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One Dimensional Contaminant Transport with Turbulence Effect: Modeling and Solutions

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Abstract: This paper presents a one-dimensional model for atmospheric contaminant transport that accounts for advection, diffusion, and turbulence effects. The classical advection-diffusion equation is extended through Reynolds decomposition and hence averaging to incorporate turbulence via eddy diffusivity. While analytical solutions for such models are typically intractable under real-world conditions with complex boundaries, we derive an exact solution for idealized cases with general initial condition and Dirichlet boundary conditions, providing a valuable benchmark for numerical validation. To address more realistic scenarios, numerical solutions are developed using finite difference (FD) and Crank-Nicolson (CN) methods. This study explores the impact of eddy diffusivity and temporal dynamics on pollutant concentrations within idealized scenarios, benchmarking numerical methods against a derived analytical solution. The analysis reveals that the CN method outperforms FD method in accuracy, particularly in diffusion-dominated regimes ($Pe \ll 1$), owing to its unconditional stability and second-order temporal precision. By combining analytical and numerical approaches, this study provides a robust framework for simulating turbulent transport where purely analytical solutions are impractical. The findings show that both methods effectively predict pollutant concentrations under turbulent conditions, offering practical insights for environmental impact assessments and pollution mitigation strategies.

Keywords: Advection, Diffusion, Eddy diffusivity, Analytical solution, Numerical solutions

1 Introduction

Advection refers to the movement of matter within a flowing fluid from one location to another, serving as a significant mechanism for transportation [17, 20]. Diffusion is the process where molecules transition from areas of high concentration to those of lower concentration, driven by a force [21]. The rate of mass transfer attributed to molecular diffusion is described by Fick's law [12, 20, 21] and explains that the rate at which the mass transported by molecular diffusion is directly proportional to the concentration gradient in that direction. Defining turbulence precisely is not easy; however, turbulent flows share several key traits as unpredictability, rapid diffusion, high levels of fluctuating vorticity, and the dissipation of kinetic energy [21]. Turbulent diffusion effectively reduces the concentrations of contaminants released into the environment at a fast pace. Despite extensive research spanning numerous years, precise forecasts of these concentrations remain elusive [1]. Many mathematical models of turbulent diffusion, especially those in engineering, typically anticipate only time-averaged concentrations [10, 27].

A major challenge in studying turbulence is unraveling the connections among the structure, movement dynamics, and statistical characteristics across both small and large motion scales [22]. One notable aspect of turbulence that has been extensively explored in recent decades is scale invariance. Scale invariance refers to the consistency of certain flow features across various scales of motion. This symmetry suggests a straightforward relationship between small and large scales, making it a valuable component in turbulence modeling. The concept of scale invariance in turbulence traces its roots back to Richardson's work in 1922 [16]. Eddy diffusivity, or turbulent diffusivity, measures how quickly pollutants and other substances spread due to atmospheric turbulence, which varies with factors like wind shear and atmospheric stability [2]. It is lower in stable conditions and higher in turbulent, unstable ones, serving as a critical concept in fluid dynamics to describe the diffusion of momentum, heat, or mass in turbulent flows [22]. This parameter is essential in models for turbulent transport in fields like atmospheric science and engineering [1].

Air pollution involves harmful solid, liquid, or gaseous substances in the atmosphere, stemming from industry, transport, agriculture, and natural events. Key pollutants—such as particulate matter, NO_2, SO_2, CO, ozone, and VOCs contribute to climate change, acid rain, and ecosystem damage [14, 26]. Prolonged exposure causes serious health issues, including respiratory and cardiovascular diseases, lung cancer, and premature death [5, 13]. Therefore, mathematical models and corresponding solutions are vital for analyzing and mitigating air pollution effectively.

