Analysis of Convection-Diffusion Problems at Various Peclet Numbers Using Finite Volume and Finite Difference Schemes

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Abstract

Convection-diffusion problems arise frequently in many areas of applied sciences and engineering. In this paper, we solve a convection-diffusion problem by central differencing scheme, upwinding differencing scheme (which are special cases of finite volume scheme) and finite difference scheme at various Peclet numbers. It is observed that when central differencing scheme is applied, the solution changes rapidly at high Peclet number because when velocity is large, the flow term becomes large, and the convection term dominates. Similarly, when velocity is low, the diffusion term dominates and the solution diverges, *i.e.*, mathematically the system does not satisfy the criteria of consistency. On applying upwinding differencing scheme, we conclude that the criteria of consistency is satisfied because in this scheme the flow direction is also considered. To support our study, a test example is taken and comparison of the numerical solutions with the analytical solutions is done.

Keywords: Finite volume method, Partial differential equation

1. Introduction

Mathematical models of physical [2, 7], chemical, biological and environmental phenomena are governed by various forms of differential equations. The partial differential equations describing the transport phenomena in fluid dynamics are difficult to solve, particularly, due to the convection terms. Such equations represent the hyperbolic conservation law for which their solutions always contain discontinuity and high gradient. Thus accurate numerical solutions are very difficult to obtain. Special treatment must be applied to suppress spurious oscillations of the computed solutions for both the convection and convection-dominated problems. In the present scenario, better ways to approximate the convection term are still needed, and thus development of accurate numerical modeling for the convection-diffusion equations remains a challenging task in computational fluid dynamics. In recent years (see [7]), with the rapid development of energy resources and environmental science, it is very important to study the numerical computation of underground fluid flow and the history of its changes under heat. In actual numerical simulation, the nonlinear three-dimensional convection-dominated diffusion problems need to be considered.

When velocity is higher, that is, flow term is larger, a simple convection-diffusion problem is converted to convection-dominated diffusion problem because Peclet number is greater than two. A Peclet number is a dimensionless number relevant in the study of transport phenomena in fluid flows. It is defined to be the ratio of the rate of advection of a physical quantity by the flow to the rate of diffusion of the same quantity driven by an appropriate gradient. In the context of the transport of heat, Peclet number is equivalent to the product of Reynolds number and Prandtl number. In the context of species or mass dispersion, Peclet number is the product of Reynolds number and Schmidt number. For diffusion of heat (thermal diffusion), Peclet number is defined as $P_e = \frac{F}{D}$, where F is the flow term and D is the diffusion term.

In most of the problems with engineering applications (see [4]), Peclet number is often very large. In such situations, the dependency of the flow upon downstream locations is diminished and variables in the flow tend to become 'one-way' properties. Thus, when modeling certain situations with high Peclet numbers, simpler computational models can be adopted. A flow can often have different Peclet numbers for heat and mass. This can lead to the phenomenon of double diffusive convection. In the context of particulate motion, Peclet numbers are also called Brenner numbers, with symbol B_r, in honors of Howard Brenner.

2. Discretization Algorithms Using Central Differencing Scheme and Upwinding Differencing Scheme

The general transport equation for any fluid property is given by

$$\frac{\partial(\rho\varphi)}{\partial t} + div(\rho\varphi u) = div(\Gamma grad\varphi) + S\varphi, \qquad (1)$$

where φ is a general property of fluid, ρ is the density and u is the velocity of the fluid. In equation (1), the rate of change term and the convective term are on the left hand side and the diffusive term (Γ is the diffusion coefficient) and the source term *S* respectively are on the right hand side. In problems, where fluid flow plays a significant role [1], we must account for the effects of convection. In nature, diffusion always occurs alongside convection, so here we examine a method to predict combined convection and diffusion. The steady convection-diffusion equation can be derived from transport equation (1) for a general property by deleting transient term:

