High Order Finite Difference Schemes for Solving Advection-Diffusion Equation

Abdulrahman Yaghoubi

Department of Applied Mathematics, Saravan Branch, Islamic Azad University, Saravan, Iran. *Corresponding author email: abyaghoobi@phd.guilan.ac.ir

Abstract: In this paper we solve one-dimensional advection diffusion equation (ADE) by high order finite difference formula and compare the results with the exact solution. The basis of analysis of the method considered here is the modified equivalent partial differential equation (MEPDE) approach, developed from the 1974 work of Warming and Hyett.

Keywords: advection-diffusion equation, finite difference schemes.

1. Introduction

Advection Diffusion Equation arises in a wide range of science and industry such as biology, astrophysics, aerospace sciences, environmental problems and particularly in fluid dynamics and transport problems. So this equation has been the focus of many studies [1-13].

One-dimensional ADE with constant coefficient is in the following form

$$\frac{\partial \tau(x,t)}{\partial t} + u \frac{\partial \tau(x,t)}{\partial x} - \alpha \frac{\partial^2 \tau(x,t)}{\partial x^2} = 0.$$
 (1)

This equation describes the change in a scalar function τ caused by diffusion in the x direction, governed by the positive coefficient α and advection in the x direction caused by a fluid moving with a velocity u in the positive xdirection. In this work we use the MEPDE approach to obtain a high order finite-difference formula for solving ADE. In the numerical methods, we need to know the relative accuracy of the resulting approximate solutions. The concept of order of convergence gives a qualitative idea of accuracy. High-order schemes are much more accurate than those of lower order, for a given value of Δx and s. Thus a fourthorder formula is more accurate than a second-order formula, and will be more efficient. When compared with, for example, the Crank-Nicolson formula, the fourth-order formula that we will apply for solving ADE is very much more accurate, but it has much more complicated coefficients and is more restricted in its range of useful (c, s)values.

2. Analysis of the method

Consider the following approximations of the derivatives in the advection-diffusion equation (1)

$$\frac{\partial \tau}{\partial t}\Big|_{i}^{j} \approx \gamma \big[FT \ at \ (i-1,j)\big] + (1-2\gamma)[FT \ at \ (i,j)] + \gamma \big[FT \ at \ (i+1,j)\big],$$

$$\frac{\partial \tau}{\partial x}\Big|_{i}^{j} \approx \theta \Big\{ \phi \big[BS \ at \ (i,j+1) \big] + \Big(1 - \phi \Big) \big[CS \ at \ (i,j+1) \big] \Big\}$$
$$+ (1 - \theta) \Big\{ \phi \big[BS \ at \ (i,j) \big] + (1 - \phi) \big[CS \ at \ (i,j) \big] \Big\},$$

$$\frac{\partial^2 \tau}{\partial x^2}\Big|_i^j \approx \theta[CS \text{ at } (i,j+1)] + (1-\theta)[CS \text{ at } (i,j)].(2)$$

In this equation, FT indicates the use of forward-time approximations, BS indicates the use of backward-space approximations and CS indicates the use of centered-space approximations. γ , θ and ϕ are the weights. Substituting these forms in (1) yield the following finite-difference approximation [14-16].

$$a_{-1}\tau_{i-1}^{j+1} + a_0\tau_i^{j+1} + a_1\tau_{i+1}^{j+1} = b_{-1}\tau_{i-1}^j + b_0\tau_i^j + b_1\tau_{i+1}^j. \eqno(3)$$

where

$$\tau_i^j \approx \tau(x_i, t_i) = \tau(i\Delta x, j\Delta t),$$

$$a_{-1} = 2\gamma - 2\theta s - \theta c(1 + \phi),$$

$$a_0 = 2(1 - 2\gamma + \theta(2s + \phi c))$$

$$a_1 = 2\gamma - 2\theta s - \theta c (1 - \phi),$$

$$b_{-1} = 2\gamma - 2s(\theta - 1) - c(\theta - 1)(1 + \phi), \tag{4}$$

$$b_0 = 2(1 - 2\gamma + (\theta - 1)(2s + \phi c)),$$

$$b_1 = 2\gamma - 2s(\theta - 1) + c(\theta - 1)(1 - \phi).$$

where

$$c = \frac{u\Delta t}{\Delta x}$$
, $s = \frac{\alpha \Delta t}{(\Delta x)^2}$.

