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Comparative Study of Uniform and Graded Meshes for Solving Convection-Diffusion Equation with Quadratic Source

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Abstract: Due to its fundamental nature, the problems of convection-diffusion are discussed in various aviation, science and engineering applications. Among major applications are in the study of the dynamics of aircraft wake vortex and its interaction with turbulent jet which is a very serious hazard in aviation. Other applications include those in the investigation of intrusive sampling of jet engine exhaust gases, and the effectiveness of hot fluid injection in the removal of ice on aircraft wings. The numerical solutions of convection-diffusion require proper meshing schemes. Among major meshes in computational fluid dynamics are those of uniform, piecewise-uniform, graded, and hybrid over which the solutions of discretized governing equations are found. Bad solutions as spurious fluctuations, over- or under-predictions, and excessive computation time might be the results of unwitting application of the meshes. Accentuating comparative effectiveness of two meshes, namely uniform mesh and graded mesh with mesh expansion factor, this paper takes the solution of a convection-diffusion equation with quadratic source term into account. The problem is solved by assigning several values of mesh expansion factor to graded mesh, while mesh number is kept constant. The factors are calculated based on the generalization of their logarithmically linear relationship with low Peclet numbers derived in previous work. Based on the values of Peclet number, five test cases are considered. Graded mesh is proven relatively more robust, particularly due the solution on the mesh being free from spurious fluctuation. Furthermore, the accuracy level of the solution of up to two order of magnitude higher is obtained. The mesh expansion factor therefore contributes to a stable and highly accurate solution corresponding to all interested Peclet numbers.

Keywords: Convection-diffusion, quadratic source, graded mesh

1. Introduction

1.1 Engineering and Aviation Applications

In fluid mechanics, the most fundamental phenomena include the transport of heat, mass and momentum since it is a universally and fundamentally natural problem [1, 2]. It is extremely important to model and describe the phenomena in various engineering disciplines, aviation [3-8], meteorology, and physical sciences [1,2,9,10]. The mathematical framework for heat and mass transfer are of same kind, and basically encompassed by advection and diffusion effects. Such general scalar transport equations are broadly termed as convection-diffusion equation, and extensively used for computational simulations, such as wake vortex simulation in aviation [5,6], petroleum reservoir simulation and global weather prediction, in which an initially discontinuous profile is propagated by diffusion and convection (or advection), the latter with a speed [1, 9, 10].

Convection-diffusion equation about some passive conservative variables such as water vapor and potential temperature can be used to describe the dynamics of aircraft wake vortex which is a very serious hazard in aviation [5].

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More advanced study includes the wake vortex interaction with turbulent jet which shows that, by solving the convection–diffusion equation, the passive scalar of interest's ability to penetrate inside the vortex core is recognized depending on the distance between the jet and the vortex axis [6].

Aviation applications also include the intrusive sampling of jet engine exhaust gases where particulate losses due to convection, diffusion and thermophoresis inside a particulate probe are investigated and quantified [7]. Moreover, the equation, when coupled with a nonlinear singular integro-differential equation and Stefan condition, is useful to describe the effectiveness of hot fluid injection in the removal of ice on aircraft wings [8].

The equation is very useful in many aspects of petroleum reservoir engineering where it governs, for instance, tracer transport as one of the most representative problems. Qualitative information about flow barriers, directional flow trends, and communication between reservoirs are extracted by injecting the tracers through the underground porous media [11].

Given a velocity field which is known a priori, the method for solving convection-diffusion problem of the second order which initially appeared in 1990 in the environmental science and engineering literature is generic, linear, and of steady-state. It was then independently developed and published in engineering literature in 1993 [2].

If the expression of derivatives depends only on the local characteristic of the function, then the governing differential convection-diffusion equations are of integer order. In a more advanced method, nonlinear fractional differential equations have a so-called memory effect, where the whole information of the function is accumulated in a weighted form [10]. The study the equations' efficient numerical solutions are a popular research topic due to its widespread usage [3].

