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Error Estimation of an Explicit Finite Difference Scheme for a Water Pollution Model

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Abstract: *In this paper, we present the solution of one dimensional advection diffusion equation for initial condition in infinite space analytically by transform to heat equation via coordinate transformation. A comparison among explicit upwind difference scheme, explicit centered difference scheme and explicit downwind difference scheme is projected herein with a variety of numerical results and relative errors. Our goal is to investigate the efficient numerical schemes for advection diffusion equation.*

Keywords: *Advection Diffusion Equation, Explicit Scheme, Relative Errors.*

I. Introduction

The mathematical model describing the transport and diffusion processes is the one dimensional advection-diffusion equation (ADE): $\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}=D\frac{\partial^2 C}{\partial x^2}$ with constant coefficients. Mathematical modeling of heat transport, pollutants, and suspended matter in water and soil involves the numerical solution of an Advection diffusion equation. Many researchers are involved for solving the model equation (ADE) by using the finite difference scheme. Agusto and Bamigbola (2007) studied on the Numerical treatment of the mathematical model for water pollution. This study was examined by various mathematical models involving water pollutant. The authors used the implicit centered difference scheme in space and a forward difference method in time for the evaluation of the generalized transport equation. Kumar et al (2009) presented an analytical solution of one dimensional advection diffusion equation with variable coefficients in a finite domain using Laplace transformation technique. The authors introduced new independent space and time variables in this process. In this study the analytical solution was compared with the numerical solution in case the dispersion is proportional to the same linearly interpolated velocity. Kumar et al (2011) made an Analytical solution of the advection diffusion equation with temporally dependent Coefficients. Park et al (2008) performed an analytical solution of the advection diffusion equation for a ground level finite area source using superposition method. Van Genuchten et al studied an Analytical solution of the advection diffusion transport equation using a change of variable and integral transform technique. Thongmoon and Mckibbin (2006) compared some Numerical Methods for the Advection-Diffusion Equation. The authors reported that the finite difference methods (FTCS, Crank Nicolson) give better point-wise solutions than the spline methods. Yuste et al (2005) described an explicit finite difference method and a new Von Numann-type stability analysis for fractional diffusion equations. Changiun Zhu et al (2010) conducted a study on a Numerical Simulation of Hybrid Finite Analytic Method for Ground Water Pollution.

Therefore, in section II, we present the derivation of advection diffusion equation on the principle of conservation law of mass using Fick's law based on ([1], [2], [3], [7]). In section III, we solve one dimensional advection diffusion equation for initial condition in infinite space analytically by transform to heat equation via coordinate transformation based on ([1], [5], [11]). Based on the study of the general finite difference method for the second order linear partial differential equation ([7], [14], [16], [17]) we develop a explicit finite difference scheme for ADE as an IBVP with two sided boundary conditions in section IV. In this section, we also establish the stability condition of the explicit centered difference scheme for advection diffusion equation. In section V, we present an algorithm for the numerical solution and we implement the numerical scheme in order to perform the numerical features of error estimation. Our goal is to investigate the efficient numerical schemes for advection diffusion equation. Finally the conclusions of the paper are given in last section.

II. Fundamental Conservation Law

Many partial differential equation models with a physical motivation develop from a conservation law. A conservation law is just a mathematical formulation of the basics fact that the rate at which a quantity changes in a given domain must equal the rate at which the quantity flows across the boundary plus the rate at which the quantity is created or destroyed within the domain. Let $C = C(x,t)$ denote the density of a given quantity (energy, mass, Automobiles, etc), density is usually measured in amount per unit volume or some time amount per unit length. Further, we let $q = q(x,t)$ denote the flux of the quantity crossing the section at x and at time t and its unit are given in amount per unit area, per unit time. Thus, $Aq(x,t)$ is the actual amount of the quantity that is crossing the section at x at time t. Where A is the cross sectional area of the tube. Finally $f = f(x,t)$ denote the given rate at which the quantity is created or destroyed within the section at x at time t. The function f is called the source term if it is positive, and a sink if it is negative, it is measured in amount per unit volume per unit time. We can derive the law by assuming a fixed time but arbitrary, section $[x_1, x_2]$ of the tube and requiring that the rate of change of the total amount of the quantity in the section must equal the rate at which it flows in at $x = x_1$, minus the rate at which it flows out at $x = x_2$, plus the rate at which it is created within $[x_1, x_2]$.

In mathematically, we can define the conservation law.

$$\frac{d}{dt}\int_{x_1}^{x_2} C(x,t)Adx = Aq(x_1,t) - Aq(x_2,t) + \int_{x_1}^{x_2} f(x,t)Adx \qquad \ldots\ldots\ldots \qquad (1)$$

This is one integral form of conservation law. Here A is constant, it may be cancelled from the formula. However, if the function C and q are sufficiently smooth, then it may reformulated as a PDE model.

$$\frac{d}{dt}\int_{x_1}^{x_2} C(x,t)dx = q(x_1,t) - q(x_2,t) + \int_{x_1}^{x_2} f(x,t)dx$$

$$\int_{x_1}^{x_2} C_t(x,t)dx = -\int_{x_1}^{x_2} q_x(x,t) + \int_{x_1}^{x_2} f(x,t)dx$$

$$\int_{x_1}^{x_2} C_t(x,t)dx + \int_{x_1}^{x_2} q_x(x,t) - \int_{x_1}^{x_2} f(x,t)dx = 0$$

We conclude that the integrand must be identically zero.

$$C_t(x,t) + q_x(x,t) - f(x,t) = 0$$

$$C_t(x,t) + q_x(x,t) = f(x,t) \qquad (2)$$

The equation (2) is the fundamental conservation law.