The terms of (3) may be replaced by their Taylor expansions about the point $(i\Delta x, j\Delta t)$, we obtain

$$2\Delta t \left[\frac{\partial \tau}{\partial t} + u \frac{\partial \tau}{\partial x} - \left(\alpha + u \phi \frac{\Delta x}{2} \right) \frac{\partial^2 \tau}{\partial x^2} + \frac{\Delta t}{2} \frac{\partial^2 \tau}{\partial t^2} + \theta \frac{\partial^2 \tau}{\partial t \partial x} + u \frac{(\Delta x)^2}{6} \frac{\partial^3 \tau}{\partial x^3} + \frac{(\Delta t)^2}{6} \frac{\partial^3 \tau}{\partial t^3} + \frac{(\Delta t)^3}{24} \frac{\partial^4 \tau}{\partial t^4} - (\alpha + u \phi \Delta x) \frac{(\Delta x)^2}{12} \frac{\partial^4 \tau}{\partial x^4} + \cdots \right]_i^j = 0. (5).$$

Therefore at the $(i,j)^{th}$ grid point, the partial differential equation actually being solved bythe formula (3) is

$$\frac{\partial \tau}{\partial t} + u \frac{\partial \tau}{\partial x} - \left(\alpha + u\phi \frac{\Delta x}{2}\right) \frac{\partial^2 \tau}{\partial x^2} + \frac{\Delta t}{2} \frac{\partial^2 \tau}{\partial t^2} + \theta \frac{\partial^2 \tau}{\partial t \partial x} + u \frac{(\Delta x)^2}{6} \frac{\partial^3 \tau}{\partial x^3} + \frac{(\Delta t)^3}{6} \frac{\partial^3 \tau}{\partial t^3} + \frac{(\Delta t)^3}{24} \frac{\partial^4 \tau}{\partial t^4} (\alpha + u\phi \Delta x) \frac{(\Delta x)^2}{12} \frac{\partial^4 \tau}{\partial x^4} + \dots = 0.$$
 (6)

This equation may be written in a more convenient form by the following procedure, which converts all time derivatives except $\frac{\partial \tau}{\partial t}$ into the spatial derivatives. For elimination term $\frac{\Delta t}{2} \frac{\partial^2 \tau}{\partial t^2}$ we differentiate with respect to time from equation (6) and then multiplying by $-\frac{\Delta t}{2}$, addition of result with (6) yield

$$\frac{\partial \tau}{\partial t} + u \frac{\partial \tau}{\partial x} - \left(\alpha + u \phi \frac{\Delta x}{2}\right) \frac{\partial^2 \tau}{\partial x^2} + u \frac{(\Delta x)^2}{6} \frac{\partial^3 \tau}{\partial x^3} - \left(\alpha + u \phi \Delta x\right) \frac{(\Delta x)^2}{12} \frac{\partial^4 \tau}{\partial x^4} + \left(\theta - u \frac{\Delta t}{2}\right) \frac{\partial^2 \tau}{\partial t^2} - \frac{(\Delta t)^2}{6} \frac{\partial^3 \tau}{\partial t^3} + \dots = 0.$$
(7)

In similar way we can eliminate all time derivatives and obtain the following equation.

$$\begin{split} &\frac{\partial \tau}{\partial t} + u \frac{\partial \tau}{\partial x} - \left(\alpha + u \frac{\Delta x}{2} (c - \phi - 2c\theta)\right) \frac{\partial^2 \tau}{\partial x^2} + u \frac{(\Delta x)^2}{6} [(1 - 6s + 2c^2) - 3c\phi + 6(2s - c^2)\theta - 6\gamma + 6c^2\theta^2 + 6c\theta\phi] \frac{\partial^3 \tau}{\partial x^3} + u \frac{(\Delta x)^3}{24} [2c^{-1}(s - 6c^2 + 12sc^2 - 2c^2 - 3c^4) - (1 - 12s + 12c^2)\phi - 8c^{-1}(3s^2 - 9sc^2 + c^2 + 3c^4)\theta + 24c^{-1}(s - c^2)\gamma + 3c\phi^2 - 36c(2s - c^2)\theta^2 + 12(3c^2 - 2s)\phi\theta + 12\phi\gamma + 48c\theta\phi\gamma - 24c^3\theta^3 - 6c\phi^2\theta - 36c^2\phi\theta^2] \frac{\partial^4 \tau}{\partial x^4} + \dots = 0. \end{split} \tag{8}$$

