ME 7310 – Project 3
Finite Volume
Convection-Diffusion Equation

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Abstract

In this project five different finite volume schemes are used to discretize the governing equation for the steady-state convection-diffusion ordinary differential equation (ODE). The schemes implemented were Central Differencing, Upwind, Hybrid Upwind and Central Differencing, Power-law, and the Quadratic Upstream Interpolation for Convective Kinematics (QUICK).

To verify the accuracy of the numerical scheme developed, a mesh refinement study is conducted for the Central Differencing scheme. In order to validate the solution, the results obtained from the finite volume schemes are compared to those obtained from the analytical solution.

1 Problem Definition

In this project the one-dimensional, steady-state, convection-diffusion equation for laminar incompressible flow is solved. The governing form is:

$$\frac{d}{dx}(\rho u \varphi) = \frac{d}{dx}\left(\Gamma \frac{d\varphi}{dx}\right) \tag{1}$$

where Γ = 0.1*kg/m-s*, u = 2.5 *m/s*, ρ = 1 *kg/m*^{3}, and L = 1 *m*. The boundary conditions are given as: $\varphi_0 = 1$ at $x = 0$ and $\varphi_L = 0$ at $x = L$.

For the boundary conditions above, the analytical solution is obtained as:

$$\frac{\varphi - \varphi_0}{\varphi_L - \varphi_0} = \frac{exp(\rho u x/\Gamma) - 1}{exp(\rho u L/\Gamma) - 1} \tag{2}$$

2 Numerical Solution Procedure

Numerical solutions of the governing ODE were obtained using five different finite volume schemes. The general form of the finite volume equation (FVE) for Equation (1) can be expressed as:

$$\rho_e u_e \varphi_e - \rho_w u_w \varphi_w = \frac{\Gamma_e}{\Delta x_{PE}}(\varphi_E - \varphi_P) - \frac{\Gamma_w}{\Delta x_{PW}}(\varphi_P - \varphi_W) \quad (3)$$

where the lower case subscripts ‘e’ and ‘w’ denote properties at the east and west faces of the 1-D finite volume cell in Figure 1 below, and ‘E’, ‘P’, and ‘W’ represent properties at the east, central, and west nodes.

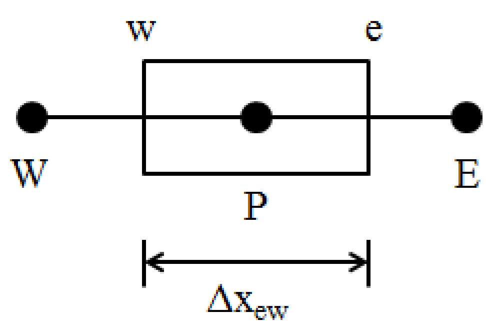

Figure 1: 1-D Finite Volume Cell

To simplify the formulation of specific finite volume schemes, constants can be combined into single expressions. The constant $\rho_e u_e$ can be replaced with F_e, the constant $\rho_w u_w$ can be replaced with F_w, the term $\frac{\Gamma_e}{\Delta x_{PE}}$ can be replaced with D_e and the term $\frac{\Gamma_w}{\Delta x_{PW}}$ can be replaced with D_w.

The first finite volume scheme investigated was the Central Differencing scheme, which utilizes a central difference approximation for the properties at the cell faces [1].

$$\varphi_e = \frac{\varphi_P + \varphi_E}{2} + O(\Delta x^2) \quad (4)$$

$$\varphi_w = \frac{\varphi_P + \varphi_W}{2} + O(\Delta x^2) \quad (5)$$

Substituting the second order accurate approximations for the properties at the faces from Equations (4) and (5), along with F_e, F_w, D_e, and D_w, from above into Equation (3), the FVE for the Central Differencing scheme takes the form:

$$\frac{F_e}{2}(\varphi_P + \varphi_E) - \frac{F_w}{2}(\varphi_P + \varphi_W) = D_e(\varphi_E - \varphi_P) - D_w(\varphi_P - \varphi_W) \quad (6)$$

Equation (6) can be further simplified into the following form by rearranging the properties at the nodes and faces. The simplified form of Equation (6) is expressed as:

$$a_P\varphi_P = a_E\varphi_E + a_W\varphi_W \tag{7}$$

where the coefficients are:

$$a_W = D_w + \frac{F_w}{2} \tag{8}$$

$$a_E = D_e - \frac{F_e}{2} \geq 0 \tag{9}$$

$$a_P = a_E + a_W \tag{10}$$

It should be noted from Equation (9) that the coefficient for the east node must be greater than or equal to zero. The central differencing scheme is second order accurate.

