

Two-Dimensional Transient Finite Volume Diffusional Approach to Transport Equations

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Abstract. This paper aims at presenting the Diffusional Method coupled with the Finite Volume scheme as an alternative approach for solving convection-diffusion equations, which under high Peclet numbers may configure a hard numerical task. It is also intended to test the proposed methodology for a case where analytical solution is known and for another one characterized by a high gradient profile. For the last case, results show that false diffusion effects are present. Comparisons of the Diffusional Method with other numerical schemes are also presented.

1. Introduction

The problem of solving convection-diffusion equations is well established in the literature [5, 8, 9]. The convection-diffusion equations are obtained in several engineering systems and also in some economic problems which can be represented by means of stochastic differential equations.

It is also well known the difficulties found in solving this kind of equations under high Peclet numbers, or under high gradient flow problems. Numerical errors arising from predominant convective problems by means of the Finite Volume Method (FVM), the Finite Difference Method (FDM) or the Finite Element Method (FEM) have been called false dispersion or false diffusion [4].

Recently, a new alternative method, named the Diffusional Method, was presented [3] to solve the convection-diffusion equation.

FORTES and FERREIRA [1] presented the Diffusional Method with FVM for one dimensional problems. This paper aims at presenting the Diffusional Method together with the FVM to solve two dimensional problems under various Peclet numbers.

2. The diffusional two-dimensional method

The model equation employed in this study is the convection-diffusion equation in an incompressible flow field. In two dimensions, the transient convection-diffusion

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equation (CDE) can be written in the non-conservative form as

$$\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} + v \frac{\partial \phi}{\partial y} - \frac{\partial}{\partial x} \left(\Gamma_x \frac{\partial \phi}{\partial x} \right) - \frac{\partial}{\partial y} \left(\Gamma_y \frac{\partial \phi}{\partial y} \right) + Q = 0, \quad (2.1)$$

where ϕ denotes the dependent variable, Γ_x and Γ_y are the diffusion coefficients in the x -direction and y -direction, respectively, Q is the source term, u and v are the velocity components in the x -direction and y -direction, respectively, t is time. Values of Q , u , v , Γ_x and Γ_y may depend on ϕ , t , x and y . A new methodology for solving equation (2.1) has been proposed [3] which is natural and independent of the numerical scheme.

Based on the just cited author, let us accept and use the obvious fact that linear and non-linear Diffusion Problems (elliptic and parabolic problems) can, in general, and in the absence of strong non-linearities, be accurately solved by means of any of the classical numerical methods, that is, Finite Differences, Finite Elements and Finite Volumes. For this purpose, let us transform equation (2.1) into a diffusion equation. Let

$$u \frac{\partial \phi}{\partial x} - \frac{\partial}{\partial x} \left(\Gamma_x \frac{\partial \phi}{\partial x} \right) = A_x \frac{\partial}{\partial x} \left(\Gamma_x B_x \frac{\partial \phi}{\partial x} \right), \quad \text{and} \quad (2.2)$$

$$v \frac{\partial \phi}{\partial y} - \frac{\partial}{\partial y} \left(\Gamma_y \frac{\partial \phi}{\partial y} \right) = A_y \frac{\partial}{\partial y} \left(\Gamma_y B_y \frac{\partial \phi}{\partial y} \right), \quad \text{so that,} \quad (2.3)$$

$$A_x \Gamma_x \frac{\partial B_x}{\partial x} = u; \quad A_x B_x = -1 \Rightarrow B_x = B_0(y) e^{-\int_0^x \frac{u}{\Gamma_x} dx}, \quad \text{and} \quad (2.4)$$

$$A_y \Gamma_y \frac{\partial B_y}{\partial y} = v; \quad A_y B_y = -1 \Rightarrow B_y = B_1(x) e^{-\int_0^y \frac{v}{\Gamma_y} dy}, \quad (2.5)$$

where $B_0(y)$, $B_1(x)$, Γ_x and Γ_y are constants.

