SCIREA Journal of Mathematics

http://www.scirea.org/journal/Mathematics

April 26, 2019

Volume 4, Issue 2, April 2019

Difference solution and parameter estimation of one dimensional convection-diffusion equation

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Abstract

The Crank-Nicolson and upwind difference schemes are used to solve the one dimensional convection-diffusion equation. Then the numerical solutions obtained and the exact solution are implemented to estimate the parameters, i.e. the convection and diffusion coefficients in this type equation by the least squares method. The simulation results demonstrate that the estimation error by using Crank-Nicolson numerical solution is smaller than that by the upwind difference format. This conclusion tells us that the good accuracy of numerical solution can improve the validity of the estimation parameters in the convection-diffusion equation.

Keywords: Convection-diffusion equation; Crank-Nicolson difference scheme; upwind difference method; parameter estimation.

1. Introduction

The convection-diffusion equation has been widely used in science and engineering. Many physical phenomena such as the distribution of pollutants in pollution, the flow of fluids and heat conduction in fluids [1-8]. It can be used to describe river pollution, air pollution and the mathematical model of viscous fluid flow etc. Therefore, finding a stable and practical numerical method has important theoretical and practical significance.

It is known that upwind difference format is required to be stable under conditions [7-12]. In order to relax the stability conditions and decrease the error in numerical calculation, we apply the Crank-Nicolson implicit difference scheme to solving this type equation [13-18]. In this paper, we use the upwind difference format and the Crank-Nicolson implicit difference scheme to simulate the distribution of the substance with different time and space and compare the errors of the numerical solutions of the windward difference format and the Crank-Nicolson format.

Finally, the two type difference solutions are applied to estimating the convection and diffusion coefficients and time $t = 0.02\text{s}$ and $t = 0.2\text{s}$ by the least squares technique, respectively. By comparison, the result of estimation parameters by the Crank-Nicolson implicit difference format is better than that by the upwind difference solution.

2. Convection-diffusion equation and its difference solution

In this section, we first introduce the one dimensional convection-diffusion equation. Then we specifically analyze the Crank-Nicolson implicit difference format how to applied to solving this type equation.

2.1. One dimensional convection-diffusion equation

we consider the case that the convection-diffusion equation [1]

$$\frac{\partial u}{\partial t} = -v\frac{\partial u}{\partial x} + \mu\frac{\partial^2 u}{\partial x^2}, \qquad x \in R, \quad 0 < t \le T \tag{1}$$

with the initial condition of a Gaussian distribution of the substance in an infinite medium

$$u(x,0) = a\exp\left[-\frac{(x-x_0)^2}{4l_0^2}\right], \tag{2}$$

where v and μ are parameters of velocity component of the fluid and diffusion coefficient, respectively. The constants a, x_0 and l_0 are the initial amplitude, the abscissa of the gravity centre of the profile and a measure of the width of the Gaussian profile, respectively. Thus in a perfect solution, the original bump will move off at a constant speed and widen and decrease in amplitude and the convenient analytical solution is denoted by [1-7]

$$u(x,t) = \frac{al_0}{\sqrt{l_0^2 + \mu t}}\exp\left[-\frac{(x - vt - x_0)^2}{4(\mu t + l_0^2)}\right]. \tag{3}$$

We now return to analyze the Crank-Nicolson type implicit difference format solution of this type equation.

2.2. Preliminaries of difference scheme

For clarity, we begins with a discretization of the spatial and time domains $[0,1] \subset R$ and $[0,T]$, respectively. We subdivide the spatial interval $[0,1]$ into M sub-intervals and the time interval $[0,T]$ into N sub-intervals such that $Mh = 1$ and $N\tau = T$, where h is spatial step and τ denotes time step, respectively. Consequently, the grid points (x_j, t_n) are defined as

$$x_j = jh, \quad j = 0,1,2,\cdots,M, \qquad t_n = n\tau, \quad n = 0,1,2,\cdots,N.$$

Note that solving the numerical solution of Eq.(1) is to find the difference approximation values u_j^n of $u(x,t)$ at the points (x_j, t_n).