The second finite volume scheme investigated was the Upwind scheme. For the conditions $u_e > 0$, and $u_w > 0$ which are satisfied for the problem investigated (u = 2.5 *m/s*), the coefficients for the simplified Equation (7) applied to the Upwind scheme are:

$$a_W = D_w + F_W \tag{11}$$

$$a_E = D_e \tag{12}$$

Unlike the Central Differencing scheme, the Upwind scheme is first order accurate, $O(\Delta x^2)$.

The third scheme investigated was a Hybrid Upwind and Central Differencing Scheme. For the Peclet Number defined as:

$$Pe = \frac{F}{D} \tag{13}$$

a central differencing scheme, $O(\Delta x^2)$, is utilized for $Pe<2$, and an upwind scheme is utilized for $Pe>2$, $O(\Delta x)$. The coefficients for the FVE of the Hybrid scheme are:

$$a_W = \max[F_{w,} \left(D_w + \frac{F_w}{2}\right), 0] \tag{14}$$

$$a_E = \max[-F_{E,} \left(D_e - \frac{F_e}{2}\right), 0] \tag{15}$$

As with the Upwind scheme, the Hybrid scheme is only first order accurate, $O(\Delta x)$.

The fourth finite volume scheme implemented was the Power-law. The coefficients for the west and east nodes of the FVE for the Power-law are:

$$a_W = D_w \max[0, (1 - 0.1|Pe_w|)^5] + max[F_{w,0}] \tag{16}$$

$$a_E = D_e \max[0, (1 - 0.1|Pe_e|)^5] + max[-F_{e,0}] \tag{17}$$

The Power-law is a very accurate scheme, but due to the exponents, the scheme is numerically expensive.

The final scheme investigated was the Quadratic Upstream Interpolation for Convective Kinetics (QUICK). This higher order-scheme for interpolation implements a parabolic fit through two grid points upstream of the *e* face, and one downstream [1]. This scheme is third order accurate. The additional upstream and downstream nodes are denoted with subscripts *EE* and *WW* respectively. From the parabolic fit, and the condition that u>0, the resulting values of the properties φ at the west and east faces are given as:

$$u_w > 0: \varphi_w = \frac{6}{8}\varphi_W + \frac{3}{8}\varphi_P - \frac{1}{8}\varphi_{WW} \tag{18}$$

$$u_e > 0: \varphi_E = \frac{6}{8}\varphi_P + \frac{3}{8}\varphi_E - \frac{1}{8}\varphi_W \tag{19}$$

The form of the FVE for the QUICK Scheme is:

$$a_P\varphi_P = a_E\varphi_E + a_W\varphi_{W+}a_{EE}\varphi_{EE} + a_{WW}\varphi_{WW} \tag{20}$$

Because of the additional nodes implemented in the Finite Volume (FV) scheme, Equation (20) will yield a five band matrix, unlike the previous schemes which are all tri-diagonal matrices. The coefficients for QUICK are:

$$a_W = D_w + \frac{6}{8}\alpha_w F_w - \frac{1}{8}\alpha_e F_e + \frac{3}{8}(1 - \alpha_w)F_w \tag{21}$$

$$a_{WW} = -\frac{1}{8}\alpha_w F_w \tag{22}$$

$$a_E = D_e - \frac{3}{8}\alpha_e F_e - \frac{6}{8}(1 - \alpha_e)F_e - \frac{1}{8}(1 - \alpha_w)F_w \tag{23}$$

$$a_{EE} = \frac{1}{8}(1 - \alpha_e)F_e \tag{24}$$

where α is subject to the following conditions:

$$\begin{cases} \alpha_w = 1 : \ F_w > 0 \ ; \ \alpha_e = 1 : \ F_e > 0 \\ \alpha_e = 0 : \ F_w < 0 \ ; \ \alpha_e = 0 : \ F_e < 0 \end{cases} \tag{25}$$

For purposes of verification, a grid refinement study was performed by decreasing step size (cell size) in the *x* dimension. Three different grid sizes were implemented and compared with results from the analytical solution.