$$div(\rho u\Phi) = div(\Gamma grad\Phi) + s_\Phi \qquad (2)$$

Formal integration over control volume gives

$$\int_A n.(\rho u\Phi)dA = \int_A n(\Gamma grad\Phi)dA + \int_{CV} S_\Phi dV.$$

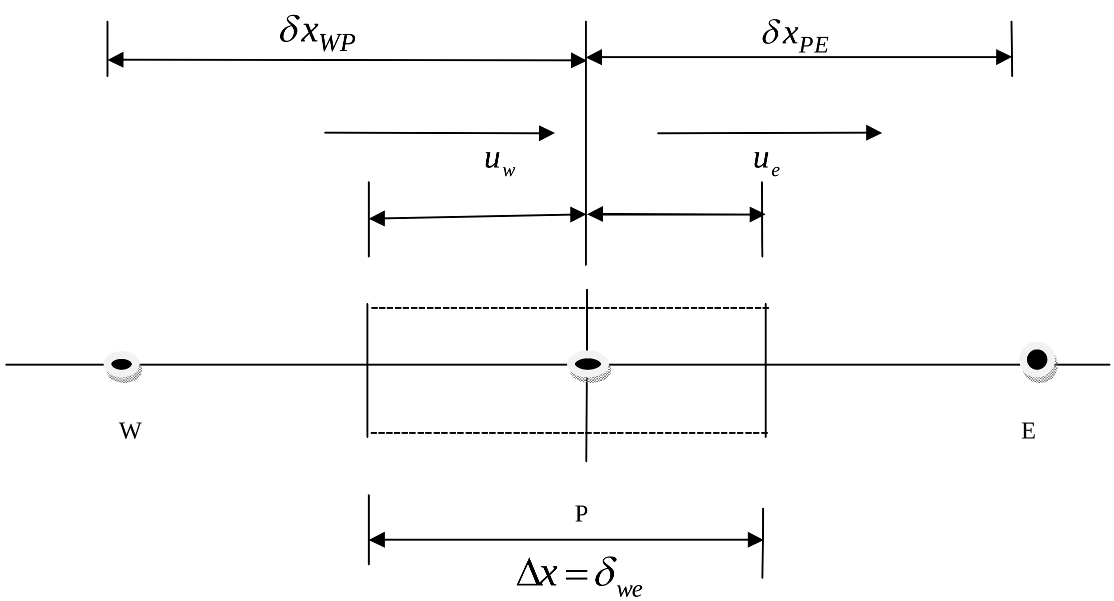

Figure 1: P is a general point around which discussions takes place, W and E are west and east nodal points respectively

In the absence of sources (see [5]), the steady convection and diffusion of a property in a given one dimensional flow field u is governed by:

$$\frac{d}{dx}(\rho u\Phi)=\frac{d}{dx}\left(\Gamma\frac{d\Phi}{dx}\right), \tag{3}$$

and continuity equation becomes $\frac{d(\rho u)}{dx}=0.$ Integrating equation (3), we have

$$(\rho uA\Phi)_e-(\rho uA\Phi)_w=\left(\Gamma A\frac{\partial\Phi}{\partial x}\right)_e-\left(\Gamma A\frac{\partial\Phi}{\partial x}\right)_w, \tag{4}$$

and continuity equation becomes $(\rho uA)_e-(\rho uA)_w=0.$

To obtain discretized equation, we shall take some assumptions:

Let $F=\rho u$ represent convective mass flux per unit area and $D=\frac{\Gamma}{\delta x}$ represent diffusion conductance. Now we are taking $A_w=A_e=A$ and applying the central differencing, the integrated convection-diffusion becomes. Here u represents velocity of fluid.

$$F_e\Phi_e-F_w\Phi_w=D_e(\Phi_E-\Phi_P)-D_w(\Phi_P-\Phi_W), \tag{5}$$

and continuity equation becomes

$$F_e-F_w=0. \tag{6}$$

Central Differencing Scheme

The central differencing approximation has been used to discretize the diffusion which appears in equation (5).

