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A Comparative Analysis of Numerical Schemes for the Convection-Diffusion Equation using the Finite Volume Method

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This study explores Computational Fluid Dynamics (CFD) schemes for convection-diffusion equations to describe the transfer of scalar quantities, such as heat, and compares the results with analytical solutions. The research delves into the fundamental concepts of numerical schemes, specifically central differencing (CD), upwind, and hybrid schemes, applying these techniques via the Finite Volume Method (FVM). The analysis identifies the strengths and limitations of each scheme, particularly revealing that while Central Differencing offers high accuracy, it exhibits instability at Peclet numbers greater than 2. Conversely, the Upwind scheme provides stability at the cost of accuracy due to numerical diffusion, while the Hybrid scheme offers an effective compromise. The study aims to provide insights into the efficacy of these schemes for solving steady-state convection-diffusion problems.

Keywords: Computational Fluid Dynamics; Finite Volume Method; Convection–Diffusion Equation; Central Differencing; Upwind Scheme; Hybrid Scheme.

1. Introduction

Computational Fluid Dynamics (CFD) emerged as a distinct scientific discipline in the early 1970s, driven by the convergence of fluid mechanics, numerical mathematics, and computer science. Its initial development was enabled by the increasing availability of powerful mainframe computers, and its continued evolution has remained closely linked to advances in computational hardware and numerical algorithms. Early CFD applications focused on the simulation of transonic flows using nonlinear potential flow equations. By the early 1980s, advances in numerical methods and computing power made it possible to solve the two-dimensional and three-dimensional Euler equations. The introduction of acceleration techniques such as multigrid methods, together with the rapid growth of supercomputing capabilities, enabled the simulation of inviscid flows around complete aircraft configurations and within turbomachinery. During the mid-1980s, research emphasis shifted toward the more challenging simulation of viscous flows governed by the Navier–Stokes equations. This transition led to the development of a wide range of turbulence models, differing in both computational complexity and predictive accuracy.

Among these, Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES) represent state-of-the-art approaches to turbulence modeling. Despite their accuracy, the high computational cost of DNS and LES continues to limit their widespread application in routine engineering design [1]. CFD provides a theoretical and computational framework for the analysis of fluid flow, heat transfer, and mass transfer phenomena through computer-based simulations. It enables detailed investigation of fundamental flow structures such as boundary layers, flow separation, wake formation, and vortex shedding, which are characterized by the temporal and spatial variation of flow variables including velocity, pressure, and temperature. In this regard, CFD serves as a complementary tool to analytical methods and experimental measurements. Although CFD is formally a subfield of fluid mechanics, it relies heavily on numerical analysis and computer science for the discretization and solution of the governing equations [2]. This interdisciplinary nature has introduced new perspectives and challenges to the study of fluid mechanics, while maintaining strong connections to classical theoretical and experimental foundations. Despite its rapid growth in recent decades, CFD is rooted in a rich historical and intellectual tradition stemming from fundamental developments in applied mathematics and physical theory [3]. Today, CFD is widely used for the analysis of systems involving fluid flow, heat transfer, and related phenomena, including chemical reactions. Its versatility and predictive capability have made it an indispensable tool across a broad range of industrial and non-industrial applications.

2. Mathematical Formulation

2.1 Governing Equations The dynamical behavior of a fluid is determined by conservation laws: mass, momentum, and energy. For a general property ϕ, the steady convection-diffusion equation is derived from the transport equation by removing the transient term:

$$div(\rho \mathrm{u}\emptyset) = div(\Gamma\ grade\ \emptyset) + S_{\emptyset} \quad (1)$$

Where ρ is density, u is the velocity vector, Γ is the diffusion coefficient, and $\emptyset$ is the source term. In a one-dimensional steady-state analysis, this reduces to:

$$\frac{d}{dx}(\rho \mathrm{u}\emptyset) = \frac{d}{dx}\left(\Gamma\ \frac{d\emptyset}{dx}\right) \quad (2)$$