2.1 advection diffusion equation

Consider the flux of the chemical past some point x in the tube or steam. In addition to the advective flux $q = uC$ there is also a net flux due to diffusion whenever the concentration profile is not flat at point x. The flux is determine by fourier's law of heat conduction (heat diffuses in much the same way as the chemical concentration), which says that the diffusive flux is simply proportional to the gradient of concentration.

Diffusive flux, $J = -D\frac{\partial C}{\partial x}$

Combining this flux with the advective flux $q = uC$ gives the net flux function

$$q_{net} = q + J$$

$$= uc - D\frac{\partial c}{\partial x}$$

We substitute this quantity at the conservation law (2) in the absence of source. And the conservation law becomes

$$C_t(x,t) + (uC - D\frac{\partial C}{\partial x})_x = 0$$

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} - D\frac{\partial^2 C}{\partial x^2} = 0$$

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2}$$

The advection diffusion equation is a parabolic type partial differential equation.

2.2 Derivation of the Mathematical model (ADE)

The derivation of the advection diffusion equation relies on the principle of superposition; advection and diffusion can be added together if they are linearly independent. Diffusion is a random process due to molecular motion. Due to diffusion, each molecule in time δt will move.

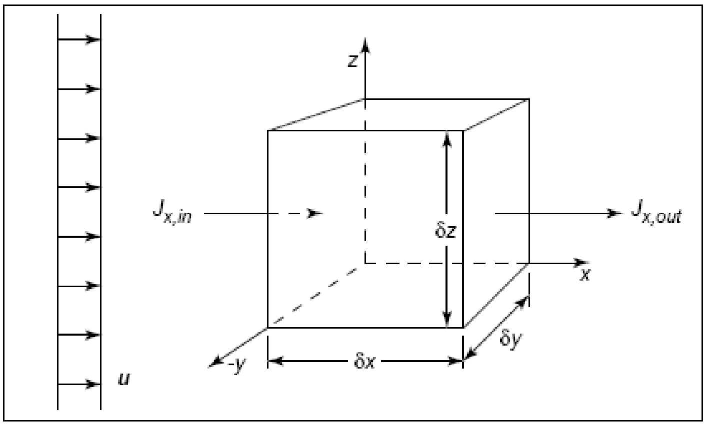

Figure 2.1: Schematic of a control volume with cross flow

Either one step to the left or one step to the right (i.e. $\pm\delta x$). Due to advection, each molecule will also move $u\delta t$ in the cross-flow direction. These processes are clearly additive and independent; the presence of the cross flow does not bias the probability that the molecule will take a diffusive step to the right or the left; it just adds something to that step. The net movement of the molecule is $u\delta t \pm \delta x$, and thus, the total flux in the x-direction J_x (above shown in graph), including the advection transport and a Fickian diffusion term, must be

$$J_{x-direction} = uc + J$$

$$= uc - D\frac{\partial c}{\partial x}$$

Where, uc the correct form of the advection term.

We now use this flux law and the conservation of mass to derive the advection diffusion equation. Consider a cross flow velocity, $u = (u, v, w)$ as shown in Figure 2.1 .From the conservation of mass, the net flux through the control volume is

$$\frac{\partial M}{\partial t} = \sum \dot{m}_{in} - \sum \dot{m}_{out} \qquad (3)$$

and for the x-direction, we have

$$\delta\dot{m}\big|_x = (uc - D\frac{\partial c}{\partial x})\Big|_1 \delta y\delta z - (uc - D\frac{\partial c}{\partial x})\Big|_2 \delta y\delta z$$

We use linear Taylor series expansion to combine the two flux terms, giving

$$uc\big|_1 - uc\big|_2 = uc\big|_1 - (uc\big|_1 + \frac{\partial(uc)}{\partial x}\Big|_1 \delta x)$$

$$= -\frac{\partial(uc)}{\partial x}\delta x$$

And $$-D\frac{\partial c}{\partial x}\bigg|_1 + D\frac{\partial c}{\partial x}\bigg|_2 = -D\frac{\partial c}{\partial x}\bigg|_1 + (D\frac{\partial c}{\partial x}\bigg|_1 + \frac{\partial}{\partial x}(D\frac{\partial c}{\partial x})\bigg|_1 \delta x)$$

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

Thus, for the x -direction

$$\delta\dot{m}\big|_x = -\frac{\partial(cu)}{\partial x}\delta x\delta y\delta z + D\frac{\partial^2 c}{\partial x^2}\delta x\delta y\delta z$$

The y and z -directions are similar, but with v and w for the velocity components, giving

$$\delta\dot{m}\big|_y = -\frac{\partial(cv)}{\partial y}\delta y\delta x\delta z + D\frac{\partial^2 c}{\partial y^2}\delta y\delta x\delta z$$

$$\delta\dot{m}\big|_z = -\frac{\partial(cw)}{\partial z}\delta z\delta x\delta y + D\frac{\partial^2 c}{\partial z^2}\delta z\delta x\delta y$$

Substituting these results into (3) and recalling that

$$M = c\delta x\delta y\delta z$$

We obtain

$$\frac{\partial c}{\partial t} + \nabla.(cu) = D\nabla^2 c$$

or in Einsteinian notation

$$\frac{\partial c}{\partial t} + \frac{\partial cu_i}{\partial x_i} = D\frac{\partial^2 c}{\partial x_i^2}$$

This is the desired advection diffusion equation (ADE).