So $\Phi_e=(\Phi_P+\Phi_E)/2;\ \Phi_w=(\Phi_W+\Phi_P)/2.$

Putting these values in equation (5), we get

$$\begin{gathered}\frac{F_e}{2}(\Phi_P+\Phi_E)-\frac{F_e}{2}(\Phi_W+\Phi_P)=D_e(\Phi_E-\Phi_P)-D_w(\Phi_P-\Phi_W)\\ \left[\left(D_w-\frac{F_w}{2}\right)+\left(D_e-\frac{F_e}{2}\right)\right]\Phi_P=\left(D_w+\frac{F_w}{2}\right)\Phi_W+\left(D_e-\frac{F_e}{2}\right)\Phi_E\\ \left[\left(D_w+\frac{F_w}{2}\right)+\left(D_e-\frac{F_e}{2}\right)+(F_e-F_w)\right]\Phi_P=\left(D_w+\frac{F_w}{2}\right)\Phi_W+\left(D_e-\frac{F_e}{2}\right)\Phi_E\end{gathered} \tag{7}$$

Equation (7) can be written as

$$a_P\Phi_P=a_W\Phi_W+a_E\Phi_E, \tag{8}$$

where a_P, a_W and a_E are coefficients of Φ_P, Φ_W and Φ_E respectively.

3. Test Example

Example 1: The general property of a fluid Φ is transported by means of convection and diffusion through the one dimensional domain. The governing equation is given below. The boundary conditions are $\Phi_0 = 1$ at *x*=0 and $\Phi_L = 0$ at *x*=*L*. Using five equally spaced cells and the central differencing scheme for convection-diffusion problems, we calculate the distribution of Φ as a function of *x* for the following cases: **Case (1):** *u*=0.1 *m/s*,**Case (2):** *u*=2.5 *m/s.*

The following data are applying to obtain the solution of above problem by central differencing scheme.

$\rho = 1.0 kg / m^3$, $\Gamma = 0.1 kg / m / s$, Length L=1.0 m,

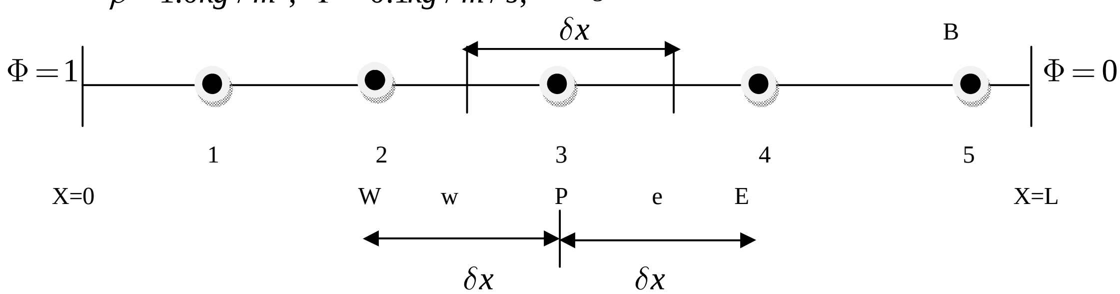

Figure 2: Discretization using five nodal points for Example (1)

Now we solve the problem by central differencing scheme and upwind differencing scheme for both the cases. Then we compare these results by finite difference method and observe the effect of schemes on the convergence rate of solution.

Solution of Example (1) by Central Differencing Scheme

Node	Distance	Finite volume solution	Analytical solution	Difference	Percentage error
1	0.1	0.9421	0.9387	-0.003	-0.36
2	0.2	0.8006	0.7963	-0.004	-0.53
3	0.3	0.6276	0.6224	-0.005	-0.83
4	0.4	0.4163	0.4100	-0.006	-1.53
5	0.5	0.1579	0.1505	-0.007	-4.91

