Estimation of Air Pollution by Numerical Simulation of Advection Diffusion Equation

Sukriti Kundu, Laek Sazzad Andallah

Abstract— This paper considers a parabolic type partial differential equation known as Advection Diffusion Equation (ADE) which has been used to estimate the concentration of pollutant. The paper reports the analytical solution of the model and studies finite difference scheme for the numerical solution of the ADE. In order to exclude any adverse effects of pollutant at environment, a problem of nitrogen diffusion into an advective air flow is an excellent model. The paper implements the numerical scheme for some real data for the flow of nitrogen gas into the air flow through uniform tube and presents the numerical results for various velocities and diffusion coefficients.

Keywords: Advection-Diffusion Equation, Air pollution, Analytical Solution, Error Estimation, Finite Difference Scheme, Numerical Implementation, Stability Condition.

1. Introduction

The smoke from vehicles (combustion in the engine) and many factories contain various compound of nitrogen which is harmful for our environment. It helps form acid rain, contributes to global warming, hampers the growth of plants. Mathematical modeling of gas flow is a challenging problem and has been of great interest to many researchers. In [10], R.N Singh describes the advection diffusion equation models in near surface geophysical and environmental sciences. In [11], advances in numerical simulations and emergence of sophisticated porous transport models have significantly improved the study and analysis of transport in living tissues. In the current perspective of global warming, climate change and air pollution, the numerical implementation of Advection Diffusion Equation has become an important issue in the field of computer simulation techniques. This gives the motivation to perform a numerical study of the Advection Diffusion Equation (ADE) in order to estimate the concentration of pollutant by computing the effect of velocity and diffusivity.

In section 2, we present the description and analytical solution of advection diffusion equation based on [2],[3],[4]. Section 3 studies the finite different schemes as two explicit centered difference schemes, implicit centered difference schemes based on [8] and Crank Nicolson's scheme followed by stability condition [8] and error estimation. Section 4 presents a computer programming code for implementation of the numerical scheme and perform numerical simulation for some real data for the transport of nitrogen gas in a uniform tube with infinitesimal cross-section and compares the results with that of [9]. At section 5, we present solution surface for nitrogen transportation in different time, different velocity and different diffusion coefficient. Although in the work of [9],

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the solution surface for nitrogen transportation was shown for analytical solution (by Green Function Method) at final time, we present the numerical solution with increase in time.

2. Mathematical Formulation

The Advection Diffusion Equation (ADE) is an important partial equation which describes the distribution of nitrogen gas in a given cross-sectional area over time. The simplest 1D advection diffusion equation is

$$\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2} \tag{1}$$

With initial condition

$$C(x,0) = C_0(x); \; for -\infty < x < \infty$$

where C is the concentration of the transport substance, D is the diffusion constant (here assume uniform in space) and v is the velocity field. The velocity field in turn couples to the pressure field of the medium through the Navier-Stokes Equations.

We will define a new coordinate system η, (convective coordinates or Lagrangian Coordinates) $\eta = x - vt$ and using this we obtain the analytical solution of (1) is

$$C(x,t) = \frac{1}{\sqrt{4\pi D\tau}} e^{-\frac{(x-vt)^2}{4Dt}}$$

This is called the fundamental solution to the advection-diffusion equation. Though we can solve the problem analytically in steady state with simple boundary conditions, most physically relevant ADEs appear within sets of nonlinear couple's equations or with nontrivial boundary conditions where analytical solutions are not possible. Most solvers use either finite difference method (FDM) or finite element method (FEM).

Numerical Solution of Advection-Diffusion Equation:

The one−dimensional linear advection- diffusion equation is

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

where $x \in (a, b)$, $t \in (0, T)$

with initial condition $C(x, 0) = 0$ and boundary condition $C(0, t) = 1$, $C_x(\infty, t) = 0$.

We discretize space:

$$a = x_{-\frac{1}{2}} < x_{\frac{1}{2}} < x_{\frac{3}{2}} < \cdots\cdots\cdots\cdots < x_{l-\frac{1}{2}} = b$$

We discretize the time:

$$t = t^0 < t^1 < t^2 < \cdots\cdots\cdots\cdots < t^N = T$$

By using Forward difference formula in space we obtain that $\frac{\partial C(x_j^n)}{\partial x} \approx \frac{C_{j+1}^n - C_j^n}{\Delta x}$.

