution of convection-diffusion equation. 9(5): 916-924.