In the one-dimensional case, $u = (u,0,0)$ and there are no concentration gradients in the y -direction or z -direction, leaving us with

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

Since u is constant, then

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} \tag{4}$$

It is well known Advection diffusion equation

2.3 Formulation of Diffusion Equation from Advection diffusion equation by transform technique

Without loss of generality, we will consider one dimensional problem where the advection takes place in the direction $x > 0$. Again, the initial concentration along the domain is assumed to be zero everywhere at the initial time $t = 0$.

i.e. we consider advection diffusion equation as the following

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} \tag{5}$$

with initial condition $c(0,x) = c_0(x)$, for $-\infty < x < \infty$

We need to solve the above IVP. To solve this equation, we will employ the logic that if we imagine ourselves as observers travelling along with the fluid at the fluid velocity u, we then observe the diffusion process only.

After the coordinate transformation, we show that the advection diffusion equation become exactly the same as the diffusion equation.

Coordinate transformation

If this logic is correct, then we can apply the solution of the diffusion equation that we obtained earlier to this situation. As a consequence we define a new coordinate system, η (convective coordinate or Lagrangian coordinate) $\eta = x - ut$.

This coordinate system, essence, translates any given fixed location x, to the distance between fixed location and observer's location, which is described by ut. In addition, we will let $\tau = t$ and then $C(x,t)$ becomes $C(\eta,\tau)$. Using the chain rule, we have

$$\frac{\partial c}{\partial x} = \frac{\partial \eta}{\partial x}\frac{\partial c}{\partial \eta} + \frac{\partial \tau}{\partial x}\frac{\partial c}{\partial \tau} = \frac{\partial c}{\partial \eta}$$

and $$\frac{\partial^2 c}{\partial x^2} = \frac{\partial^2 c}{\partial \eta^2}$$

Similarly, the time derivative term can be expressed as

$$\frac{\partial c}{\partial t} = \frac{\partial \eta}{\partial t}\frac{\partial c}{\partial \eta} + \frac{\partial \tau}{\partial t}\frac{\partial c}{\partial \tau} = -u\frac{\partial c}{\partial \eta} + \frac{\partial c}{\partial \tau}$$

Substituting of the above expression to the advection diffusion equation leads to the following expression

$$-u\frac{\partial c}{\partial \eta} + \frac{\partial c}{\partial \tau} + u\frac{\partial c}{\partial \eta} = D\frac{\partial^2 c}{\partial \eta^2}$$

Which leads to a final form

$$\frac{\partial c}{\partial \tau} = D\frac{\partial^2 c}{\partial \eta^2} \qquad (6)$$

Which is known as the diffusion equation

Therefore, solutions for advection diffusion equation are the same as those for diffusion equation of various initial and boundary conditions with the exception that we must replace η by $x - ut$.

III. Analytic Solution Of The Heat Equation (Diffusion) As A Cauchy Problem

The diffusion equation is

$$\frac{\partial c}{\partial \tau} = D\frac{\partial^2 c}{\partial \eta^2} \qquad (7)$$

With $$c(0,\eta) = c_0(\eta) \qquad (8)$$

Driving the solution of (7)-(8) is accomplished in two steps. First we will solve the problem for a special step function $c_0(\eta)$, and then we will construct the solution to (7)-(8) using the special solution

So firstly we consider the problem

$$\frac{\partial c}{\partial \tau} = D\frac{\partial^2 c}{\partial \eta^2} \qquad (9)$$

With $c(0,\eta) = c_0$ for $\eta > 0$

and $c(0,\eta) = 0$ for $\eta < 0$ (10)

Where we have taken the initial condition to be a step function with jump c_0

3.1 The fundamental Solution of the Heat Equation

We persuade our approach to the solution (9)-(10) with a simple idea from the subject of dimensional analysis. Dimensional analysis deals with the study of units (seconds, meters, kilogram, and so forth) and dimensions (time, length, mass and so forth) of the quantities in a problem and how relate to each other. Equations must be dimensionally consistent (one cannot add apples or oranges), and important conclusions can be drawn from this fact. The cornerstone result in dimensional analysis is called the pi theorem. The pi theorem guarantees that whenever there is a physical law dimensionless quantities $q_1, q_2, q_3, \ldots\ldots\ldots\ldots, q_m$ then there is an equivalence physical law relating the independent dimensionless quantities that can be formed from $q_1, q_2, q_3, \ldots\ldots\ldots\ldots, q_m$. By a dimensional quantity we mean one in which all the dimensions (time, length, mass and so forth) cancel out. As an example take the law

$$h = -\frac{1}{2}gt^2 + ut$$

That gives the height h of an object at time t when something is thrown upwind with initial velocity u; the constant g is the acceleration due to gravity. Here the dimensioned quantities are h, t, u and g, having dimensions length, time, length per time, and length per time squared. This law can be rearranged and written equivalently as

$$\frac{h}{ut} = -\frac{gt}{2u} + 1$$

$$\pi_1 \equiv \frac{h}{ut} \text{ and } \pi_2 \equiv \frac{gt}{u}$$

For example, h is length and ut, also a length. So π_1 has no dimensions and similarly π_2 is dimensionless.

