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Explicit Numerical Solution of Three-Dimensional Advection-Diffusion Equation Using Simultaneously Temporal and Spatial Weighted Parameters

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Abstract: Two numerical techniques have been developed and compared for solving the three-dimensional advection-diffusion equation with constant coefficients. These techniques are based on the finite difference methods (FDM). By changing the values of temporal and spatial weighted parameters, solutions are obtained for explicit techniques such as FTCS, FTBSCS schemes. Numerical solution is given for a special case which has been dealt with in the literature and for which an analytical solution has been provided. Comparison of the results has confirmed that the FTBSCS numerical approach matches successfully with the analytical solution while the other technique result in some levels of discrepancy.

Key words: Finite difference methods; advection–diffusion equation; spatial weight; temporal weight explicit techniques.

INTRODUCTION

The significant applications of advection–diffusion equation lie in fluid dynamics (Kumar, 1988), heat transfer (Isenberg, 1972) and mass transfer (Guvanasen, 2004) models. Various approaches are available for solving three-dimensional advection–diffusion partial differential equations. Analytical solutions (Ahmad, 2005; Bear,1990; Dehghan, 2004; Noye. 1988; Zheng, 1995) to solve engineering problems are highly desirable due to the elegant connection that becomes visible between physical and mathematical principles. But the analytical solution of these equations containing complex initial and boundary conditions are usually unavailable. Graphical methods (Welty, 2001), finite element methods (Badrot-Nico, 2007; Hajri, 2007) and finite difference methods (Bear, 1990; Kinzelbach, 1986;Remson, 19871; Wang, 1982; Zheng, 1995) are other approaches for solve partial differential equations (PDEs). Because the analytical solution of partial differential equations containing complex initial and boundary conditions are very difficult, it seems that the finite difference methods are appropriate for solving these equations. In previous work, we solved “one-dimensional” advection-diffusion equation by using the temporal and spatial weighted parameters (Mohammadi). Eq. (1) shows the mathematical form of three-dimensional advection–diffusion phenomenon.

$$\frac{\partial c}{\partial t}+u_x\frac{\partial c}{\partial x}+u_y\frac{\partial c}{\partial y}+u_z\frac{\partial c}{\partial z}=D_x\frac{\partial^2 c}{\partial x^2}+D_y\frac{\partial^2 c}{\partial y^2}+D_z\frac{\partial^2 c}{\partial z^2} \tag{1}$$

with initial condition

$$c(x,y,z,0)=f(x,y,z) \tag{2}$$

and boundary conditions

$$c(0,y,z,t)=g_0(y,z,t) \tag{3}$$

$$c(L_x,y,z,t)=g_1(y,z,t) \tag{4}$$

$$c(x,0,z,t)=h_0(x,z,t) \tag{5}$$

$$c(x,L_y,z,t)=h_1(x,z,t) \tag{6}$$

$$c(x,y,0,t)=k_0(x,y,t) \tag{7}$$

$$c(x,y,L_z,t)=k_1(x,y,t) \tag{8}$$

Where f , g_0, g_1, h_0, h_1, k_0 and k_1 are known functions. u and D are the speed of advection and diffusivity respectively. The domains are $0\le x\le L_x, 0\le y\le L_y$, $0\le z\le L_z$ and $0\le t\le T$.

By changing only the values of temporal ϕ , and spatial θ , weighted parameters, Eq. (1) can be solve by various explicit finite difference methods [Ahmad, 2005; Karhan, 2006; Karhan, 2007).

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Numerical Solution:

The mesh of grid-lines are introduced as

$$x_i = i\Delta x \qquad i = 0,1,2,\ldots,M_x \tag{9}$$

$$y_j = j\Delta y \qquad j = 0,1,2,\ldots,M_y \tag{10}$$

$$z_k = k\Delta z \qquad k = 0,1,2,\ldots,M_z \tag{11}$$

$$t_n = n\Delta t \qquad n = 0,1,2,\ldots,N \tag{12}$$

The constant spatial and temporal grid-spacing are $\Delta x = \frac{L_x}{M_x}, \Delta y = \frac{L_y}{M_y}, \Delta z = \frac{L_z}{M_z}$ and $\Delta t = \frac{T}{N}$, respectively (Karhan, 2006).

Where M denotes the total number of spatial grid-spacing and N denotes the total number of temporal grid-spacing.

