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# Numerical Solution of a 3-D Advection-Dispersion Model for Pollutant Transport

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**Abstract :** This paper describes a mathematical model for transport of a pollutant in a street tunnel. The three-dimensional advection-diffusion (advection-dispersion) equation is solved by using a finite difference (FTCS) method. Results show the concentration of pollutant within the tunnel for various pollution source configurations.

**Keywords :** advection-diffusion equation, finite difference FTCS method

## 1 Introduction

Partial differential equations are the basis of many mathematical models of physical, chemical and biological phenomena, and their use has also spread into economics, financial forecasting and other fields. Because exact analytical solutions are not generally able to be found, it is often necessary to resort to numerical methods to find approximate solutions of these partial differential equations, in order to investigate the predictions of the mathematical models.

Sousa [1] studies the conditions that ensure stability for various finite difference schemes for the advection-diffusion equation, while Hindmarsh *et al.* [2] examined the stability criteria for the multidimensional advection-diffusion equation.

Dehghan [3] defines and calculates the stability conditions for several numerical methods [ e.g. Forward in Time, Centre in Space (FTCS); Forward in Time, Backward in Space (FTBS); Lax-Wendroff; Backward in Time, Centre in Space (BTCS); and Crank-Nicolson methods ] for the three-dimensional advection-diffusion equation and compares the numerical and analytical solutions.

Choo-in [4] used a Box Model to determine the pollutants in a street tunnel in Thailand.

In this study, we solve the 3-D advection-diffusion equation by using the Forward in Time, Centre in Space (FTCS) finite difference method. The domain of this study is a typical street tunnel. Pollutant dispersal patterns within the tunnel are calculated. Numerical results for several different pollutant source configurations are presented and discussed.

# 2 PROBLEM DEFINITION AND THE GOVERNING EQUATION

## 2.1 Problem Definition

The street tunnel configuration is shown in Figure 1. Typically such a "tunnel" is formed by the covering of a normal downtown city street by an overhead railway or similar. This provides a roof over a certain length of the street. In the schematic shown, the street runs along the $x$-direction and the tunnel is fully-open on the ends at $x = 0$ and $x = L$. The tunnel is assumed fully-closed on the pavement and roof at $z = 0$ and $z = H$ respectively.

The sides of the street are composed of sections of buildings, between which are side streets, pathways, gateways or doorways that provide paths for wind flow. We assume that these are somewhat randomly-distributed, but that they allow a wind flow across the street, as well as that along it. The average fraction of each of the street-sides that is open is assumed the same for both sides.

The pollutant source is taken to be outside, but near to the tunnel. The pollutant may be from traffic exhausts entering, or being generated inside, the tunnel region. Some other toxic source may occur at a street-entrance to the tunnel, or in one of the side-streets.

Two cases are examined in this study. First, we suppose that there is wind flow only in $x$-direction. Secondly, we allow for a crosswind through the gaps in the side-walls of the tunnel, with wind inflow in $x$ and $y$-directions. The wind speed in $y$-direction is taken to be a uniform value averaged over the tunnel side-walls. The actual wind-speed through the side openings will be greater than this average cross-tunnel wind-speed. Then the problem domain of this study is:

$$\Omega = \{(x, y, z); 0 \le x \le L, 0 \le y \le W, 0 \le z \le H\}$$

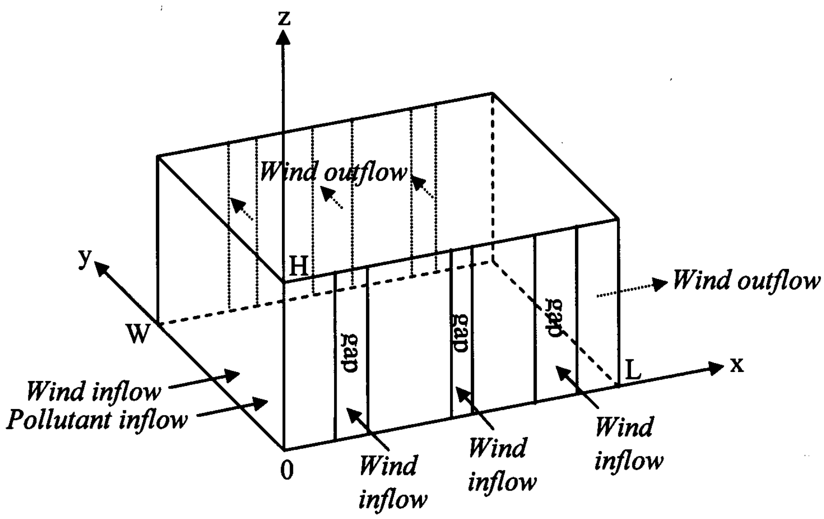



Figure 1: The domain for street tunnel

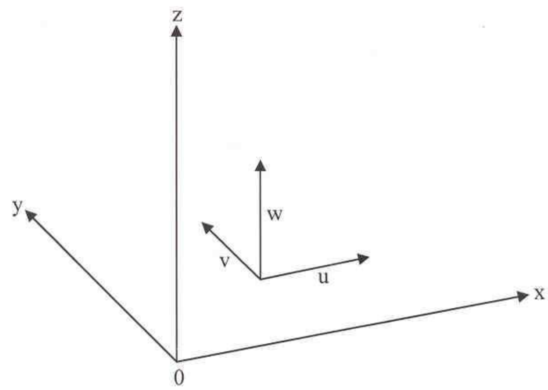



Figure 2: Wind direction for three-dimensional model

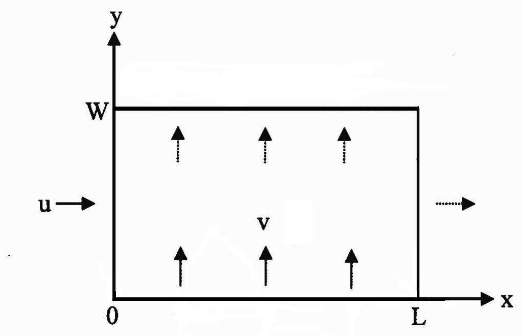



Figure 3: The structure of domain on the top

In Figures 1 and 2, the schematics show the Cartesian axes system and the wind-components. Here,

| | |
|---|---|
| $L$ | is the length of tunnel |
| $W$ | is the width of tunnel |
| $H$ | is the height of tunnel |