Table 1: The solution of problem by central differencing scheme for *u*=0.1

Node	Distance	Finite volume Solution	Analytical solution	Difference	Percentage error
1	0.1	1.0356	1.0000	-0.0035	-3.56
2	0.2	0.8694	0.9999	0.131	13.03
3	0.3	1.2573	0.9999	-0.257	-25.74
4	0.4	0.3521	0.9994	0.647	64.70
5	0.5	2.4644	0.9179	-1.546	-168.48

Table2: The solution of problem by central differencing scheme for u=2.5

Solution of Problem by Upwind Differencing Scheme

One of the major inadequacies of the central differencing scheme is its inability to identify the flow direction. The value of property Φ at west cell face is always influenced by both Φ_P and Φ_W in central differencing. In a strongly convective flow from west to east, the above treatment is not suitable because the west cell face should receive much stronger influencing from node W than from node P. The upwind differencing and donor cell differencing schemes takes into account the flow direction when determining the value at cell face: the convicted value of Φ at a cell face is taken to be equal to the value at upstream node. We show the nodal values used to calculate cell face values when the flow is in the positive direction in Figure 2 those for the negative direction.

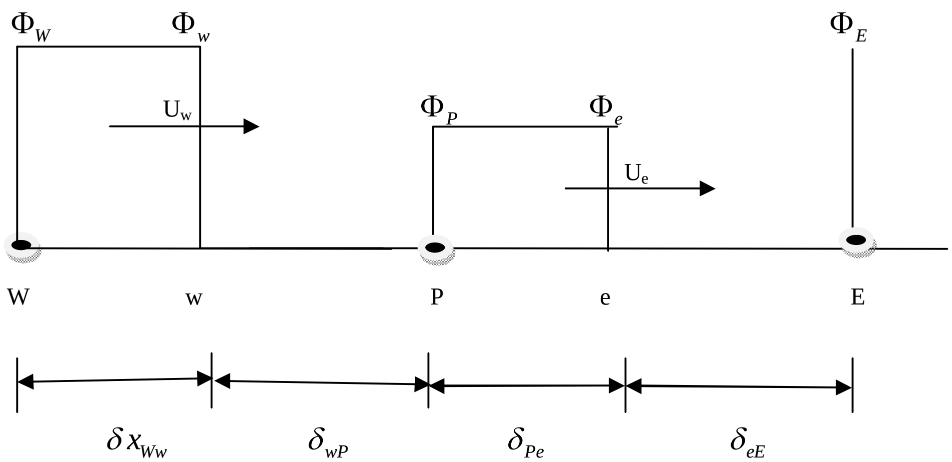

Figure 3: Discretization technique for upwinding differencing scheme

When the flow is in positive direction, $u_w > 0, u_e > 0 (F_w > 0, F_e > 0)$, the upwind schemes sets

$$\Phi_w = \Phi_W \ and \ \Phi_e = \Phi_P. \tag{8}$$

And the discretized equation (5) becomes $F_e\Phi_P - F_w\Phi_W = D_e(\Phi_E - \Phi_P) - D_w(\Phi_P - \Phi_W)$.

This may be written as

$$\left(D_w + D_e + F_e\right)\Phi_P = \left(D_w + F_w\right)\Phi_W + D_e\Phi_E,$$

which gives

$$[\left(D_w + F_w\right) + D_e + (F_e - F_w)]\Phi_P = \left(D_w + F_w\right)\Phi_W + D_e\Phi_E \tag{9}$$