1.2 Diversity of Mesh Generation

Diversity of mesh generation can be seen in, for instance, mesh minimization [12-14], coarsening and refinement, 2-mesh schemes, and multimesh techniques [15-18]. These meshes on which discretized governing equations are numerically solved in fluid dynamics have been extensively discussed with the aims to achieve high accuracy results [18-22] and mesh effectiveness with regard to computation time [12, 22, 23].

Unwanted results as spurious fluctuation which is unacceptable physically might be due to over-coarsening the mesh and should be avoided by careful use of a meshing technique. One of the successful methods is a modification of the finite difference method where fluid flow problem is solved using the finite difference-arbitrary mesh procedures [12]. The method enables local condensation of the mesh. Another finite difference scheme called component-wise splitting method, on the other hand, involves relatively simple equations of which the successive integration replaces the integration of the interested initial equation, and is proven absolutely stable [13]. The base idea is to have a sequence of the operators of the simplest structure which are splitted from a complex one. When the irregular mesh size is introduced in both methods, the analysis system mesh number is greatly reduced. A time-domain algorithm of second-order finite-difference was also introduced which greatly reduces the needed mesh number despite there is a slight increment in the computational load per step of time. In comparison to conventional algorithm, the corresponding solution on the relatively coarse mesh has error that is 10^{-4} smaller [14]. Another effective mesh scheme is a hybrid Shishkin-graded (SG) mesh with constant transition parameter, where a sufficiently fine equidistant mesh is defined in a boundary layer and is connected to a graded mesh. The results of test cases affirm that whenever the conventional Shishkin mesh fails to support the non-oscillatory solutions, the SG might not.

An excellent candidate for solving the convection dominated diffusion equation is the improved rearward hybrid difference method, particularly in the handling of major issues pertaining fluctuation, and clearly picturing the problem [24]. It is also noteworthy that physically realistic calculation results could effectively be produced by applying SMART, MINMOD, and Superbee which are discretization schemes of second-order [19]. Among schemes of high order of accuracy, there is an extensive sixth-order accuracy numerical procedure on the fine mesh in solving convection-diffusion equation which involves integrating the use of a compact difference scheme of the fourth-order, the employment of technique of Richardson extrapolation, and the application of interpolation scheme of an operator [20,21].

It was found that both Lattice Boltzmann (LBS) and one-step Lax-Wendrof of second-order schemes achieve equally in the aspect of simulation time decrease [22, 23].

1.3 Model of Interest

The model of interest in differential form and its boundary conditions are given by

$$-D\partial_x^2\kappa + c(x)\partial_x\kappa + d(x)\kappa = -4y^2 + 4y, \text{ for } x \in (0,1), y \in (0,1) \tag{1}$$

and

$$\kappa(0) = \kappa(1) = 0, \tag{2}$$

where $-D\partial_x^2\kappa$, $c(x)\partial_x\kappa$, $d(x)\xi$, and the expression on the right side of the equation are diffusive, convective, reactive, and source terms, respectively, $c(x)$ and $d(x)$, are sufficiently smooth functions, and parameter κ is unknown. It is assumed that

$$\begin{gathered} D > 0, \\ c(x) > 0 \text{ for all } x \in [0,1], \\ d(x) \geq 0 \text{ in } [0,1] \end{gathered} \tag{3}$$

Without convection, reaction and source, the solution of Eq. (1) is linear in space. We are not interested in such pure diffusion process. The equation is important with regard to convection only if $c(x)$ is nonzero for all $x \in [0,1]$. Note that the solution of Eq. (1) remains when $c(x) < 0$ in $[0,1]$, and the variable transformation is imposed on x such that it becomes $1 - x$.

The error of finite difference technique is indicated by the consistency and stability of Eq. (1) which are significantly affected by a boundary layer that appears at $x = 1$ if D is small. Enhancement of the consistency of the technique is possible if boundary values are given such that the boundary layer vanishes, but its stability is not guaranteed [25-27].

Equation (1) is simplified in this paper into

$$-D\partial_x^2\kappa + c(x)\partial_x\kappa = -4y^2 + 4y, \tag{4}$$

where the reactive term is neglected.