## 2.2 Governing Equation

The concentration of a pollutant in a given domain may be described by the advection-diffusion equation:

$$\frac{\partial C}{\partial t} + \boldsymbol{V}\cdot\nabla C = \nabla\cdot(\bar{K}\otimes\nabla C) \tag{2.1}$$

where $C(x, y, z, t)$ is the concentration (mass per unit volume) of pollutant at point $(x, y, z)$ in Cartesian coordinates and at time $t$. $\boldsymbol{V}$ is the (average) wind velocity field and $\bar{K}$ is the eddy-diffusivity or dispersion tensor. The air turbulence acts as a mechanical dispersion mechanism within the flow, tending to spread and dilute highly-concentrated material.

With the assumption that the wind flow is horizontal, that the wind and dispersion tensor components are uniformly constant within the tunnel, and that the dispersion is horizontally isotropic, the three-dimensional advection-diffusion equation may be written:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} = D_h\frac{\partial^2 C}{\partial x^2} + D_h\frac{\partial^2 C}{\partial y^2} + D_v\frac{\partial^2 C}{\partial z^2} \quad (2.2)$$

where

| | |
|---|---|
| $u$ | is a constant wind speed in the $x-$direction |
| $v$ | is a constant wind speed in the $y-$direction |
| $D_h$ | is a constant dispersion coefficient in the horizontal direction |
| $D_v$ | is a constant dispersion coefficient in the $z-$direction (vertical) |

with the appropriate initial and boundary conditions.

# 3 FINITE DIFFERENCE METHODS

The main idea behind the finite difference method for obtaining the solution of a given partial differential equation is to approximate the derivatives appearing in the equation by a set of values of the function at a selected number of points. The most usual way to generate these approximations is through the use of Taylor series.

The solution domain of the problem over a time $0 \le t \le T$ is covered by a mesh of uniformly-spaced grid-lines:

$$x_j = j\Delta x, j = 0, 1, 2, \ldots, N; \quad (3.1)$$

$$y_i = i\Delta y, i = 0, 1, 2, \ldots, M; \quad (3.2)$$

$$z_k = k\Delta z, k = 0, 1, 2, \ldots, O; \quad (3.3)$$

$$t_n = n\Delta t, n = 0, 1, 2, \ldots, R; \quad (3.4)$$

parallel to the space and time coordinate axes, respectively. Approximations $C^n_{i,j,k}$ to $C(i\Delta y, j\Delta x, k\Delta z, n\Delta t)$ are calculated at the point of intersection of these lines, namely, $(i\Delta y, j\Delta x, k\Delta z, n\Delta t)$ which is referred to as the $(i, j, k, n)$ grid point. The uniform spatial and temporal grid-spacings are $\Delta y = W/M, \Delta x = L/N, \Delta z = H/O$ and $\Delta t = T/R$ where $W$ is the width, $L$ is the length and $H$ is the height of the tunnel.

The finite difference scheme approximates the solution of Equation (2.2) for the inner points; we use the FTCS scheme as described above, with errors of first order in the time interval and second order in spatial coordinate grid spacings:

$$\frac{C^{n+1}_{i,j,k}-C^n_{i,j,k}}{\Delta t} + u(\frac{C^n_{i,j+1,k}-C^n_{i,j-1,k}}{2\Delta x}) + v(\frac{C^n_{i+1,j,k}-C^n_{i-1,j,k}}{2\Delta y}) =$$

$$D_h(\frac{C^n_{i,j+1,k}-2C^n_{i,j,k}+C^n_{i,j-1,k}}{(\Delta x)^2}) + D_h(\frac{C^n_{i+1,j,k}-2C^n_{i,j,k}+C^n_{i-1,j,k}}{(\Delta y)^2}) + D_v(\frac{C^n_{i,j,k+1}-2C^n_{i,j,k}+C^n_{i,j,k-1}}{(\Delta z)^2}). \quad (3.5)$$

Rearrangement of Equation (3.5) gives,

$$\begin{aligned} C_{i,j,k}^{n+1} &= (\tfrac{D_h\Delta t}{\Delta x^2} + \tfrac{u\Delta t}{2\Delta x})C_{i,j-1,k}^{n} + (\tfrac{D_h\Delta t}{\Delta y^2} + \tfrac{v\Delta t}{2\Delta y})C_{i-1,j,k}^{n} + (\tfrac{D_v\Delta t}{\Delta z^2})C_{i,j,k-1}^{n} \\ &+(\tfrac{D_h\Delta t}{\Delta x^2} - \tfrac{u\Delta t}{2\Delta x})C_{i,j-1,k}^{n} + (\tfrac{D_h\Delta t}{\Delta y^2} - \tfrac{v\Delta t}{2\Delta y})C_{i-1,j,k}^{n} + (\tfrac{D_v\Delta t}{\Delta z^2})C_{i,j,k-1}^{n} \\ &+(1 - 2\tfrac{D_h\Delta t}{\Delta x^2} - 2\tfrac{D_h\Delta t}{\Delta y^2} - 2\tfrac{D_v\Delta t}{\Delta z^2})C_{i,j,k}^{n}. \end{aligned} \tag{3.6}$$

The finite difference scheme used here is stable [2, 3] if both

$$D_h\frac{\Delta t}{(\Delta x)^2} + D_h\frac{\Delta t}{(\Delta y)^2} + D_v\frac{\Delta t}{(\Delta z)^2} \le \frac{1}{2}$$

and

$$\frac{u^2\Delta t}{D_h} + \frac{v^2\Delta t}{D_h} \le 3$$

are satisfied.