Subject to the continuity equation $\frac{d}{dx}(\rho \mathrm{u}) = 0$

2.2 Finite Volume Discretization

The domain is divided into discrete control volumes. Integration of the governing equation over a control volume yields:

$$(\rho \mathrm{uA}\emptyset)_e - (\rho \mathrm{uA}\emptyset)_w = \left(\Gamma \mathrm{A}\ \frac{d\emptyset}{dx}\right)_e - \left(\Gamma \mathrm{A}\ \frac{d\emptyset}{dx}\right)_w \quad (3)$$

Defining the convective mass flux F = rho u and diffusion conductance $D = \frac{\Gamma}{dx}$, the integrated equation becomes:

$$F_e\emptyset_e - F_w\emptyset_w = D_e(\emptyset_E - \emptyset_P) - D_w(\emptyset_P - \emptyset_W) \quad (4)$$

3. Numerical Schemes

The determination of the face values $\emptyset_e$ and $\emptyset_w$ depends on the chosen numerical scheme.

3.1 Central Differencing Scheme (CDS)

The CDS employs linear interpolation to compute cell face values. For a uniform grid:

$$\emptyset_e = \frac{\emptyset_P - \emptyset_E}{2} \quad (5)$$

While CDS is second-order accurate, it fails to account for flow direction. It is known to produce oscillatory solutions when the local Peclet number (Pe = F/D) exceeds 2.

3.2 Upwind Differencing Scheme (UDS)

The UDS accounts for flow direction (transportiveness). The value at a cell face is taken to be equal to the value at the upstream node.

For positive flow (u > 0):

$$\emptyset_w = \emptyset_W \; and \; \emptyset_e = \emptyset_P \quad (6)$$

This scheme is unconditionally stable but is only first-order accurate and introduces false diffusion (numerical diffusion).

3.3 Hybrid Differencing Scheme

The Hybrid scheme combines CDS and UDS. It utilizes CDS for small Peclet numbers (|Pe| < 2) to maintain second-order accuracy and switches to UDS for large Peclet numbers (|Pe| > 2) to ensure stability. The net flux through a west face is given by:

$$q_w = F_w \, \emptyset_w \; and \; Pe_w \geq 2 \quad (7)$$

$$q_w = F_w \left[\frac{1}{2}\left(1 + \frac{2}{Pe_w}\right)\emptyset_W + \frac{1}{2}\left(1 - \frac{2}{Pe_w}\right)\emptyset_P\right] \; for - 2 < Pe_w < 2 \quad (8)$$

4. Results and Discussion

A property Temperature is transported by means of convection and diffusion through the one-dimensional and two-dimensional domain. The governing equation is (4.3); the boundary conditions are T_1 = 35 at x = 0 and T_2 = 25 at x = L. Using Twenty equally spaced cells and the central differencing scheme for convection and using the upwind differencing scheme and using the hybrid scheme, calculate the distribution of T as a function of x for with velocity in fixed in all case and compare the results with the analytical solution

4.2 Case 1 simulation of the temperature distribution in 1-D

Describe the case study and boundary conditions also the analytical solution, In a case 1 study of temperature distribution, the boundary conditions of the system are determined. These thermal boundary conditions include the amount of heat consumed, the amount of heat lost, the desired temperature in the system, and other factors that may affect the distribution of temperature, this simulation is carried out using mathematical models that rely on equations of convection and diffusion. Analytical solutions rely on obtaining an exact solution to the equations of motion and heat in an analytical way, and the analytical solution can be used to predict the distribution of temperature in the system.

We have defined the variables required for simulation, such as the length of the material (L), the initial and final temperatures of the material (T_1 and T_2), and the thermal conductivity of the material (k). We have divided the material into small equal parts, where the temperature in each part is estimated. Then we calculate the amount of heat transferred using the heat balance equation to calculate the amount of heat transferred through each part of the material. This solution includes thermal conductivity and temperature differences between parts. Then we update the temperatures of each part based on the amount of heat transferred.