The motion of fluid element's responsibility to carry along the scalar concentration κ in the convection process, and κ's ability to spread within the fluids are confirmed by the presence of convection and diffusion terms, respectively, in Eq. (4). Interestingly, over a defined distance, a sudden change in κ is observed after its initial gradual growth in x if D is small and appropriate boundary conditions are applied. Computational fluid dynamics is challenged by the sharp drop of κ with respect to discretization method, and the computational domain mesh structure.

We consider in this paper a convection-diffusion problem as a model which is solved on uniform and graded meshes after being discretized using finite difference technique. The use of graded mesh is supported by the numerical analysis results. We observe κ which is obtained by solving Eq. (1) on both types of mesh in order to reduce time of pre-computation yet produce solution of the flow problem that is accurate. This is caused by the need to keep mesh number as minimum as possible without letting κ profile, where κ is the unknown quantity, from being physically unacceptable. We compare the solutions on both type of meshes in several cases especially in the region where κ changes abruptly. In the case where mesh expansion factor is applicable, its selection has to be made with care in order to preserve the accuracy of the results. An effort is made to generalize the previous works on the relationship between mesh structure and Peclet number for the solution of convection-diffusion equation with zero source term [28,29].

It is apparent that broad study on various mesh schemes has been sparked by many factors including the need to solve numerically the system of equations. Detailed comparative study of mesh structure effectiveness in preserving the accuracy of the solutions of convection-diffusion equation with quadratic source term for low Peclet number Pe, however, is still open to research. Examining graded mesh is essential to appreciate its flexibility against uniform mesh in solving the governing equation of interest even if the mesh is relatively coarse, thus save computation time. Proving the effectiveness of r_e to solve the equation of interest with minimum mesh number N is the aim of this research.

2. Methodology

Boundary conditions of representation in Eq. (4) of the model problem are given as

$$\begin{gathered} \kappa(0) = 0 \\ \kappa(1) = 0 \end{gathered} \tag{5}$$

Graded mesh is used in the corresponding domain of solution. The interval number is given by $(N-1)$, where an odd integer N is the mesh number. In order to define the atoms for the mesh, let first discretize a defined independent variable x domain in such a way that $x = [0,1]$.

The atoms $x_0, \dots, x_{N-1}$ for the mesh is defined as

$$x_{i+1} = x_i + r_e \Delta x_i, \tag{6}$$

where $0 \leq i \leq (N-1), i \in \mathbb{Z}$, and mesh expansion factor $r_e > 0$.

Clearly $\sum \Delta x_i = 1$. Illustration of the mesh is presented in Fig. 1.

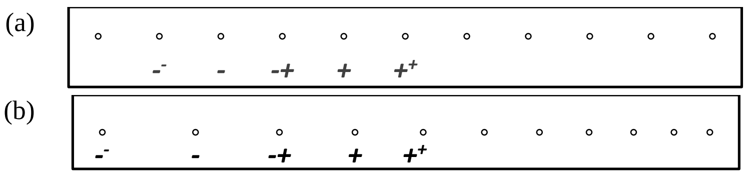


Fig. 1 - computational atoms (a) uniform mesh; (b) graded mesh

With a given and neighboring atoms being assigned to the variables of interest, Eq. (4) solution can be approximated by means of the algebraic equations. This is done by approximating partial derivatives at every single atom by nodal algebraic expression resulting from discretizing Eq. (4) as

$$C_{-+}\kappa_{-+} + \sum_{m} C_m \xi_m = Q_{-+} \tag{7}$$

The atoms which are denoted by $'-+'$ are assigned to Eq. (7). The instant left and right atoms are denoted by m. Three $n \times n$ array allocates the matrix C elements, where C is a bidiagonal matrix (the nonzero elements are represented by C_{ii}, C_{-}, and C_{+}). Thus, Eq. (7) becomes

$$C_{-+}\kappa_{-+} + C_{+}\kappa_{i+1} + C_{-}\kappa_{i-1} = Q_{-+} \tag{8}$$

after using three-point computational atoms.

It is possible to use central difference scheme in order to discretize the diffusive term's outer and inner derivatives, and the convective term's derivative in Eq. (4) [25,26].