By using backward difference formula in space we obtain that $\frac{\partial C(x_j^n)}{\partial x} \approx \frac{C_j^n - C_{j-1}^n}{\Delta x}$.

By using central difference formula in space we obtain that $\frac{\partial C(x_j^n)}{\partial x} \approx \frac{C_{j+1}^n - C_{j-1}^n}{2\Delta x}$.

By substitution the values of $\frac{\partial C(x_j^n)}{\partial t}$, $\frac{\partial C(x_j^n)}{\partial x}$ and $\frac{\partial^2 C(x_j^n)}{\partial x^2}$ (which are obtained by 1st order forward difference in time, backward difference in space and centered difference in space respectively) into (2), we obtain

$$C_j^{n+1} = (\alpha + C_r)u_{j-1}^n + (1 - 2\alpha - C_r)u_j^n + \alpha C_{j+1}^n \qquad (3)$$

Where $\alpha = \frac{D\Delta t}{\Delta x^2}$ and $C_r = \frac{v\Delta t}{\Delta x}$

which is the explicit centered difference scheme and it is also known as FTBSCS techniques.

Again by substitution the values of $\frac{\partial C(x_j^n)}{\partial t}$, $\frac{\partial C(x_j^n)}{\partial x}$ and $\frac{\partial^2 C(x_j^n)}{\partial x^2}$ (which are obtained by 1st order forward difference in time and centered difference in space respectively) into (2), we obtain

$$C_j^{n+1} = (\alpha - C_r/2)C_{j+1}^n + (1 - 2\alpha)C_j^n + (\alpha + C_r/2)C_{j-1}^n \qquad (4)$$

Where $\alpha = \frac{D\Delta t}{\Delta x^2}$ and $C_r = \frac{v\Delta t}{\Delta x}$.

Stability Condition:

The stability condition of 1D diffusion equation

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} \text{ is } \frac{D\Delta t}{\Delta x^2} \leq \frac{1}{2}.$$

The stability condition of 1D advection equation $\frac{\partial C}{\partial t} + v\frac{\partial C}{\partial x} = 0$ is

$$\frac{v\Delta t}{\Delta x} \leq 1$$

For the stability condition of advection-diffusion equation,

since the second order diffusive term $D\frac{\partial^2 C}{\partial x^2}$ dominates the 1st order term $v\frac{\partial C}{\partial x}$. Therefore the explicit central difference scheme is stable if the analytical and numerical method is also characterized due to the 2nd order diffusion term of numerical solution. Thus for large D the stability condition of advection-diffusion equation can be considered as the same as diffusion equation.

Therefore the stability condition for explicit centered difference scheme of advection-diffusion equation is given by $\frac{D\Delta t}{\Delta x^2} \leq \frac{1}{2}$.

Error Estimation:

We have discussed different types of explicit difference scheme and analytical solution of advection-diffusion equation. Now we shall compute the relative error between exact solution and different types of explicit difference scheme to determine which scheme is best. We compute the relative error in $L_1 - norm$ which is defined by

$$err = \frac{\|C_e - C_n\|_1}{\|C_n\|},$$

for all time $t = 0$ to $t = 7$. Where C_e is the exact solution and C_n is the numerical solution computed by the finite difference scheme.
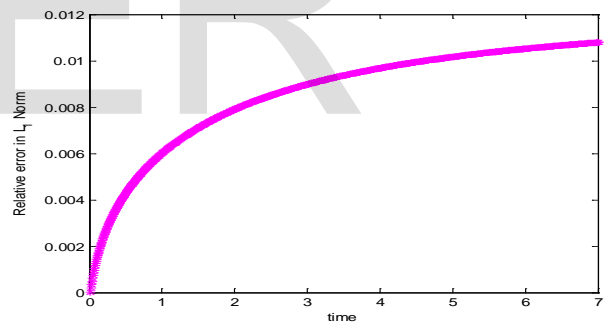

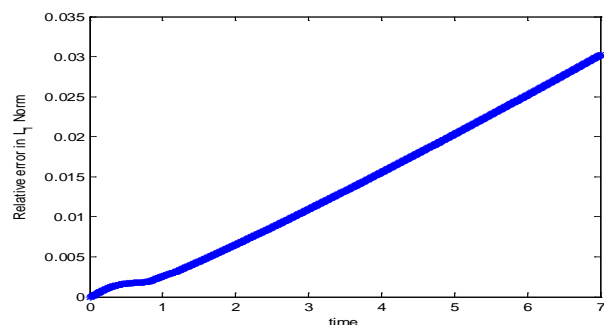Fig1: Error estimation for scheme (3)