When flow is in the negative direction, $u_w<0$, $u_e<0$ ($F_w <0$, $F_e<0$),

$$\Phi_w = \Phi_P \ \ and \ \ \Phi_e = \Phi_E$$

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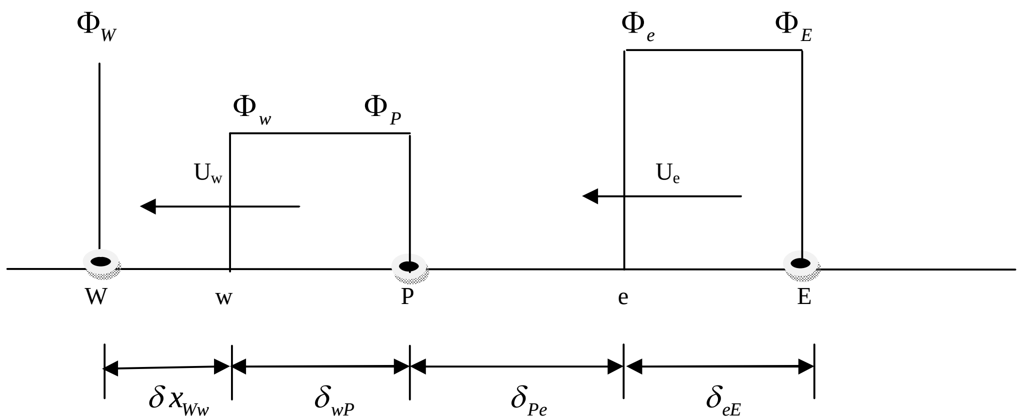

Figure 4: Discretization Technique for Upwinding Differencing Scheme for Example (1)

Now the discretized equation is

$$F_e\Phi_E - F_w\Phi_P = D_e(\Phi_E - \Phi_P) - D_w(\Phi_P - \Phi_W)$$

Or $[D_w + (D_e - F_e) + (F_e - F_w)]\Phi_P = D_w\Phi_W + (D_e - F_e)\Phi_e$ (10)

Identifying coefficients of Φ_W and Φ_E as a_w and a_E, the Equations (9) and (10) can be written in the general form as

$$a_P\Phi_P = a_W\Phi_W + a_E\Phi_E, \tag{11}$$

with central coefficients $a_P = a_W + a_E + (F_e - F_w)$.

The grid shown in above figure is used for discretization. The discretization equation at internal nodes 2,3 and 4 and relevant neighbor coefficient are given by (11). Note that in this example

$F = F_e = F_w = \rho u \ and \ D = D_e = D_w = \dfrac{\Gamma}{\delta x}$ everywhere.

At the boundary node (1), the use of upwind differencing scheme for the convective terms gives

$$F_e\Phi_P - F_A\Phi_A = D_e(\Phi_E - \Phi_P) - D_A(\Phi_P - \Phi_A),$$

and at node (5),

$$F_B\Phi_P - F_w\Phi_W = D_B(\Phi_B - \Phi_P) - D_w(\Phi_P - \Phi_W).$$

At the boundary nodes we have $D_A = D_B = \dfrac{2\Gamma}{\delta x} = 2D \ and \ F_A = F_B = F$ and as usual boundary condition enter the discretized equation as source contribution: $a_P\Phi_P = a_W\Phi_W + a_E\Phi_E + S_u$ with $a_P = a_W + a_E + (F_e - F_w) - S_P$.

Node	a_W	a_E	S_P	S_u
1	*0*	*D*	*-(2D+F)*	$(2D+F)\Phi_A$
2,3,4	*D+F*	*D*	*0*	*0*
5	*D+F*	*0*	*-2D*	$2D\Phi_B$

Table 3: Determination of coefficients aw, aE, Sp and Su

Node	a_W	a_E	S_P	S_u	a_P
1	0	0.5	-1.1	1.1	1.6
2,3,4	0.6	0.5	0	0	1.6
5	0.6	0	-1	0	1.6

Table 4: Determination of coefficients aw, aE, Sp, Su and aP for U=0.1 m/s

Case 1: U=0.1 m/s: $F=\rho u=0.1, D=\dfrac{\Gamma}{\delta x}=0.1/0.2=0.5\ so\ P_e=\dfrac{F}{D}=0.2$ where P_e is known as Peclet number. The coefficients are given in Table 4.