We use similar reasoning to guess the form of the IVP (9)-(10). First we list all the variables and constants in the problem η, τ, c, c_0, D. These have dimensions length, time, degrees, and length squared per time respectively. We notice that $\frac{c}{c_0}$ is a dimensionless quantity (degrees divided by degrees), the only other dimensionless quantity in the problem is $\frac{\eta}{\sqrt{4D\tau}}$

We accept therefore that the solution can be written as some combination of these dimensionless variables, or $\frac{c}{c_0} = f(\frac{\eta}{\sqrt{4D\tau}})$ for some function f to be determined.

So let us substitute $c = f(z)$, $z = \frac{\eta}{\sqrt{4D\tau}}$ into the PDE (9). We have taken $c_0 = 1$ for simplicity. The chain rule allows us to compute the partial derivatives as

$$c_\tau = f'(z)z_\tau = -\frac{1}{2}\frac{\eta}{\sqrt{4D\tau^3}}f'(z)$$

$$c_\eta = f'(z)z_\eta = \frac{1}{\sqrt{4D\tau}}f'(z)$$

$$c_{\eta\eta} = \frac{1}{\sqrt{4D\tau}}f''(z)\frac{1}{\sqrt{4D\tau}} = \frac{1}{4D\tau}f''(z)$$

Substituting these quantities into (9) then gives,

$$D\frac{1}{4D\tau}f''(z) = -\frac{1}{2}\frac{\eta}{\sqrt{4D\tau^3}}f'(z)$$

$$\frac{1}{4\tau}f''(z) = -\frac{1}{2}z\frac{1}{\tau}f'(z)$$

$$\frac{1}{4\tau}f''(z) = -\frac{1}{2}z\frac{1}{\tau}f'(z)$$

$$f''(z) = -2zf'(z)$$

$$f''(z) + 2zf'(z) = 0, \text{ for } f(z)$$

This is an ODE

Here integrating factor is e^{z^2}. The equation is easily solved by multiplying through by integrating factor e^{z^2} and integrating.

We get $f'(z) = k_1 e^{-z^2}$, where k_1 is integrating constant.

Integration from 0 to z gives

$$f(z) = k_1\int_0^z e^{-r^2}dr + k_2, \quad \text{where } k_2 \text{ is another integrating constant.}$$

Therefore the solution of (6) is

$$c(\eta,\tau)=k_1\int_0^{\frac{\eta}{\sqrt{4D\tau}}} e^{-r^2}dr+k_2,$$

To determine the constant k_1 and k_2 we apply the initial condition. For a fixed $\eta<0$ we take the limit as $\tau\to 0$ to get

$$0=c(\eta,0)=k_1\int_0^{-\infty} e^{-r^2}dr+k_2,$$

For a fixed $\eta>0$ we take the limit as $\tau\to 0$ to get

$$1=c(\eta,0)=k_1\int_0^{\infty} e^{r^{-2}}dr+k_2$$

Recalling that $\int_0^{\infty} e^{-r^2}dr=\frac{\sqrt{\pi}}{2}$

By solving last two equation, $k_1=\frac{1}{\sqrt{\pi}}$ and $k_2=\frac{1}{2}$

Therefore the solution to (9)-(10) with $c_0=1$ is $c(\eta,\tau)=\frac{1}{\sqrt{\pi}}\int_0^{\frac{\eta}{\sqrt{4D\tau}}} e^{-r^2}dr+\frac{1}{2}$

This solution can be presented by the special function called the error function as

$$c(\eta,\tau)=\frac{1}{2}\left(1+erf\left(\frac{\eta}{\sqrt{4D\tau}}\right)\right)$$

Where the error function is defined by

$$erf(z)=\frac{2}{\sqrt{\pi}}\int_0^{z} e^{-r^2}dr$$

Firstly if a function c satisfies the heat equation, then the function c_η satisfies the heat equation.

$$0=(c_\tau-Dc_{\eta\eta})_\eta=(c_\tau)_\eta-D(c_{\eta\eta})_\eta=(c_\eta)_\tau-D(c_\eta)_{\eta\eta}$$

{Since $(c_\tau)_\eta=-\frac{1}{2}\frac{1}{\sqrt{4D\tau^3}}[f'(z)+zf''(z)]$ and $(c_\eta)_\tau=-\frac{1}{2}\frac{1}{\sqrt{4D\tau^3}}[f'(z)+zf''(z)]$

Hence $(c_\tau)_\eta=(c_\eta)_\tau$ }

Therefore the function

$G(\eta,\tau)\equiv c_\eta(\eta,\tau)$ is the solution of heat equation.

By the direct differentiation

We find that $G(\eta,\tau)=\frac{1}{\sqrt{4\pi D\tau}}e^{-\eta^2/4D\tau}$ (11)

The function is called the fundamental solution to the heat equation.

3.1.1 The Fundamental solution of Advection Diffusion equation

Putting the relation $\eta=x-ut$, and $\tau=t$ in (11), we get

$$G(x,t)=\frac{1}{\sqrt{4\pi Dt}}e^{-(x-ut)^2/4Dt}$$

is called the fundamental solution to the advection diffusion equation.

IV. Finite Difference Scheme

In this section, the study investigates a finite difference scheme for the water pollution model as a parabolic second order partial differential equation. This chapter contains the analysis of the condition of stability of the explicit finite difference scheme.