Pasquill (1961) [18] presents a comprehensive method for estimating the dispersion of wind borne pollutants based on empirical observations and statistical analysis and emphasizes the importance of understanding atmospheric stability, wind speed, and turbulence in predicting the spread of pollutants from a source. Appadu (2013) [3] compares standard and nonstandard finite difference schemes for solving the one-dimensional advection-diffusion equation and evaluates the accuracy, stability, and efficiency of these numerical methods in capturing the behavior of the solution under different conditions. Hanna et al. (1982) [10] overview the processes of pollutant dispersion in the atmosphere, covering advection, diffusion, deposition, and chemical transformation. The book discusses various dispersion models, from simple Gaussian to complex numerical approaches for predicting pollutant spread. Goyal and Kumar (2011) [8] developed a mathematical model to simulate the transport, dispersion, and transformation of air pollutants in the study area and validated their air pollution model using observational data from monitoring stations located within the study area. Taylor (1922) [25] introduced a mathematical framework for solute dispersion in fluids, showing how velocity profiles in laminar and turbulent flows affect dispersion rates. His work is foundational for understanding pollutant transport in the environments. Wissocq and Abgrall (2023) [28] introduced a kinetic method for linear and non-linear convection-diffusion problems, offering insights into finite kinetic speeds in 1D cases. Additionally, Bedrossian et al. (2019) [4] investigated mixing and dissipation properties in ADEs under stochastic Navier-Stokes advection, providing valuable perspectives on enhanced dissipation and exponential mixing.

Most existing studies on advection-diffusion equations (ADEs) rely on numerical methods suited for simplified, laminar flows, often overlooking turbulence effects and lacking analytical validation. This limits their accuracy in realistic contexts such as atmospheric or riverine pollutant transport. While analytical solutions can provide exact expressions, they are typically constrained by idealized boundary and initial conditions, reducing their applicability to complex real-world scenarios. Addressing these limitations, the present study derives an exact solution to the 1D turbulent ADE using Reynolds decomposition to account for turbulence, under homogeneous Dirichlet boundary conditions and general initial conditions. This analytical framework enables the determination of concentration profiles throughout the domain and reveals how eddy diffusivity and time influence contaminant decay, especially under low Peclet number conditions. To complement the analytical model and extend its applicability, numerical simulations using Crank–Nicolson and finite difference methods are performed. This integrated approach not only validates the analytical solution but also provides a comprehensive understanding of transport dynamics in the presence of turbulence and complex boundaries.

2 Extended Mass Transport Model

The advection-diffusion equation (ADE) finds extensive use in operational atmospheric dispersion models for forecasting average concentrations of pollutants within the planetary boundary layer (PBL). Essentially, this equation allows for the theoretical modeling of dispersion from a continuous point source [6]. The general linear form of one dimensional ADE in cartesian system is [11]

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}(D\frac{\partial C}{\partial x}) - \frac{\partial}{\partial x}(uC), \tag{1}$$

where C is the concentration and D is the diffusivity of the pollutants at position x of the domain at any time t. u is the mean advective velocity along the x direction.

The mass conservation equation for turbulent flows can be obtained from the ADE by considering that turbulence is significant enough to break down the mean advective velocity u and the concentration C into a temporal mean taken over consecutive time intervals $T = t_2 - t_1$ and an instantaneous deviation from this mean as [1, 10, 23]

$$\frac{\partial(\overline{C} + C')}{\partial t} = \frac{\partial}{\partial x}[D\frac{\partial(\overline{C} + C')}{\partial x}] - \frac{\partial}{\partial x}((\overline{u} + u')(\overline{C} + C')), \tag{2}$$

where u', and C' denote the instantaneous deviations from the time means $\overline{u}$, and $\overline{C}$ due to eddy fluctuations. Further,

$$\overline{u} = \frac{1}{T}\int_{t_1}^{t_2} u(t)dt, \text{where} \quad u = \overline{u} + u', \text{and} \quad \overline{C} = \frac{1}{T}\int_{t_1}^{t_2} C(t)dt, \text{where} \quad C = \overline{C} + C' \tag{3}$$

Applying the sum rule of differentiation after multiplying the second term on right hand side, and on the remaining terms of equation (2), we obtain

$$\frac{\partial \overline{C}}{\partial t} + \frac{\partial C'}{\partial t} = \frac{\partial}{\partial x}(D\frac{\partial \overline{C}}{\partial x}) + \frac{\partial}{\partial x}(D\frac{\partial C'}{\partial x}) - \frac{\partial}{\partial x}(\overline{u}\overline{C}) - \frac{\partial}{\partial x}(\overline{u}C') - \frac{\partial}{\partial x}(u'\overline{C}) - \frac{\partial}{\partial x}(u'C') \tag{4}$$