2.3. Crank-Nicolson implicit difference format

It is known that the Crank-Nicolson type implicit difference format can be described as [1]

$$\frac{u_j^{n+1}-u_j^n}{\tau}=-\frac{v}{2}\left(\frac{u_{j+1}^n-u_{j-1}^n}{2h}+\frac{u_{j+1}^{n+1}-u_{j-1}^{n+1}}{2h}\right)+\frac{\mu}{2}\left(\frac{u_{j+1}^n-2u_j^n+u_{j-1}^n}{h^2}+\frac{u_{j+1}^{n+1}-2u_j^{n+1}+u_{j-1}^{n+1}}{h^2}\right). \quad (4)$$

Its approximation accuracy is second order $\mathrm{O}\left(\tau^2+h^2\right)$ and another difference form can be demonstrated that

$$\begin{cases}(-\frac{v\tau}{4h}-\frac{\mu\tau}{2h^2})u_{j-1}^{n+1}+(1+\frac{\mu\tau}{h^2})u_j^{n+1}+(\frac{v\tau}{4h}-\frac{\mu\tau}{2h^2})u_{j+1}^{n+1}=(\frac{v\tau}{4h}+\frac{\mu\tau}{2h^2})u_{j-1}^n+(1-\frac{\mu\tau}{h^2})u_j^n-(\frac{v\tau}{4h}+\frac{\mu\tau}{2h^2})u_{j+1}^n, & \\ u_j^0=f(x_j), & j=0,1,2,\cdots,M, \\ u_0^n=g_1(0,t_n),\quad u_1^n=g_2(1,t_n), & n=0,1,2,\cdots,N,\end{cases} \quad (5)$$

where f, g_1 and g_2 are the initial and boundary conditions decided by the analytical solution.

In order to solve the numerical solution u_j^{n+1} from the u_j^n in (5) , we should solve the following linear algebraic systems

$$Au^{n+1}=b(u^n)\,, \quad (6)$$

$$A=\begin{pmatrix} 1+\mu\tau/h^2 & v\tau/4h-\mu\tau/2h^2 & \cdots & 0 & 0 \\ -v\tau/4h-\mu\tau/2h^2 & 1+\mu\tau/h^2 & \cdots & 0 & 0 \\ \cdots & \cdots & \ddots & \cdots & 0 \\ 0 & \cdots & -v\tau/4h-\mu\tau/2h^2 & 1+\mu\tau/h^2 & v\tau/4h-\mu\tau/2h^2 \\ 0 & 0 & \cdots & -v\tau/4h-\mu\tau/2h^2 & 1+\mu\tau/h^2 \end{pmatrix},$$

$$u^{n+1}=\begin{pmatrix} u_1^{n+1} \\ u_2^{n+1} \\ u_3^{n+1} \\ \vdots \\ u_{M-1}^{n+1} \end{pmatrix},$$

$$b(u^n)=\begin{pmatrix} (v/4h+\mu/2h^2)\tau(u_0^{n+1}+u_0^n)+(1-\mu\tau/h^2)u_1^n+(-v/4h+\mu/2h^2)\tau u_2^n \\ (v/4h+\mu/2h^2)\tau u_1^n+(1-\mu\tau/h^2)u_2^n+(-v/4h+\mu/2h^2)\tau u_3^n \\ (v/4h+\mu/2h^2)\tau u_2^n+(1-\mu\tau/h^2)u_3^n+(-v/4h+\mu/2h^2)\tau u_4^n \\ \vdots \\ (v/4h+\mu/2h^2)\tau u_{M-2}^n+(1-\mu\tau/h^2)u_{M-1}^n+(-v/4h+\mu/2h^2)\tau(u_M^n+u_M^{n+1}) \end{pmatrix},$$

where u_j^0 is computed by the initial condition and u_0^{n+1}, u_M^{n+1} can be calculated by the boundary conditions at different time.