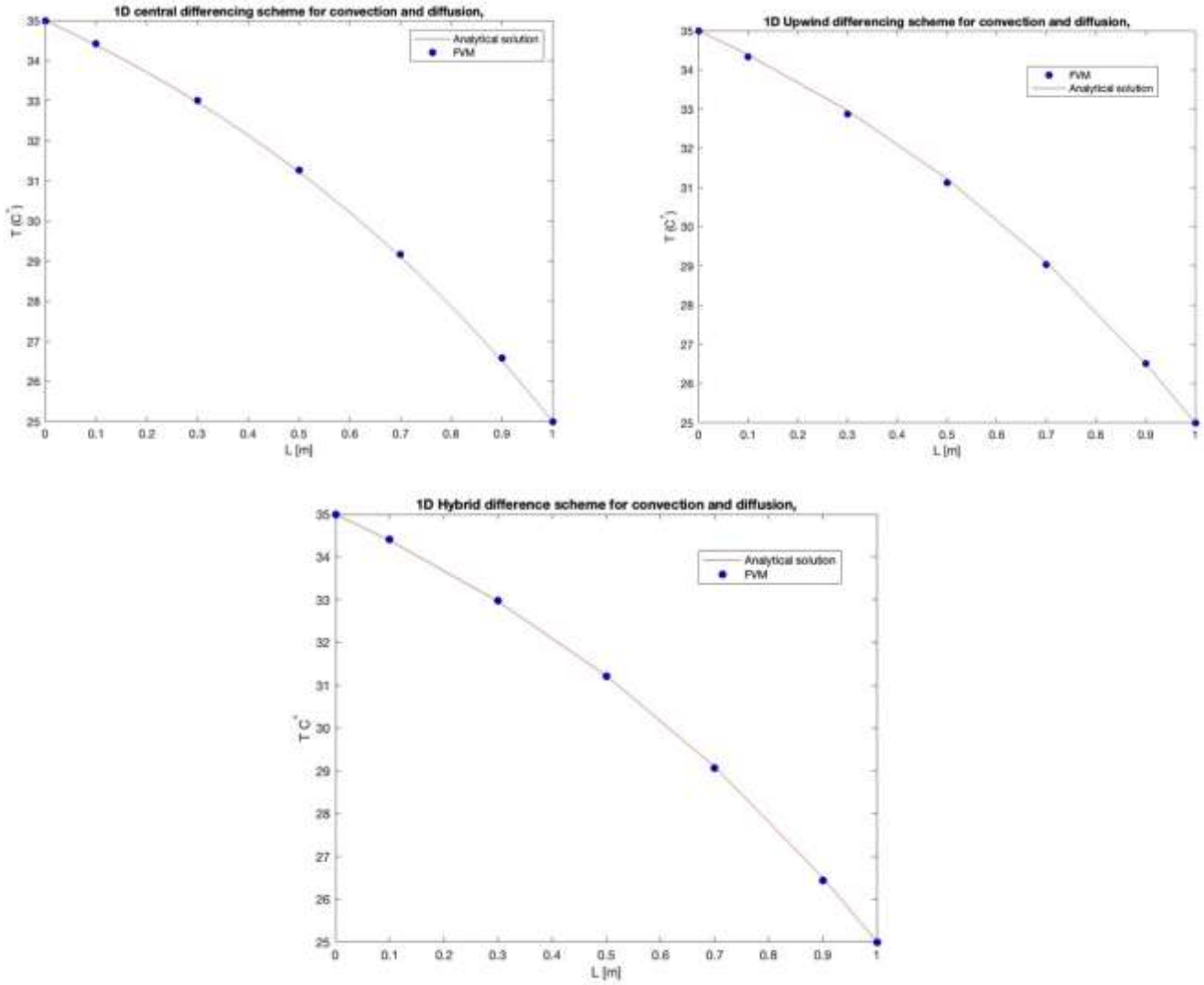


Figure 4. 1 compared central differences, upwind and hybrid scheme results at u = 0.1 (coarse grid)

The comparison between the numerical and analytical solutions is well-done and can be seen in Figure 4.1. Despite the grid being rough, the central differencing (CD) method shows a satisfactory level of agreement with the analytical solution.