In this notation, the diffusional formulation of (2.1) is

$$\frac{\partial \phi}{\partial t} + A_x \frac{\partial}{\partial x} \left(\Gamma_x B_x \frac{\partial \phi}{\partial x} \right) + A_y \frac{\partial}{\partial y} \left(\Gamma_y B_y \frac{\partial \phi}{\partial y} \right) + Q = 0. \quad (2.6)$$

The substitution of equations (2.4) and (2.5) into equation (2.6) leads to

$$\frac{\partial \phi}{\partial t} - e^{-\int_0^x \frac{u}{\Gamma_x} dx} \frac{\partial}{\partial x} \left(\Gamma_x e^{-\int_0^x \frac{u}{\Gamma_x} dx} \frac{\partial \phi}{\partial x} \right) - e^{-\int_0^y \frac{v}{\Gamma_y} dy} \frac{\partial}{\partial y} \left(\Gamma_y e^{-\int_0^y \frac{v}{\Gamma_y} dy} \frac{\partial \phi}{\partial y} \right) + Q = 0 \quad (2.7)$$

and rearranging one arrives to the general two-dimensional diffusional form of the CDE

$$\begin{aligned} e^{-\left(\int_0^x \frac{u}{\Gamma_x} dx + \int_0^y \frac{v}{\Gamma_y} dy\right)} \left(\frac{\partial \phi}{\partial t} + Q \right) & - e^{-\int_0^y \frac{v}{\Gamma_y} dy} \frac{\partial}{\partial x} \left(\Gamma_x e^{-\int_0^x \frac{u}{\Gamma_x} dx} \frac{\partial \phi}{\partial x} \right) \\ & - e^{-\int_0^x \frac{u}{\Gamma_x} dx} \frac{\partial}{\partial y} \left(\Gamma_y e^{-\int_0^y \frac{v}{\Gamma_y} dy} \frac{\partial \phi}{\partial y} \right) = 0. \end{aligned} \quad (2.8)$$

If one assumes u/Γ_x and v/Γ_y to be constant or an average within the integration range, then the above equation can be written in terms of the global Peclet numbers in both directions, $P_x = uL_x/2\Gamma_x$ and $P_y = vL_y/2\Gamma_y$ as the simplified two-dimensional diffusional form of the CDE

$$e^{-\left(\frac{2P_{xx}}{L_x} + \frac{2P_{yy}}{L_y}\right)} \left(\frac{\partial \phi}{\partial t} + Q \right) - e^{-\frac{2P_{yy}}{L_y}} \frac{\partial}{\partial x} \left(\Gamma_x e^{-\frac{2P_{xx}}{L_x}} \frac{\partial \phi}{\partial x} \right) - e^{-\frac{2P_{xx}}{L_x}} \frac{\partial}{\partial y} \left(\Gamma_y e^{-\frac{2P_{yy}}{L_y}} \frac{\partial \phi}{\partial y} \right) = 0, \quad (2.9)$$

where L_x and L_y are the characteristic lengths in x - and y -direction, respectively.

The above equations (2.8) and (2.9) are in an excellent form, well suited to be solved by any numerical technique, and more particularly, by the finite volume method. Worthy to note is the equivalence of finite element, volume and difference methods used to solve one dimensional convection diffusion problems [2].

3. The finite volume diffusional method for the two-dimensional convection-diffusion equation

Consider the two-dimensional control volume shown in Figure 1. The key step of the finite volume method is the integration of equation (2.9) over the control volume [8], which is done by writing equation (2.9) in terms of local Peclet numbers, Pe_x and Pe_y . For simplicity, the standard Finite Volume notation δx_{we} is denoted by h_x and δx_{sn} is denoted by h_y .

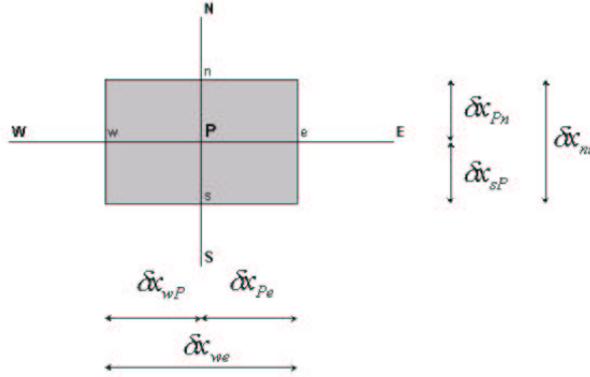


Figure 1: Two-dimensional control volume.