We utilize Jacobian iterative method to solve the above linear algebraic systems [1-7]. To be specific, the iterative format is described as

$$u_i^{(k+1)} = \frac{1}{a_{ii}}\left(b_i - \sum_{l=1, l\neq i}^{M-1} a_{il} u_i^{(k)}\right), \tag{7}$$

where a_{il} is the represented element of the matrix A and b_i is the i th element of the constant column $b(u^n)$. Additionally, the condition of stopping iteration is

$$\sum_{i=1}^{M-1} \left|u_i^{(k+1)} - u_i^{(k)}\right| < \varepsilon, \tag{8}$$

where ε is the approximation accuracy.

3. Numerical simulation

In this section , we set the parameters and constants in (1) and (2) as $v=1$, $\mu = 0.01$, $a=1$, $x_0 = -0.5$ and $l_0^2 = 0.003125$, respectively. The the concrete form of Eq.(1) and Eq.(2) is represented as

$$\begin{cases} \dfrac{\partial u}{\partial t} = -\dfrac{\partial u}{\partial x} + 0.01\dfrac{\partial^2 u}{\partial x^2}, & 0<x<1,\quad 0<t<1, \\ u(x,0) = \exp[-(x+0.5)^2/0.00125], & 0<x<1, \end{cases} \tag{9}$$

and its exact solution is

$$u(x,t) = \frac{0.025}{\sqrt{0.000625+0.02t}} \exp[-(x+0.5-t)^2/(0.00125+0.04t)]. \tag{10}$$

and the boundary conditions are decided by the analytical solution (10).

In this example, the spacial and time steps of the difference grid points are set as $\Delta x = h = 0.01$, $\Delta t = \tau = 0.01$, respectively. Then Eq.(9) is numerically solved by the the Crank-Nicolson difference method and the corresponding numerical solution is depicted in Figure 1.

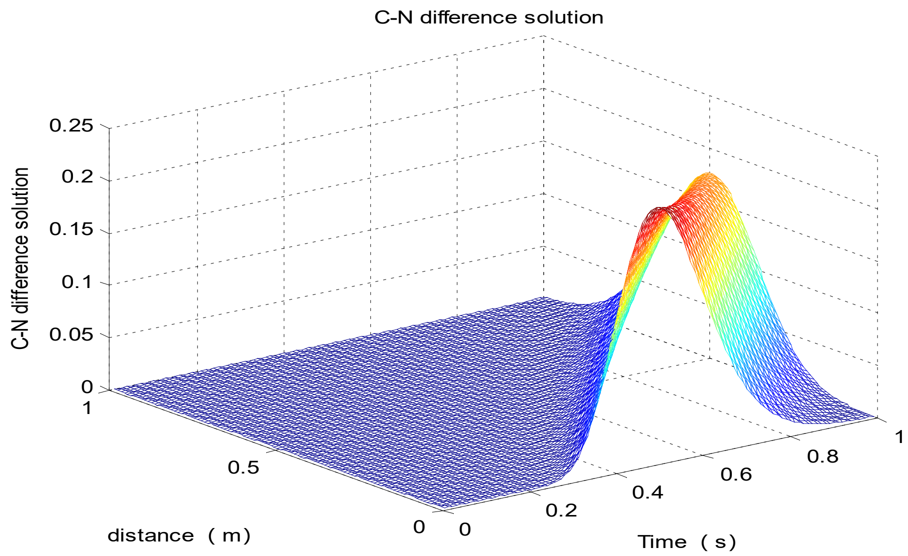

Figure 1. The Crank-Nicolson difference solution at different space and time

Accordingly, Figure 2 describes the absolute errors between the Crank-Nicolson difference and the exact solutions are described at the grid points. Correspondingly, the L_1 error of this scheme is 0.0037.