Validation of the FV schemes was obtained by comparing results from the five different FV schemes with those obtained from the analytical solution.

3 Numerical Results

In order to verify the Central Differencing FV scheme, the grid refinement study given in Table 3-1 was implemented. As can be seen in Figure 3-1, as the grid is refined, the solution obtained from the FV scheme closely approximates the analytical solution. This is to be expected for the second order accurate Central Differencing scheme.

Table 3-1: Grid refinement study for the Central Differencing scheme

Grid Number	Number of Cells	Step Size Δx [m]
1	20	0.05
2	40	0.025
3	80	0.0125

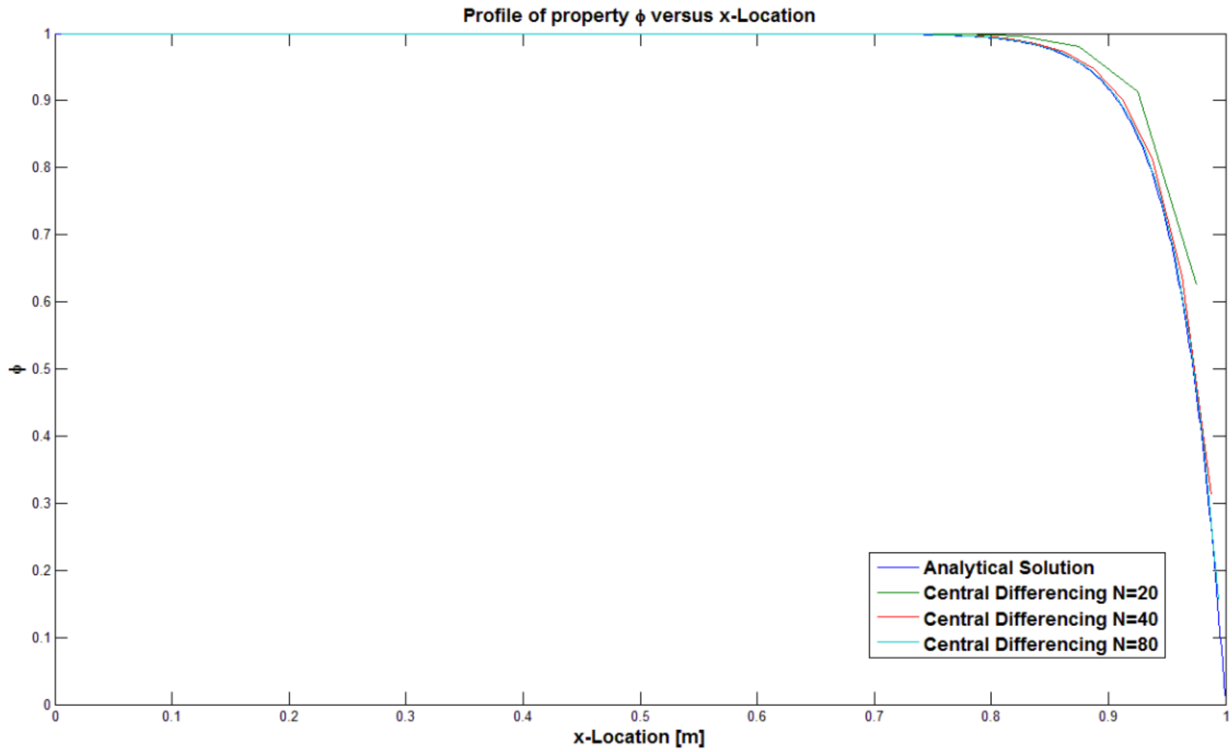

Figure 3-1: Grid refinement study for the Central Differencing scheme

To validate the numerical schemes, two different grids were implemented. The first grid implemented was $\Delta x = 0.2$ m (5 cells). Results are plotted in Figure 3-2 below.