The two-dimensional steady state diffusional scheme takes the form

$$\int_s^n \int_w^e \left[-e^{-\frac{2P_y y}{h_y}} \frac{\partial}{\partial x} \left(\Gamma_x e^{-\frac{2P_x x}{h_x}} \frac{\partial \phi}{\partial x} \right) - e^{-\frac{2P_x x}{h_x}} \frac{\partial}{\partial y} \left(\Gamma_y e^{-\frac{2P_y y}{h_y}} \frac{\partial \phi}{\partial y} \right) + e^{-\left(\frac{2P_x x}{h_x} + \frac{2P_y y}{h_y}\right)} Q \right] dx dy = 0. \quad (3.1)$$

Using centred difference and assuming an uniform grid spacing in both directions, the integration leads to

$$\begin{aligned} & -\frac{h_y}{2Pe_y} \frac{\Gamma_x}{h_x} (e^{Pe_y} - e^{-Pe_y}) [e^{Pe_x} \Phi_W - (e^{Pe_x} + e^{-Pe_x}) \Phi_P + e^{-Pe_x} \Phi_E] \\ & -\frac{h_x}{2Pe_x} \frac{\Gamma_y}{h_y} (e^{Pe_x} - e^{-Pe_x}) [e^{Pe_y} \Phi_S - (e^{Pe_y} + e^{-Pe_y}) \Phi_P + e^{-Pe_y} \Phi_N] \\ & + \frac{h_x}{2Pe_x} \frac{h_y}{2Pe_y} (e^{Pe_x} - e^{-Pe_x}) (e^{Pe_y} - e^{-Pe_y}) Q = 0, \end{aligned} \quad (3.2)$$

that can be rearranged as

$$\begin{aligned} & -\frac{2Pe_x \Gamma_x}{h_x^2} \left[\left(\frac{e^{Pe_x}}{e^{Pe_x} - e^{-Pe_x}} \right) \Phi_W - (\coth Pe_x) \Phi_P + \left(\frac{e^{-Pe_x}}{e^{Pe_x} - e^{-Pe_x}} \right) \Phi_E \right] \\ & -\frac{2Pe_y \Gamma_y}{h_y^2} \left[\left(\frac{e^{Pe_y}}{e^{Pe_y} - e^{-Pe_y}} \right) \Phi_S - (\coth Pe_y) \Phi_P + \left(\frac{e^{-Pe_y}}{e^{Pe_y} - e^{-Pe_y}} \right) \Phi_N \right] + Q = 0. \end{aligned} \quad (3.3)$$

Substituting α_x and α_y defined as

$$\alpha_x = \coth Pe_x - \frac{1}{Pe_x} \quad \text{and} \quad \alpha_y = \coth Pe_y - \frac{1}{Pe_y} \quad (3.4)$$

in equation (3.3) to give after algebraic manipulations

$$\begin{aligned} & \frac{\Gamma_x}{h_x^2} \{ -[Pe_x(\alpha_x + 1) + 1] \Phi_W + [2Pe_x \alpha_x + 2] \Phi_P - [Pe_x(\alpha_x - 1) + 1] \Phi_E \} + \\ & \frac{\Gamma_y}{h_y^2} \{ -[Pe_y(\alpha_y + 1) + 1] \Phi_S + [2Pe_y \alpha_y + 2] \Phi_P - [Pe_y(\alpha_y - 1) + 1] \Phi_N \} + Q = 0. \end{aligned} \quad (3.5)$$

The above equation is the discretised equation for node P. For eventual comparisons, equation (3.5) can be represented by the following form:

$$a_s \Phi_W + f_s \Phi_S + b_s \Phi_P + c_s \Phi_E + g_s \Phi_N + d_i = 0, \quad (3.6)$$

where

$$a_s = -\frac{\Gamma_x}{h_x^2} [Pe_x(\alpha_x + 1) + 1] \quad \text{and} \quad f_s = -\frac{\Gamma_y}{h_y^2} [Pe_y(\alpha_y + 1) + 1]; \quad (3.7)$$

$$b_s = (2Pe_x \alpha_x + 2) + (2Pe_y \alpha_y + 2); \quad (3.8)$$

$$c_s = -\frac{\Gamma_x}{h_x^2} [Pe_x(\alpha_x - 1) + 1]; \quad g_s = -\frac{\Gamma_y}{h_y^2} [Pe_y(\alpha_y - 1) + 1]; \quad (3.9)$$