The finite difference scheme for the first and second normal derivatives at the left-hand end $x = 0$ and the right-hand end $x = L$ are taken to be the one-sided forms:

$$\frac{\partial C}{\partial x}(y_i, x_1, z_k) = \frac{-3C_{i,1,k} + 4C_{i,2,k} - C_{i,3,k}}{2\Delta x}; \tag{3.7}$$

$$\frac{\partial^2 C}{\partial x^2}(y_i, x_1, z_k) = \frac{C_{i,1,k} - 2C_{i,2,k} + C_{i,3,k}}{(\Delta x)^2} \tag{3.8}$$

$$\frac{\partial C}{\partial x}(y_i, x_N, z_k) = \frac{3C_{i,N,k} - 4C_{i,N-1,k} + C_{i,N-2,k}}{2\Delta x}; \tag{3.9}$$

$$\frac{\partial^2 C}{\partial x^2}(y_i, x_N, z_k) = \frac{2C_{i,N,k} - 5C_{i,N-1,k} + 4C_{i,N-2,k} - C_{i,N-3,k}}{(\Delta x)^2}, \tag{3.10}$$

respectively. The first and second derivatives at the corresponding end points in $y-$ and $z-$directions are obtained in the same way. These have the same discretization errors as the central difference forms used in Equation (3.6).

# 4 NUMERICAL EXPERIMENTS

In this section we present four example calculations. In Example 1 we assume that the wind flows steadily only in the $x-$direction and there is no cross wind flow in$y-$ direction ($v = 0$), a distributed pollution source is across part of the inflow end of the tunnel and that turbulent dispersion takes place in three dimensions. Example 2 is similar to Example 1 with the addition of a pollution source on the side wall of the tunnel. In Example 3 we consider Example 2 again and add a cross-wind flow in the $y-$direction. In Example 4 we consider Example 3 but use different dispersion coefficients and some condition of source on the plane $x = 0$.

For simplicity, we assume the tunnel is cubic in shape, and so consider advection and dispersion in the domain $0 \le x \le 1, 0 \le y \le 1$ and $0 \le z \le 1$, with initial and boundary conditions as set out below for each particular example.

## 4.1 Example 1

The three-dimensional advection-diffusion equation:

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}=D_h\frac{\partial^2 C}{\partial x^2}+D_h\frac{\partial^2 C}{\partial y^2}+D_v\frac{\partial^2 C}{\partial z^2} \tag{4.1}$$

is solved with the initial and boundary conditions:

$$\begin{array}{lcll} C(x,y,z,0) & = & 0 & 0\le x\le 1; 0\le y\le 1; 0\le z\le 1\\ C(0,y,z,t) & = & 1 & 0.5\le y\le 1; 0\le z\le 1\\ C(L,y,z,t) & = & 0 & 0\le y\le 1; 0\le z\le 1\\ \frac{\partial C}{\partial y}(x,y,z,t) & = & 0 & on \quad y=0,1; t>0\\ \frac{\partial C}{\partial z}(x,y,z,t) & = & 0 & on \quad z=0,1; t>0. \end{array} \tag{4.2}$$

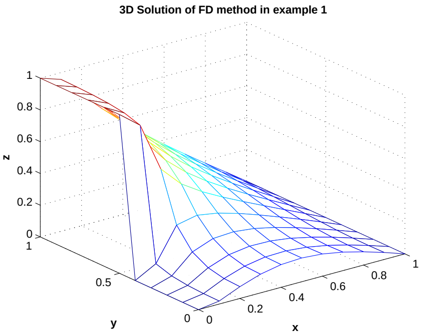
The latter boundary conditions reflect the conditions that there be no dispersive flux of the pollutant through the (solid) side-walls nor through the base and roof. The finite difference scheme for the given equation is:

$$\begin{aligned} \frac{C^{n+1}_{i,j,k}-C^n_{i,j,k}}{\Delta t}+u\left(\frac{C^n_{i,j+1,k}-C^n_{i,j-1,k}}{2\Delta x}\right) &= D_h\left(\frac{C^n_{i,j+1,k}-2C^n_{i,j,k}+C^n_{i,j-1,k}}{(\Delta x)^2}\right)\\ &+D_h\left(\frac{C^n_{i+1,j,k}-2C^n_{i,j,k}+C^n_{i-1,j,k}}{(\Delta y)^2}\right)\\ &+D_v\left(\frac{C^n_{i,j,k+1}-2C^n_{i,j,k}+C^n_{i,j,k-1}}{(\Delta z)^2}\right). \end{aligned}$$

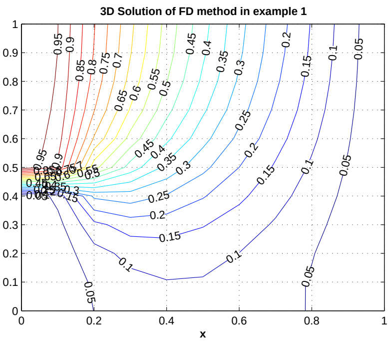
This equation is used to calculate values of $C$ at the internal points $i=2,3,\ldots,M-1; j=2,3,\ldots,N-1; k=2,3,\ldots,O-1$.
Since $\frac{\partial C}{\partial y}=0$ on $y=0,W$, then for $i=2,3,\ldots,M-1; j=1$ and for $k=2,3,\ldots,O-1$ we use the numerical scheme as follows:

$$\begin{array}{lcl} C^n_{i,1,k} & = & \frac{(4C^n_{i,2,k}-C^n_{i,3,k})}{3};\\ C^n_{i,L,k} & = & \frac{(4C^n_{i,L-1,k}-C^n_{i,L-2,k})}{3};\\ C^n_{1,j,k} & = & \frac{(4C^n_{2,j,k}-C^n_{3,j,k})}{3};\\ C^n_{W,j,k} & = & \frac{(4C^n_{W-1,j,k}-C^n_{W-2,j,k})}{3};\\ C^n_{i,j,1} & = & \frac{(4C^n_{i,j,2}-C^n_{i,j,3})}{3};\\ C^n_{i,j,O} & = & \frac{(4C^n_{i,j,O-1}-C^n_{i,j,O-2})}{3}. \end{array}$$

The numerical results are shown in Figure 4. Figure 4 shows the numerical solutions of Example 1 in the case where $\Delta x=\Delta y=\Delta z=0.1\ m; \Delta t=0.01\ s; D_h=D_v=0.1\ m^2\cdot s^{-1}; u=0.02\ m\cdot s^{-1}$ and for the time $T=20\ s$. Note that the boundary conditions ensure that $C$ depends only on $x$ and $y$, but is independent of $z$. The solution shown in Figure 4 is that for all heights $z$ in the tunnel. The results are reasonable, with the boundary conditions satisfied; the concentration decreases away from the source, and is less than one-half of that of the source value over more than three-quarters of the tunnel.