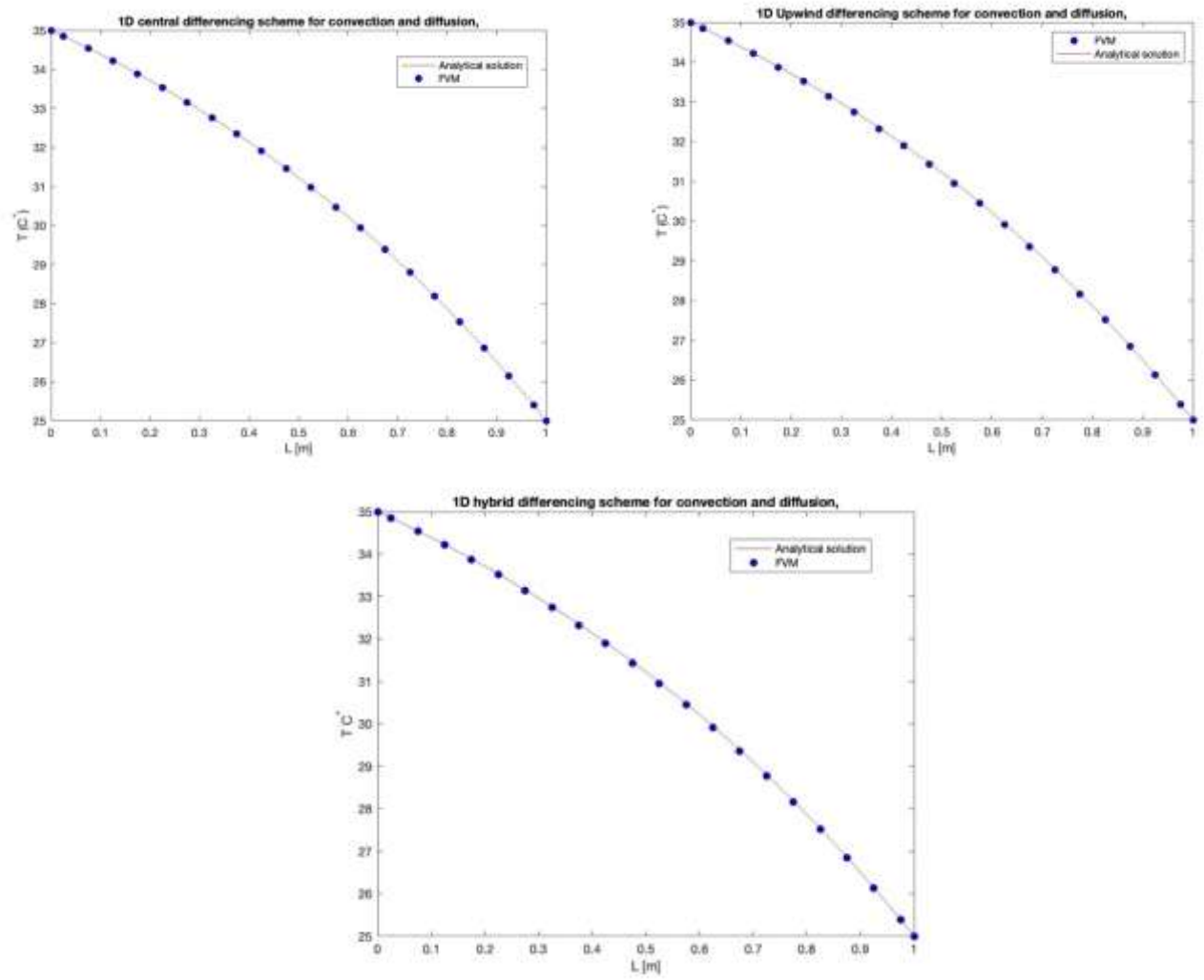


Figure 4. 2 compared central diffrences, uwind and hybrid scheme results at u = 0.1 (fine grid)

Figure 4.2 shows the comparison between the central difference and upwind schemes on a fine grid confirms that the former is more precise. The central difference scheme's precision is attributed to its ability to capture the flow's subtle features accurately. So the results demonstrate that all three schemes remain effective in simulating fluid flow and heat transfer with a high degree of accuracy. On the other hand, the upwind scheme is less sensitive to small perturbations in the flow field, making it more robust in some cases. The hybrid scheme's effectiveness is demonstrated in figure 4.2, where it produces results that are in excellent agreement with the analytical solution.