$$\begin{aligned}1.6\Phi_1&=0.5\Phi_2+1.1\\1.1\Phi_2&=0.6\Phi_1+0.5\Phi_3\\1.1\Phi_3&=0.6\Phi_2+0.5\Phi_4\\1.1\Phi_4&=0.6\Phi_3+0.5\Phi_5\\1.6\Phi_5&=0.6\Phi_4+1.6\end{aligned}$$ or, $$\begin{bmatrix}1.6000 & -0.5000 & 0 & 0 & 0\\ -0.6000 & 1.1000 & -0.5000 & 0 & 0\\ 0 & -0.6000 & 1.1000 & -0.5000 & 0\\ 0 & 0 & -0.6000 & 1.1000 & -0.5000\\ 0 & 0 & 0 & -0.6000 & 1.6000\end{bmatrix}\begin{bmatrix}\Phi_1\\\Phi_2\\\Phi_3\\\Phi_4\\\Phi_5\end{bmatrix}=\begin{bmatrix}1.1000\\0\\0\\0\\0\end{bmatrix}$$, or, $$\begin{bmatrix}\Phi_1\\\Phi_2\\\Phi_3\\\Phi_4\\\Phi_5\end{bmatrix}=\begin{bmatrix}0.9337\\0.7879\\0.6130\\0.4031\\0.1512\end{bmatrix}$$

Node	**Distance**	**Upwind solution**	**Analytical solution**	**Central Differencing solution**	**Finite difference solution**
1	0.1	0.9337	0.9387	0.9421	0.9048
2	0.2	0.7879	0.7963	0.8006	0.7884
3	0.3	0.6130	0.6224	0.6276	0.6461
4	0.4	0.4031	0.4100	0.4163	0.4722
5	0.5	0.1512	0.1505	0.1579	0.2597

Table 4: Comparison for various results for U=0.1 m/s

Case 2: U=2.5 m/s: $F=\rho u=2.5, D=\dfrac{\Gamma}{\delta x}=0.1/0.2=0.5\ so\ P_e=\dfrac{F}{D}=5$ where $P_e>2$. Due to this reason upwinding differencing scheme provide better convergence. In this case, the coefficients are given below:

Node	$\mathbf{a_W}$	$\mathbf{a_E}$	$\mathbf{S_P}$	$\mathbf{S_u}$	$\mathbf{a_P}$
1	0	0.5	-3.5	3.5	4.0
2,3,4	3.0	0.5	0	0	3.5
5	3.0	0	-1.0	0	4.0

Table 7: Determination of coefficients aw, aE, Sp, Su and aP for U=2.5 m/s

$$\begin{aligned} 4\Phi_1 &= 0.5\Phi_2 + 3.5 \\ 3.5\Phi_2 &= 3\Phi_1 + 0.5\Phi_3 \\ 3.5\Phi_3 &= 3\Phi_2 + 0.5\Phi_4 \\ 3.5\Phi_4 &= 3\Phi_3 + 0.5\Phi_5 \\ 4\Phi_5 &= 3\Phi_4 \end{aligned}, \text{ or } \begin{bmatrix} 4.0000 & -0.5000 & 0 & 0 & 0 \\ -3.0000 & 3.5000 & -0.5000 & 0 & 0 \\ 0 & -3.0000 & 3.5000 & -0.5000 & 0 \\ 0 & 0 & -3.0000 & 3.5000 & -0.5000 \\ 0 & 0 & 0 & -3.0000 & 4.0000 \end{bmatrix} \begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \Phi_4 \\ \Phi_5 \end{bmatrix} = \begin{bmatrix} 3.5000 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \text{ or } \begin{bmatrix} \Phi_1 \\ \Phi_2 \\ \Phi_3 \\ \Phi_4 \\ \Phi_5 \end{bmatrix} = \begin{bmatrix} 0.9998 \\ 0.9987 \\ 0.9921 \\ 0.9524 \\ 0.7143 \end{bmatrix}$$

Node	Distance	Upwinding solution	Central Differencing Solution	Analytical solution	Finite difference solution
1	0.1	0.9998	1.0356	1.0000	1.0208
2	0.2	0.9987	0.8694	0.9999	0.9723
3	0.3	0.9921	1.2573	0.9999	1.0854
4	0.4	0.9524	0.3521	0.9994	0.8214
5	0.5	0.7143	2.4644	0.9179	1.4375