4.1 Explicit Upwind difference schemes for Advection Diffusion Equation

We consider our second order water pollution model

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} \qquad (12)$$

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

The discreetization of $\frac{\partial c}{\partial t}$ is obtained by first order forward difference in time

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

The discreetization of $\frac{\partial c}{\partial x}$ **i**s obtained by first order backward difference in space

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

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

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

The simplest numerical discretization of (12) is

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

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

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

$$c_i^{n+1} = (\lambda + \gamma)c_{i-1}^n + (1 - \gamma - 2\lambda)c_i^n + \lambda c_{i+1}^n \qquad (13)$$

where $\gamma = u\frac{\Delta t}{\Delta x}$, $\lambda = D\frac{\Delta t}{\Delta x^2}$

Which is the explicit upwind difference scheme and it is also known as FTBSCS techniques. The stability condition is controlled by $\gamma = u\frac{\Delta t}{\Delta x}$, $\lambda = D\frac{\Delta t}{\Delta x^2}$

4.2 Explicit centered difference scheme for Advection Diffusion Equation

We consider our second order water pollution model

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} \qquad (14)$$

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 can be obtained from

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

Centered difference discretization in spatial derivative:

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

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

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

The simplest numerical discretization of (14) is

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

$$\Rightarrow \; c_i^{n+1} = (\frac{D\Delta t}{\Delta x^2} + \frac{u\Delta t}{2\Delta x})c_{i-1}^n + (1 - 2\frac{D\Delta t}{\Delta x^2})c_i^n + (\frac{D\Delta t}{\Delta x^2} - \frac{u\Delta t}{2\Delta x})c_{i+1}^n \qquad (15)$$

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

This is the explicit centered difference scheme of 1 D advection diffusion equation and it is also known as FTCSCS

4.3 Explicit downwind difference scheme for Advection Diffusion Equation

We consider our second order water pollution model

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} \qquad (16)$$

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

The discreetization of $\frac{\partial c}{\partial t}$ is obtained by first order forward difference in time

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

The discreetization of $\frac{\partial c}{\partial x}$ **i**s obtained by first order forward difference in space

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

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

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

The simplest numerical discretization of (16) is

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

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

$$c_i^{n+1} = \lambda c_{i-1}^n + (1 + \gamma - 2\lambda)c_i^n + (\lambda - \gamma)c_{i+1}^n \qquad (17)$$

Which is the explicit downwind difference scheme and it is also known as FTFSCS techniques. The stability condition is controlled by $\gamma = u\frac{\Delta t}{\Delta x}$, $\lambda = D\frac{\Delta t}{\Delta x^2}$

Now we can write the general form of an explicit finite difference scheme of advection diffusion equation as
$c_i^{n+1} = A_0 c_{i-1}^n + A_1 c_i^n + A_2 c_{i+1}^n$

Values of Coefficients of three different schemes at a glance

Coefficients of an explicit finite difference scheme			
	A_0	A_1	A_2
EUDS/FTBSCS	$(\lambda+\gamma)$	$(1-\gamma-2\lambda)$	λ
ECDS	$(\lambda+\frac{\gamma}{2})$	$(1-2\lambda)$	$(\lambda-\frac{\gamma}{2})$
EDDS/FTFSCS	λ	$(1+\gamma-2\lambda)$	$(\lambda-\gamma)$

Lemma 4.3-1*:* Stability of the explicit centered difference scheme (15) of Advection Diffusion equation is given by the conditions

$$0 \le u\frac{\Delta t}{\Delta x} \le 1\ , \quad 0 \le D\frac{\Delta t}{\Delta x^2} \le \frac{1}{2}$$

Proof: The explicit centered difference scheme for (14) is given

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

$$=> c_i^{n+1} = (\lambda + \frac{\gamma}{2})c_{i-1}^n + (1-2\lambda)c_i^n + (\lambda - \frac{\gamma}{2})c_{i+1}^n \qquad (18)$$

where $\gamma = u\frac{\Delta t}{\Delta x}$, $\lambda = D\frac{\Delta t}{\Delta x^2}$

The equation (18) implies that for

$$0 \le \lambda + \frac{\gamma}{2} \le 1 \qquad (i)$$

$$0 \le 1-2\lambda \le 1 \qquad (ii)$$

$$0 \le \lambda - \frac{\gamma}{2} \le 1 \qquad (iii)$$

The new solution is a convex combination of the two previous solutions. That is the solution at new time-step $(n+1)$ at a spatial node i is an average of the solutions at the previous time-step at the spatial-nodes $i-1$, i and $i+1$. This means that the extreme value of the new solution is the average of the extreme values of the previous two solutions at the three consecutive nodes.
In our model the characteristics speed u is assumed to positive.

Then we have $\gamma = \frac{u\Delta t}{\Delta x} \ge 0$

From equation (ii), $0 \le 1-2\lambda \le 1$

$$-1 \le -2\lambda \le 1-1$$

$$0 \le \lambda \le \frac{1}{2}$$

And from (i),

$$0 \le \lambda + \frac{\gamma}{2} \le 1$$

$$0 \le \frac{1}{2} + \frac{\gamma}{2} \le 1$$

It is clear that $\gamma \le 1$

We can conclude that the explicit centered difference scheme (18) is stable for

Where $0 \le \gamma = u\dfrac{\Delta t}{\Delta x} \le 1$ and $0 \le \lambda = D\dfrac{\Delta t}{\Delta x^2} \le \dfrac{1}{2}$

V. Algorithm For The Numerical Solution

To find out the numerical solution of the model, we have to accumulate some variables which are offered in the following algorithm.