We set

$$\eta_2(c,s) = c - \phi - 2c\theta$$

$$\eta_3(c,s) = (1 - 6s + 2c^2) - 3c\phi + 6(2s - c^2)\theta - 6\gamma + 6c^2\theta^2 + 6c\theta\phi, \tag{9}$$

$$\begin{split} \eta_4(c,s) &= 2c^{-1}(s-6c^2+12sc^2-2c^2-3c^4) \\ &-(1-12s+12c^2)\phi \\ &-8c^{-1}(3s^2-9sc^2+c^2+3c^4)\theta \\ &+24c^{-1}(s-c^2)\gamma+3c\phi^2-36c(2s-c^2)\theta^2 \\ &+12(3c^2-2s)\phi\theta+12\phi\gamma+48c\theta\phi\gamma \\ &-24c^3\theta^3-6c\phi^2\theta-36c^2\phi\theta^2. \end{split}$$

Therefore, we have

$$\frac{\partial^{\tau}}{\partial t} + u \frac{\partial^{\tau}}{\partial x} - \left(\alpha + u \frac{\Delta x}{2} \eta_{2}(c, s)\right) \frac{\partial^{2} \tau}{\partial x^{2}} + u \frac{(\Delta x)^{2}}{6} \eta_{3}(c, s) \frac{\partial^{3} \tau}{\partial x^{3}} + u \frac{(\Delta x)^{3}}{24} \eta_{4}(c, s) \frac{\partial^{4} \tau}{\partial x^{4}} + \dots = 0.$$
(10)

This equation is called modified equivalent partial differential equation. By setting different coefficients in equation (4) equal to zero and eliminating different leading error terms in (10) by setting corresponding values of $\eta_q(c,s)$ equal to zero we obtain different finite difference formula.

In this work we set

$$\eta_2 = \eta_3 = \eta_4 = 0. \tag{11}$$

Therefore we obtain the following values for the weights γ , θ and ϕ .

$$\gamma = \frac{720c^{2}s^{4} + (24c^{6} - 36c^{2})s^{2} + c^{4}(c^{6} - 3c^{2} + 2)}{1728s^{4} + 128(c^{2} - 1)c^{2}s^{2}},$$

$$\theta = \frac{12s^{2} + (4c^{2} - 2)s + c^{2}(c^{2} - 1)}{24s^{2} + 2c^{2}(c^{2} - 1)},$$

$$\phi = -\frac{2c(2c^{2} - 1)s}{12s^{2} + c^{2}(c^{2} - 1)}.$$
(12)

Substituting these values into (4), it gives the following values

$$\begin{aligned} a_{-1}(c,s) &= c^2(1-c)^2(2-c)(1+c) - 6c(1-c)(1+c - c^2)s - 12(1-3c+3c^2)s^2 + 72s^3, \\ a_0(c,s) &= 2c^2(1-c)(2-c)(1+c)(2+c) - 12c^4s - 24(5-3c^2)s^2 - 144s^3, \end{aligned}$$

$$a_1(c,s) = a_{-1}(-c,s),$$

$$b_{-1}(c,s) = a_{-1}(-c,-s), \tag{13}$$

$$b_0(c,s) = a_0(c,-s),$$

$$b_1(c,s) = a_{-1}(c,-s).$$

By these values we obtain fourth-order formula for solving equation (1).

3. Stability analysis

Carrying out a Von Neuman stability of (3) gives the amplification factor

$$G = \frac{b_{-1} \exp(-i\beta) + b_0 + b_1 \exp(i\beta)}{a_{-1} \exp(-i\beta) + a_0 + a_1 \exp(i\beta)}$$

It follows that

$$|G|^2 - 1 = \frac{F(\chi)}{D(\chi)}$$

where

$$\chi = \cos \beta$$
, so $|\chi| \le 1$ and

$$D(\chi) = (a_0 + (a_{-1} + a_1)\chi)^2 + (a_{-1} - a_1)^2 (1 - \chi^2),$$

$$F(\chi) = 4(b_{-1}b_1 - a_{-1}a_1)\chi^2 + 2(b_0(b_{-1} + b_1) - a_0(a_{-1} + a_1))\chi + (b_0 - a_0)(b_0 + a_0) + (b_{-1} - b_1)^2(a_{-1} - a_1)^2.$$

Since $D(\chi)$ is non-negative then the requirement for stability, namely $|G| \le 1$ for all β , becomes $F(\chi) \le 0$ for all $|\chi| \le 1$.

F(1) = 0 and F'(1) > 0, and since $F(\chi)$ is a quadratic function in χ , to have $F(\chi) \le 0$ requires only $F(-1) \le 0$, or

$$384s(12s^2 - c^4)(12s^2(3c^2 - 2) + c^2(c^2 - 1)^2) \le 0.$$

Firstly since s > 0, we consider case

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$$(12s^2 - c^4) \le 0$$
, $(12s^2(3c^2 - 2) + c^2(c^2 - 1)^2) \ge 0$.