Since u' and C' are the eddy fluctuations and the time means of the eddy fluctuations $\overline{u'}$, and $\overline{C'}$ become zero, i.e.,

$$\overline{u'} = \frac{1}{T}\int_{t_1}^{t_2} u'(t)dt = \frac{1}{T}\int_{t_1}^{t_2}(u(t) - \overline{u})dt = 0, \text{and} \quad \overline{C'} = \frac{1}{T}\int_{t_1}^{t_2} C'(t)dt = \frac{1}{T}\int_{t_1}^{t_2}(C(t) - \overline{C})dt = 0 \tag{5}$$

By employing Reynolds averaging principles and averaging across the time span T, equation (4) after using equation (5) , takes the following specific form [10, 23]

$$\frac{\partial \overline{C}}{\partial t} = \frac{\partial}{\partial x}(D\frac{\partial \overline{C}}{\partial x}) - \frac{\partial}{\partial x}(\overline{u}\overline{C}) - \frac{\partial}{\partial x}(\overline{u'C'}) \tag{6}$$

This equation (6) illustrates how the eddy fluctuations influence the temporal variation of $\overline{C}$ and how $\overline{C}$ relies on the eddy fluctuations u' and C'.
From the statistical perspective, the quantity $\overline{u'C'} = \overline{(u - \overline{u})(C - \overline{C})}$ represents the covariance between the variables u and C, and it becomes zero only when u and C are not correlated [23].
Since turbulent fluxes are presumed to be proportional to the mean concentration gradient of the temporal mean of C, akin to Fick's law [10, 15, 27]. i.e.,

$$\overline{u'C'} = -K\frac{\partial \overline{C}}{\partial x}, \tag{7}$$

where K denotes the eddy diffusion constant or eddy diffusivity and has unit m^2s^{-1}. Utilizing this equation (7), the prior equation (6) can be reformulated as

$$\frac{\partial \overline{C}}{\partial t} = \frac{\partial}{\partial x}(D\frac{\partial \overline{C}}{\partial x}) - \frac{\partial}{\partial x}(\overline{u}\overline{C}) + \frac{\partial}{\partial x}(K\frac{\partial \overline{C}}{\partial x}) \tag{8}$$

If we assume that the air maintains a constant velocity and that the coefficients D and K remain consistent, the equation (8) is simplified to

$$\frac{\partial \overline{C}}{\partial t} + \overline{u}\frac{\partial \overline{C}}{\partial x} = D\frac{\partial^2 \overline{C}}{\partial x^2} + K\frac{\partial^2 \overline{C}}{\partial x^2}. \tag{9}$$

Replacing the sum of D and K by a constant λ and simply drop out the bar of C and u, equation (9) takes the form

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = \lambda\frac{\partial^2 C}{\partial x^2} \tag{10}$$

This is the extended mass transport model which incorporates the mechanisms of advection, diffusion, and turbulence for transporting pollutants in the atmosphere. The primary innovation of this enhanced model lies in its ability to provide a more precise description of pollutant dispersion in the atmosphere. Its solution is expected to offer the most accurate measurement of pollutant concentration and produce superior results compared to those derived from the advection-diffusion equation.

3 Result and Discussion

3.1 Analytical solution

The general initial condition and the homogeneous Dirichlet boundary conditions under which the specific solution of the above model(10) is planned to be obtained are

$$C(x,0) = f(x), \quad C(0,t) = C(L,t) = 0 \tag{11}$$

To transform the developed model (10) into a pure diffusion equation, let the nontrivial solution of (10) be given by [7]

$$C(x,t) = A(x,t)V(x,t). \tag{12}$$

The objective is to identify a function $A(x,t)$ such that the advection term in (10), i.e., uC_x, vanishes. Plugging (12) into (10) and omitting all the details of algebra, we obtain

$$V_t = \lambda V_{xx}, \tag{13}$$

which is the transformed pure diffusion equation.

The transformed initial condition is

$$V(x,0) = \exp\left(-\frac{ux}{2\lambda}\right) f(x). \tag{14}$$

The transformed Dirichlet boundary conditions are

$$V(0,t) = 0, \tag{15}$$

$$V(L,t) = 0. \tag{16}$$

Using the separation of variables method along with the principle of superposition, the general solution of equation (13) is the linear combination of the form [7, 20]

$$V(x,t) = \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{L}\right) \exp\left(-\lambda \left(\frac{n\pi}{L}\right)^2 t\right). \tag{17}$$

where b_n are constants and can be calculated by using the initial condition as

$$V(x,0) = \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{L}\right) \Rightarrow \exp\left(-\frac{ux}{2\lambda}\right) f(x) = \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{L}\right) \tag{18}$$

which is a half range Fourier Sine series and

$$b_n = \frac{2}{L}\int_0^L \exp\left(-\frac{ux}{2\lambda}\right) f(x) \sin\left(\frac{n\pi x}{L}\right) dx \tag{19}$$