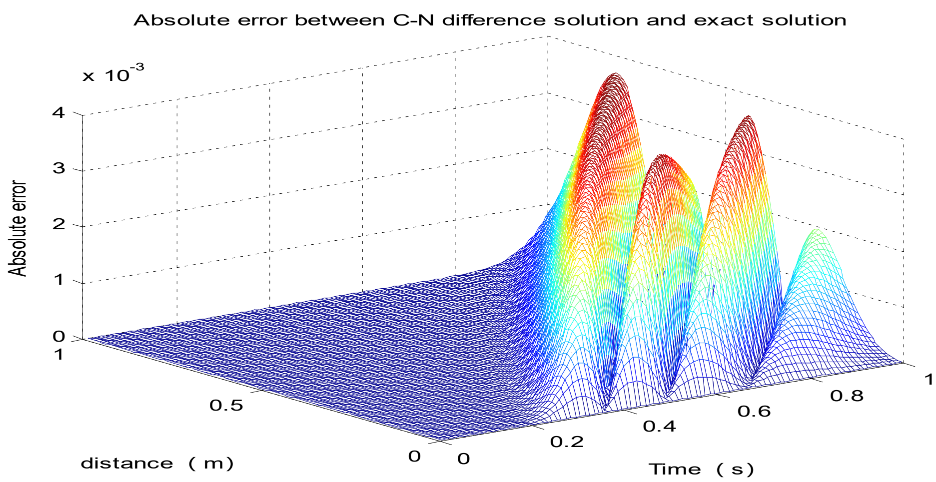

Figure 2. The error of the Crank-Nicolson difference solution compared with exact solution

We also consider the situation that the extended spacial and time domains to $[0,5]\times[0,5]$. Similarly, the numerical solution is demonstrated in Figure 3 and the L_1 error of this scheme is 0.027.

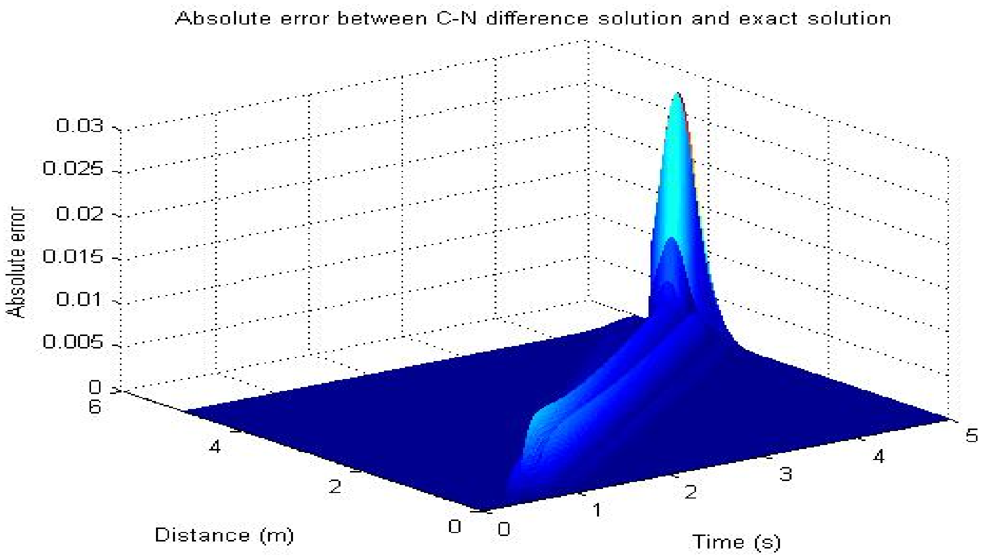

Figure 3. The error of the Crank-Nicolson difference solution compared with exact solution in extended domains

Furthermore, we fixed the time $t = 0.75$ and compare the two types difference solutions with the analytical solution. The comparison results are shown in Figure 4 and the the L_1 errors of the the Crank-Nicolson difference scheme and the upwind difference method are 0.0037 and 0.0334, respectively.