Fig1: Error estimation for scheme (4)

Comparison of two schemes:

Now we compute our numerical methods by plotting their relative errors simultaneously.
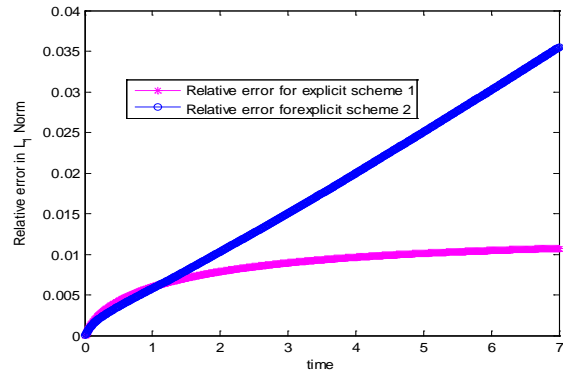

Fig 3: Comparisons of two Explicit Centered Difference Scheme for v=0.1cm/s, D=0.01cm^2/s, $\Delta x = 0.04, \Delta t = 0.007, \alpha = 0.04$

From the above figure we observe that the relative errors for two explicit centered difference scheme and these error for both scheme is shown as below by table 1.

Serial	Time	Error for scheme 3	Error for scheme 4
1	t=.5	0.004	0.003
2	t=1	0.006	0.005
3	t=1.25	0.007	0.007
4	t=4	0.008	0.018
5	t=6	0.009	0.03
6	t=7	0.011	0.035

From the above table we observe that scheme 4 is more accurate then scheme 3. So we implement explicit centered difference scheme 3 for nitrogen gas flow in any tube.

4. Results and Discussion

A 1D channel is designed to contain a uniform advective air flow, as shown in figure 4. At the end of the channel, nitrogen is injected into the air flow. Another end is assumed to be far enough. The pressure is 0.1013 Mpa the temperature 298.15K. by defining the mass fraction of nitrogen as the solved variable $C = C(x,t)$, the advection diffusion process can be formulated as,

$$C_t + vC_x - C_{xx} = 0, 0 < x < \infty, 0 < t < \infty$$

$$C(x,0) = 0, \qquad C(1,t) = 1$$

Fig 4: One dimensional advection diffusion of nitrogen into air flow

This is a boundary value problem in a Dirichlet type, defined in a semi-infinite domain. Here we present numerical simulation results for nitrogen transportation with time increasing, diffusion increasing and for different cell size. Our aim is to show that for the environment pollution, any substance with bigger diffusion than another causes great harm. Here we shall show that a bigger D results in a wider nitrogen front, or a bigger diffusion distance. For different coefficients ranging from 0.001 cm^2/s to 1 cm^2/s, as shown in Fig 7 to 10.

If $D = 1 cm^2/s$ and $v = 2 cm/s$, the theoretical nitrogen mass friction distribution at time $t = 5sec$, for the numerical scheme (which is described at the previous section) is shown in **Figure 5** which show that how the nitrogen concentration distributed within the tube.
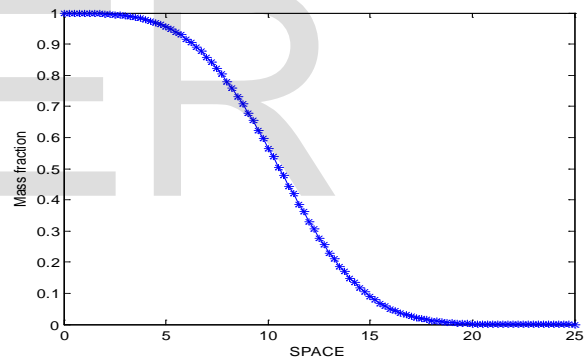

Fig 5: One dimensional advection diffusion with $D = 1 cm^2/s$ at time t = 5sec with $v = 2 cm/s$.