(a)$(i)$




(a)$(ii)$

Figure 4: The numerical solution for Example 1. The solution is independent of height $z$. (a)$(i)$ mesh plot on $z = z_1(= 0)$. (a)$(ii)$ contour plot on $z = z_3(= 0.2)$.

## 4.2 Example 2

The three-dimensional advection-diffusion equation:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D_h\frac{\partial^2 C}{\partial x^2} + D_h\frac{\partial^2 C}{\partial y^2} + D_v\frac{\partial^2 C}{\partial z^2} \tag{4.3}$$

is solved with the initial and boundary conditions:

$$\begin{array}{rcll} C(x,y,z,0) & = & 0 & 0 < x \le 1; 0 < y \le 1; 0 < z \le 1 \\ C(0,y,z,t) & = & 1 & 0.5 \le y \le 1; 0 \le z \le 1 \\ C(x,0,z,t) & = & 1 & 0.3 \le x \le 0.6; 0 \le z \le 1 \\ \frac{\partial C}{\partial x}(0,y,z,t) & = & 0 & 0 < y \le 1; 0 < z \le 1 \\ \frac{\partial C}{\partial y}(x,y,z,t) & = & 0 & \mathit{on} \quad y = 0,1; t > 0 \\ \frac{\partial C}{\partial z}(x,y,z,t) & = & 0 & \mathit{on} \quad z = 0,1; t > 0. \end{array} \tag{4.4}$$

The finite difference scheme for $y_1 = 0 < y_i < y_M = 1$ becomes:

$$\frac{C^{n+1}_{i,j,k} - C^n_{i,j,k}}{\Delta t} + u\left(\frac{C^n_{i,j+1,k} - C^n_{i,j-1,k}}{2\Delta x}\right) =$$

$$D_h\left(\frac{C^n_{1,j+1,k} - 2C^n_{i,j,k} + C^n_{i,j-1,k}}{(\Delta x)^2}\right) + D_h\left(\frac{C^n_{i+1,j,k} - 2C^n_{i,j,k} + C^n_{i-1,j,k}}{(\Delta y)^2}\right) + D_v\left(\frac{C^n_{i,j,k+1} - 2C^n_{i,j,k} + C^n_{i,j,k-1}}{(\Delta z)^2}\right). \tag{4.5}$$

For $x = x_N = 1$ and $y = y_1 = 0$, we use the finite difference scheme:

$$\frac{C^{n+1}_{1,N,k} - C^n_{1,N,k}}{\Delta t} + u(\frac{3C^n_{1,N,k} - 4C^n_{1,N-1,k} + C^n_{1,N-2,k}}{2\Delta x})$$
$$= D_h(\frac{C^n_{1,3,k} - 2C^n_{1,2,k} + C^n_{1,1,k}}{(\Delta x)^2}) + D_h(\frac{C^n_{3,N,k} - 2C^n_{2,N,k} + C^n_{1,N,k}}{(\Delta y)^2}) \tag{4.6}$$
$$+D_v(\frac{C^n_{i,j,k+1} - 2C^n_{i,j,k} + C^n_{i,j,k-1}}{(\Delta z)^2}).$$

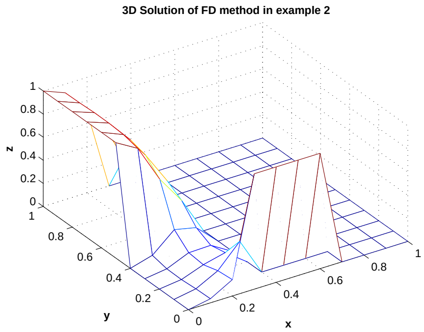
For $x = x_N = 1$ and $y_1 < y_i < 1$, we use the scheme:

$$\frac{C^{n+1}_{i,N,k} - C^n_{i,N,k}}{\Delta t} + u(\frac{3C^n_{i,N,k} - 4C^n_{i,N-1,k} + C^n_{i,N-2,k}}{2\Delta x})$$
$$= D_h(\frac{C^n_{i,N,k} - 2C^n_{i,N,k} + C^n_{i,N,k}}{(\Delta x)^2}) + D_h(\frac{C^n_{i+1,N,k} - 2C^n_{i,N,k} + C^n_{i-1,N,k}}{(\Delta y)^2}) \tag{4.7}$$
$$+D_v(\frac{C^n_{i,N,k+1} - 2C^n_{i,N,k} + C^n_{i,N,k-1}}{(\Delta z)^2}).$$

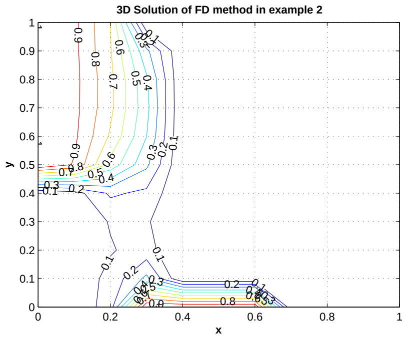
For $x = x_N = 1$ and $y_M = 1$ we use the scheme:

$$\frac{C^{n+1}_{M,N,k} - C^n_{(M,N,k)}}{\Delta t} + u(\frac{3C^n_{M,N,k} - 4C^n_{M,N-1,k} + C^n_{M,N-2,k}}{2\Delta x})$$
$$= D_h(\frac{C^n_{M,N,k} - 2C^n_{M,N,k} + C^n_{M,N,k}}{(\Delta x)^2}) + D_h(\frac{C^n_{M,N,k} - 2C^n_{M-1,N,k} + C^n_{M-2,N,k}}{(\Delta y)^2}) \tag{4.8}$$
$$+D_v(\frac{C^n_{M,N,k+1} - 2C^n_{M,N,k} + C^n_{M,N,k-1}}{(\Delta z)^2})$$