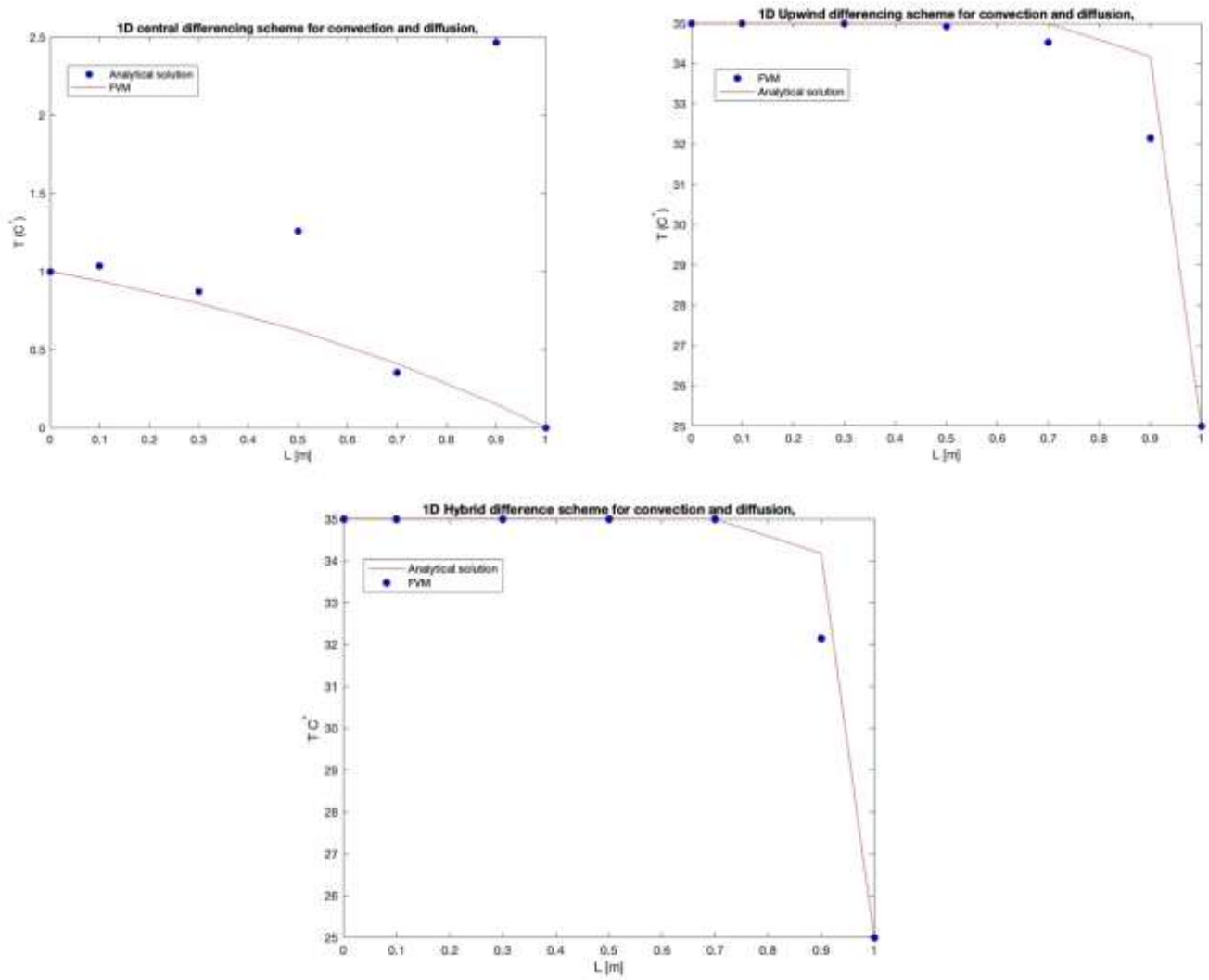


Figure 4. 3 compared central diffrences, uwind and hybrid scheme results at u = 2.5 (coarse grid)

The simulation results at a velocity of 2.5 m/s are presented in the figure, which clearly shows the limitations of the central difference scheme. The wiggling results observed in this scheme are attributed to its inability to perform well when the Prandtl number exceeds 2 or when the flux term F is double or more than the diffusion term D. Overall, this study emphasizes the importance of carefully selecting a numerical scheme that is appropriate for the specific problem being addressed. While each scheme has its strengths and limitations.