$$d_i = Q. \quad (3.10)$$

In an **unsteady-flow**, the discretization equation is derived by integrating equation (2.9) over the control volume and over the time interval from t to $t + \Delta t$. Thus,

$$\int_t^{t+\Delta t} \int_s^n \int_w^e \left[e^{-\left(\frac{2Pe_x x}{h_x} + \frac{2Pe_y y}{h_y}\right)} \left(\frac{\partial \Phi}{\partial t} + Q \right) - e^{-\frac{2Pe_y y}{h_y}} \frac{\partial}{\partial x} \left(\Gamma_x e^{-\frac{2Pe_x x}{h_x}} \frac{\partial \phi}{\partial x} \right) - e^{-\frac{2Pe_x x}{h_x}} \frac{\partial}{\partial y} \left(\Gamma_y e^{-\frac{2Pe_y y}{h_y}} \frac{\partial \phi}{\partial y} \right) \right] dx dy dt = 0. \quad (3.11)$$

If the dependent variable at the node is assumed to prevail over the whole control volume, integration of transient term can be written as

$$\int_t^{t+\Delta t} \int_s^n \int_w^e \left[e^{-\left(\frac{2Pe_x x}{h_x} + \frac{2Pe_y y}{h_y}\right)} \left(\frac{\partial \Phi}{\partial t} \right) \right] dx dy dt = \frac{h_y}{2Pe_x} \frac{h_y}{2Pe_y} (e^{Pe_x} - e^{-Pe_x}) (e^{Pe_y} - e^{-Pe_y}) \left(\frac{\Phi_P^{n+1} - \Phi_P^n}{\Delta t} \right), \quad (3.12)$$

where indices n and $n + 1$ refer to time levels.

Spatial integration of the other terms of equation (3.11) is given by equations (3.2) and (3.3). The time integration can be evaluated using the mean value theorem. Making the same simplification done between equation (3.2) and equation (3.3), for the transient term given by equation (3.12), the result of the integration of equation (3.11) can be written as

$$\begin{aligned} \frac{\Phi_P^{n+1} - \Phi_P^n}{\Delta t} &+ \theta \left(\frac{\Gamma_x}{h_x^2} \{ -[Pe_x(\alpha_x + 1) + 1]\Phi_W^{n+1} + [2Pe_x\alpha_x + 2]\Phi_P^{n+1} \} \right) \\ &+ \theta \left(\frac{\Gamma_x}{h_x^2} \{ -[Pe_x(\alpha_x - 1) + 1]\Phi_E^{n+1} \} \right) \\ &+ \theta \left(\frac{\Gamma_y}{h_y^2} \{ -[Pe_y(\alpha_y + 1) + 1]\Phi_S^{n+1} \} \right) \\ &+ \theta \left(\frac{\Gamma_y}{h_y^2} \{ [2Pe_y\alpha_y + 2]\Phi_P^{n+1} - [Pe_y(\alpha_y - 1) + 1]\Phi_N^{n+1} \} + Q^{n+1} \right) \\ &= -(1 - \theta) \left(\frac{\Gamma_x}{h_x^2} \{ -[Pe_x(\alpha_x + 1) + 1]\Phi_W^n + [2Pe_x\alpha_x + 2]\Phi_P^n \} \right) \\ &\quad - (1 - \theta) \left(\frac{\Gamma_x}{h_x^2} \{ -[Pe_x(\alpha_x - 1) + 1]\Phi_E^n \} \right) \\ &\quad - (1 - \theta) \left(\frac{\Gamma_y}{h_y^2} \{ -[Pe_y(\alpha_y + 1) + 1]\Phi_S^n \} \right) \\ &\quad - (1 - \theta) \left(\frac{\Gamma_y}{h_y^2} \{ [2Pe_y\alpha_y + 2]\Phi_P^n - [Pe_y(\alpha_y - 1) + 1]\Phi_N^n \} + Q^n \right), \end{aligned} \quad (3.13)$$

where $0 \leq \theta \leq 1$, for which there are some popular choices: $\theta = 0$, $\theta = 1/2$ and $\theta = 1$, associated with the explicit, Crank Nicholson and fully implicit scheme, respectively.