Scalar concentration κ in Eq. (4) is found numerically by solving the approximate algebraic Eq. (8) using block elimination method. Note that Eq. (8) represents a linear system of differential equation, where it contains only linear terms. Thus, there is no requirement for linearization of Eq. (4) solution. We choose that

$$c = 1.0, N = 11 \tag{9}$$

Peclet number $Pe = 1/D$ of interest is defined in a sequence

$$\begin{aligned} &Pe_l, \\ &Pe_{l+1} = Pe_l/q, \\ &Pe_{l+2} = Pe_{l+1}/q, \\ &Pe_{l+3} = Pe_{l+2}/q, \\ &. \\ &. \\ &. \\ Pe_n &= Pe_{n-1}/q, \end{aligned} \tag{10}$$

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

Let

$$q = 2, Pe_1 = 100, n = 6, l = 1 \tag{11}$$

Thus, the sequence in Eq. (10) becomes

$$100, 50, 25, 12.5, 6.25, 3.125 \tag{12}$$

We use the following equation [28]

$$r_e = m \lg Pe + b, \tag{13}$$

where

$$m = \frac{.5}{(\lg\ .03125)}, \tag{14}$$

and

$$b = 1. -(m \lg 3.125), \tag{15}$$

are curve slope and a constant, respectively, in order to systematically set the values of r_e. Equation (13) was initially used for the solution of convection-diffusion equation with zero source, and boundary conditions of $\kappa(0) = 0, \kappa(1) = 1$. Here generalization is made to extent the equation when quadratic source term and boundary conditions of $\kappa(0) = \kappa(1) = 0$ are considered.

The value of r_e needs to be found in order to preserve the accuracy of the solution with respect to Pe since N is kept constant. The inaccuracy could also include fluctuation as shown in Fig. 2. The fluctuation as shown in the figure indicates nonphysical solution of Eq. (4) caused by inappropriate choice of r_e and/or N.

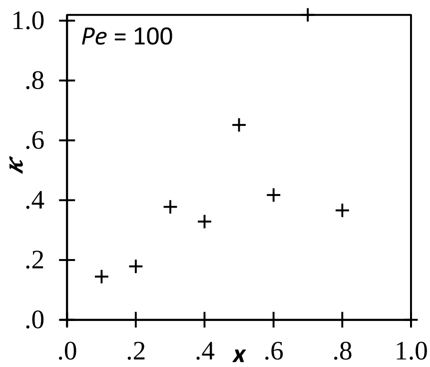


Fig. 2 - inappropriate mesh expansion factor and or mesh number leads to inaccurate κ profile over computational domain; physically correct profile does not fluctuate

3. Result and Discussion

Graded mesh is only applied in *x*-coordinates, while uniform mesh in both *x*- and *y*-coordinates. This is due to the derivatives in Eq. (4) are those with respect to *x* only, thus non-uniform mesh in *y*-coordinates is unnecessary. Mesh expansion factor r_e affects the distance between two neigbouring computational atoms Δx as illustrated in Fig. 3 of graded meshes. The distance between the atoms on the coarse part of mesh increases, while that on the fine part decreases when r_e decreases. The change in the distance is exponential. For $r_e = 1$, graded and uniform meshes are identical, where all neighboring computational atoms are equally spaced from one another.

Over-reduction of r_e would result in significant lost of information on the coarse part. This occurs in two ways; firstly, the line curvature over the part is insufficient, and secondly, the overall profile of κ is under-predicted. On the other hand, under-reduction of r_e would cause a more serious accuracy issue involving spurious fluctuation/s in the solution. Although the number of meshing interval is constant where $(N-1) = 10$, computational atoms on the fine part are extremely densed for $r_e = .5$ such that they are not easily distinguishable. For $r_e \to 1$ and $r_e \to 0$, $\Delta x \to (1/N-1)$ and $(\Delta x)_{coarse} \to 1$, respectively, where $(\Delta x)_{coarse}$ is the distance between the atoms on the coarse part.