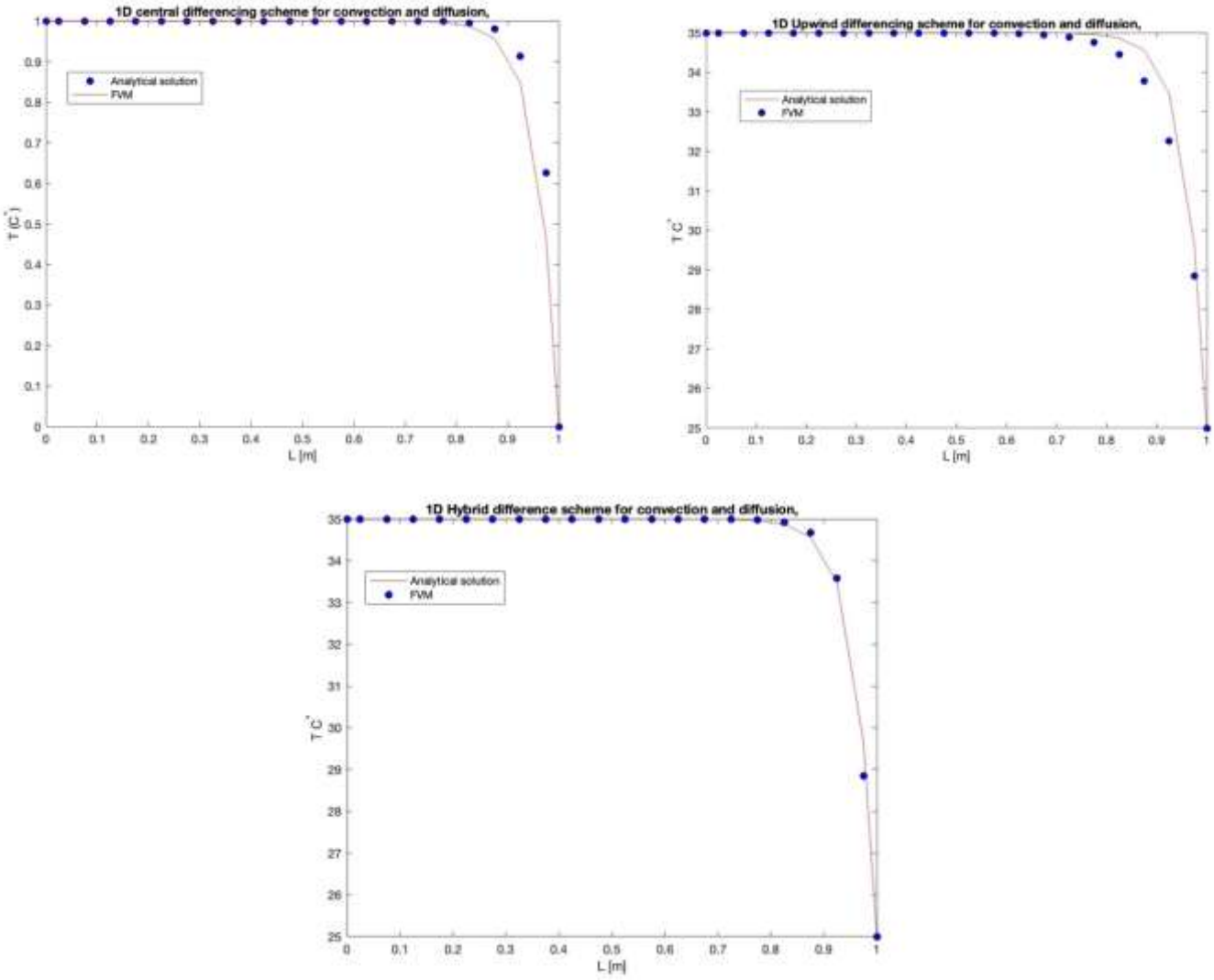


Figure 4. 4 compared central diffrences, uwind and hybrid scheme results at u = 2.5 (fine grid)

