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Numerical Solution of Diffusion Equation by Finite Difference Method

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Abstract: *In this work error estimation for numerical solution of Diffusion equation by finite difference method is done. The Explicit centered difference scheme is described to find the numerical approximation of the Diffusion equation. The numerical scheme is implemented in order to perform the numerical features of error estimation. To get analytic solution, we present the variable separation method. We develop a computer program to implement the finite difference method in scientific programming language. An example is used for comparison; the numerical results are compared with analytical solutions.*

Keywords*: Analytic solution, Diffusion equation, Finite difference scheme, Initial value problem (IVP), Relative error.*

I. Introduction

In Mathematics, the finite difference methods are numerical methods for approximating the solutions to differential equations using finite difference equations to approximate derivatives. Our goal is to approximate solutions to differential equations.i, e. to find a function (or some discrete approximation to this functions) which satisfies a given relationship between several of its derivatives on some given region of space /and or time, along with some boundary conditions along the edges of this domain. A finite difference method proceeds by replacing the derivatives in the differential equation by the finite difference approximations. This gives a large algebraic system of equations to be solved in place of the differential equation, something that is easily solved on a computer.

In (A.N. Richmond, 2006), the authors develop the analytical solutions of non-trivial examples of a well-known class of initial-boundary value problems which, by the choice of parameters, can be reduced to regular or singular Sturm-Liouville problems. In (Sweilam et. al, 2012) the author presents the C-N-FDM to solve the linear time fractional diffusion equation. They claimed that the C-N-FDM gives good results. The authors studied the Spectral methods for solving the one dimensional parabolic heat equation (Juan- Gabriel et. al 2006). In (Hikment Koyunbakan and Emrah Yilmaz, 2010), the Authors claimed that The ADM method is more accurate. In (Subir et. al, 2011), the authors present the Adomian Decomposition method to solve the nonlinear diffusion equation with fractional time derivatives. With the above discussion in view, our intention is to investigate mathematical models, to establish the stability condition of the numerical scheme and to analyze the error of the scheme.

In section 2, present a short discussion on the derivation of Diffusion equation as IBVP. In section 3, the analytical solution of diffusion equation is illustrated by variable separation method. We describe an explicit centered difference scheme for Diffusion equation as an IBVP with two sided boundary conditions in section 4. In section 4, we also set up the stability condition of the numerical scheme. In section 5, we develop a computer program in scientific programming language for the implementation of the numerical scheme and perform numerical simulations in order to verify the behavior for various parameters. Finally the conclusions of the paper are given in the last section.

II. Governing Equation And Its Derivation:

In this study we consider the governing equation as IBVP

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$

c is the concentration at the point x at the time t , D is the diffusive constant in the x direction, t is the time.
With appropriate initial and boundary condition

$$c(t_0, x) = c_0(x); a \le x \le b$$

$$c(t, a) = c_a(t); t_0 \le t \le T$$

$$c(t, b) = c_b(t)$$

Consider the equation of mass conservation of the tracer. The continuity equation states that divergence of mass flux equals change in mass in a control volume.

$$-\nabla \bullet \rho \bar{q} = \frac{\partial \rho c}{\partial t}$$

If we assume that ρ is constant in time and space, the continuity equation can be written as

$$-\nabla \bullet \bar{q} = \frac{\partial c}{\partial t}$$

Using Fick's law for $\bar{q}$, we have a general Diffusion equation

$$\nabla \bullet D\nabla c = \frac{\partial c}{\partial t}$$

If D is constant, the diffusion equation is given by as

$$D\nabla^2 c = \frac{\partial c}{\partial t}$$

The diffusion coefficient theoretically is a tensor. However, for most cases, we assume it is a scalar. The diffusion equation written in the Cartesian coordinate system in a one dimensional.

$$D\frac{\partial^2 c}{\partial x^2} = \frac{\partial c}{\partial t}$$

III. Analytical Solution Of The Governing Equation By The Method Of Variable Separation:

Consider $c = XT$ be the solution of the diffusion equation

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \quad t_0 \le t \le T \quad a \le x \le b \tag{1}$$

with the homogeneous boundary condition

Initial condition $c(x,0) = c_0$, and boundary condition $c(0,t) = 0$, $c(L,t) = 0$, $0 \le x \le L$

Then $\frac{\partial c}{\partial t} = XT'$, $\frac{\partial c}{\partial x} = X'T$ and $\frac{\partial^2 c}{\partial x^2} = X''T$.