Consider the following approximations of the derivatives in the advection–diffusion equation which incorporate time and space weights ϕ and θ as follows:

$$\frac{\partial c}{\partial t} = \frac{c(i,j,k,n+1) - c(i,j,k,n)}{\Delta t} \tag{13}$$

$$\begin{aligned} u_x \frac{\partial c}{\partial x} &= (1-\phi)\left\{\frac{u_x}{\Delta x}\left[(1-\theta)c(i,j,k,n) + \theta c(i+1,j,k,n) - (1-\theta)c(i-1,j,k,n) - \theta c(i,j,k,n)\right]\right\} \\ &+ \phi\left\{\frac{u_x}{\Delta x}\left[(1-\theta)c(i,j,k,n+1) + \theta c(i+1,j,k,n+1) - (1-\theta)c(i-1,j,k,n+1) - \theta c(i,j,k,n+1)\right]\right\} \end{aligned} \tag{14}$$

$$\begin{aligned} u_y \frac{\partial c}{\partial y} &= (1-\phi)\left\{\frac{u_y}{\Delta y}\left[(1-\theta)c(i,j,k,n) + \theta c(i,j+1,k,n) - (1-\theta)c(i,j-1,k,n) - \theta c(i,j,k,n)\right]\right\} \\ &+ \phi\left\{\frac{u_y}{\Delta y}\left[(1-\theta)c(i,j,k,n+1) + \theta c(i,j+1,k,n+1) - (1-\theta)c(i,j-1,k,n+1) - \theta c(i,j,k,n+1)\right]\right\} \end{aligned} \tag{15}$$

$$\begin{aligned} u_z \frac{\partial c}{\partial z} &= (1-\phi)\left\{\frac{u_z}{\Delta z}\left[(1-\theta)c(i,j,k,n) + \theta c(i,j,k+1,n) - (1-\theta)c(i,j,k-1,n) - \theta c(i,j,k,n)\right]\right\} \\ &+ \phi\left\{\frac{u_z}{\Delta z}\left[(1-\theta)c(i,j,k,n+1) + \theta c(i,j,k+1,n+1) - (1-\theta)c(i,j,k-1,n+1) - \theta c(i,j,k,n+1)\right]\right\} \end{aligned} \tag{16}$$

$$\begin{aligned} D_x \frac{\partial^2 c}{\partial x^2} &= (1-\phi)\left\{\frac{D_x}{\Delta x^2}\left[c(i-1,j,k,n) - 2c(i,j,k,n) + c(i+1,j,k,n)\right]\right\} \\ &+ \phi\left\{\frac{D_x}{\Delta x^2}\left[c(i-1,j,k,n+1) - 2c(i,j,k,n+1) + c(i+1,j,k,n+1)\right]\right\} \end{aligned} \tag{17}$$

$$\begin{aligned} D_y \frac{\partial^2 c}{\partial y^2} &= (1-\phi)\left\{\frac{D_y}{\Delta y^2}\left[c(i,j-1,k,n) - 2c(i,j,k,n) + c(i,j+1,k,n)\right]\right\} \\ &+ \phi\left\{\frac{D_y}{\Delta y^2}\left[c(i,j-1,k,n+1) - 2c(i,j,k,n+1) + c(i,j+1,k,n+1)\right]\right\} \end{aligned} \tag{18}$$

$$\begin{aligned} D_z \frac{\partial^2 c}{\partial z^2} &= (1-\phi)\left\{\frac{D_z}{\Delta z^2}\left[c(i,j,k-1,n) - 2c(i,j,k,n) + c(i,j,k+1,n)\right]\right\} \\ &+ \phi\left\{\frac{D_z}{\Delta z^2}\left[c(i,j,k-1,n+1) - 2c(i,j,k,n+1) + c(i,j,k+1,n+1)\right]\right\} \end{aligned} \tag{19}$$

Where ϕ is a time weighting factor and θ is the spatial weighting factor. Substituting Eqs. (13-19) into Eq. (1) gives:

$$c(i,j,k,n+1)=\frac{-1}{A_1}\left[A_0c(i,j,k,n)+B_0c(i+1,j,k,n)+B_1c(i+1,j,k,n+1)\right.$$
$$+D_0c(i-1,j,k,n)+D_1c(i-1,j,k,n+1)+E_0c(i,j+1,k,n)+E_1c(i,j+1,k,n+1) \quad (20)$$
$$+F_0c(i,j-1,k,n)+F_1c(i,j-1,k,n+1)+G_0c(i,j,k+1,n)+G_1c(i+1,j,k+1,n+1)$$
$$\left.+H_0c(i,j,k-1,n)+H_1c(i,j,k-1,n+1)\right]$$