If use is made of the terminology defined above for steady-state terms such as a_s , b_s , c_s , f_s and g_s , a new analogous transient coefficient is defined (with the subscript t) and denoted b_t . Then, regardless of which value is specified for θ , equation (3.14) can be rewritten in the form:

$$\begin{aligned} a_s \theta \Phi_W^{n+1} &+ f_s \theta \Phi_S^{n+1} + (b_t + b_s \theta) \Phi_P^{n+1} + c_s \theta \Phi_E^{n+1} + g_s \theta \Phi_N^{n+1} \\ &= -d_i - a_s (1 - \theta) \Phi_W^n - f_s (1 - \theta) \Phi_S^n + (b_t - b_s (1 - \theta)) \Phi_P^n \\ &\quad - c_s (1 - \theta) \Phi_E^n - g_s (1 - \theta) \Phi_N^n, \end{aligned} \quad (3.14)$$

with the coefficients a_s and f_s , b_s , c_s and g_s given by equations (3.7) to (3.9), respectively and

$$b_t = \frac{1}{\Delta t}, \quad (3.15)$$

$$d_i = [\theta Q^{n+1} + (1 - \theta) Q^n]. \quad (3.16)$$

4. Example problems

4.1. Analytical Study

The problem solved in this section was proposed by SHEU et al. [7]. This problem was chosen to evaluate the described algorithm under conditions that lead to known analytical results. The problem consists in solving equation (2.1), where holds $0 \leq x \leq 1$; $0 \leq y \leq 1$; $\Gamma_x = \Gamma_y = \Gamma$; and the following boundary conditions:

$$\begin{aligned} x = 1 &\Rightarrow \Phi = 0, \\ y = 1 &\Rightarrow \Phi = 0, \\ x = 0 &\Rightarrow \Phi = \frac{1 - e^{(x-1)\frac{u}{\Gamma}}}{1 - e^{-\frac{u}{\Gamma}}}, \\ y = 0 &\Rightarrow \Phi = \frac{1 - e^{(y-1)\frac{v}{\Gamma}}}{1 - e^{-\frac{v}{\Gamma}}}. \end{aligned} \quad (4.1)$$

Here, the transport problem is uncoupled with the flow problem since the velocities u and v are assumed prescribed and constant all over the domain.

The problem consists in solving boundary value problem (2.1) and (4.1) under the diffusional scheme, previously described.

First, the L_2 error norms [6] were computed with different diffusive coefficients Γ , ranging from 1 to 10^{-5} . Equally spaced grids ranging from 11 to 41 nodes in each direction were also used, for the particular case where u and v equals unity. Results obtained for the L_2 norm under explicit formulation for the Diffusional scheme and those obtained by SHEU [7] for the characteristic Galerkin finite-element and Legendre-polynomial finite-element are summarised at Table 1.

Comparisons of the above results allow saying that the Diffusional scheme offered better results than the Legendre polynomial scheme, particularly for more diffusive problems. It is also clear that the presented formulation leads to inferior L_2 norm

h	$\Gamma = 1$		$\Gamma = 0.1$	
	Diffusional	Legendre	Diffusional	Legendre
0.1	9.153E-11	1.175E-09	8.434E-16	1.217E-09
0.05	1.202E-12	1.095E-09	4.945E-16	1.156E-09
0.025	1.449E-14	1.073E-09	7.055E-18	1.112E-09

h	$\Gamma = 0.01$		
	Diffusional	Legendre	Galerkin
0.1	8.182E-17	4.407E-06	1.125E-01
0.05	7.991E-17	5.885E-08	7.616E-02
0.025	5.866E-18	2.865E-10	5.483E-02

h	$\Gamma = 0.001$		$\Gamma = 0.0001$	
	Diffusional	Galerkin	Diffusional	Galerkin
0.1	8.316E-18	1.508E-02	1.284E-26	1.575E-04
0.05	4.206E-17	2.184E-03	4.432E-18	2.569E-07
0.025	4.132E-5	1.455E-04	8.259E-19	2.966E-12

Table 1: Compilation of results for Diffusional Method, Legendre Polynomials and Characteristic Galerkin.

errors than the characteristic Galerkin for predominantly convective problems. So, no matter what Peclet numbers we shall work with, the presented methodology showed better accuracy than those methods studied by the cited authors.

It is also important to say that, when diffusive coefficients are smaller than 10^{-3} , the increasing error with refining the meshes can be explained by the truncation errors. Despite this behaviour, the L_2 errors under this conditions are extremely small.

