ME 7310 – Project 2
Convection-Diffusion PDE

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Abstract

In this project three different finite difference schemes are used to discretize the governing equation for the convection-diffusion partial differential equation (PDE). The schemes implemented include a first-order forward-time and second-order central space (FTCS) scheme for convection and diffusion, first order upwind for convection and FTCS for diffusion, and a MacCormack method for convection and second order central space for diffusion. The convection portion of the governing equation is of the form of a hyperbolic PDE, while the diffusion term is of the form of a parabolic PDE.

To verify the accuracy of the numerical scheme developed, a mesh refinement study is conducted. Both the truncation error and stability conditions for the FTCS scheme are investigated. In order to validate the solution, the results obtained from the numerical scheme are compared to those obtained from the analytical solution.

1 Problem Definition

In this project the one-dimensional wave propagation for laminar incompressible flow is solved. Also known as the convection-diffusion equation, the governing form is:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = \alpha\frac{\partial^2 u}{\partial x^2} \tag{1}$$

where the wave speed, a, is 2.5 *m/s*, the kinematic viscosity, α, is 0.005 m^2/s, the final time is 0.2 *s*, and the domain $0 \le x \le 1\ m$ are all given. The flow is subject to the following initial condition:

$$u(x,0) = \begin{cases} 1.0 \text{ if } x < 0.2 \\ 0.5 \text{ if x} = 0.2 \\ 0.0 \text{ if x} > 0.2 \end{cases} \tag{2}$$

and the boundary conditions:

$$u(0,t) = 1\ m/s;\ u(1,t) = 0 \tag{3}$$

Given the initial condition and boundary conditions above, the analytical solution is obtained as:

$$u_a(x,t) = 1 - \frac{1}{2}\left[1 + erf\left(\frac{x - x_0 - at}{2\sqrt{\alpha t}}\right)\right];\ x_0 = 0.2\ m \tag{4}$$

2 Numerical Solution Procedure

Numerical solutions of the governing PDE were obtained using three different explicit finite-difference schemes. The first scheme implemented was a first-order forward-time and second-order central space (FTCS) scheme. The numerical scheme, as derived from the Taylor Series [1], is:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = \alpha\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} + O((\Delta t),(\Delta x)^2) \tag{5}$$

As $\Delta t \rightarrow 0$ and $\Delta x^2 \rightarrow 0$, the truncation error vanishes, thus the FTCS scheme is consistent. Rearranging (5), the explicit form of the equation can be expressed as:

$$u_i^{n+1} = u_i^n - \frac{a\Delta t}{2\Delta x}(u_{i+1}^n - u_{i-1}^n) + \frac{\alpha\Delta t}{(\Delta x)^2}(u_{i+1}^n - 2u_i^n + u_{i-1}^n) \tag{6}$$

where the term $\frac{a\Delta t}{2\Delta x}$ represents the Courant number, *c*, and the term $\frac{\alpha\Delta t}{(\Delta x)^2}$ represents the Fourier number, *d*. Performing algebraic substitutions using the Courant number and Fourier number, Equation (6) can be rewritten in the form:

$$u_i^{n+1} = u_i^n - \frac{c}{2}(u_{i+1}^n - u_{i-1}^n) + d(u_{i+1}^n - 2u_i^n + u_{i-1}^n) \tag{7}$$

The final explicit form of the FTCS scheme represented by Equation (7) was implemented using a computer program whose algorithm marches forward in time. It is important to note that the following stability condition, known as the *mesh Reynolds number* [1], was implemented as part of the FTCS algorithm:

$$Re_{\Delta x} = \frac{a\Delta x}{\alpha} \leq 2 \tag{8}$$

The second finite-difference scheme implemented was a first-order upwind for convection, and FTCS for diffusion scheme. As before, the numerical scheme can be derived from the Taylor Series. The resulting finite difference scheme is:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a\frac{u_i^n - u_{i-1}^n}{\Delta x} = \alpha\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{(\Delta x)^2} + O((\Delta t),(\Delta \mathrm{x})) \tag{9}$$