Where

$$A_0=-1+(1-\phi)\ \{(a_x+a_y+a_z)(1-2\theta)+2(s_x+s_y+s_y)\} \quad (21)$$
$$A_1=1+\phi\ \{(a_x+a_y+a_z)(1-2\theta)+2(s_x+s_y+s_y)\} \quad (22)$$
$$B_0=(1-\phi)\ [a_x\theta-s_x] \quad (23)$$
$$B_1=\phi\ [a_x\theta-s_x] \quad (24)$$
$$D_0=-(1-\phi)\ [a_x(1-\theta)+s_x] \quad (25)$$
$$D_1=-\phi\ [a_x(1-\theta)+s_x] \quad (26)$$
$$E_0=(1-\phi)\ [a_y\theta-s_y] \quad (27)$$
$$E_1=\phi\ [a_y\theta-s_y] \quad (28)$$
$$F_0=-(1-\phi)\ [a_y(1-\theta)+s_y] \quad (29)$$
$$F_1=-\phi\ [a_y(1-\theta)+s_y] \quad (30)$$
$$G_0=(1-\phi)\ [a_z\theta-s_z] \quad (31)$$
$$G_1=\phi\ [a_z\theta-s_z] \quad (32)$$
$$H_0=-(1-\phi)\ [a_z(1-\theta)+s_z] \quad (33)$$
$$H_1=-\phi\ [a_z(1-\theta)+s_z] \quad (34)$$

and

$$a_x=u_x\frac{\Delta t}{\Delta x} \quad (35)$$
$$a_y=u_y\frac{\Delta t}{\Delta y} \quad (36)$$
$$a_z=u_z\frac{\Delta t}{\Delta z} \quad (37)$$
$$s_x=D_x\frac{\Delta t}{\Delta x^2} \quad (38)$$
$$s_y=D_y\frac{\Delta t}{\Delta y^2} \quad (39)$$
$$s_z=D_z\frac{\Delta t}{\Delta z^2} \quad (40)$$

Explicit Finite Difference Schemes:

The FTCS Technique:

This scheme uses the forward-difference routine for the time-derivative and centered-difference routine for all spatial derivatives. Application of the technique on solving Eq. (20) for $\phi=0$ and $\theta=0.5$ is depicted below.

$$c(i,j,k,n+1)=\left(s_x+\frac{a_x}{2}\right)\ c(i-1,j,k,n)+\left(s_y+\frac{a_y}{2}\right)\ c(i,j-1,k,n)$$
$$+\left(s_y+\frac{a_y}{2}\right)\ c(i,j-1,k,n)+\left(s_z+\frac{a_z}{2}\right)\ c(i,j,k-1,n)+\left(1-2s_x-2s_y-2s_z\right)\ c(i,j,k,n) \quad (41)$$
$$+\left(s_x-\frac{a_x}{2}\right)\ c(i+1,j,k,n)+\left(s_y-\frac{a_y}{2}\right)\ c(i,j+1,n)+\left(s_z-\frac{a_z}{2}\right)\ c(i,j,k+1,n)$$

The FTBSCS Technique:

This technique - also called the *explicit Upwind* - uses the forward-difference form for the time derivative, centered-difference forms for the diffusive derivatives and backward differences forms for the spatial derivatives in the advection terms. Application of the technique on solving Eq. (20) for $\phi=0$ and $\theta=0$ is depicted below.

$$c(i,j,k,n+1)=\left(s_x+a_x\right)\ c(i-1,j,k,n)+\left(s_y+a_y\right)\ c(i,j-1,k,n) \quad (42)$$
$$+\left(s_z+a_z\right)\ c(i,j,k-1,n)+s_x c(i+1,j,k,n)+s_y c(i,j+1,k,n)$$
$$+s_z c(i,j,k+1,n)+\left(1-2s_x-2s_y-2s_z-a_x-a_y-a_z\right)\ c(i,j,k,n)$$

Numerical Applications:

Example1:

The analytical solution of the three-dimensional advection–diffusion in a region bounded by $0\le x\le 4000$, $0\le y\le 4000$, $0\le z\le 4000$ and $2000\le t\le 3000$ with initial Gaussian pulse of unit height and boundary conditions that given in Eqs. (45-50) is taken from Ref. (Sankaranarayanan, 1998) and given as

$$c(x,y,z,t)=\exp\left[-\frac{(x-1400-u_x t)^2+(y-1400-u_y t)^2+(z-1400-u_z t)^2}{4D_x t}\right] \quad (43)$$

In this example the values of various used parameters are

$$D_x=D_y=D_z=10\ \ m^2/s,\ \ u_x=u_y=u_z=0.2\ \ m/s,\ \ \Delta x=\Delta y=\Delta z=50\ \ m,\ \ \Delta t=50\ \ s$$

Where $t_0=2000s$ is the initial time, and the initial and boundary conditions are

$$c(x,y,z,t_0)=\exp\left[-\frac{(x-1400-u_x t_0)^2+(y-1400-u_y t_0)^2+(z-1400-u_z t_0)^2}{4D_x t_0}\right] \quad (44)$$

$$c(0,y,z,t)=\exp\left[-\frac{(-1400-u_x t)^2+(y-1400-u_y t)^2+(z-1400-u_z t)^2}{4D_x t}\right] \quad (45)$$

$$c(4000,y,z,t)=\exp\left[-\frac{(2600-u_x t)^2+(y-1400-u_y t)^2+(z-1400-u_z t)^2}{4D_x t}\right] \quad (46)$$

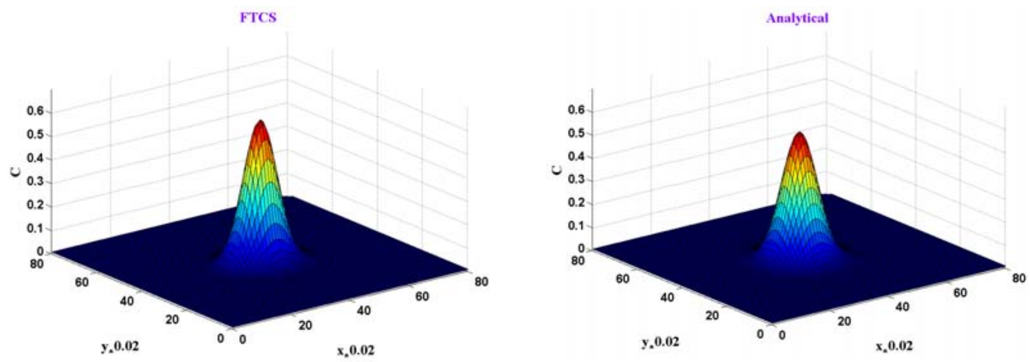
$$c(x,0,z,t)=\exp\left[-\frac{(x-1400-u_x t)^2+(-1400-u_y t)^2+(z-1400-u_z t)^2}{4D_x t}\right] \quad (47)$$

$$c(x,4000,z,t)=\exp\left[-\frac{(x-1400-u_x t)^2+(2600-u_y t)^2+(z-1400-u_z t)^2}{4D_x t}\right] \quad (48)$$

$$c(x,y,0,t)=\exp\left[-\frac{(x-1400-u_x t)^2+(y-1400-u_y t)^2+(-1400-u_z t)^2}{4D_x t}\right] \tag{49}$$

$$c(x,y,4000,t)=\exp\left[-\frac{(x-1400-u_x t)^2+(y-1400-u_y t)^2+(2600-u_z t)^2}{4D_x t}\right] \tag{50}$$

Fig. 1, shows the numerical and analytical solution of Eq. (1) for this example at $z=2000\ m$ and $T=3000\ s$. Regarding this figure, the two explicit numerical methods establish results close to the analytical solution.



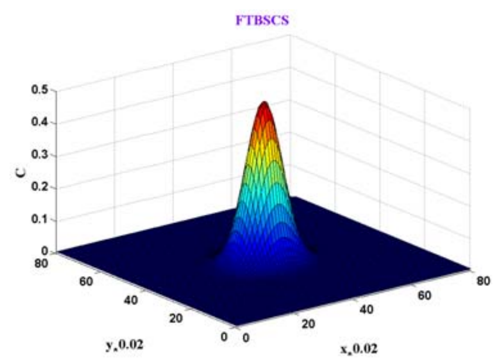


Fig. 1: Numerical and analytical solution of three-dimensional advection-diffusion equation at $z=2000m$ and $T=3000s$ for Example 1.