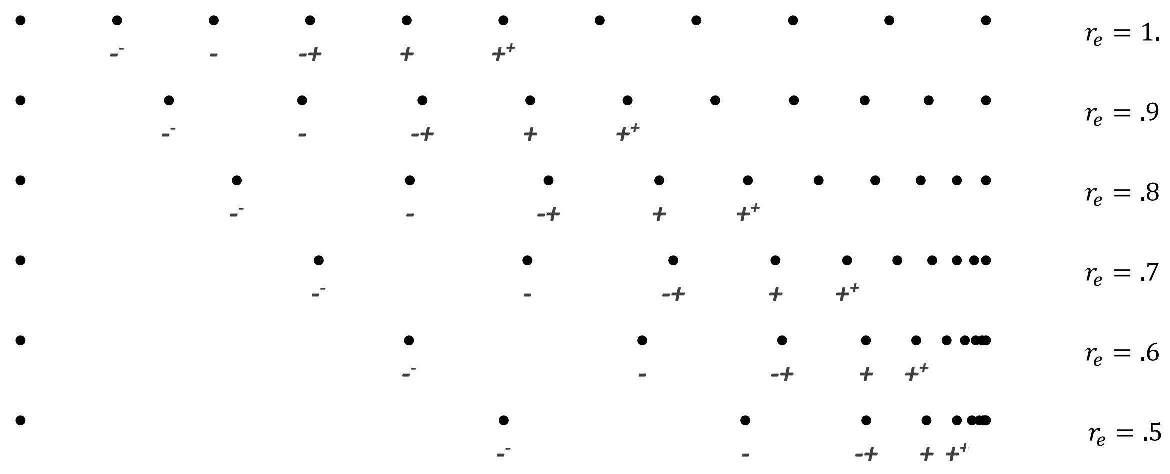


Fig. 3 - computational atoms for various mesh expansion factors

Scalar concentration κ which is numerically and analytically calculated over graded and uniform meshes at (x_i, y_3) and (x_i, y_6) was plotted against x as shown in Fig. 4. The plot generally involves six curves corresponding to; numerical solution on graded mesh at (x_i, y_3); numerical solution on graded mesh at (x_i, y_6); exact solution at (x_i, y_3); exact solution at (x_i, y_6); numerical solution on uniform mesh at (x_i, y_3); and numerical solution on uniform mesh at (x_i, y_6). Note that the exact solutions serve as benchmarks for validation of the numerical calculations. The concentration at y_3 and y_6 represents that when the source is relatively small (i.e. $e(y_3) = 0.64$) and maximum (i.e. $e(y_6) = 1$), respectively. The plot in the figure when $Pe = 3.125$ consists of only four curves since graded mesh with $r_e = 1$ is identical with uniform mesh such that their corresponding numerical results are also identical.

Applying Eq. (13) for the determination of r_e with regard to the Peclet number Pe, the resulting solutions of Eq. (4) on graded mesh are in very good agreement with the exact solutions. The extension of Eq. (13) [28] for the solution of convection-diffusion equation with boundary conditions in Eq. (2) and quadratic source term is therefore valid.

During the gradual growth of κ, the correct curvature of profiles decreases with the increment of Pe until the curves are close to linear. On the other hand, the second part of the curves whose beginnings are marked by maximum κ experience sharp drops with regard to Pe.