Finally, reducing the algebraic details, the analytical solution to the model (10) becomes

$$C(x,t) = \exp\left(-\frac{u^2 t}{2\lambda}\right) \exp\left(\frac{ux}{2\lambda}\right) \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{L}\right) \exp\left(-\lambda \left(\frac{n\pi}{L}\right)^2 t\right) \tag{20}$$

where b_n can be calculated by using equation (19).
Using the following Dirichlet homogeneous boundary conditions and a suitable initial condition

$$BCs : C(0,t) = C(L,t) = 0; \quad t \geq 0 \tag{21}$$

$$IC : C(x,0) = sin(\frac{\pi x}{L}); \quad 0 \leq x \leq L., \tag{22}$$

the solution of the above developed model (10) with the reference of (19), and (20) becomes [20]

$$C(x,t) = exp(-(\frac{u^2}{4\lambda} + \frac{\lambda\pi^2}{L^2})t) \times sin(\frac{\pi x}{L}), \text{where} \quad \lambda = D + K. \tag{23}$$

The function $C(x, t)$ represents a physical quantity evolving over space x and time t. The parameters present in the function $C(x, t)$ in equation (23) determine the behavior of the system and describes a phenomenon where C decays exponentially with time and oscillates sinusoidally with x. The combination of these two terms results in a wave-like behavior that decays over time and oscillates spatially. The visual output effectively illustrates the alterations of the function $C(x, t)$ across spatial and temporal dimensions, offering valuable insights into its dynamics and progression.

In our study, we employed a transformation approach where the concentration function C(x,t) is expressed as a product of two functions: C(x,t) = A(x,t)V (x,t).

This method allowed us to decouple the original ADE into a pure diffusion equation for V(x,t) and an associated equation for A(x,t), facilitating the derivation of an analytical solution in one dimension. Extending this specific transformation technique to two dimensions introduces significant mathematical complexity. The presence of additional spatial variables complicates the decoupling process, and the resulting equations may not be amenable to standard analytical methods. Moreover, the integration of solutions for A(x,y,t) and V(x,y,t) in two dimensions can lead to cumbersome calculations that may not yield closed-form expressions. Therefore, the particular transformation approach utilized in our study is not readily extendable to higher dimensions due to the increased mathematical intricacies involved.

3.1.1 Concentration by varying the eddy diffusivity

Richardson estimated eddy diffusivity as $K \approx 1\,\mathrm{m^2/s}$ from smoke trail studies, while Robert proposed $K \in [1, 10]\,\mathrm{m^2/s}$ based on short-range diffusion tests. Broader literature suggests a range from 0.01 to $10^7\,\mathrm{m^2/s}$ [24]. Higher K promotes turbulence and dispersion, lowering peak concentrations; lower K leads to localized pollutant buildup. Diffusivity varies with pollutant type, atmospheric conditions, and environment. Molecular diffusivity D for pollutants such as CO, CO_2, CH_4, NO_2, SO_2, and $PM_{2.5}/PM_{10}$ typically ranges from 10^{-5} to $10^{-4}\,\mathrm{m^2/s}$, increasing with turbulence [24]. At 20°C, $D_{CO_2} = 1.61 \times 10^{-5}\,\mathrm{m^2/s}$ [19], $D_{CH_4} = 1.8 \times 10^{-5}\,\mathrm{m^2/s}$ [21], and average wind speed is $u = 5\,\mathrm{m/s}$ [24]. In this study, we use $L = 1000\,\mathrm{m}$, $u = 5\,\mathrm{m/s}$, and $D = 1.61 \times 10^{-5}\,\mathrm{m^2/s}$. By varying $K = 0, 1, 10, 10^2, 500, 10^3\,\mathrm{m^2/s}$, we generate analytical 3D concentration plots, as shown in Fig. 1.