The comparison of the numerical and analytical solutions has been well-executed and can be observed in Figure 4.4. Despite the grid being coarse, the central differencing method demonstrates a satisfactory level of correspondence with the analytical solution. The agreement between the numerical outcomes and the analytical solution is now strong. When comparing the data from this situation to the one computed on the five-point grid of Case 2, it is apparent that grid refinement has decreased the F/D ratio from 5 to 1.25. The central differencing approach appears to produce precise results when the F/D ratio is low. The findings of this study demonstrate that all three numerical schemes - central difference, upwind, and hybrid - are effective in simulating fluid flow and heat transfer, even with a coarse grid. The results align well with the analytical solution, indicating that these schemes can be relied upon for accurate predictions. However, the central difference scheme does exhibit an oscillation solution when the Prandtl number exceeds 2. This limitation can be overcome by carefully manipulating the initial values, such as dx, to ensure that the Prandtl number remains below two. Furthermore, the comparison of the central difference and upwind schemes reveals that the former is more precise

than the latter. This suggests that the central difference scheme should be preferred when accuracy is of utmost importance. However, it is worth noting that the upwind scheme has its own advantages, such as being less sensitive to small perturbations in the flow field. To leverage the benefits of both schemes, a hybrid approach that combines central difference and upwind would be ideal. This approach would allow for greater accuracy while also being less sensitive to small perturbations. In summary, this study highlights the strengths and limitations of different numerical schemes for simulating fluid flow and heat transfer and provides guidance on how to choose the most appropriate scheme for a given problem.

4.4 Case 2 simulation of the temperature distribution in 2D

Central differences scheme In case 2, we study of a rectangular plate with dimensions Lx and Ly, which is initially at a uniform temperature T0. The left and right boundaries of the plate (x= 0 and x = L) are maintained at constant temperatures T_1 and T_2, respectively, while the top and bottom boundaries (y = 0 and y = Ly) are Insulated, meaning there is no heat transfer across these boundaries. We can substitute this into the convection-diffusion equation and obtain ordinary differential equations. Let us move on to numerical methods for simulating the temperature distribution In 2-D, which approximate the derivatives in the convection-diffusion equation using discrete differences. Three such methods are the central differences scheme, the upwind scheme and the hybrid scheme. The upwind scheme Is a first-order accurate method that approximates the second derivatives using forward or backward differences, depending on the direction of the temperature gradient, and the hybrid scheme, which combines the central differences scheme and the upwind scheme. It uses the central differences scheme when the temperature gradient is small and the upwind scheme when the temperature gradient is large. For the Simulation of the temperature distribution in 2-D, we will use highly accurate methods, such as finite difference methods. The analytical solution can be obtained using the separation of variables and satisfies the boundary conditions of the problem. Finite volume methods, such as the central differences scheme, the upwind scheme, and the hybrid scheme, approximate the derivatives In the convection-diffusion equation using discrete differences and solve the resulting system of linear equations iteratively.