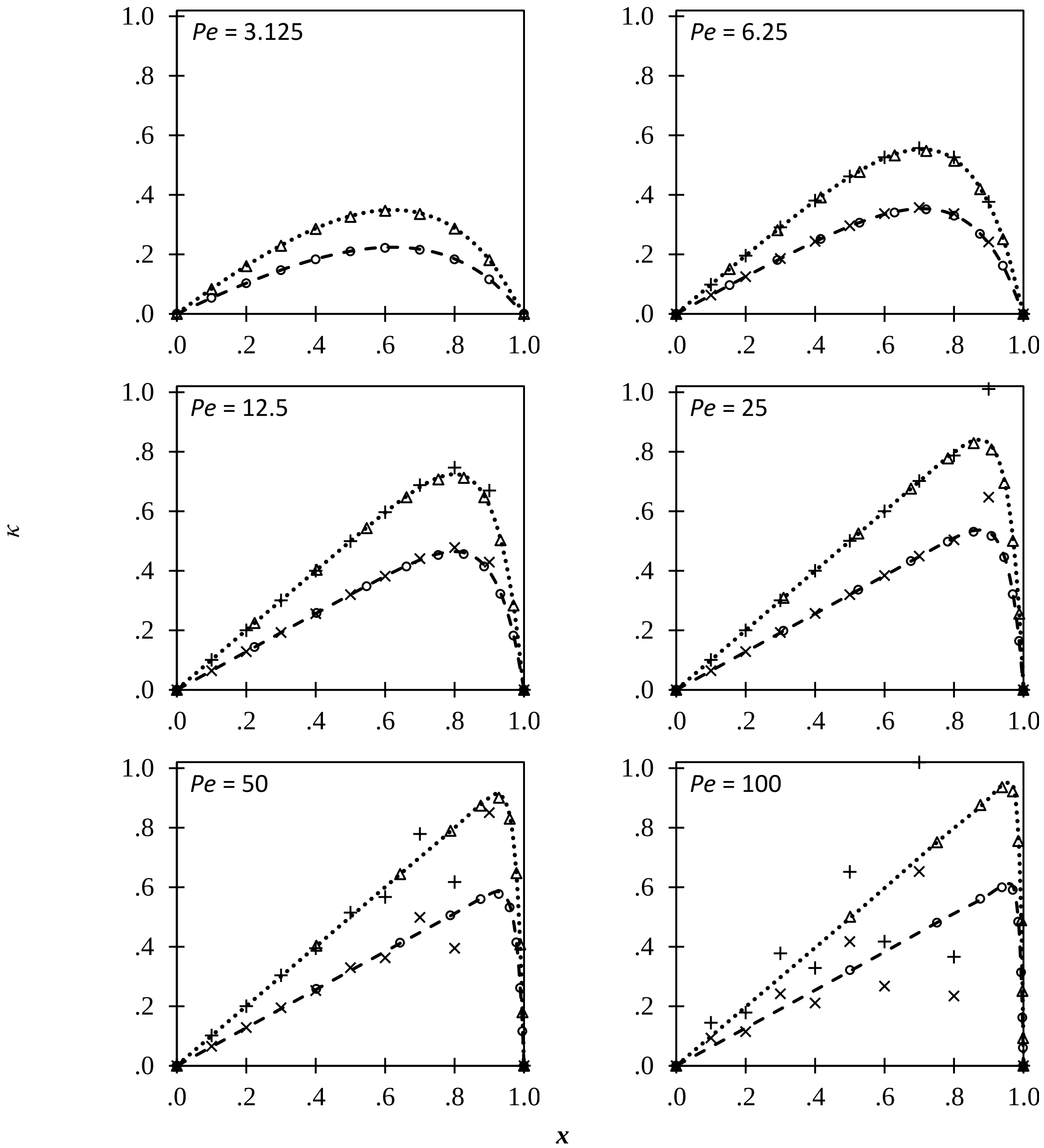


Fig. 4 - Profiles of κ; - - - - - Numerical solution on graded mesh at (x_i, y_3); ……... Numerical solution on graded mesh at (x_i, y_6); o Exact solution at (x_i, y_3); Δ Exact solution at (x_i, y_6); x Numerical solution on uniform mesh at (x_i, y_3); + Numerical solution on uniform mesh at (x_i, y_6)

The numerical solutions on uniform mesh both at y_3 and y_6 are in very good agreement with the exact solutions only when $Pe = 3.125$ and $Pe = 6.25$, as can be seen in Fig. 4. When $Pe = 12.5$ and $Pe = 25$, the curves of the numerical and exact solutions no longer coincide, and scalar concentrations κ are over-predicted. More seriously, there are fluctuations in the solutions when $Pe = 50$ and $Pe = 100$.

It is confirmed now that graded mesh offers more flexibility to the solutions than uniform mesh when mesh number N is constant.