Input: nx and nt the number of spatial and temporal mesh points respectively.

t_f , the right end point of $(0,T)$

(x_d), the right end point of $(0,b)$

C_0, the initial concentration density, apply as a initial condition

C_a, Left hand boundary condition

C_b, Right hand boundary condition

D, Diffusion rate

u, velocity

Output: $c(x,t)$ the solution matrix

Initialization: $dt = \dfrac{T-0}{nt}$, the temporal grid size

$dx = \dfrac{b-0}{nx}$, the spatial grid size

$gm = u * \dfrac{dt}{dx}$, the courant number

$ld = D * \dfrac{dt}{(dx)^2}$

Step1. Calculation for numerical solution of ADE by explicit centered difference scheme

For $n = 1$ to nt

For $i = 2$ to nx

$C(n+1,i) = (\lambda + \gamma/2) * C(n,i-1) + (1 - 2*\lambda) * C(n,i) + (\lambda - \gamma/2) * C(n,i+1)$

end

end

Step2; Output $c(x,t)$

Step3: Figure Presentation

Step4: Stop

5.1 Relative Error Estimation of the Numerical Scheme

In this section we compute the relative error between analytic solution and different types of explicit finite difference scheme to determine which scheme is best.

We compute the relative error in L_1 -norm defined by

$$\|e\|_1 = \frac{\|C_e - C_N\|_1}{\|C_e\|_1}$$

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

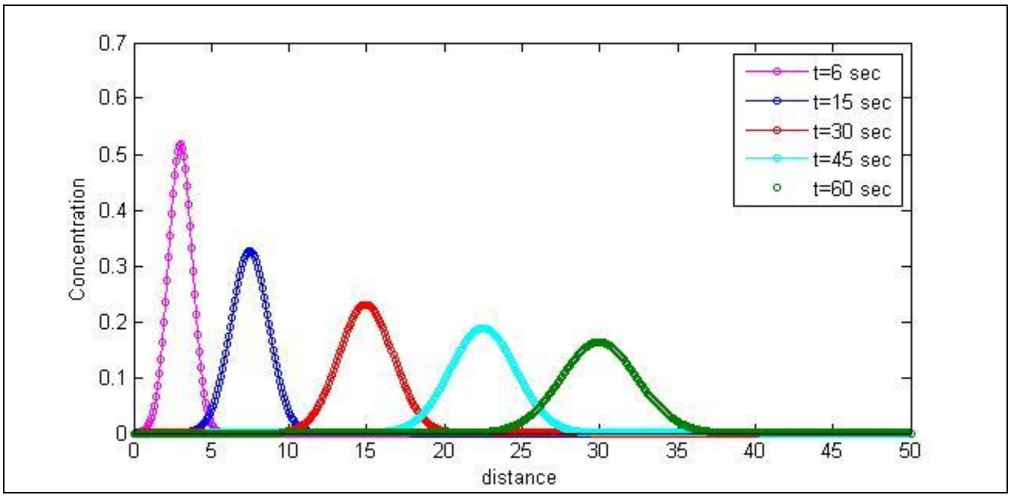

Figure 5: Analytic solution for Advection diffusion equation at different time

5.1.1 Relative error for explicit upwind difference scheme

We present explicit upwind difference scheme for $u = 0.5$ and $D = 0.05$ up to time $t = 60$ in temporal grid size $\Delta t = 0.06$ in spatial domain [0, 50] with spatial grid size $\Delta x = 0.1$

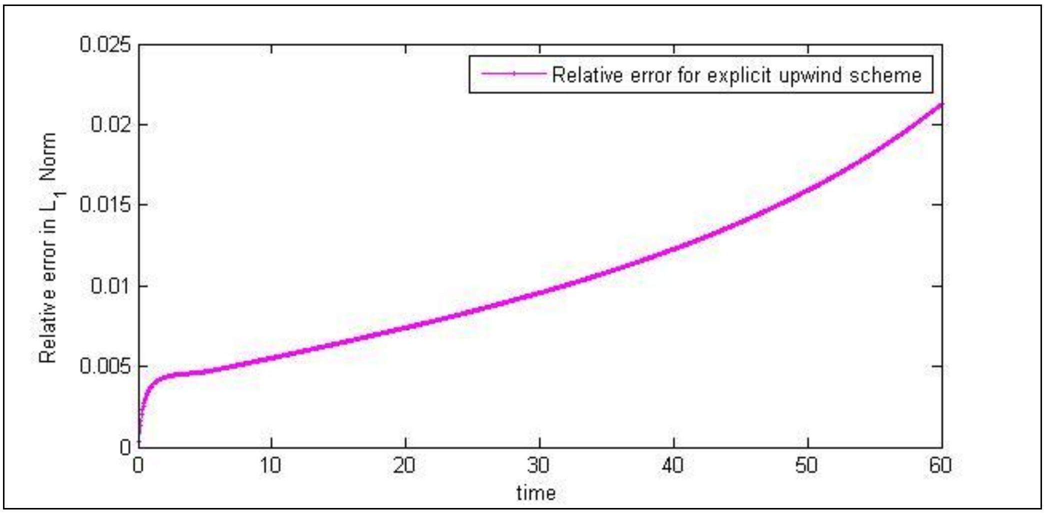

Figure 5.1: Relative errors of explicit upwind difference scheme

5.1.2 Relative error for explicit centered difference scheme

we perform explicit centered difference scheme for $u = 0.5$ and $D = 0.05$ up to time $t = 60$ in temporal grid size $\Delta t = 0.06$ in spatial domain [0, 50] with spatial grid size $\Delta x = 0.1$ which guarantees the stability condition , $0 \le \gamma \le 1$, $\lambda \le \frac{1}{2}$ where $\lambda = D\frac{\Delta t}{\Delta x^2} = 0.30$, $\gamma = u\frac{\Delta t}{\Delta x} = 0.30$