The profiles of φ for $y = 0.5$ are examined at Figure 2, for the case where $\Gamma = 10^{-5}$. As expected, the numerical solution converges to the analytic profile as the meshes are refined.

4.2. Skew Convection Problem

The second test problem was also proposed by SHEU et al. [7]. Here, we investigate the effectiveness of diffusional scheme under high gradient solution profile in the flow. The boundary conditions for this problem are summarised at Figure 3.

The profile of the dependent variable for $\Gamma = 10^{-5}$, $u = v = 1$ and $y = 0.5$ for various meshes are plotted in Figure 4. False diffusion effects are representative for the fine mesh of 160 spacing grids in each direction, as used by SHEU et al. [7], which under the Characteristic Galerkin Scheme, offered better results than the proposed scheme. For this last one, further meshes refinements are so justified. Comparisons between the profile under 320×320 and 640×640 spacing grids indicate that more refinements are necessary, since solution field has not converged.

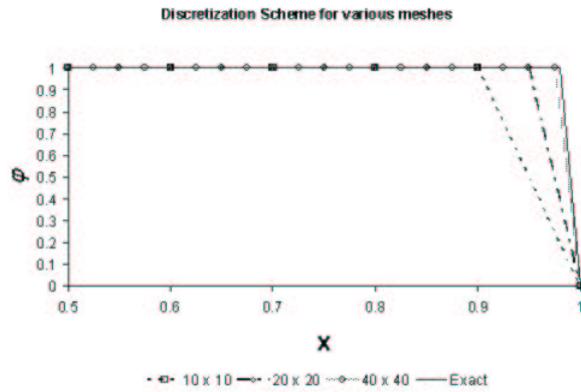


Figure 2: Computed solution at $y = 0.5$ for the analytical test, for the case of $\Gamma = 10^{-5}$.

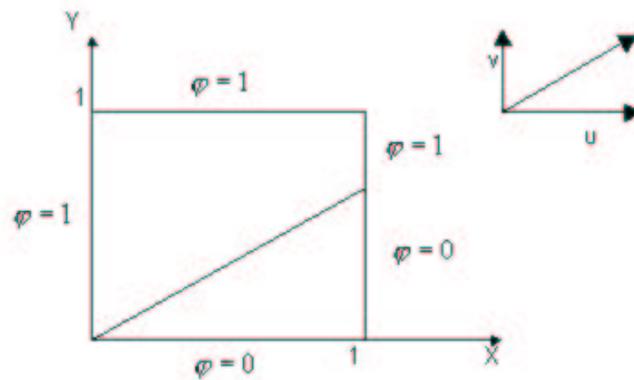


Figure 3: Illustration of the skew-convection diffusion problem.

The response is also plotted in Figure 5 for the case with $u = 0.5$, $v = 1$ and $\Gamma = 10^{-5}$. Here, as in the last case, false diffusion effects are present even for extremely refined mesh.

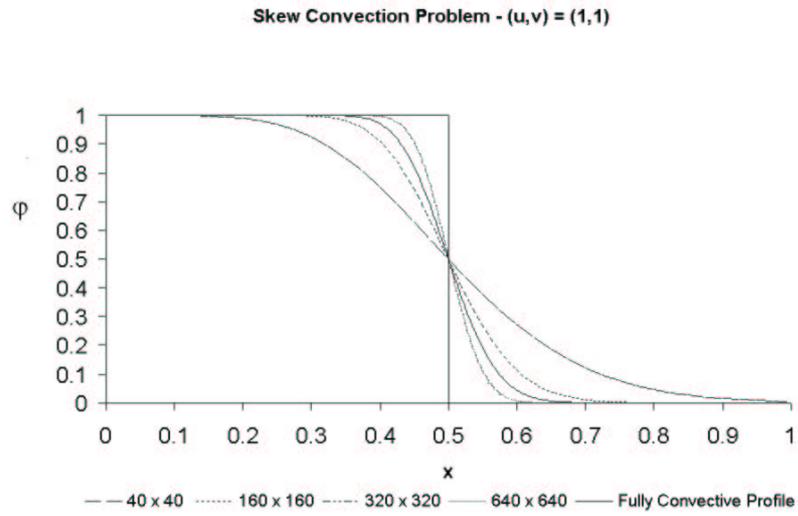


Figure 4: Profile of the dependent variable for $\Gamma = 10^{-5}$, $y = 0.5$ and $v, u = 1$.