3.1.2 Concentration with different time points

The feasibility of the analytical solution can be demonstrated more distinctly through the corresponding 2D plots at various time points. The 2D plots illustrate the analytical solution $c(x,t) = e^{-\lambda t} \sin\left(\frac{\pi x}{1000}\right)$, where λ depends on diffusivity and eddy diffusivity. A larger λ causes quicker decay in pollutant concentration. In cases of low diffusivity without eddy diffusivity (Figs. 2A–C), the concentration drops to zero rapidly, rendering the solution ineffective due to large peclet number. With increased eddy diffusivity (Figs. 2D–F), decay is slower, improving concentration estimation. Accurate predictions occur when $\left(\frac{u^2}{4\lambda} + \frac{\lambda\pi^2}{L^2}\right) t \approx 10^{-2}$, using realistic CO_2 parameters, eddy diffusivity $K \in [1, 1000]\,\mathrm{m^2/s}$, and advective velocity $u \approx 5\,\mathrm{m/s}$. The small value of the advection velocity relative to the effective diffusivity results in a low Peclet number, indicating a diffusion-dominated transport regime. Consequently, the concentration profiles in the simulations exhibit characteristics typical of diffusion processes, such as symmetric spreading, with minimal advection-induced asymmetry. This behavior aligns with theoretical expectations for systems where diffusion and turbulence are the primary transport mechanisms.

3.2 Numerical Methods

3.2.1 Finite difference method

The finite difference method (FDM) substitutes the continuous derivatives in differential equations with finite difference approximations, transforming the differential equation into a system of algebraic equations