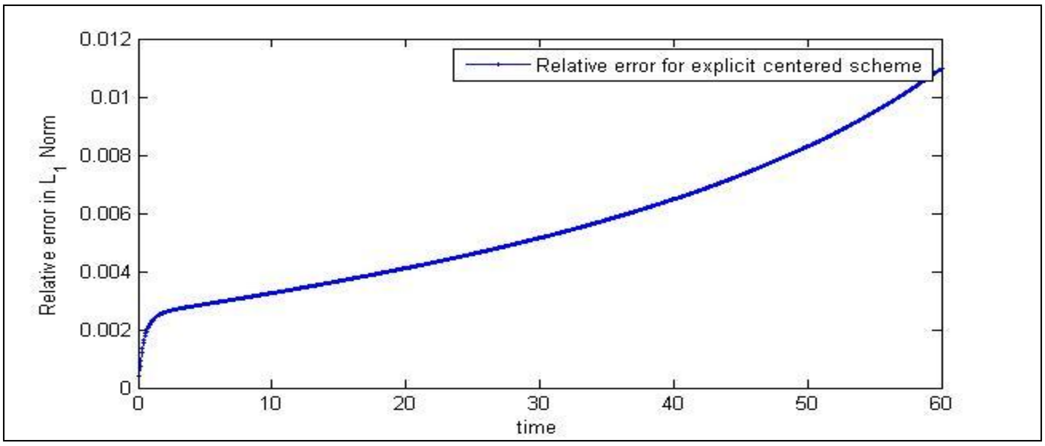

Figure 5.2: Relative errors of explicit centered difference scheme

5.1.3 Relative error for explicit downwind difference scheme

We execute explicit downwind difference scheme for $u = 0.5$ and $D = 0.05$ up to time $t = 60$ in temporal grid size $\Delta t = 0.06$ in spatial domain [0, 50] with spatial grid size $\Delta x = 0.1$.

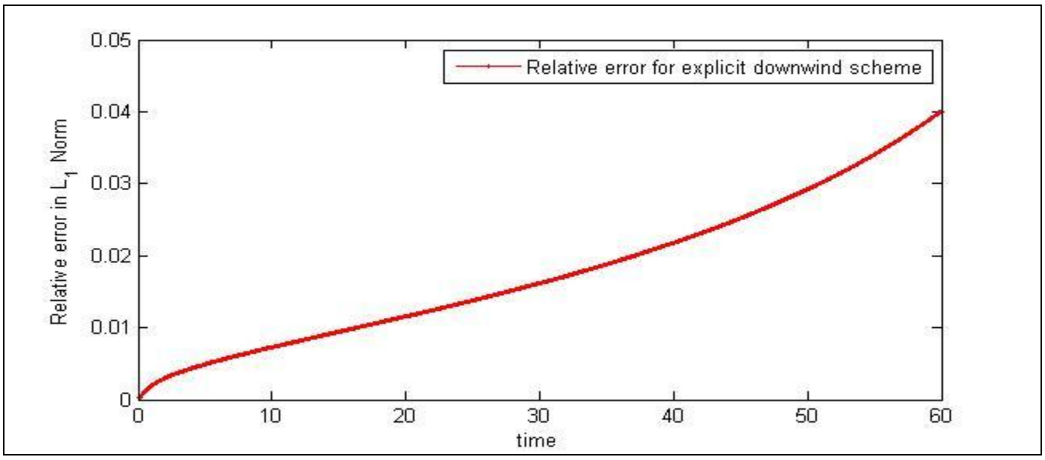

Figure 5.3: Relative error for explicit downwind difference scheme

5.1.4 Comparison of explicit upwind difference scheme, explicit centered difference scheme and explicit downwind difference scheme

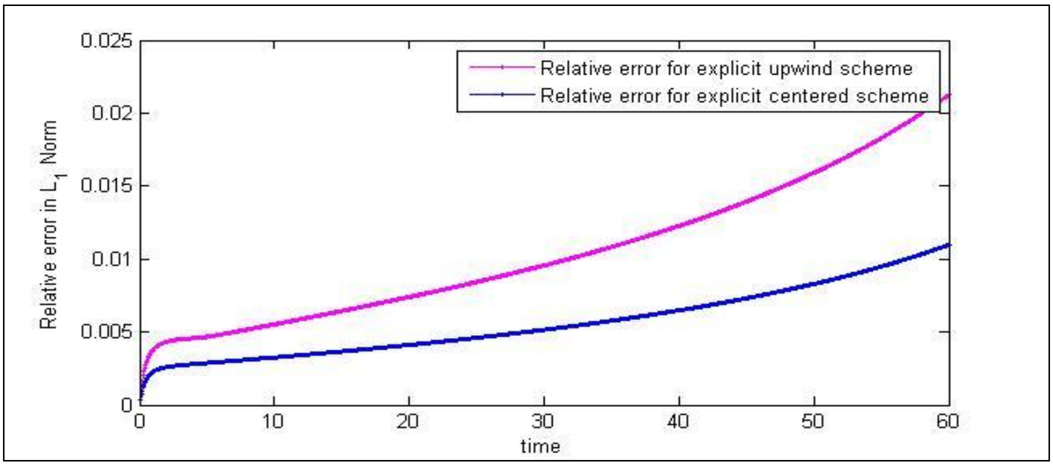

Figure 5.4: Comparison of Relative errors between explicit upwind difference scheme and explicit centered difference scheme