Now from the given equation, we have

$$\frac{T'}{DT} = \frac{X''}{X} \tag{2}$$

Each side of (2) must be constant,

$$\frac{T'}{DT} = \frac{X''}{X} = -\lambda^2 \text{ (say)}$$

Then $T' + D\lambda^2 T = 0$ and $X'' + \lambda^2 X = 0$ whose solution are,

$T = C_1 e^{-D\lambda^2 t}$ and $X = A_1 \cos\lambda x + B_1 \sin\lambda x$

Thus a solution of the partial differential equation is

$$c(x,t) = (A_1 \cos\lambda x + B_1 \sin\lambda x) C_1 e^{-D\lambda^2 t} = e^{-D\lambda^2 t}(A\cos\lambda x + B\sin\lambda x) \qquad (3)$$

Applying the boundary condition

Since $c(0,t) = 0$, $\Rightarrow 0 = Ae^{-D\lambda^2 t}$

$A = 0$, since $e^{-D\lambda^2 t} \neq 0$.

Thus from (3), we have

$$c(x,t) = Be^{-D\lambda^2 t} \sin\lambda x \qquad (4)$$

Since $c(L,t) = 0$, $\Rightarrow 0 = Be^{-D\lambda^2 t} \sin\lambda L$

If $B = 0$ the solution is identically zero, so we must have $\sin\lambda L = 0$ since $B \neq 0$, $e^{-D\lambda^2 t} \neq 0$ $\lambda = \frac{n\pi}{L}$, $n = 0, \pm 1, \pm 2, \ldots\ldots\ldots$

By the principle of superposition

The solution is

$$c(x,t) = \sum_{n=1}^{\infty} B_n e^{-\frac{n^2\pi^2}{L^2}Dt} \sin\frac{n\pi}{L}x \qquad (5)$$

In order to satisfy the last condition, $c(x,0) = \sum_{n=1}^{\infty} B_n \sin\frac{n\pi}{L}x$

Using Fourier series, $B_n = \frac{2}{L}\int_0^L c(x,0)\sin\frac{n\pi}{L}x dx$

The solution of the governing equation can be written as follows

$$c(x,t) = \sum_{n=1}^{\infty} \left(\frac{2}{L}\int_0^L c(x,0)\sin\frac{n\pi}{L}x dx\right) e^{-\frac{n^2\pi^2}{L^2}Dt} \sin\frac{n\pi}{L}x \qquad (6)$$

IV. Formulation Of The Diffusion Equation

We would like to consider the diffusion equation as an initial and homogeneous boundary value problem

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \ , \ t_0 \le t \le T \ , \ a \le x \le b$$

Initial condition $c(x,0) = c_0$, and boundary condition $c(0,t) = 0$, $c(L,t) = 0$

In order to develop the scheme, we discretize the $x - t$ plane by choosing a mesh width $h \equiv \Delta x$ space and a time step $k \equiv \Delta t$. The finite difference methods we will develop produce approximations $c_i^n \in R^n$ to the solution $c(x_i, t_n)$ at the discrete points by

$$x_i = ih \ , \quad i = 0,1,2,3.....$$
$$t_n = nk \ , \quad n = 0,1,2,3.....$$

Let the solution $c(x_i, t_n)$ be denoted by C_i^n and its approximate value by c_i^n.

Simple approximations to the first derivative in the time direction by forward difference can be obtained from

$$\frac{\partial c}{\partial t} \approx \frac{C_i^{n+1} - C_i^n}{\Delta t} + o(\Delta t)$$

Discretization of $\frac{\partial^2 c}{\partial x^2}$ is obtain from second order central difference in space.

$$\frac{\partial^2 c}{\partial x^2} \approx \frac{C_{i-1}^n - 2C_i^n + C_{i+1}^n}{\Delta x^2} + o(\Delta x^2)$$

We obtain

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = D\frac{C_{i-1}^n - 2C_i^n + C_{i+1}^n}{\Delta x^2} + o(\Delta t + \Delta x^2) \qquad (7)$$

The terms $o(\Delta t + \Delta x^2)$ denote the order of the method. Neglecting the error terms and simplifying. We obtain the difference methods

$$\Rightarrow c_i^{n+1} = \frac{D\Delta t}{\Delta x^2}c_{i-1}^n + (1 - 2\frac{D\Delta t}{\Delta x^2})c_i^n + \frac{D\Delta t}{\Delta x^2}c_{i+1}^n \qquad (8)$$

This is the required explicit centered difference scheme for the IBVP

$$c_i^{n+1} = \lambda c_{i-1}^n + (1 - 2\lambda)c_i^n + \lambda c_{i+1}^n \qquad (9)$$

This scheme uses a second order central difference in space and the first order forward Euler scheme in time.