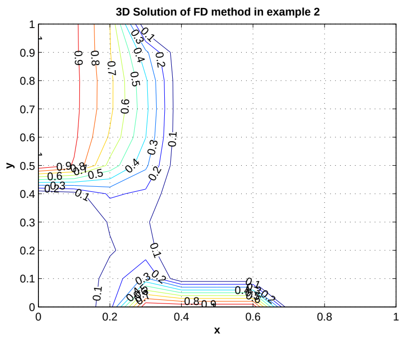
The numerical results are shown in Figure 5. Figure 5 shows the numerical solutions of Example 2 in the case where $\Delta x = \Delta y = \Delta z = 0.1 \quad m; \Delta t = 0.01 \quad s; D_h = D_v = 0.2 \quad m^2 \cdot s^{-1}; u = 1 \quad m \cdot s^{-1}$ and for the time $T = 50 \quad s$. As for Example 1, the boundary conditions are independent of height $z$, so also is the concentration field.



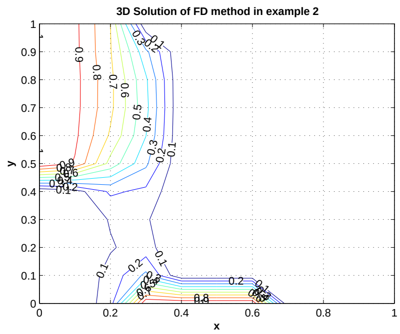

(a)$(i)$




(a)$(ii)$




(a)$(iii)$




(a)$(iv)$

Figure 5: The numerical solution for Example 2. (a)$(i)$ Mesh plot on $z = z_1(= 0)$. (a)$(ii)$ contour plot on $z = z_1$. (a)$(iii)$ contour plot on $z = z_3(= 0.2)$. (a)$(iv)$ contour plot on the top ($z = 1$).

## 4.3 Example 3

The three-dimensional advection-diffusion equation:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} = D_h\frac{\partial^2 C}{\partial x^2} + D_h\frac{\partial^2 C}{\partial y^2} + D_v\frac{\partial^2 C}{\partial z^2} \tag{4.9}$$

is solved with the initial and boundary conditions:

$$\begin{array}{rcll} C(x,y,z,0) & = & 0 & 0 < x \leq 1; 0 < y \leq 1; 0 < z \leq 1 \\ C(0,y,z,t) & = & 1 & 0.5 \leq y \leq 1; 0 \leq z \leq 1 \\ C(x,0,z,t) & = & 1 & 0.3 \leq x \leq 0.6; 0 \leq z \leq 1 \\ \frac{\partial C}{\partial x}(0,y,z,t) & = & 0 & \\ \frac{\partial C}{\partial y}(x,y,z,t) & = & 0 & on \quad y = 0,1 \\ \frac{\partial C}{\partial z}(x,y,z,t) & = & 0 & on \quad z = 0,1. \end{array} \tag{4.10}$$

The finite difference scheme for the given equation is:

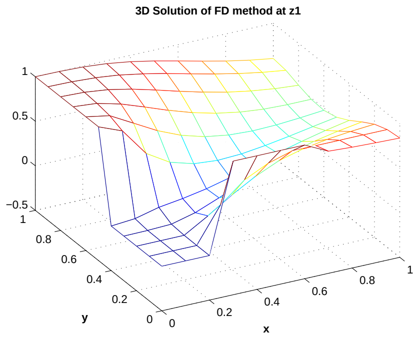
$$\begin{aligned} &\tfrac{C^{n+1}_{i,j,k} - C^n_{i,j,k}}{\Delta t} + u(\tfrac{C^n_{i,j+1,k} - C^n_{i,j-1,k}}{2\Delta x}) + v(\tfrac{C^n_{i+1,j,k} - C^n_{i-1,j,k}}{2\Delta y}) \\ &= D_h(\tfrac{C^n_{1,j+1,k} - 2C^n_{i,j,k} + C^n_{i,j-1,k}}{(\Delta x)^2}) + D_h(\tfrac{C^n_{i+1,j,k} - 2C^n_{i,j,k} + C^n_{i-1,j,k}}{(\Delta y)^2}) \\ &+ D_v(\tfrac{C^n_{i,j,k+1} - 2C^n_{i,j,k} + C^n_{i,j,k-1}}{(\Delta z)^2}). \end{aligned} \tag{4.11}$$

For $x = x_N = 1; y = y_1 = 0; 0 < z_k < O$, we use the finite difference scheme:

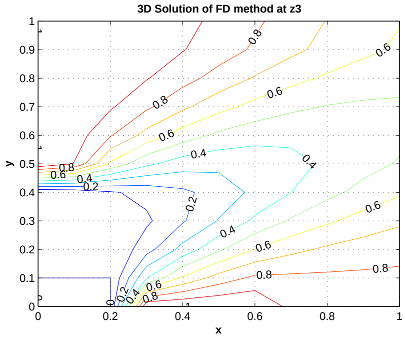
$$\begin{aligned} &\tfrac{C^{n+1}_{1,N,k} - C^n_{1,N,k}}{\Delta t} + u(\tfrac{3C^n_{1,N,k} - 4C^n_{1,N-1,k} + C^n_{1,N-2,k}}{2\Delta x}) + v(\tfrac{-3C^n_{1,N,k} + 4C^n_{2,N,k} - C^n_{3,N,k}}{2\Delta y}) \\ &= D_h(\tfrac{2C^n_{1,N,k} - 5C^n_{1,N-1,k} + 4C^n_{1,N-2,k} - C^n_{1,N-3,k}}{(\Delta x)^2}) + D_h(\tfrac{C^n_{1,N,k} - 2C^n_{2,N,k} + C^n_{3,N,k}}{(\Delta y)^2}) \\ &+ D_v(\tfrac{C^n_{1,N,k+1} - 2C^n_{1,N,k} + C^n_{1,N,k-1}}{(\Delta z)^2}). \end{aligned} \tag{4.12}$$