This scheme is first-order accurate in both time and space. As $\Delta t \rightarrow 0$ and $\Delta x \rightarrow 0$, the truncation error vanishes, thus the FTCS scheme is consistent. Rearranging (9) and performing substitutions for the Courant and Fourier number, the numerical scheme can be written in the following explicit form:

$$u_i^{n+1} = u_i^n - c(u_i^n - u_{i-1}^n) + d(u_{i+1}^n - 2u_i^n + u_{i-1}^n) \tag{10}$$

The third finite-difference scheme implemented was the MacCormack method for convection, and second-order central space for diffusion. The MacCormack method is a two-step, explicit, predictor-corrector method [1]. As applied to the governing convection-diffusion equation, the resulting algorithm is expressed in explicit form as:

Predictor:

$$u_i^{\overline{n+1}} = u_i^n - c(u_{i+1}^n - u_i^n) + d(u_{i+1}^n - 2u_i^n + u_{i-1}^n) \tag{11}$$

Corrector:

$$u_i^{n+1} = \frac{1}{2}\left[u_i^n + u_i^{\overline{n+1}} - c\left(u_i^{\overline{n+1}} - u_{i-1}^{\overline{n+1}}\right) + d(u_{i+1}^{\overline{n+1}} - 2u_i^{\overline{n+1}} + u_{i-1}^{\overline{n+1}}\right] \tag{12}$$

where $u_i^{\overline{n+1}}$is a temporary value, *c* is the Courant number, and *d* is the Fourier number. The resulting scheme is second-order accurate in both time and space, with a truncation error of $O((\Delta t)^2, (\Delta x)^2)$. As with the previous schemes, as $\Delta t \rightarrow 0$ and $\Delta x \rightarrow 0$, the truncation error vanishes, thus the scheme is consistent.

In order to verify the numerical schemes, a grid refinement study was performed by decreasing the grid steps in both time and space (Δt and Δx, respectively). This was done by varying Courant and Fourier number for all three numerical schemes. An additional verification was done independently for the MacCormack method.

Validation of the numerical schemes was obtained by comparing results from the numerical solutions with those obtained from the analytical solution at different values of time, Courant, and Fourier number.

3 Numerical Results

For purposes of validation, the numerical solutions from the three finite difference schemes previously developed were compared with results obtained from the analytical solution. Results of the numerical and analytical solutions for velocity profile were plotted for various combinations of Courant and Fourier Numbers as the solutions evolved over time. Given the need to satisfy the stability criteria of the mesh Reynolds number (8) for the FTCS scheme, as well as implement the values of interest given for Courant and Fourier number, the grid was essentially predetermined for the different scenarios investigated.

The first scenario investigated was that for which c=0.3 and d=0.3 at different final times ranging from 0.05 s to 0.20 s. Results for the velocity profile are plotted in Figure 1, and information regarding discretization of the numerical schemes is shown in Table 1.