Table 8: Comparison for various results for U=2.5 m/s

4. Discretization Algorithm for Finite Difference Method

For solving any given boundary value problems, we can divide the range $[x_0, x_n]$ in to *n* equal subintervals of width h so that $x_i = x_0 + ih$, i=1, 2… *n*. The finite difference approximations of derivatives of any fluid property Φ at $x = x_i$ are given by

$$\Phi'_i = \frac{\Phi_{i+1} - \Phi_{i-1}}{2h} + O(h^2) \qquad \text{and} \qquad \Phi''_i = \frac{\Phi_{i-1} - 2\Phi_i + \Phi_{i-1}}{h^2} + o(h^2)$$

On the basis of above discussion, we now solve the given convection dominated diffusion problem in Example (1) by finite difference method for equal spacing.

Case1: **U=0.1**

Node	Distance	Finite volume Solution	Analytical solution	Finite difference solution
1	0.1	0.9421	0.9387	0.9048
2	0.2	0.8006	0.7963	0.7884
3	0.3	0.6276	0.6224	0.6461
4	0.4	0.4163	0.4100	0.4722
5	0.5	0.1579	0.1505	0.2597

Table 9: Comparison for various results for U=0.1 m/s

Case2: U=2.5

Node	Distance	Finite volume Solution	Analytical solution	Finite difference solution
1	0.1	1.0356	1.0000	1.0208
2	0.2	0.8694	0.9999	0.9723
3	0.3	1.2573	0.9999	1.0854
4	0.4	0.3521	0.9994	0.8214
5	0.5	2.4644	0.9179	1.4375

Table 10: Comparison for various results for U=2.5 m/s

5. Graphical Representation of Convergence for Example (1)

The graphical result of Table 9 and Table 10 are shown in fig. 5 which describes convergence criteria for various methods

Case 1: *U* = 0.1

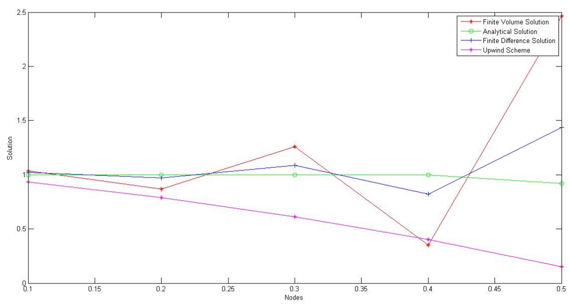

Figure 5: Convergence criteria for various methods for U=0.1

Case2: *U* = 2.5

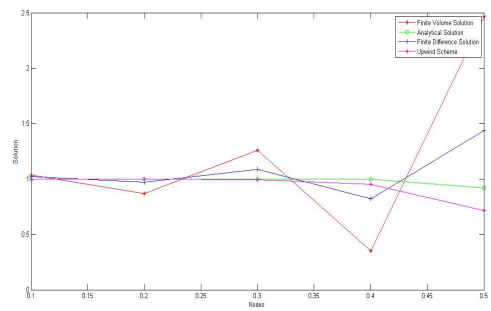

Figure 6: Convergence criteria for various methods for U=2.5

6. Concluding Remark

When U=2.5, we observe that result show better convergence since $a_E = D_e - \frac{F_e}{2}$ and the convective contribution to the east coefficient is negative. Thus, the solution converges faster towards the exact solution for large Peclet number. If the convection dominates, a_E can be negative. Given that $F_w > 0$ and $F_e > 0$ (*i.e.,* flow is unidirectional), for a_E to be positive D_e and F_e must satisfy the condition: $\frac{F_e}{D_e} = p_e < 2.$ If P_e is greater than 2 the east coefficient will be negative. This violates one of the requirements for boundedness and may lead to physically impossible solution.

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