The average errors as shown in Table 1 and Table 2 are generally related to Pe. When the results corresponding to y_3 and y_6 obtained from the solutions on graded mesh are compared with those on uniform mesh, the latter average error is found to be larger than the former by up to two order of magnitude.

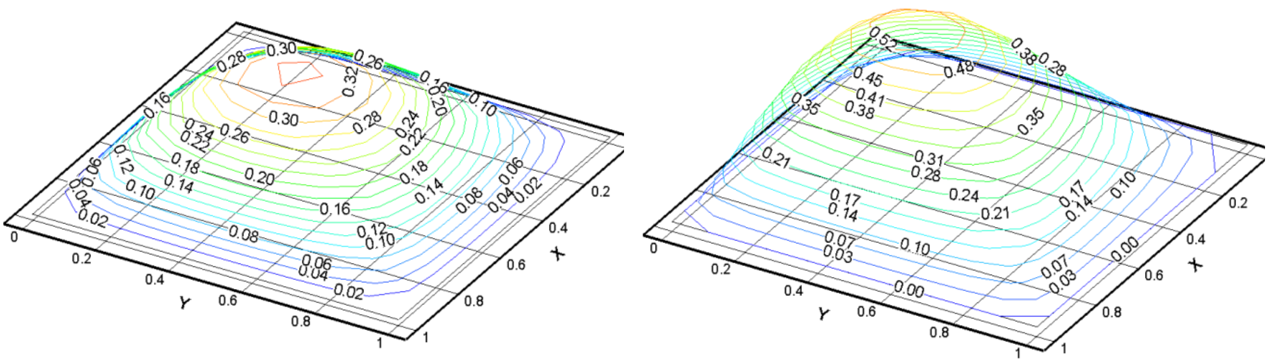
Table 1 - Numerical errors for at y_3

	Uniform mesh	Graded mesh
Pe	**Error**	**Error**
3.125	8.0 x 10^{-4}	
6.25	2.8 x 10^{-3}	1.6 x 10^{-3}
12.5	5.9 x 10^{-3}	2.1 x 10^{-3}
25	1.2 x 10^{-2}	2.1 x 10^{-3}
50	4.4 x 10^{-2}	2.3 x 10^{-3}
100	1.2 x 10^{-1}	2.7 x 10^{-3}

Table 2 - Numerical errors for at y_6

	Uniform mesh	Graded mesh
Pe	**Error**	**Error**
3.125	1.3 x 10^{-3}	
6.25	4.4 x 10^{-3}	2.5 x 10^{-3}
12.5	9.2 x 10^{-3}	3.2 x 10^{-3}
25	1.8 x 10^{-2}	3.3 x 10^{-3}
50	6.9 x 10^{-2}	3.5 x 10^{-3}
100	1.8 x 10^{-1}	4.3 x 10^{-3}

3-d surface plots of concentration κ are given in Fig. 5 and Fig. 6. The scalar quantity is initially concentrated about the center of the computation domain especially when $Pe = 3.125$, and moves in the flow direction with respect to Pe. This is due to relatively low diffusivity at higher Pe such that convection becomes more dominant. Note that in the case of extremely high Pe, the scalar would form a boundary layer. It is also interesting to note that the maximum value of κ (i.e. κ_{max}) increases with Pe. For instance, κ_{max} is maximum at $Pe = 100$.



(a) (b)