At $x = x_N = 1; y_1 < y_i < 1; 0 < z_k < O$, we use the scheme:

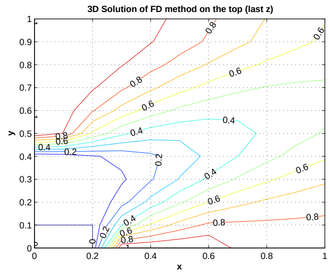
$$\begin{aligned} &\tfrac{C^{n+1}_{1,N,k} - C^n_{1,N,k}}{\Delta t} + u(\tfrac{3C^n_{1,N,k} - 4C^n_{1,N-1,k} + C^n_{1,N-2,k}}{2\Delta x}) + v(\tfrac{C^n_{i+1,N,k} - C^n_{i-1,N,k}}{2\Delta y}) \\ &= D_h(\tfrac{2C^n_{1,N,k} - 5C^n_{1,N-1,k} + 4C^n_{1,N-2,k} - C^n_{1,N-3,k}}{(\Delta x)^2}) + D_h(\tfrac{C^n_{i+1,N,k} - 2C^n_{i,N,k} + C^n_{i-1,N,k}}{(\Delta y)^2}) \\ &+ D_v(\tfrac{C^n_{1,N,k+1} - 2C^n_{1,N,k} + C^n_{1,N,k-1}}{(\Delta z)^2}). \end{aligned} \tag{4.13}$$




(a)($i$)




(a)($ii$)




(a)($iii$)

Figure 6: The numerical solution of Example 3. (a)($i$) mesh plot on $z = z_1(=0)$. (a)($ii$) contour plot on $z = z_3(= 0.2)$. (a)($iii$) contour plot on the top ($z = 1$).

At $x = x_N = 1; y = y_M = 1; 0 < z_k < O$ we use the scheme:

$$\frac{C^{n+1}_{1,N,k} - C^n_{1,N,k}}{\Delta t} + u\left(\frac{3C^n_{1,N,k} - 4C^n_{1,N-1,k} + C^n_{1,N-2,k}}{2\Delta x}\right) + v\left(\frac{3C^n_{M,N,k} - 4C^n_{M-1,N,k} + C^n_{M-2,N,k}}{2\Delta y}\right)$$

$$= D_h\left(\frac{2C^n_{1,N,k} - 5C^n_{1,N-1,k} + 4C^n_{1,N-2,k} - C^n_{1,N-3,k}}{(\Delta x)^2}\right) + D_h\left(\frac{2C^n_{M,N,k} - 5C^n_{M-1,N,k} + 4C^n_{M-2,N,k} - C^n_{M-3,N,k}}{(\Delta y)^2}\right)$$

$$+ D_v\left(\frac{C^n_{1,N,k+1} - 2C^n_{1,N,k} + C^n_{1,N,k-1}}{(\Delta z)^2}\right). \tag{4.14}$$

The numerical results are shown in Figure 6. Figure 6 shows the numerical solutions of Example 3 in the case of $\Delta x = \Delta y = \Delta z = 0.1\ \ m; \Delta t = 0.01\ \ s; D_h = 0.2\ \ m^2{\cdot}s^{-1}, D_v = 0.3\ \ m^2{\cdot}s^{-1}; u = 4\ \ m{\cdot}s^{-1}, v = 2\ \ m{\cdot}s^{-1}$ and for the time $T = 10\ \ s$.

## 4.4 Example 4

The three-dimensional advection-diffusion equation:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} = D_h\frac{\partial^2 C}{\partial x^2} + D_h\frac{\partial^2 C}{\partial y^2} + D_v\frac{\partial^2 C}{\partial z^2} \tag{4.15}$$

is solved with the initial and boundary conditions:

$$\begin{array}{lcll} C(x,y,z,0) & = & 0 & 0 < x \leq 1; 0 < y \leq 1; 0 < z \leq 1 \\ C(0,y,z,t) & = & 1 & 0.5 \leq y \leq 1; 0 \leq z \leq 0.5 \\ C(x,0,z,t) & = & 0.5 & \quad 0.3 \leq x \leq 0.6; 0 \leq z \leq 1 \\ \frac{\partial C}{\partial x}(0,y,z,t) & = & 0 & \\ \frac{\partial C}{\partial y}(x,y,z,t) & = & 0 & on \qquad y = 0,1 \\ \frac{\partial C}{\partial z}(x,y,z,t) & = & 0 & on \qquad z = 0,1; t > 0. \end{array} \tag{4.16}$$

The finite difference scheme for the internal points $y_1 = 0 < y_i < y_M = 1; x_1 = 0 < x_j < x_N = 1$ and $z_1 = 0 < z_k < z_O = 1$ becomes,

$$\frac{C^{n+1}_{i,j,k} - C^n_{i,j,k}}{\Delta t} + u(\frac{C^n_{i,j+1,k} - C^n_{i,j-1,k}}{2\Delta x}) + v(\frac{C^n_{i+1,j,k} - C^n_{i-1,j,k}}{2\Delta x})$$

$$= D_h(\frac{C^n_{i,j+1,k} - 2C^n_{i,j,k} + C^n_{i,j-1,k}}{(\Delta x)^2}) + D_h(\frac{C^n_{i+1,j,k} - 2C^n_{i,j,k} + C^n_{i-1,j,k}}{(\Delta y)^2}) + D_v(\frac{C^n_{i,j,k+1} - 2C^n_{i,j,k} + C^n_{i,j,k-1}}{(\Delta z)^2}). \tag{4.17}$$