Fig. 2, depicts the absolute errors of various explicit numerical methods for this example at $z=2000\ m$ and $T=3000\ s$. The maximum absolute error of FTCS and FTBSCS schemes for this example are 0.0771 and 0.0708 respectively.

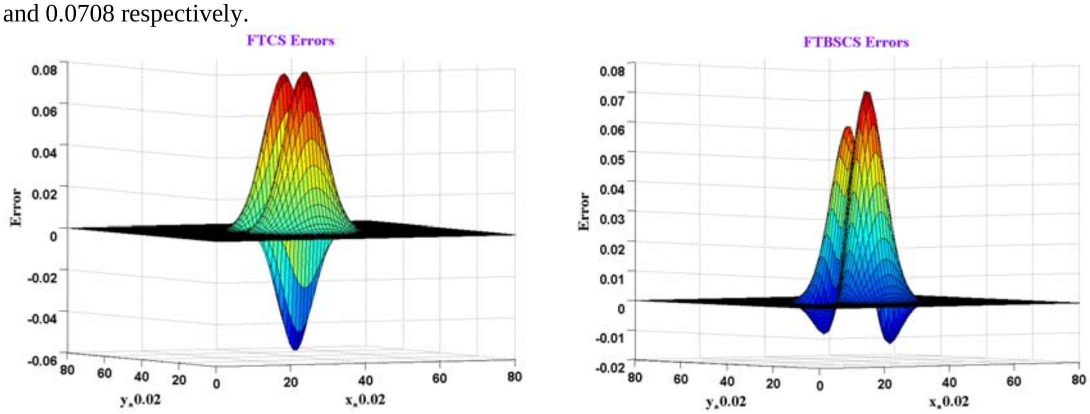


Fig. 2: absolute errors of various numerical methods for Example 1. at $z=2000m$ and $T=3000s$.

Fig. 3. shows the numerical solution of Eq. (1) at $y = 2000\ m$, $z = 2000\ m$ and $T = 3000\ s$ that are compared with analytical solution. This figure also shows the good agreement of FTBSCS scheme with the analytical solution. Fig. 4, depicts the errors of numerical methods at $y = 2000\ m$, $z = 2000\ m$ and $T = 3000\ s$.

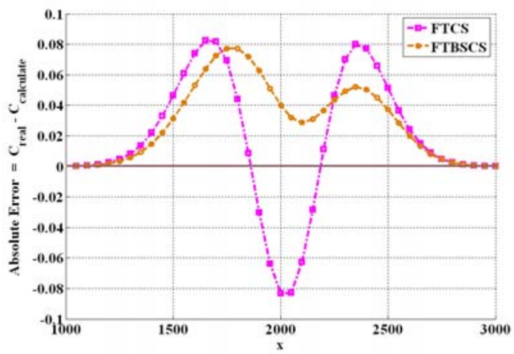


Fig. 3: Comparison of analytical and numerical solutions for Example 1. at $y = 2000m$, $z = 2000m$ and $T = 3000s$.

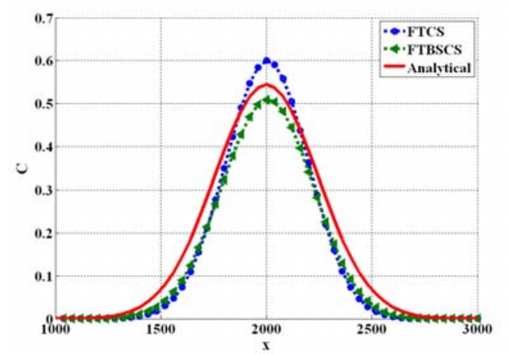


Fig. 4: Absolute errors of implicit methods for Example 1. at $y = 2000m$, $z = 2000m$ and $T = 3000s$.

Conclusions:

Two explicit numerical methods have been applied to solve a three-dimensional advection–diffusion equation. The numerical schemes satisfy this model very good. As just the values of temporal and spatial weighted parameters are changed, the solutions could be determined for explicit techniques such as FTCS and FTBSCS schemes. By comparing the two explicit techniques for determining the numerical solution, it was found that the FTBSCS scheme has a good agreement with analytical results.

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