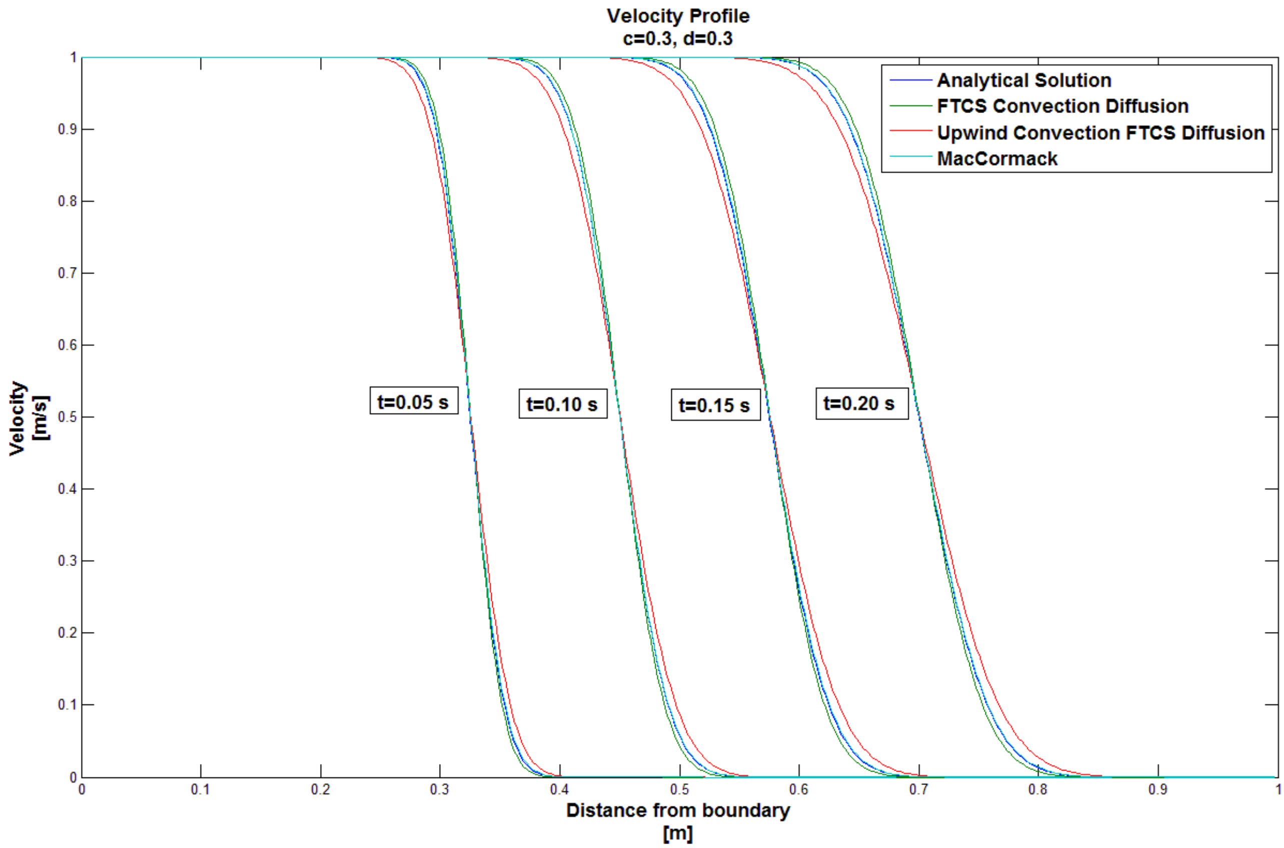

Figure 1: Velocity profile at t=0.05, 0.10, 0.15, 0.20 for c=0.3 and d=0.3

Table 1: Grid systems at t=0.05, 0.10, 0.15, and 0.20 s for c=0.3 and d=0.3

Final Time [s]	Spatial Discretization Δx [m]	Time Step Δt [s]	Grid System (N x t)	Re	c	d
0.05	0.002	0.00024	500 x 208	1	0.3	0.3
0.10	0.002	0.00024	500 x 416	1	0.3	0.3
0.15	0.002	0.00024	500 x 625	1	0.3	0.3
0.20	0.002	0.00024	500 x 833	1	0.3	0.3

The second scenario investigated was that for which c=0.4 and d=0.2, at different final times ranging from 0.05 s to 0.20 s. Results for the velocity profile are plotted in Figure 2, and information regarding discretization of the numerical schemes is shown in Table 2.