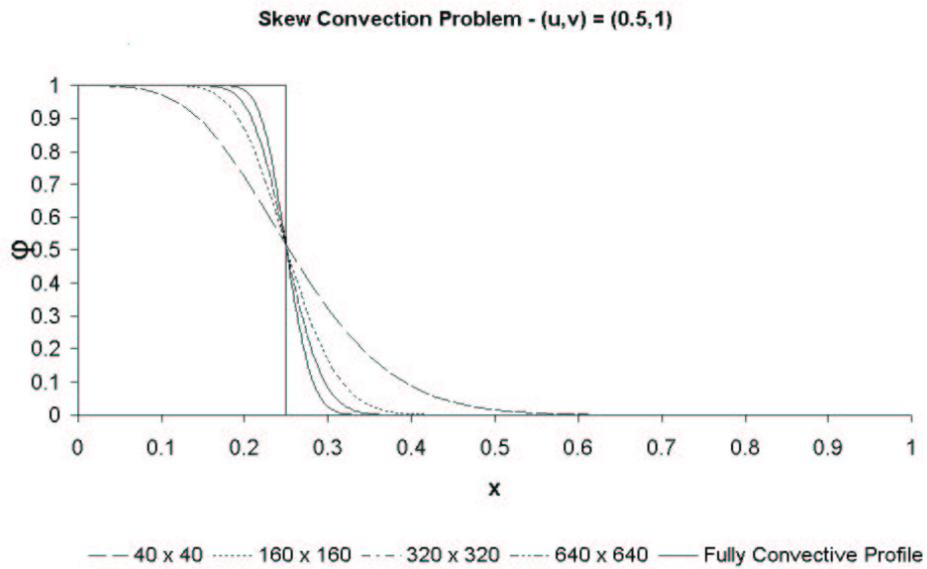


Figure 5: Profile of the dependent variable for $\Gamma = 10^{-5}$, $y = 0.5$, $u = 0.5$, $v = 1$.

5. Conclusions

The two-dimensional Diffusional method was presented to solve transport equations together with the FEM, FVM, FDM. Particularly, at the presented study, we used the diffusional method under the Finite Volume formulation.

An analytical test problem was solved by the proposed method together with the Finite Volume scheme and its performance, measured by the L_2 norm, was superior when compared to characteristic Galerkin finite-element method and also Legendre-polynomials finite-element method. In all Peclet range simulated, the diffusional method achieved superior accuracy.

A skew advection problem was also solved, and relevant false diffusion behaviour was observed. Fine meshes refinements upon to 640×640 spacing grids were made but false diffusion effects were still present, even though consistence prevailed. In this problem, the method presented worse results than the Characteristic Galerkin.

References

- [1] M. Fortes and W.R. Ferreira, Finite volume approach to transport equations by the diffusional method, in "Annals of the third SIMEC - Simpósio de Mecânica Computacional", 1, pp. 443-452, 1999.
- [2] M. Fortes and W.R. Ferreira, The one dimensional transient diffusional method: finite element solutions to convection-diffusion problems, *International Journal of Thermal Sciences*, **38** (1999), 780-796.
- [3] M. Fortes, The diffusional method for convection-diffusion equations: finite element one-dimensional solutions, *Numerical Methods in Thermal Problems*, **10** (1997), 57-68.
- [4] J.D. Hoffman, "Numerical Methods for Engineers and Scientists", McGraw-Hill, New York, 1992.
- [5] S.V. Patankar, "Numerical Heat Transfer and Fluid Flow", McGraw-Hill Book Co., NY, 1980.
- [6] J.N. Reddy, "An Introduction to the Finite Element Method", 2nd Edition, McGraw-Hill, 1993.
- [7] T.W.H. Sheu, S.F. Tsai, S.K. Wang, Monotonic, multidimensional flux discretization scheme for all Peclet numbers, *Numerical Heat Transfer*, **31** (1997), 441-457.
- [8] H.K. Versteeg and W. Malalasekera, "An Introduction to Computational Fluid Dynamics - The Finite Volume Method", Longman Scientific and Technical, 1995.
- [9] O.C. Zienkiewicz and R.L Taylor, "The Finite Element Method, Vol.2: Solid and Fluids Mechanics and Non-linearity", 4th ed., McGraw-Hill, London, 1991.