Where $\lambda = \frac{D\Delta t}{\Delta x^2}$ Note that if $0 < \lambda \le \frac{1}{2}$, then the solution at the new time is a weighted average of the solution at the old time .This implies a discrete maximum principle, and therefore numerical stability. It also implies monotonocity: if $c_{i+1}^n - c_i^n$ for all i, then

$$c_{i+1}^{n+1} - c_i^{n+1} = \lambda(c_i^n - c_{i-1}^n) + (1 - 2\lambda)(c_{i+1}^n - c_i^n) + \lambda(c_{i+2}^n - c_{i+1}^n) > 0$$

However, we must choose the time step to be small: we must have $\lambda \le \frac{1}{2}$, or equivalently that $\Delta t \le \frac{\Delta x^2}{2D}$

This time step restriction typically requires an unacceptably large number of time steps, unless the diffusion constant D is very small.

4.1 Stability of the explicit centered difference scheme (8) is given by the conditions $0 \le \frac{D\Delta t}{\Delta x^2} \le \frac{1}{2}$

Proof: The explicit centered difference scheme (8) takes the form

$$=> c_i^{n+1} = \frac{D\Delta t}{\Delta x^2} c_{i-1}^n + (1 - 2\frac{D\Delta t}{\Delta x^2}) c_i^n + \frac{D\Delta t}{\Delta x^2} c_{i+1}^n$$

$$c_i^{n+1} = \lambda c_{i-1}^n + (1-2\lambda) c_i^n + \lambda c_{i+1}^n \qquad (10)$$

Where $\lambda = \frac{D\Delta t}{\Delta x^2}$

The equation (10) implies that if $0 < \lambda \le \frac{1}{2}$, and then the solution at the new time is a weighted average of the solution at the old time. This implies a discrete maximum principle. We can conclude that the explicit centered difference scheme (10) is stable for

$$0 \le \lambda = D\frac{\Delta t}{\Delta x^2} \le \frac{1}{2}$$

V. Error Estimation Of The Scheme:

In order to perform error estimation, we consider the exact solution of the model equation with initial condition $c(x,0) = c_0(x) = x(1-x)$ and homogeneous boundary condition. We get

$$c(x,t) = \sum_{n=1}^{\infty} (\frac{2}{L} \int_0^L c(x,0) \sin\frac{n\pi}{L} x dx) e^{-\frac{n^2\pi^2}{L^2} Dt} \sin\frac{n\pi}{L} x$$

We compute the error defined by

$$\|e\| = \frac{\|C_e - C_N\|}{\|C_e\|}$$

for all time where C_e is the exact solution and c_N is the Numerical solution computed by the finite difference scheme.

5.1Results And Discussion:

We solve the diffusion equation by implementing the centered difference scheme, while varying the different parameter values.