From the first inequality we have $s \le \frac{c^2}{\sqrt{12}}$.

If $3c^2-2\geq 0$, that is $c\geq \sqrt{2/3}$, then the second inequality holds. If $3c^2-2<0$, that is $c<\sqrt{2/3}$, then the following additional inequality is required

$$0 < s \le \frac{c(c^2 - 1)}{\sqrt{12(2 - 3c^2)}},$$

This leads to two stability regions in the (c, s) plane.

i.
$$s \le c^2 / \sqrt{12}$$
, $c \ge \sqrt{2/3}$.

ii.
$$s \le c^2 / \sqrt{12}$$
, $c < \sqrt{2/3}$, $0 < s \le \frac{c(c^2 - 1)}{\sqrt{12(2 - 3c^2)}}$.

Secondly, consider the case

$$(12s^2 - c^4) \ge 0$$
, $(12s^2(3c^2 - 2) + c^2(c^2 - 1)^2) \le 0$

which requires $s \ge c^2/\sqrt{12}$ from the first inequality. The second inequality requires

$$S \le \frac{c(c^2-1)}{\sqrt{12(2-3c^2)}}$$

with
$$c \le \sqrt{\frac{2}{3}}$$
.

4. Numerical results

Consider equation (1) with the following initial and boundary values

$$\tau(x,0)=0, \ x\geq 0,$$

$$\tau(0,t) = 1, \ t > 0, \tag{14}$$

$$\frac{\partial \tau(\infty,t)}{\partial x} = 0, \ t > 0.$$

We suppose

$$u=0.1$$
 , $\alpha=0.05$, $\Delta x=0.1$, $\Delta t=0.1$,

$$x\epsilon[0,2], N=20. \tag{15}$$

Therefore

$$c = \frac{u\Delta t}{\Delta x} = 0.1, s = \frac{\alpha \Delta t}{(\Delta x)^2} = 0.5.$$
 (16)

The exact solution of (1) with condition (14) is as follows [17].

$$\tau(x,t) = \frac{1}{2} \left[erfc\left(\frac{x-ut}{\sqrt{4\alpha t}}\right) + exp\left(\frac{xu}{\alpha}\right) erfc\left(\frac{x+ut}{\sqrt{4\alpha t}}\right) \right], \tag{17}$$

In which

$$erfc(x) = 1 - erf(x),$$
 (18)

$$erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-z^2} dz.$$
 (19)

In figure 1, the numerical solutions for t = 0.5, 1, 1.5, 2, 2.5 are compared with the exact solutions and in table 1 the absolute error is given.

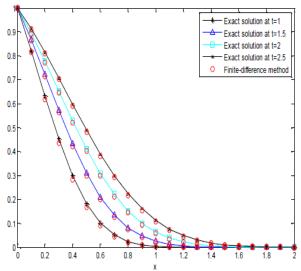


Figure 1. Comparing exact solution and finite difference method at t = 0.5, 1, 1.5, 2, 2.5

Table 1. Absolute error of the finite difference method.

<u> </u>	FD	Exact	Absolute
	method		error
0	1.0000	1.0000	0.0000
0.1	0.8155	0.8219	0.0064
0.2	0.6194	0.6316	0.0122
0.3	0.4352	0.4511	0.0158
0.4	0.2815	0.2981	0.0165
0.5	0.1669	0.1815	0.0146
0.6	0.0904	0.1015	0.0111
0.7	0.0447	0.0520	0.0073
0.8	0.0202	0.0224	0.0042
0.9	0.0083	0.0104	0.0021
1	0.0032	0.0041	0.0009
1.1	0.0011	0.0014	0.0003
1.2	0.0004	0.0005	0.0001
1.3	0.0001	0.0001	0.0000
1.4	0.0000	0.0000	0.0000
1.5	0.0000	0.0000	0.0000
1.6	0.0000	0.0000	0.0000
1.7	0.0000	0.0000	0.0000
1.8	0.0000	0.0000	0.0000
1.9	0.0000	0.0000	0.0000
2	0.0000	0.0000	0.0000

5. Acknowledgments

The authors acknowledge the financial support from Saravan Branch, Islamic Azad University.

6. Conclusion

The results of formula (4) in comparing with other finite difference formulas such as Crank-Nicolson formula, has much more complicated coefficients and is more restricted in its range of useful (c, s) values for stability and solvability, but it is very much more accurate.

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