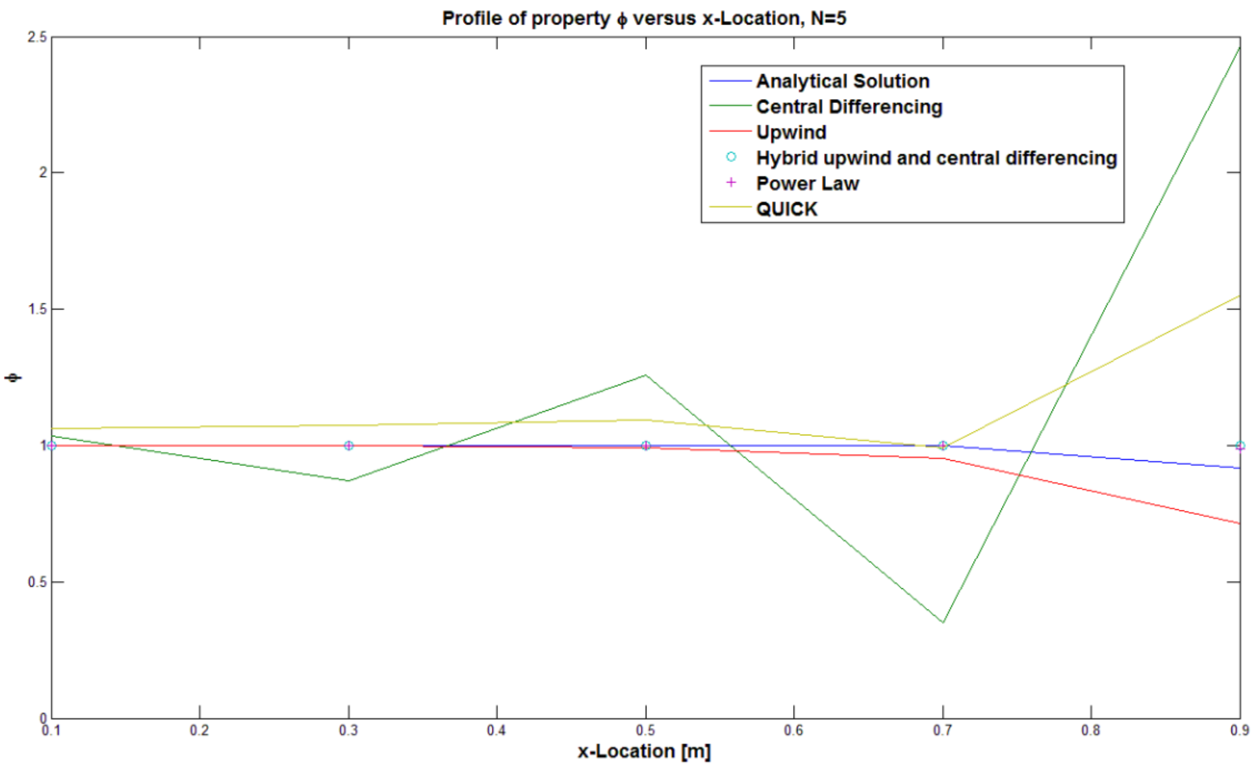

Figure 3-2: Profile of property ϕ versus x-Location for N=5

It is interesting to note that the first order accurate Upwind and Hybrid schemes more closely approximate the analytical solution than the second order central differencing scheme, and the third order QUICK scheme. Another interesting result is the fact that the Central Differencing scheme seems to "blow up" and start oscillating. This behavior is expected due to the violation of the criteria that the coefficient of the east node must be greater than or equal to zero (from Equation (9)). For the 5 cell grid, the coefficient of the east node is actually -0.75. Likewise, for the QUICK scheme, the coefficient of the east node is also negative, which could be causing the similar oscillatory behavior to that of the Central Differencing Scheme. The most accurate approximation of the analytical solution is the one obtained from the Power-law scheme.

The second grid implemented was $\Delta x = 0.05$ m (20 cells). Results are plotted in Figure 3-3.