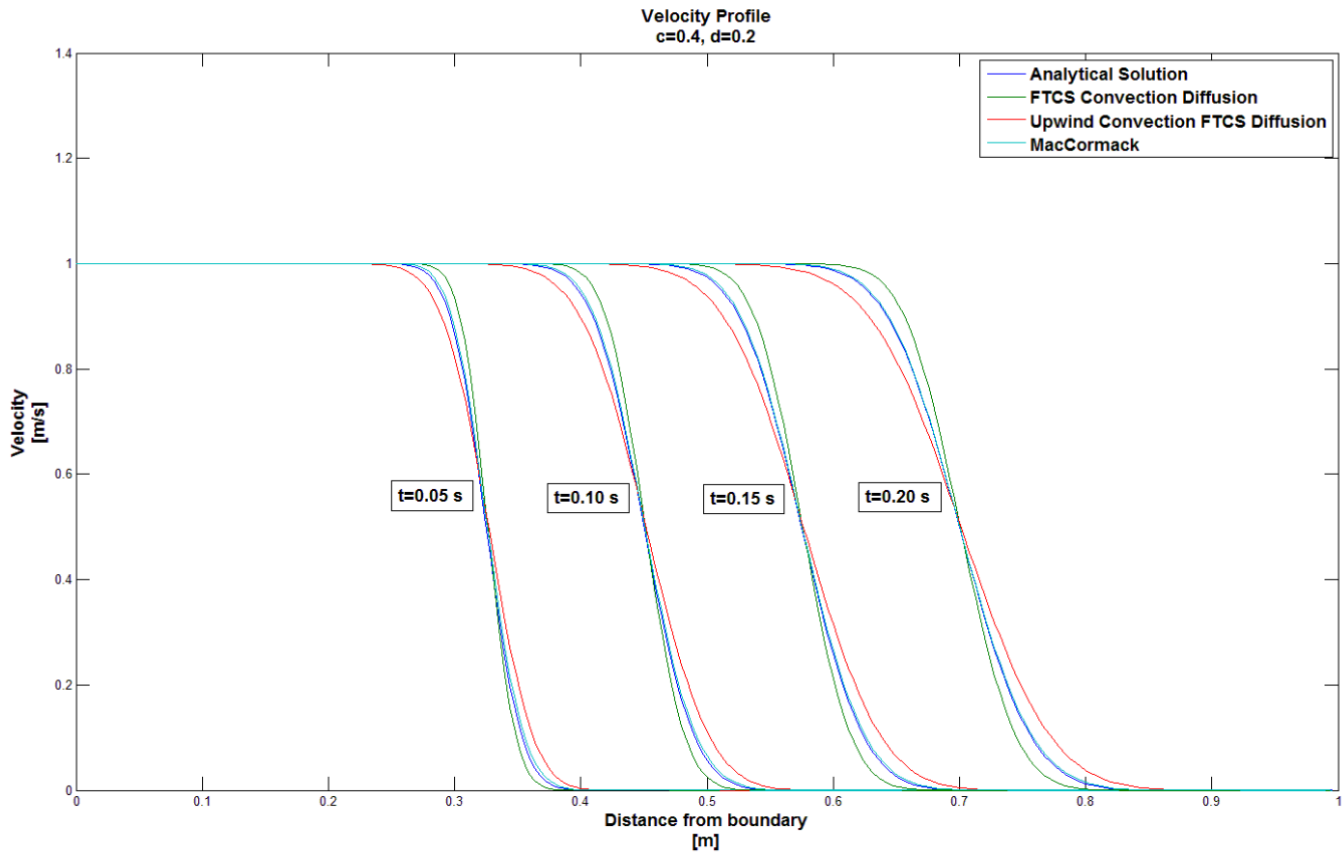

Figure 2: Velocity profile at t=0.05, 0.10, 0.15, 0.20 for c=0.4 and d=0.2

Table 2: Grid systems at t=0.05, 0.10, 0.15, and 0.20 s for c=0.4 and d=0.2

Final Time [s]	Spatial Discretization Δx [m]	Time Step Δt [s]	Grid System (N x t)	Re	c	d
0.05	0.004	0.00064	250 x 78	2	0.4	0.2
0.10	0.004	0.00064	250 x 156	2	0.4	0.2
0.15	0.004	0.00064	250 x 234	2	0.4	0.2
0.20	0.004	0.00064	250 x 312	2	0.4	0.2

It is interesting to note that the results from the numerical schemes obtained in the first scenario match more closely to the analytical solution than those obtained in scenario two. This is precisely what is expected based on the more refined grid system of scenario one, as displayed in Table 1.

The final scenario investigated was that for which c=0.2 and d=0.4, at different final times ranging from 0.05 s to 0.20 s. Results for the velocity profile are plotted in Figure 3, and information regarding discretization of the numerical schemes is shown in Table 3.