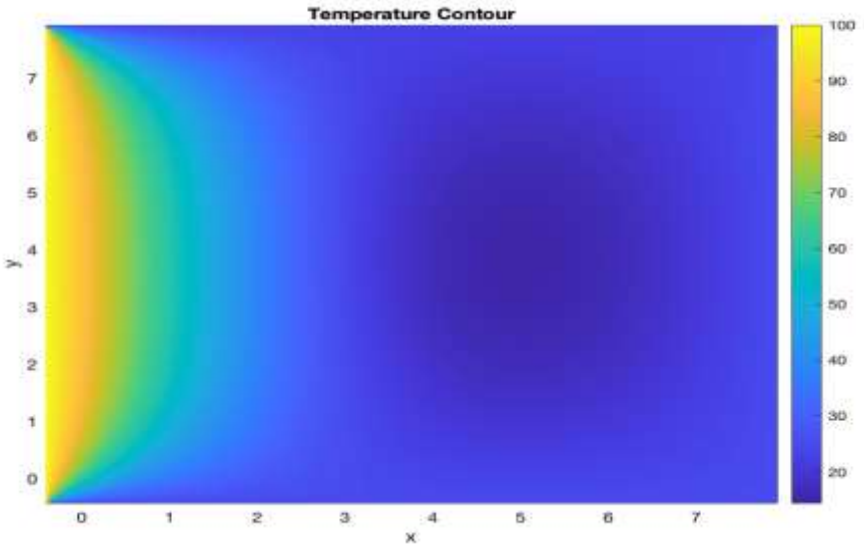


Figure 4. 5 Temperature contour for rectangular space

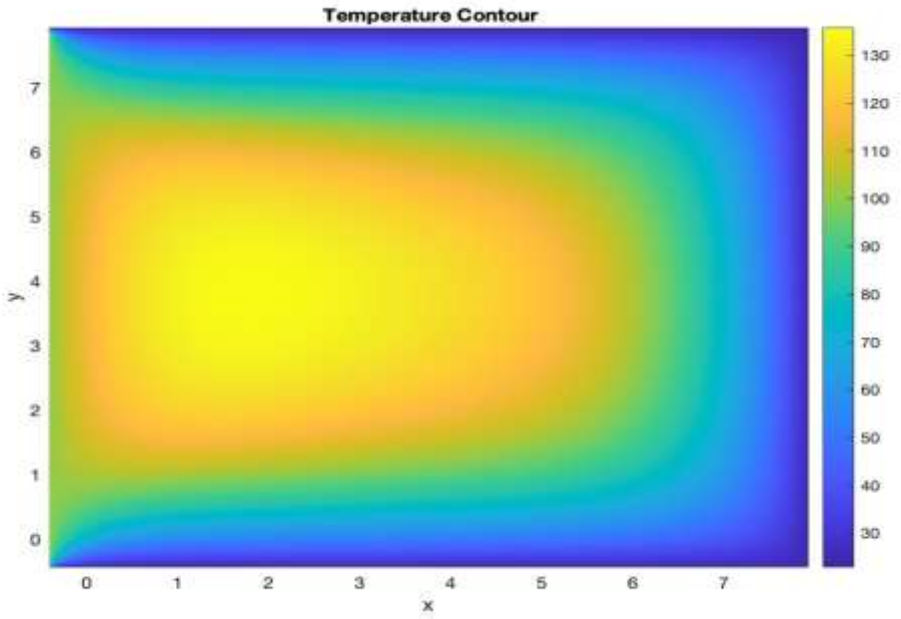


Figure 4. 6 Temperature contour for rectangular space with heat generation.

Conclusion

Finite Volume Method (FVM) is a widely used numerical technique for solving partial differential equations, including those governing convective diffusion problems. In this discussion, we will explore the application of FVM to model convective diffusion phenomena, its advantages, and some considerations for its implementation. One of the key advantages of FVM is its ability to handle complex geometries and unstructured grids. The control volumes can be defined around each cell, allowing for flexibility in representing irregular shapes and boundaries. This makes FVM suitable for simulating convective diffusion in practical engineering applications, where complex geometries are often encountered. In FVM, the convective and diffusive fluxes across the control volume faces are computed using appropriate numerical schemes. For convective fluxes, schemes like upwind, central differencing, or higher-order schemes. These schemes ensure that the direction of the flux is determined by the flow direction, capturing the convective transport accurately. Another consideration is the choice of grid resolution. The grid should be fine enough to capture the variations in concentration and flow velocity accurately. However, a very fine grid can lead to excessive computational costs. Balancing the grid resolution with computational efficiency is crucial in FVM simulations. In conclusion, the Finite Volume Method is a powerful numerical technique for modeling convective diffusion problems. Its ability to handle complex geometries, unstructured grids, and different boundary conditions makes it suitable for a wide range of engineering applications. By appropriately selecting numerical schemes, implementing boundary conditions, and validating the model, FVM can provide accurate and reliable predictions of convective diffusion phenomena.

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