At points $x = x_N = 1; y_1 < y_i < 1$ and $z_1 = 0 < z_k < z_O = 1$, we use the finite difference scheme:

$$\begin{aligned} &\frac{C^{n+1}_{i,N,k} - C^n_{i,N,k}}{\Delta t} + u(\frac{3C^n_{i,N,k} - 4C^n_{i,N-1,k} + C^n_{i,N-2,k}}{2\Delta x}) + v(\frac{C^n_{i+1,N,k} - C^n_{i-1,N,k}}{2\Delta y}) \\ &= D_x(\frac{C^n_{i,N,k} - 2C^n_{i,N,k} + C^n_{i,N,k}}{(\Delta x)^2}) + D_y(\frac{C^n_{i+1,N,k} - 2C^n_{i,N,k} + C^n_{i-1,N,k}}{(\Delta y)^2}) \\ &+ D_z(\frac{C^n_{i,N,k+1} - 2C^n_{i,N,k} + C^n_{i,N,k-1}}{(\Delta z)^2}). \end{aligned} \tag{4.18}$$

At the points $y_M = 1; x_1 = 0 < x_j < x_N$ and $z_1 = 0 < z_k < z_O = 1$, we use the scheme:

$$\begin{aligned} &\frac{C^{n+1}_{M,j,k} - C^n_{M,j,k}}{\Delta t} + u(\frac{C^n_{M,j+1,k} - C^n_{M,j-1,k}}{2\Delta x}) + v(\frac{3C^n_{M,j,k} - 4C^n_{M-1,j,k} + C^n_{M-2,j,k}}{2\Delta y}) \\ &= D_h(\frac{C^n_{M,j-1,k} - 2C^n_{M,j,k} + C^n_{M,j+1,k}}{(\Delta x)^2}) + D_h(\frac{2C^n_{M,j,k} - 5C^n_{M-1,j,k} + 4C^n_{M-2,j,k} - C^n_{M-3,j,k}}{(\Delta y)^2}) \\ &+ D_v(\frac{C^n_{i,N,k+1} - 2C^n_{i,N,k} + C^n_{i,N,k-1}}{(\Delta z)^2}). \end{aligned} \tag{4.19}$$

At the points $y_M = 1; x_N = 1$ and $z_1 = 0 < z_k < z_O = 1$, we use the scheme:

$$\frac{C^{n+1}_{M,j,k}-C^n_{M,j,k}}{\Delta t} + u(\frac{3C^n_{M,N,k}-4C^n_{M,N-1,k}+C^n_{M,N-2,k}}{2\Delta y}) + v(\frac{3C^n_{M,j,k}-4C^n_{M-1,j,k}+C^n_{M-2,j,k}}{2\Delta y})$$

$$= D_h(\frac{2C^n_{M,N,k}-5C^n_{M,N-1,k}+4C^n_{M,N-2,k}-C^n_{M,N-3,k}}{(\Delta x)^2}) + D_h(\frac{2C^n_{M,j,k}-5C^n_{M-1,j,k}+4C^n_{M-2,j,k}-C^n_{M-3,j,k}}{(\Delta y)^2})$$

$$+D_v(\frac{C^n_{i,N,k+1}-2C^n_{i,N,k}+C^n_{i,N,k-1}}{(\Delta z)^2}). \tag{4.20}$$

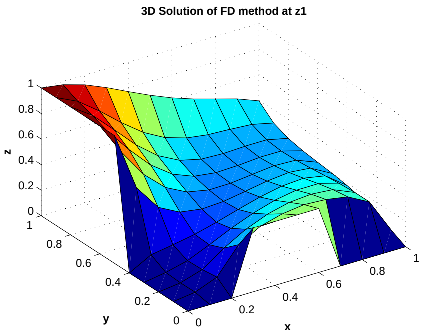
At the bottom of domain $z = z_1 = 0; 0 < x_j \leq x_N = 1$ and $0 < y_i \leq y_M = 1$, since $\frac{\partial C}{\partial z} = 0$ on $z = z_1 = 0$, we use the finite difference scheme:

$$C^n_{i,j,z_1} = \frac{4C^n_{i,j,z_2} - C^n_{i,j,z_3}}{3} \tag{4.21}$$

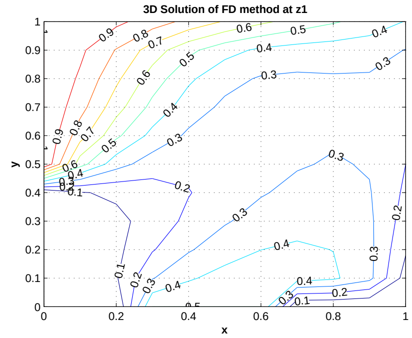
and at the top of domain $z = z_O = 1; 0 < x_j \leq x_N = 1$ and $0 < y_i \leq y_M = 1$, since $\frac{\partial C}{\partial z} = 0$ on $z = z_1 = 0$, we use the finite difference scheme:

$$C^n_{i,j,z_O} = \frac{4C^n_{i,j,z_{O-1}} - C^n_{i,j,z_{O-2}}}{3}. \tag{4.22}$$

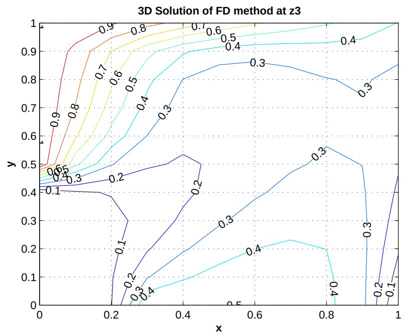
The numerical results are shown in Figure 7. Figure 7 shows the numerical solutions of Example 4 in the case where $\Delta x = \Delta y = \Delta z = 0.1 \;\; m; \Delta t = 0.01 \;\; s; D_h = D_v = 0.1 \;\; m^2 \cdot s^{-1}; u = v = 1 \;\; m \cdot s^{-1}$ and for the time $T = 10 \;\; s$. Figure 8 shows the numerical solutions of Example 4 in the case where $\Delta x = \Delta y = \Delta z = 0.1 \;\; m; \Delta t = 0.01 \;\; s; D_h = 0.2 \;\; m^2 \cdot s^{-1}, D_v = 0.1 \;\; m^2 \cdot s^{-1}; u = 4 \;\; m \cdot s^{-1}, v = 2 \;\; m \cdot s^{-1}$ and for the time $T = 10 \;\; s$.