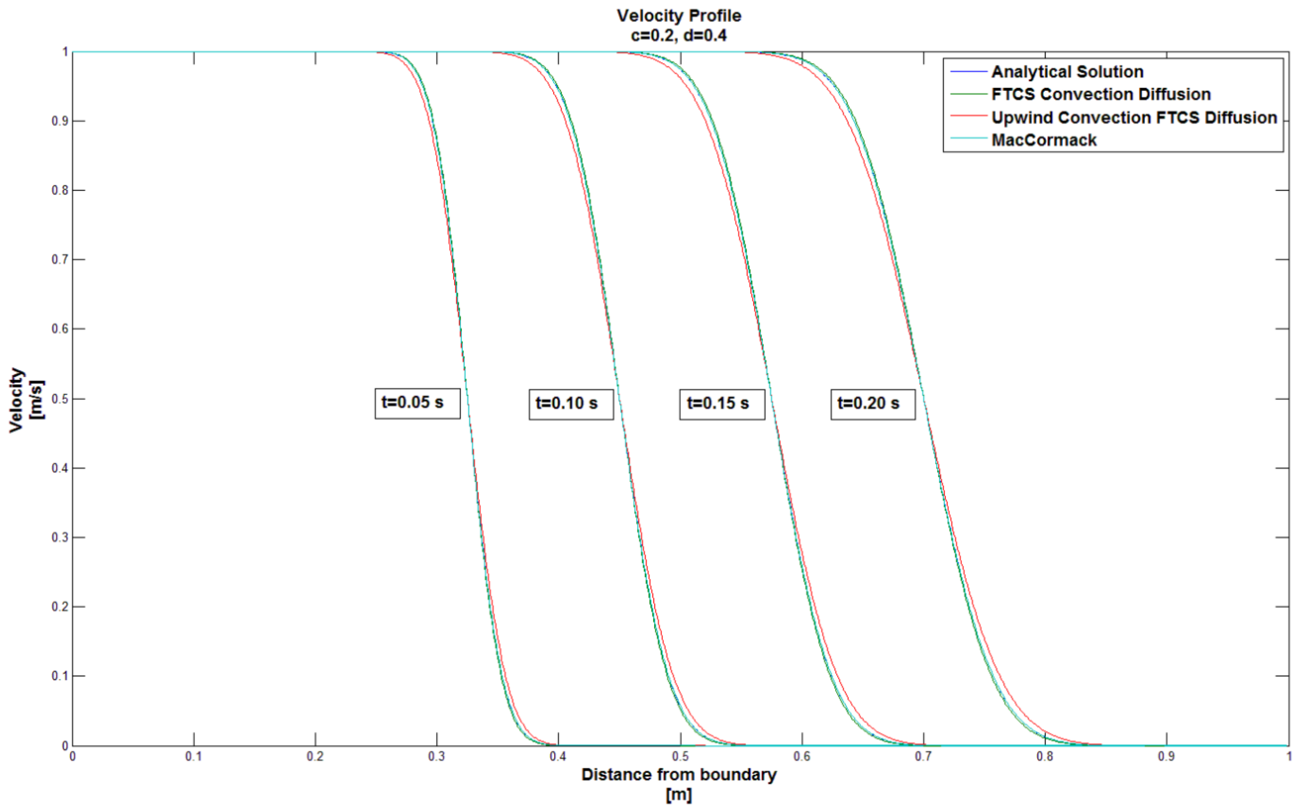

Figure 3: Velocity profile at t=0.05, 0.10, 0.15, 0.20 for c=0.2 and d=0.4

Table 3: Grid systems at t=0.05, 0.10, 0.15, and 0.20 s for c=0.2 and d=0.4

Final Time [s]	Spatial Discretization Δx [m]	Time Step Δt [s]	Grid System (N x t)	Re	c	d
0.05	0.001	0.00008	1000 x 625	0.5	0.2	0.4
0.10	0.001	0.00008	1000 x 1250	0.5	0.2	0.4
0.15	0.001	0.00008	1000 x 1875	0.5	0.2	0.4
0.20	0.001	0.00008	1000 x 2500	0.5	0.2	0.4

The third scenario yields the most accurate results, as can be seen from a comparison of the numerical results plotted from the third scenario (Figure 3) to the previous two scenarios investigated (Figure 1 and Figure 2). This was to be expected because the third scenario implements the most refined grid, as can be seen in Table 3.

In order to verify the accuracy of the MacCormack method, a grid refinement study was conducted. Results for three different refinement levels (Table 4) are plotted versus the analytical solution, as displayed in Figure 4.