Fig. 5 - 3-d surface plot of κ on graded mesh (a) $Pe = 3.125$ (b) $Pe = 6.25$

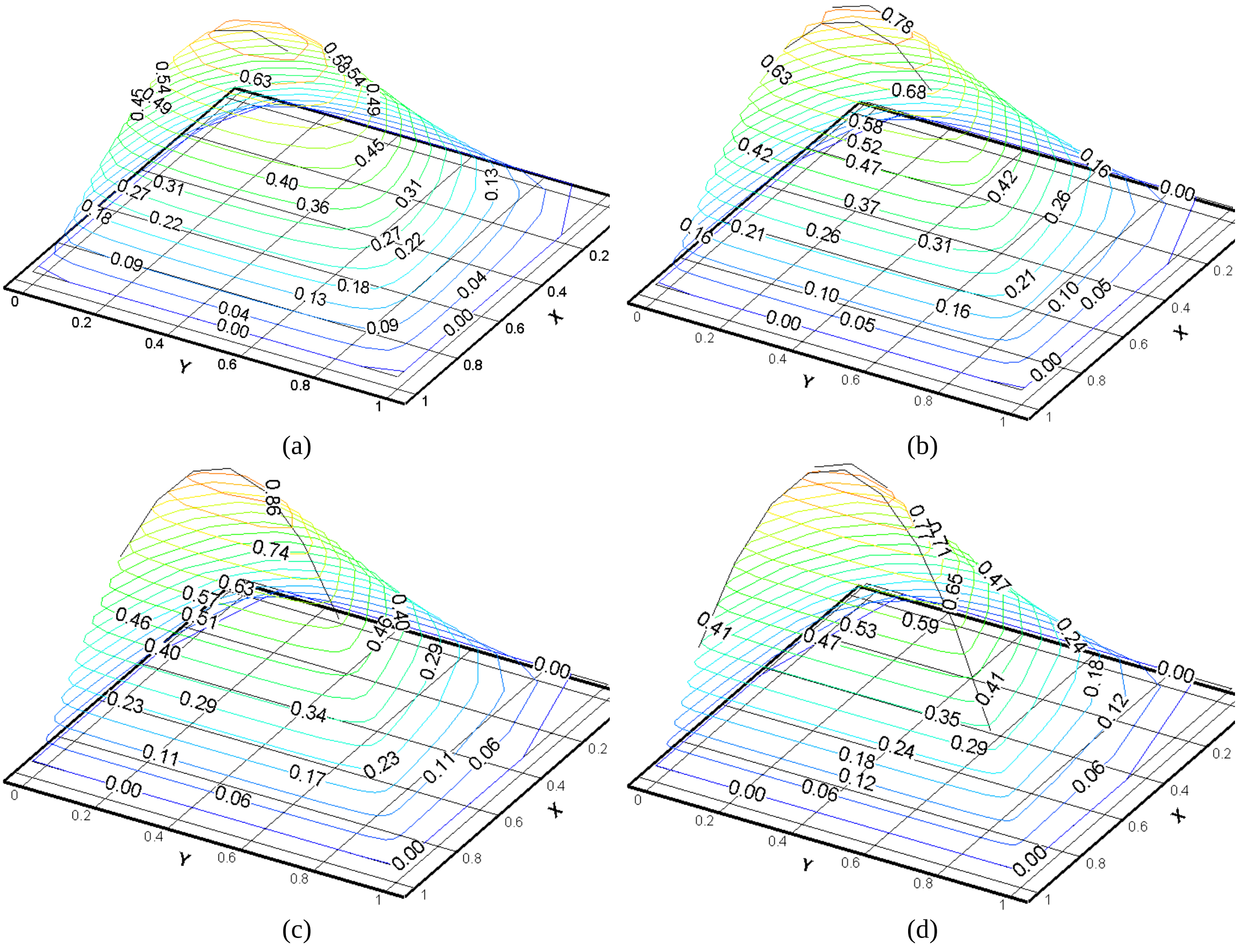


Fig. 6 - 3-d surface plot of κ on graded mesh (a) $Pe = 12.5$ (b) $Pe = 25$ (c) $Pe = 50$ (d) $Pe = 100$

4. Conclusion

Uniform mesh and that of graded with mesh expansion factor r_e for solving convection-diffusion equation with quadratic source and boundary conditions in Eq. (5) for small values of the Peclet number Pe have been comparatively studied. The results improve our understanding on the contribution of r_e to preserve highly accurate solution when Pe increases, and the robustness of graded mesh.

The expressions in Eq. (13) - (15) which were formulated for convection-diffusion equation [28] with zero source and boundary conditions of $\kappa(0) = 0, \kappa(1) = 1$ to determine r_e has been successfully generalized for the current problem (i.e. convection-diffusion equation with quadratic source and boundary conditions of $\kappa(0) = \kappa(1) = 0$).

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