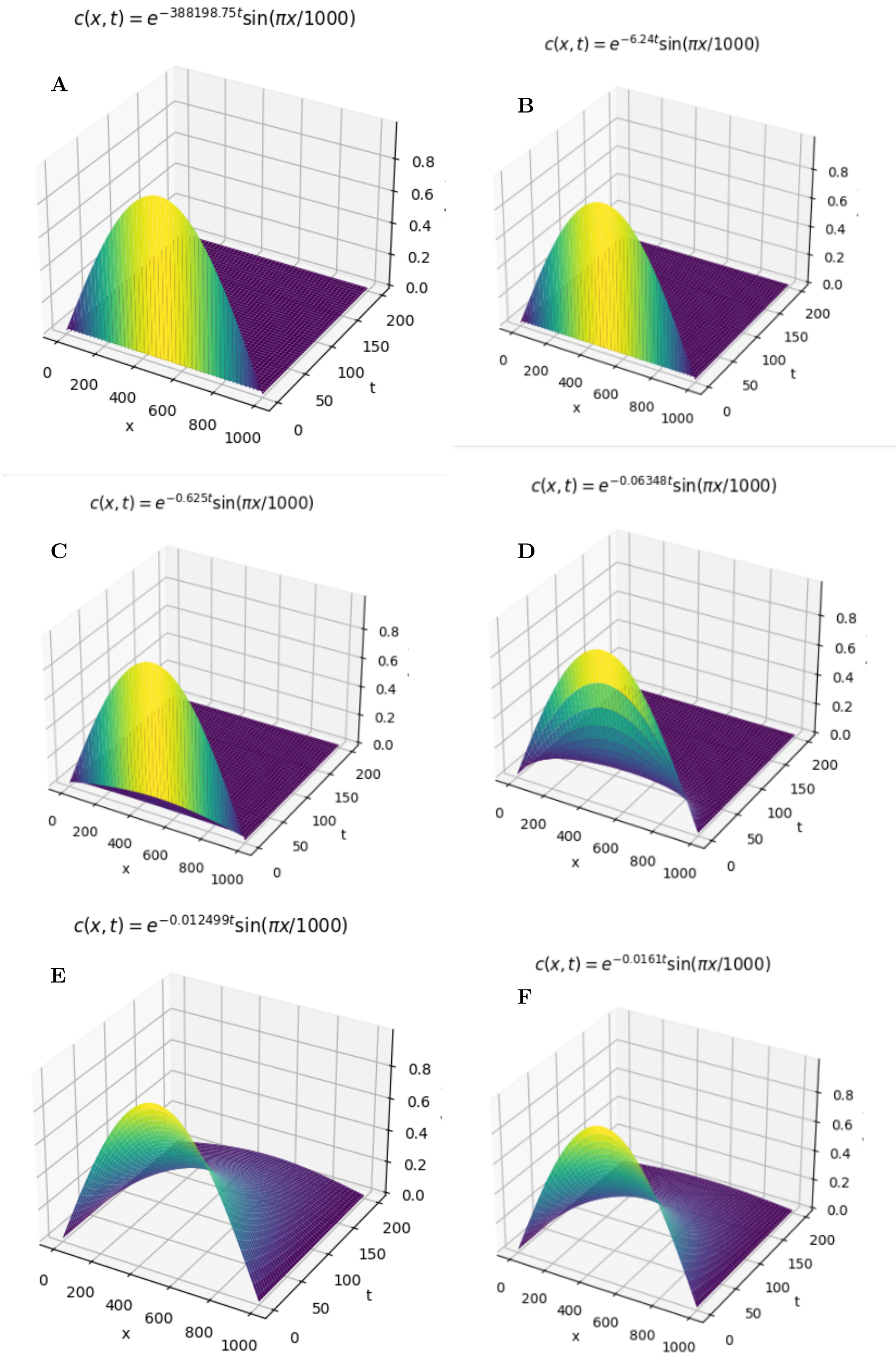

Figure 1: Dynamics of air pollutants with constant diffusivity and variable eddy diffusivity. The value of eddy diffusivity **A:** $K = 0$ m^2/s, **B:** $K = 1$ m^2/s,**C:** $K = 10$ m^2/s, **D:** $K = 100$ m^2/s,**E:** $K = 500$ m^2/s, **F:** $K = 1000$ m^2/s.