Now keeping spatial grid size, diffusion coefficient and velocity fixed we observe the following figure for different time space $t = sec, t = 2sec, t = 4sec, t = 5sec$ respectively. Then for **$D = 1 cm/s, v = 2 cm/s$**,the solution appeared is given below
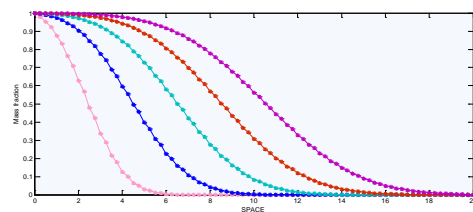

Fig 6: One dimensional advection diffusion with $D = 1 cm^2/s$ at different temporal grid size with $v = 2 cm/s$.

Figure 6 shows that as time is increasing from t=1sec to t=5sec the level of the nitrogen gas is increasing from the boundary. Now keeping spatial grid size and diffusion coefficient we observe the following figures for different temporal size and velocity. Then for $\mathbf{D = 1\ cm^2/s}$ the solution appeared is given below
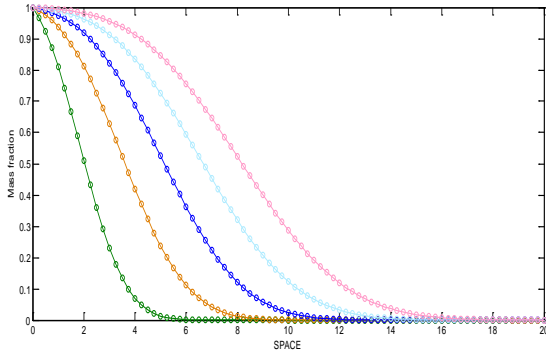

Fig 7: Nitrogen Concentration with $D = 1\ cm^2/s$ at different temporal grid size with $v = 1.5\ cm/s$.

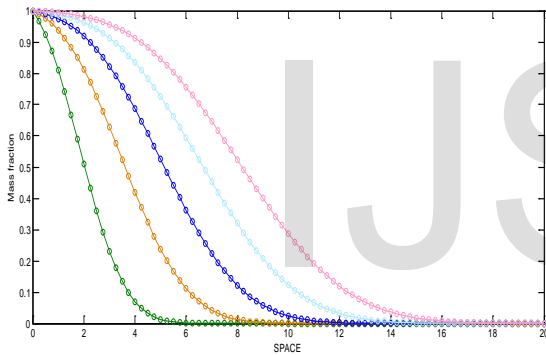Fig 8: Nitrogen Concentration with $D = 1\ cm^2/s$ at different temporal grid size with $v = 1\ cm/s$.

From figure 6, 7 and 8 we observe that with the decreasing of the value of v, the speed of nitrogen flow is decreasing.

Now keeping spatial grid size and velocity ($\mathbf{v = 2\ cm/s}$) we observe three cases by the following figures for different temporal size and different diffusion coefficients. Then for $\mathbf{v = 2\ cm/s}$ the solution appeared is given below
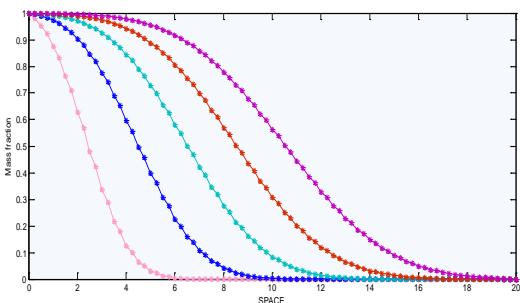

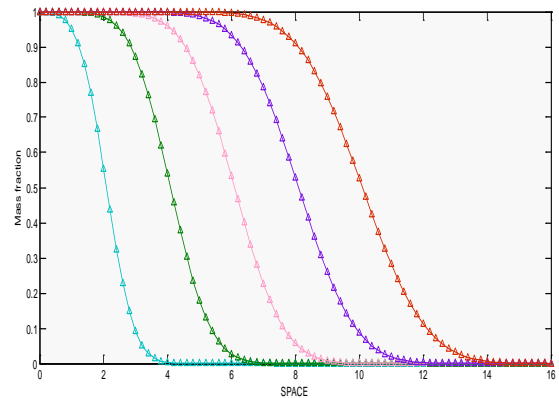Fig 9: Nitrogen Concentration with velocity $v = 2\ cm/s$ at different temporal grid size with $D = 1\ cm^2/s$