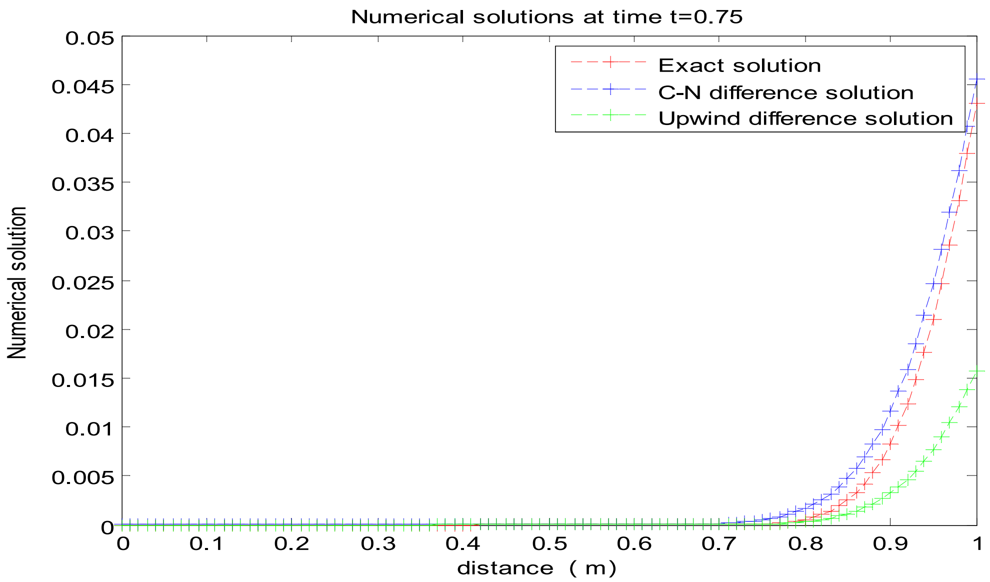

Figure 4. Comparisons of the difference methods with exact solution at *t*=0.75

From Fig. 3 and Fig. 4, we can see that the approximation solutions is obtained by using the Crank-Nicolson difference scheme is better than that by the upwind difference method.

4. Estimation parameters in convection-diffusion model

In this section, we utilize the above the Crank-Nicolson and upwind difference schemes to estimate the unknown parameters v and μ of the convection-diffusion equation.

We firstly use the values $u(x_j,t_n)$ of the analytical solution at the grid points (x_j,t_n) as given sets of data. Secondly, we solve the numerical solution u_j^n in (9) by using the Crank-Nicolson difference scheme. Finally, we apply the least squares technique to optimally adapting this model to the data $u(x_j,t_n)$ by determining the parameter values for v and μ. Then the deviation of model and data is minimized by the form

$$\arg\min_{v,\mu} \sum_{j=0}^{M}\sum_{n=0}^{N}\left|u(x_j,t_n)-u_j^n\right|^2, \tag{11}$$

where u_j^n is the Crank-Nicolson difference solution at the grind point. Then, by using this difference numerical solution at time $t = 0.02$, $t = 0.2$ and the least squares method, the estimated values Ev , $E\mu$ of the parameters v , μ in Eq.(9) are described in Table 1, respectively.

Table 1. The results of parameters estimated by the the Crank-Nicolson difference scheme

Method	t	Ev	v	$E\mu$	μ
Exact solution	**0.02**	**1**	**1**	**0.01**	**0.01**
C-N difference Solution	0.02	0.9809	1	0.0099	0.01
Upwind difference solution	0.02	0.8862	1	0.0101	0.01
Exact solution	**0.2**	**1**	**1**	**0.01**	**0.01**
C-N difference Solution	0.2	0.9984	1	0.0099	0.01
Upwind difference solution	0.2	0.7411	1	0.0126	0.01

From the results in Table 1, we know that the estimation by using the Crank-Nicolson difference solution is better than that by using the upwind difference solution. Consequently, we can find other validity methods for solving Eq.(9) to get good the parameter estimation.

5. Conclusion

In this paper, the Crank-Nicolson implicit difference scheme and the upwind difference scheme are used to solve the one-dimensional convection-diffusion equation. By using the least squares method, the parameters in Eq.(9) are estimated. The estimated values of the two parameters show that the the Crank-Nicolson difference scheme is better than upwind difference method used to estimate the parameters. Furthermore, better approximation solution to Eq.(1) developed can improve the accuracy of the parameters estimated.

Acknowledgments

This work is funded by Research Projects of Pre-research Fund of International college of Liangjiang, Chongqing University of Technology.

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