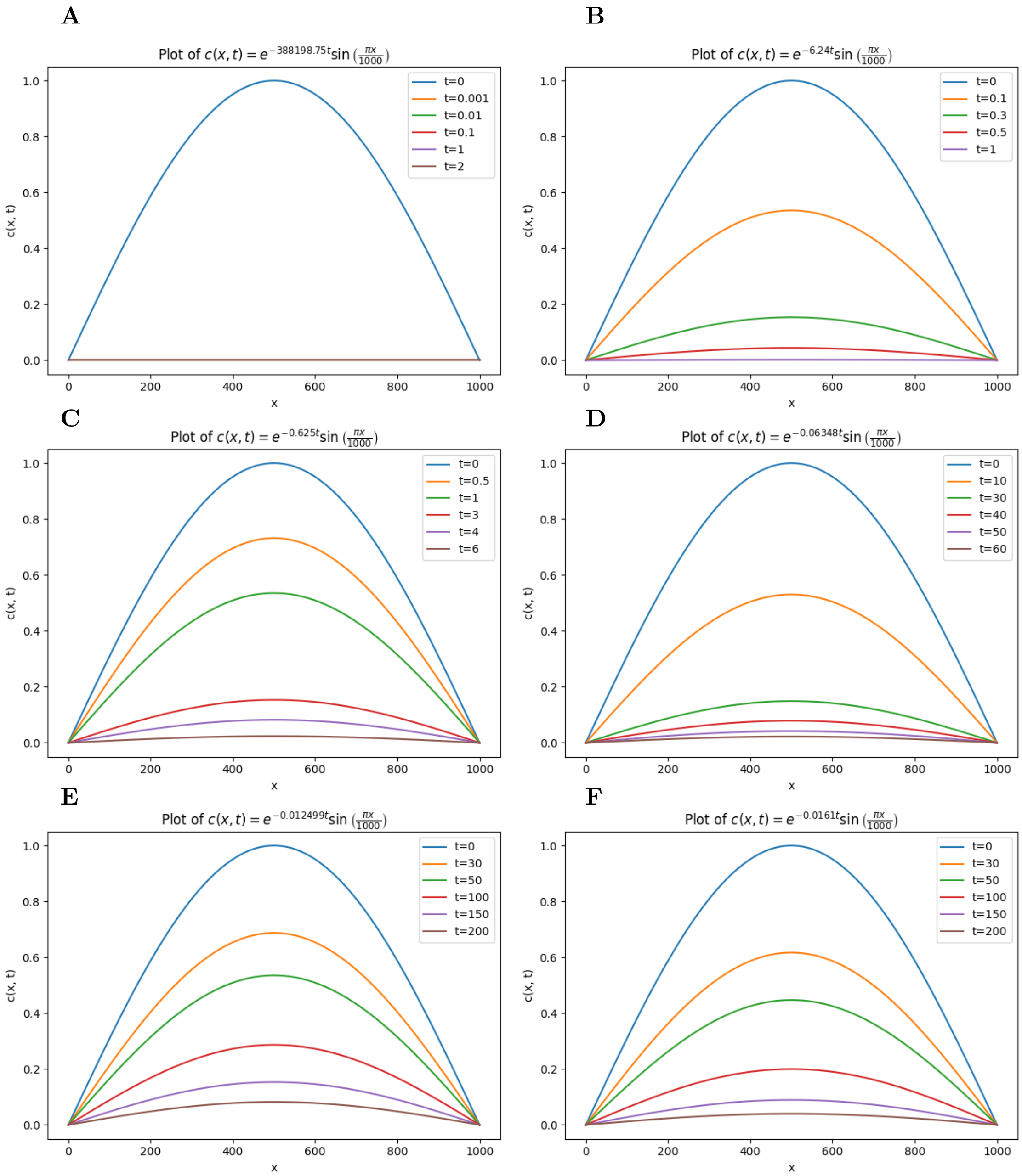

Figure 2: Concentration of pollutants with variable eddy diffusivity at different time points. The value of eddy diffusivity **A:** $K = 0$ m^2/s, **B:** $K = 1$ m^2/s, **C:** $K = 10$ m^2/s, **D:** $K = 100$ m^2/s, **E:** $K = 500$ m^2/s, **F:** $K = 1000$ m^2/s.

[9].

The explicit scheme for the model (10) is

$$C_i^{n+1} = C_i^n + \frac{\lambda \Delta t}{(\Delta x)^2}(C_{i+1}^n - 2C_i^n + C_{i-1}^n) - \frac{u\Delta t}{2\Delta x}(C_{i+1}^n - C_{i-1}^n) \tag{24}$$

The new value C_i^{n+1} is computed explicitly from C_i^n, C_{i+1}^n and C_{i-1}^n.

The explicit method is conditionally stable, meaning its stability depends on the time step Δt meeting specific criteria, known as the Courant–Friedrichs–Lewy (CFL) condition. These criteria are based on the spatial grid size Δx and the problem's parameters, such as the eddy diffusion coefficient K, diffusion coefficient D, and advection velocity u. Therefore, when applying this method to solve the differential equation, both the spatial and temporal step sizes must be chosen to ensure the following stability conditions are satisfied:

$$\frac{\lambda \Delta t}{(\Delta x)^2} \leq \frac{1}{2}, \quad \frac{u\Delta t}{\Delta x} \leq 1$$

If these conditions are not satisfied, the solution can become unstable and produce spurious oscillations or blow up.

3.2.2 Crank-Nicolson method

The Crank-Nicolson method (CN) is a midpoint strategy that integrates both the current and next time steps into its formulation. It combines the benefits of the explicit (forward time step) and implicit (backward time step) approaches, providing stability while maintaining accuracy [9].

Define the grid points $x_i = i\Delta x$ for $i = 0, 1, 2, ..., N$ and the time step $t_n = n\Delta t$ for $n = 0, 1, 2, ...$ Let $C(x_i, t_n) = C_i^n$ and represents the solution at the spatial point i and time step n.

For Crank-Nicolson Method, we have

$$\frac{\partial C}{\partial t} \approx \frac{C_i^{n+1} - C_i^n}{\Delta t}, \quad \frac{\partial C}{\partial x} \approx \frac{1}{2}(\frac{C_{i+1}^{n+1} - C_{i-1}^{n+1}}{2\Delta x} + \frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x})$$

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

Substituting these values, equation (10) becomes

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} + \frac{u}{4\Delta x}(C_{i+1}^{n+1} - C_{i-1}^{n+1} + C_{i+1}^n - C_{i-1}^n) = \frac{\lambda}{2\Delta x^2}(C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1} + C_{i+1}^n - 2C_i^n + C_{i-1}^n) \tag{25}$$

Transforming $(n+1)^{th}$ time level terms to left hand side of the equation and the known n^{th} time level terms to the right hand side, equation (25) takes the form:

$$aC_{i-1}^{n+1} + bC_i^{n+1} + mC_{i+1}^{n+1} = d_i \tag{26}$$

where,

$$a = -\frac{u\Delta t}{4\Delta x} - \frac{\lambda \Delta t}{2(\Delta x)^2}, \quad b = 1 + \frac{\lambda \Delta t}{(\Delta x)^2}, \quad m = \frac{u\Delta t}{4\Delta x} - \frac{\lambda \Delta t}{2(\Delta x)^2}$$

and d_i contains the known values from the previous n^{th} time step.
Equation (26) represents tri-diagonal system and can be efficiently solved by using the Thomas algorithm.