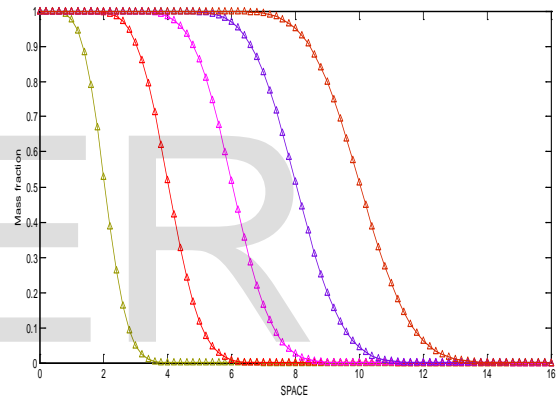Fig 10: Nitrogen Concentration with velocity $v = 2\ cm/s$ at different temporal grid size with $D = 0.1\ cm^2/s$

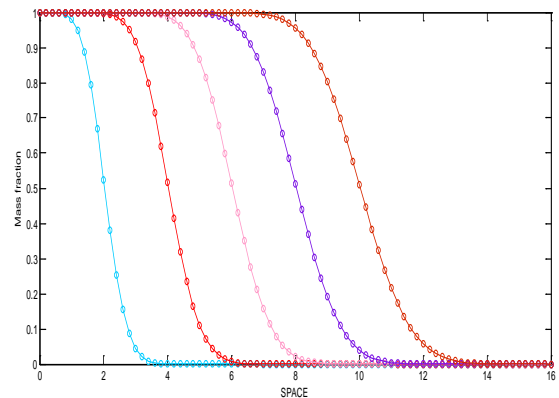Fig 11: Nitrogen Concentration with velocity $v = 2\ cm/s$ at different temporal grid size with $D = 0.01\ cm^2/s$

Fig 12: Nitrogen Concentration with velocity $v = 2\ cm/s$ at different temporal grid size with $D = 0.001\ cm^2/s$

Following figure13 shows numerical scheme for different diffusion co-efficient for fixed time $t = 5$ and velocity $v = 2 \ cm/s$.
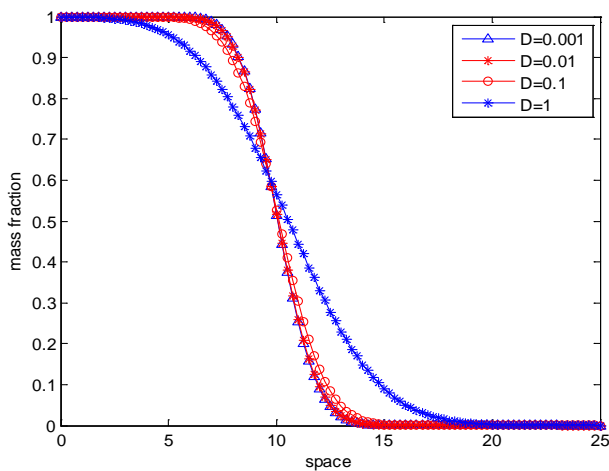

Fig 13: manifest that a bigger D results in a wider nitrogen front or a bigger diffusion coefficient.

As we know that the stability condition of advection diffusion equation is $\frac{D\Delta t}{\Delta x^2} \leq \frac{1}{2}$ the course of action will be continued until this stability condition is satisfied. Thus as diffusion coefficient is increasing from 0.001 to 1, the nitrogen wave front is becoming wider than before.

5. Conclusion

There is growing concern in understanding and evaluating the nitrogen transportation at the air. Our purpose is to estimate the nitrogen wave front for different diffusion coefficient. The problem by the PDE which is known as advection-diffusion equation. Although this problem can be solved analytically, but in order to incorporate initial and boundary data it is completely unavoidable to use numerical method .We have studied explicit differences schemes for the numerical solutions of the advection-diffusion equation of nitrogen transportation in air flow. In the numerical simulation of nitrogen transportation experiment we have used real data [9] and the results are in a very good agreement with the results presented in [9].It is thus verified that the advection-diffusion equation is a very useful mathematical model to describe nitrogen transportation in air flow and explicit finite difference scheme is quite suitable to perform the numerical simulation of the nitrogen transportation in air flow. It may be more effective experiment using 2D advection-diffusion equation passing through porous media or the Crank-Nicolson method may be better than the explicit finite difference scheme and we left this as our future work.

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