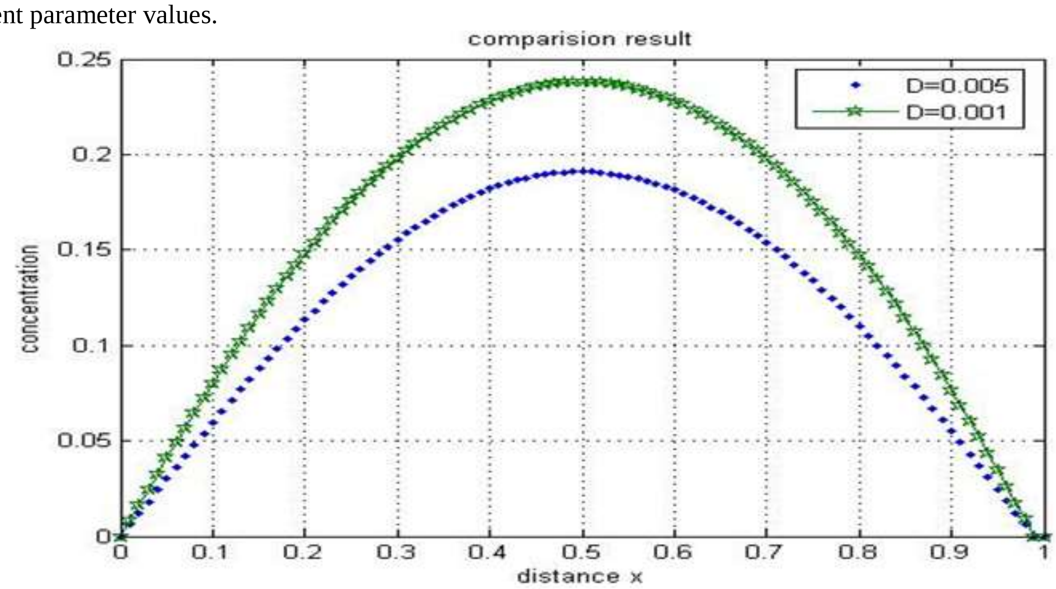

Figure 1: The behavior of numerical solution at $D = 0.001m^2/s$, $0.005m^2/s$.

Concentration distribution for each diffusion rate at time t=24 min. In figure-1, the profile for varying contaminant diffusion rate, we saw that the contaminant concentration with a higher diffusion rate decreases at a higher rate than that with a lower diffusion rate. The curve marked by "star" shows the concentration profile for diffusion rate $D = 0.001m^2/s$ and the curve visible by "dot line" represents the concentration profile for diffusion rate $D = 0.005m^2/s$

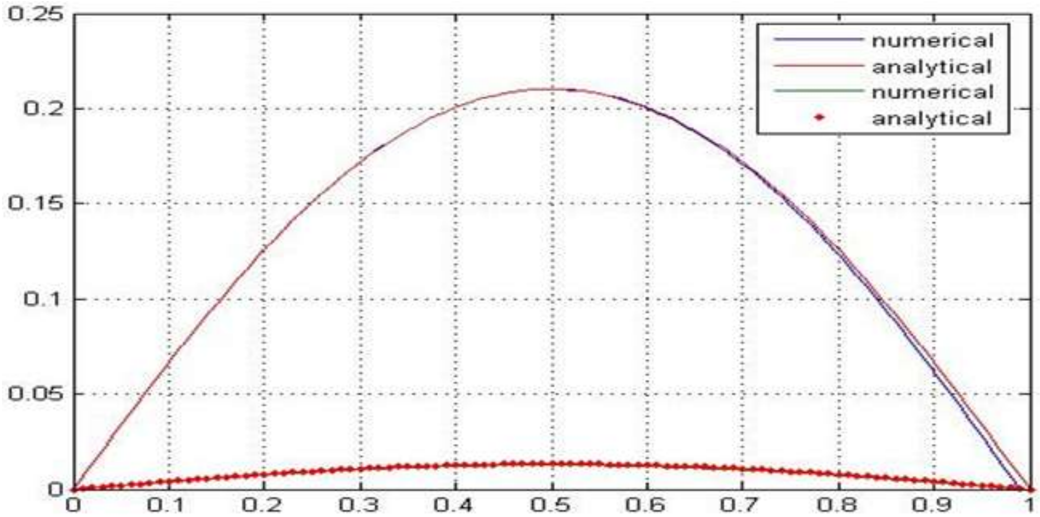

Figure 2: Analytic solution and Numerical solution at different time Analytical solution of diffusion equation is compared with the numerical solution at different time in figure-2. The curve noticeable by "blue line" shows the numerical solution, the curve visible by "red line" represents numerical solution. The results are very close.

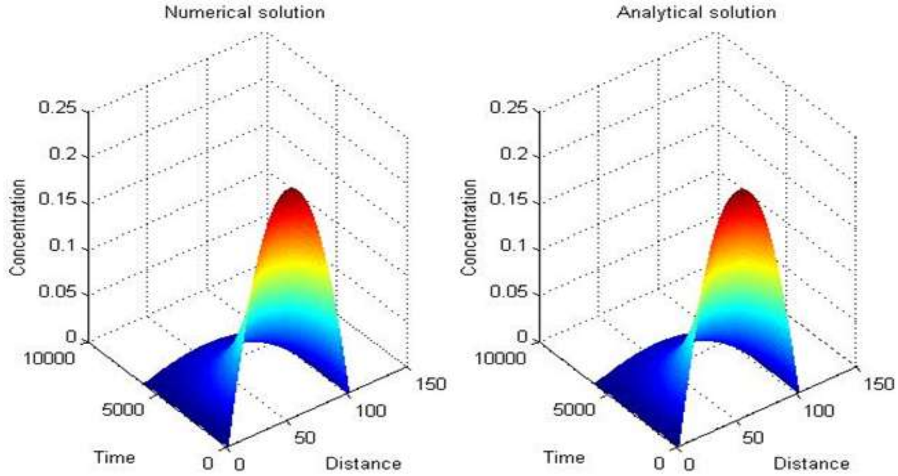

Figure 3: The Numerical solution and Analytical solution in mesh.