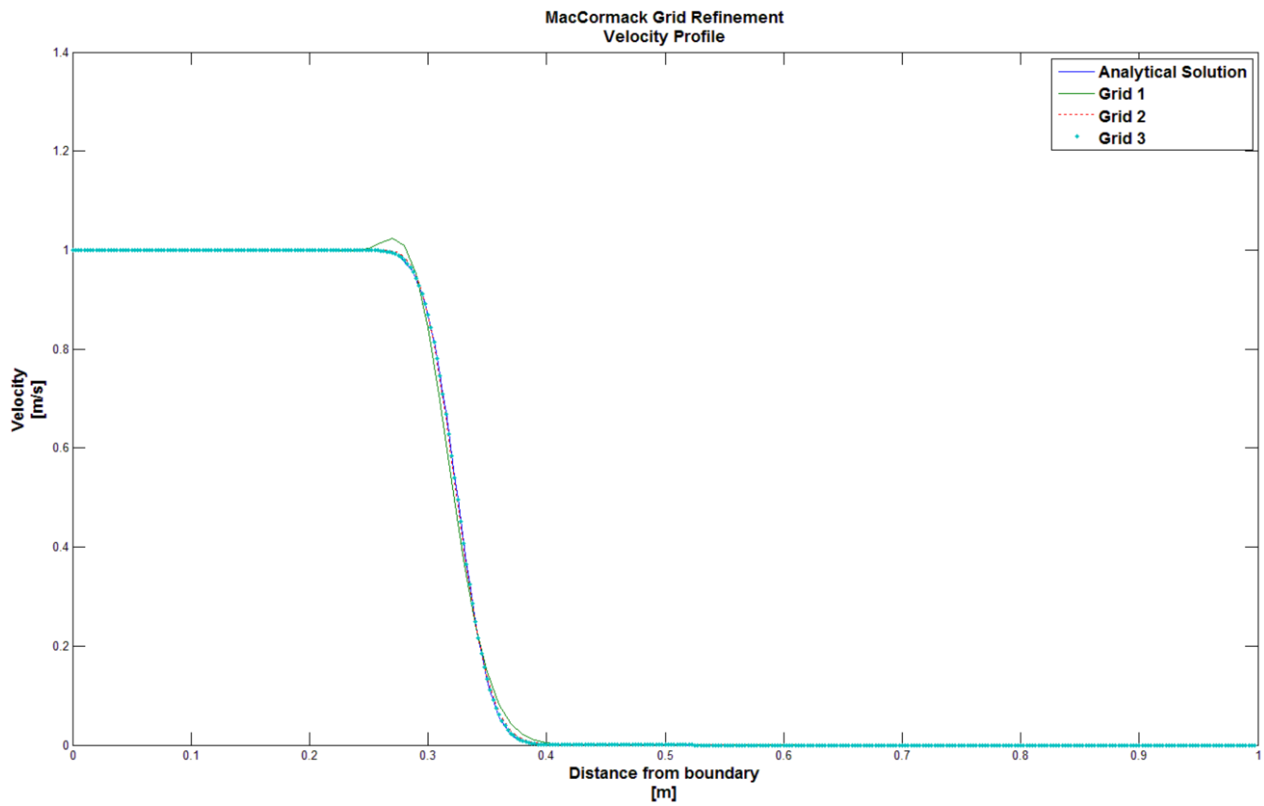

Figure 4: Grid refinement study of the MacCormack method

Table 4: Grid systems for the grid refinement study of the MacCormack method

Grid	Spatial Discretization Δx [m]	Time Step Δt [s]	Grid System (N x t)	Final Time [s]
1	0.01	0.001	100 x 50	0.05
2	0.005	0.0005	200 x 100	0.05
3	0.0025	0.00025	400 x 200	0.05

The refinement study shows that as the grid is significantly refined, the solution from the numerical scheme approaches the analytical solution.

Results from all three numerical schemes match closely with those obtained from the analytical solution, but it appears that the results from the MacCormack method are the most accurate. This is to be expected because the MacCormack method is second order accurate ($O((\Delta t)^2, (\Delta x)^2)$), while both the FTCS scheme ($O((\Delta t), (\Delta x)^2)$), and Upwind scheme($O((\Delta t), (\Delta x))$) are first order accurate.

Effects of truncation error on the solutions from the different numerical schemes were investigated through numerical experimentation. Implementing a coarser grid (50 spatial nodes x 50 time nodes) than those previously investigated, it can clearly be seen in Figure 5 that the

FTCS convection-diffusion and MacCormack schemes are dispersive, while the upwind scheme is dissipative.