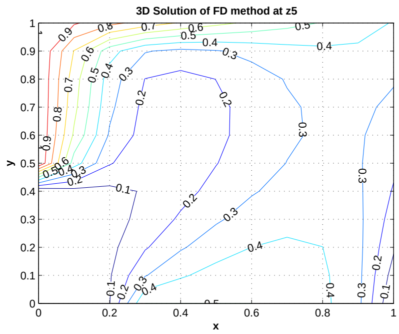

(a)$(i)$



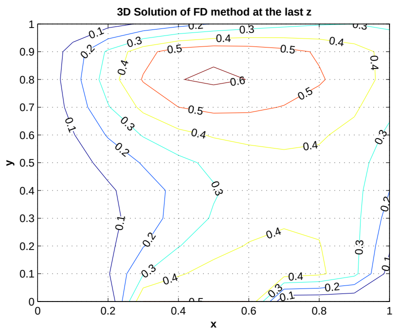

(a)$(ii)$




(a)$(iii)$

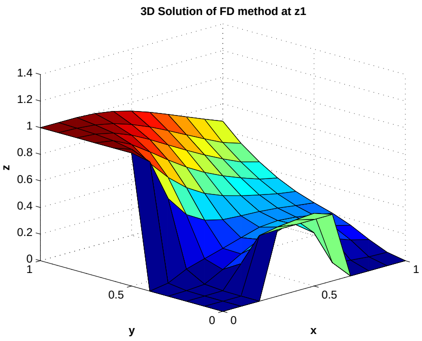



(a)$(iv)$

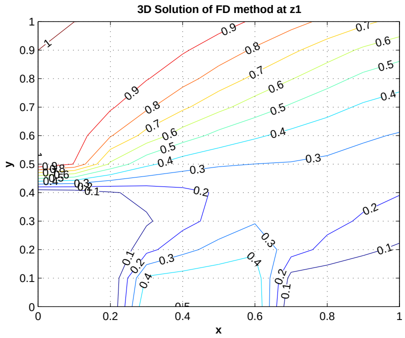



(a)$(v)$

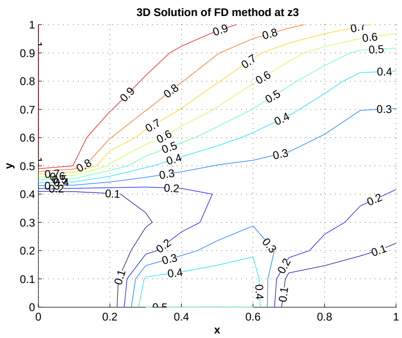
Figure 7: The numerical solution of 3D case Example 4 in the case of $D_h = D_v$. (a)$(i)$ surface plot on $z = z_1 (= 0)$. (a)$(ii)$ contour plot on $z = z_1 (= 0)$. (a)$(iii)$ contour plot on $z = z_3 (= 0.2)$. (a)$(iv)$ contour plot on $z = z_5 (= 0.4)$. (a)$(v)$ contour plot on the top $z = 1$.



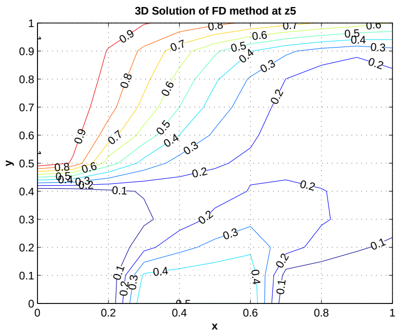

(a)($i$)



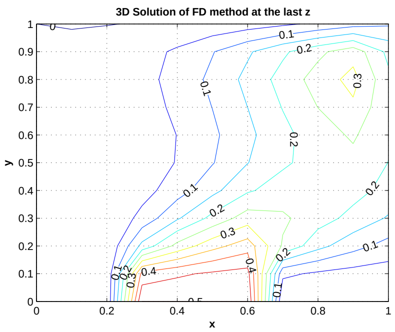

(a)($ii$)




(a)($iii$)




(a)($iv$)




(a)($v$)

Figure 8: The numerical solution of 3D case Example 4 in the case of $D_h \neq D_v$. (a)($i$) surface plot on $z = z_1(= 0)$. (a)($ii$) contour plot on $z = z_1(= 0)$. (a)($iii$) contour plot on $z = z_3(= 0.2)$. (a)($iv$) contour plot on $z = z_5(= 0.4)$. (a)($v$) contour plot on the top $z = 1$.

# 5 CONCLUSION AND DISCUSSION

We have presented some results using a finite difference (FTCS) method for the three-dimensional advection-diffusion equation. We consider two cases: first, we assume that the velocity $v$ in y-direction is equal to zero ($v = 0$) and the second we assume that the velocity $v$ in y-direction is not equal to zero. The numerical experiments of the first case are presented in Example 1 and Example 2 and the numerical experiment of the second case are presented in Example 3 and Example 4, respectively. The numerical solutions in Example 1 and Example 2 depend only on $x$ and $y$, but are independent of $z$. The numerical solutions in Example 3 and Example 4 depend on $x, y$ and $z$.

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## References

[1] E. Sousa, The controversial stability analysis. *Applied Mathematics and Computation*, **145**, 777-794, 2003.

[2] A. C. Hindmarsh, P. M. Gresho and D. F. Griffiths, The stability of explicit Euler time-integration for certain finite difference approximations of the multi-dimensional advection-diffusion equation. *Int. J. Numer. Methods Fluids*, **4**, 853-897, 1984.

[3] M. Dehghan, Numerical solution of the three-dimensional advection-diffusion equation. *Applied Mathematics and Computation*, **150**, 5-19, 2004.

[4] S. Choo-in. Mathematical Model for Determining Carbon Monoxide and Nitrogen Oxide Concentration in Street Tunnel. *M.Sc. Thesis, Thammasat University, Thailand*, 2001.

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