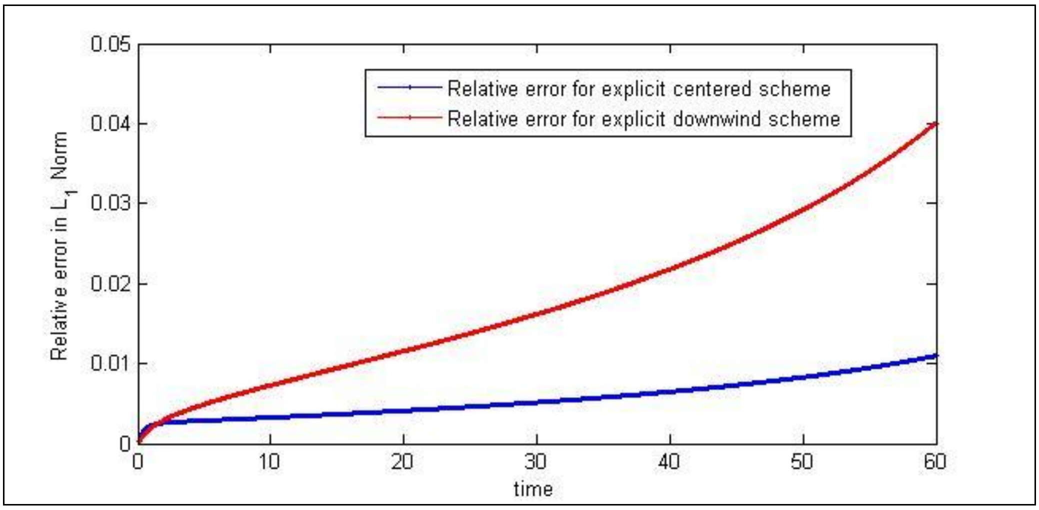

Figure 5.5: Comparison of Relative errors between explicit centered difference scheme and explicit downwind difference scheme

5.1.5 Comparison of explicit upwind difference scheme, explicit centered difference scheme and explicit downwind difference scheme

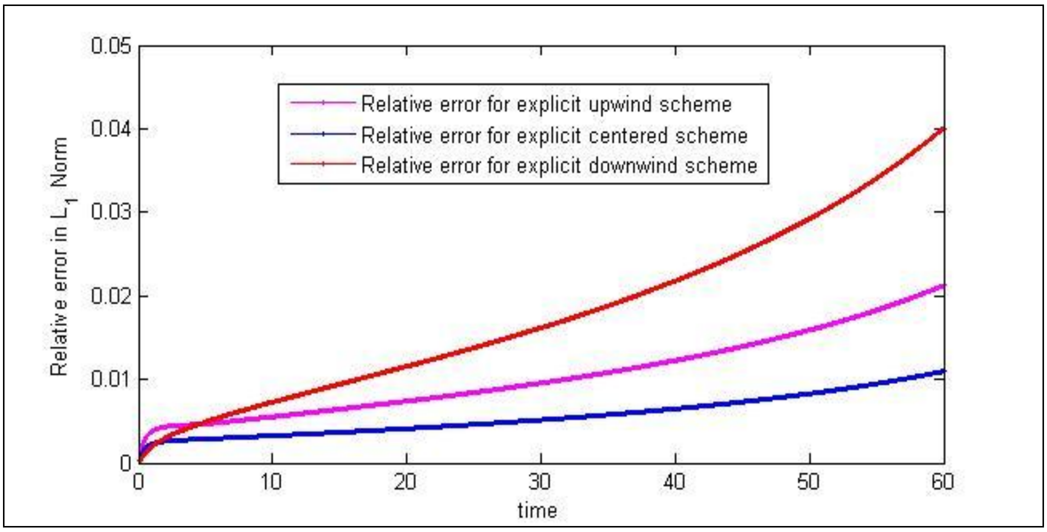

Figure 5.6: Comparison of Relative errors among explicit upwind difference scheme, explicit centered difference scheme and explicit downwind difference scheme

Figure (Figure 5.1-5.6) shows the relative error of three different schemes for advection diffusion equation. Figure 5.1 shows the relative error for EUDS, which remains below 0.0212. Figure 5.2 shows the relative error for ECDS which remains below 0.0110. Figure 5.3 shows the relative error for EDDS scheme which remains below 0.0401. ECDS provides accurate results than the EUDS and EDDS scheme with respect to discretization parameter Δx .

VI. Conclusion

The study has presented the numerical and analytical solution of Advection Diffusion equation. We have studied three explicit differences schemes for the numerical solutions of Advection Diffusion Equation. It has also compared among the three different schemes; EUDS, ECDS and EDDS scheme for estimating the relative error in advection diffusion equation. The explicit centered difference scheme is more efficient numerical scheme for ADE. The explicit centered difference scheme can be extended for two dimensional advection diffusion equations as a water pollution model which demands the further study.

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