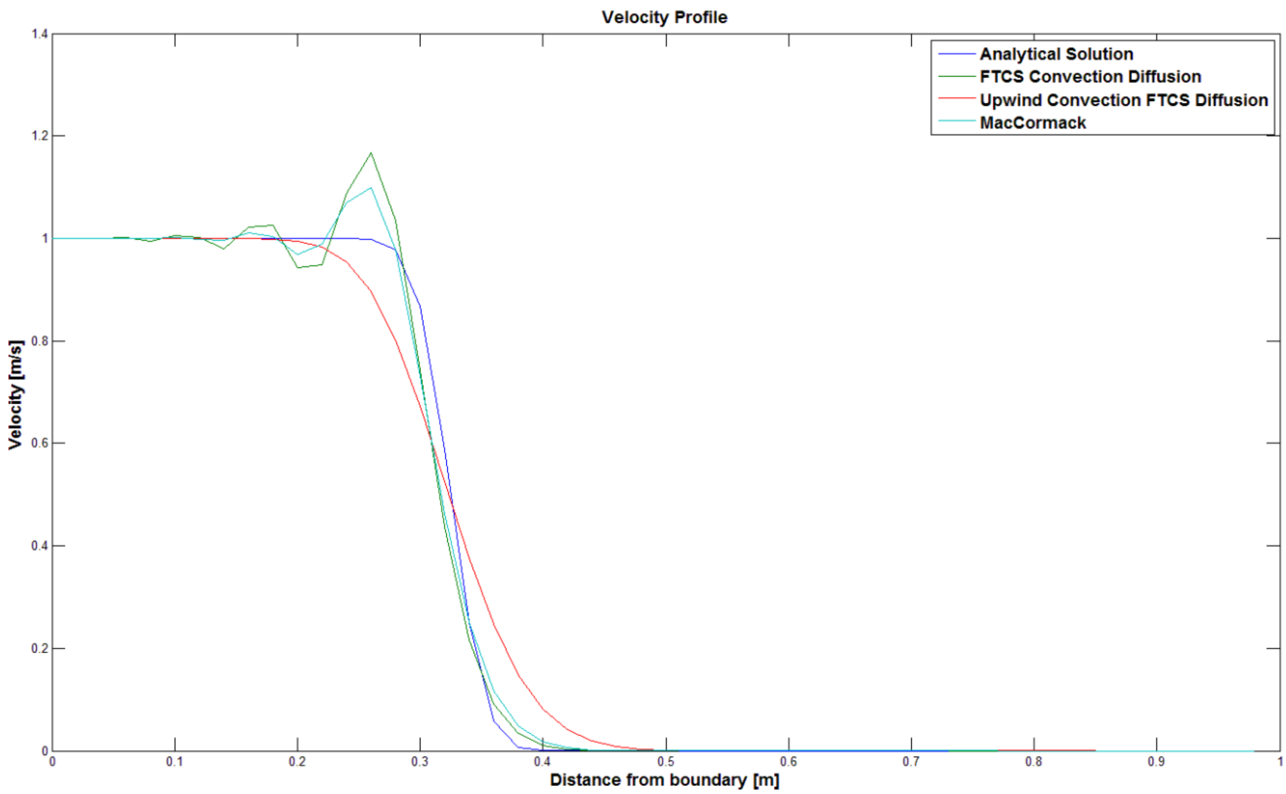

Figure 5: Numerical dispersion and dissipation in a coarse grid

Examination of the modified equation for a similar two step Lax-Wendroff method also verifies that the numerical scheme is dispersive because the lowest order derivative on the right hand side of the equation is odd [1]. The FTCS convection-diffusion scheme is more dispersive than the MacCormack scheme, which indicates that the lowest order derivative on the right hand side of the modified equation must be of lower order than that of the MacCormack scheme. The upwind scheme on the other hand seems to be dissipative, which indicates that the lowest order derivative on the right hand side of the modified equation is even.

4 References

[1] Computational Fluid Mechanics and Heat Transfer, J.C. Tannehill, D.A. Anderson, R.H. Pletcher, Taylor and Francis, 1997.