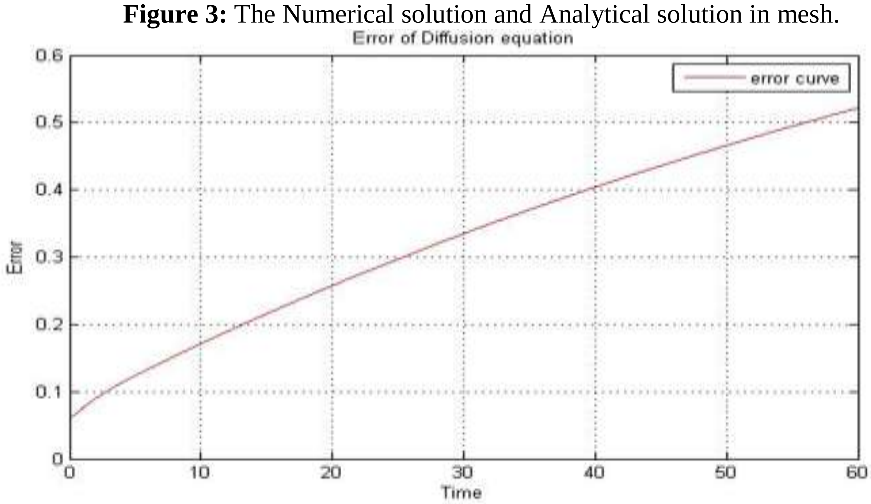

Figure 4: The error in the numerical result is shown for Δx=0.1

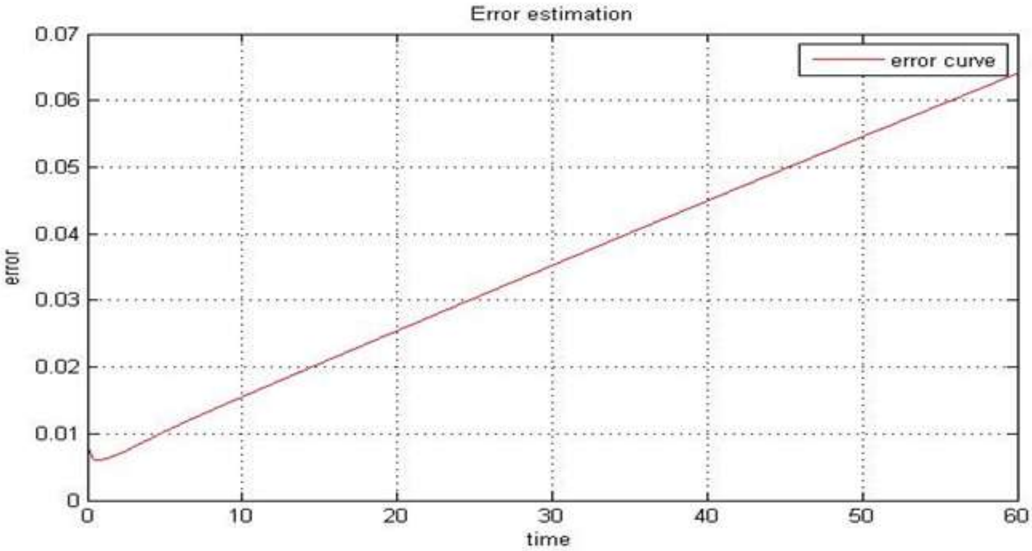

Figure 5: The error in the numerical result is shown for Δx=0.01

Figure-4 and figure-5 shows the error in the numerical solution from each of the methods when compared with the analytical solution, for the atwo cases N=10, N=100, corresponding to Δx=0.1, 0.01 respectively. Comparisons are made for the solution at different time for smaller Δx the errors reduce in size. The errors for the central difference scheme decrease as the grid size decrease.

VI. Conclusion:

The study has presented the numerical and analytical solution of Diffusion equation. The explicit centered difference scheme is used in order to perform the numerical features of error estimation. We have seen that the contaminant concentration with a higher diffusion rate decreases at a higher rate than that with a lower diffusion rate. In order to execute the numerical method we have developed a computer program in the language of scientific computing that is a very good agreement of the finite difference method for Diffusion equation.

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