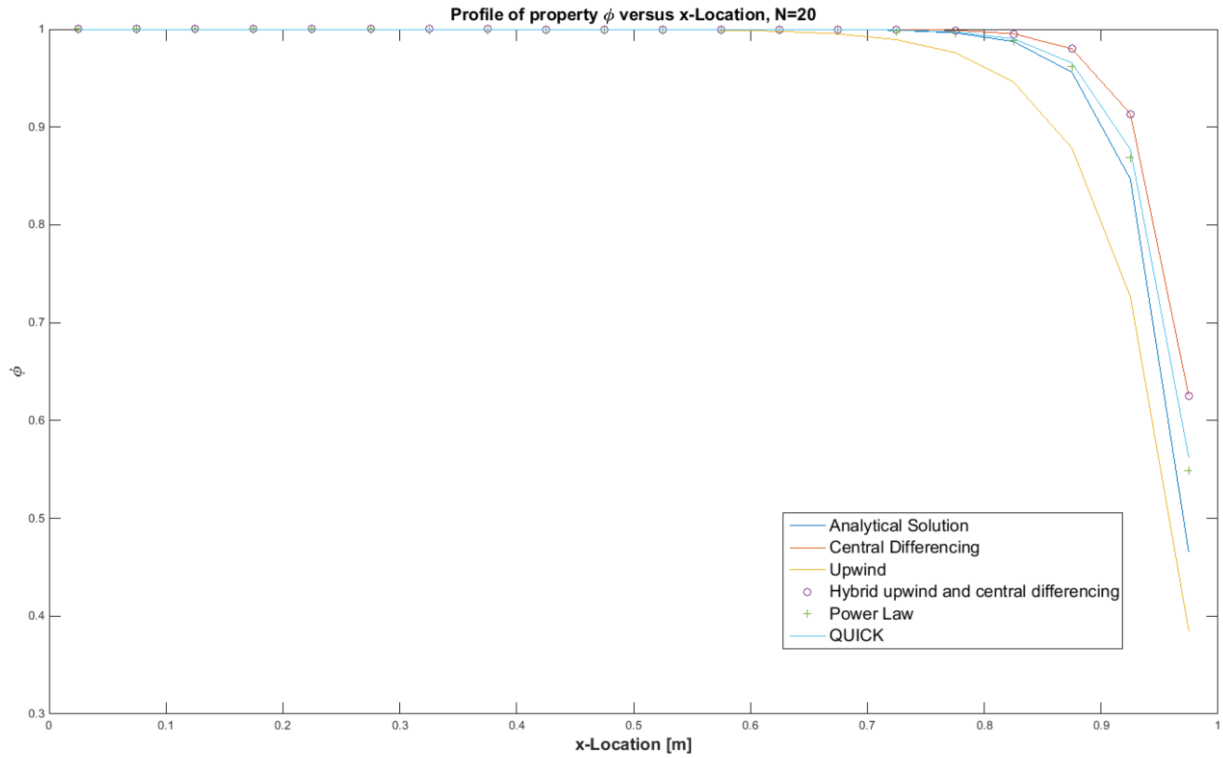

Figure 3-3: Profile of property ϕ versus x-Location for N=20

When the finer grid is implemented (N=20), the second order accurate Central Differencing scheme more closely approximates the analytical solution than the first order accurate upwind scheme, and it exactly matches that of the Hybrid scheme, which becomes second order accurate for Peclet Numbers less than 2. The third order accurate QUICK scheme seems to more accurately approximate the sharp gradient than it did in the previous scheme. As with the previous grid, the Power-law accurately approximates the analytical solution.

It is interesting to note that the lower order accuracy schemes seem to more closely approximate the analytical solution of the more coarse, 5 cell grid, while the higher order accuracy schemes better approximate the analytical solution of the finer, 20 cell grid. Another comparison can be made with regards to the Peclet Number. For the coarse grid, the Peclet Number is 5, while the Peclet Number for the finer grid is 1.25. Since the Peclet Number is a dimensionless ratio of the convective transport to the diffusive transport, one can deduce that lower order upwind schemes seem to be more appropriate for higher Peclet Number flows where convective transport dominates, while the higher order accuracy schemes seem to be more appropriate for lower Peclet Number flows where diffusive transport dominates.

4 References

[1] Essential Computational Fluid Dynamics, by O. Zikanov, John Wiley & Sons, Inc., 2010