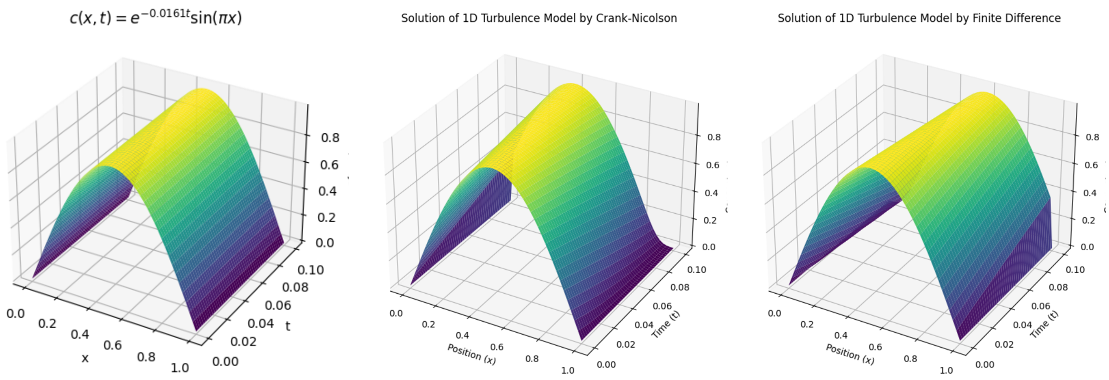

Figure 3: Comparison between the plots of analytical and numerical solutions.

4 Comparison of Analytical and Numerical Solutions

Below are the 3D plots related with the solution of extended model (10) obtained through analytical, Crank-Nicholson, and Finite Difference method respectively by taking $L = 1$, $T = 0.1$, $\lambda = 0.010016$, $u = 1$, $nx = 50$, and $nt = 500$.

To detect the appropriateness of the numerical methods, ten random points were chosen within the specified domain and time intervals. The concentrations calculated at these points from the Analytical, Crank-Nicolson, and Finite Difference methods, along with their respective percentage errors, are displayed in the table below. The above table and the plots confirms that CNM outperforms the FDM.

Table 1: Comparison of analytical, CN, and FDM solutions with percentage errors.

(x, t)	Analytical	FDM	CN	Err FDM (%)	Err CN (%)
(0.6044, 0.2674)	0.192685	0.193058	0.197418	0.19	2.46
(0.5704, 0.2372)	0.171855	0.168833	0.172997	1.76	0.66
(0.5939, 0.3368)	0.052934	0.046529	0.049165	12.10	7.12
(0.7381, 0.1109)	0.271259	0.261959	0.263760	3.43	2.76
(0.6360, 0.1029)	0.778657	0.769382	0.763783	1.19	1.91
(0.7097, 0.4376)	0.091403	0.085869	0.089884	6.05	1.66
(0.5132, 0.2049)	0.098500	0.094067	0.097140	4.50	1.38
(0.5473, 0.1412)	0.455116	0.467458	0.469374	2.71	3.13
(0.7821, 0.5638)	0.048519	0.042515	0.045490	12.37	6.24
(0.4752, 0.2640)	0.012122	0.008988	0.009680	25.86	20.14

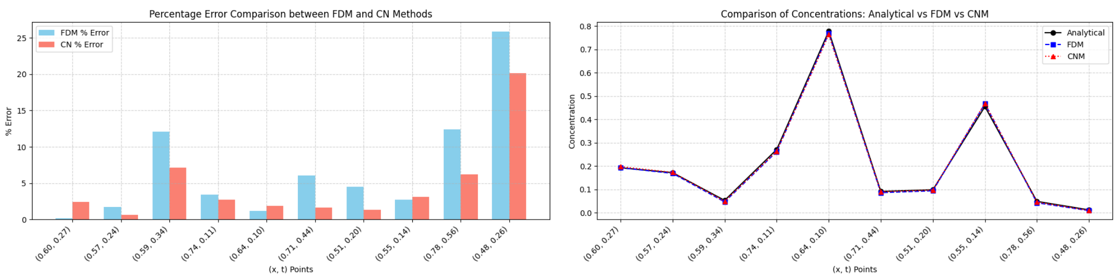

Figure 4: Comparison of Analytical, CN, and FDM Solutions with graphs.

5 Conclusion

This work presents a detailed one-dimensional mathematical model for simulating atmospheric pollutant transport, accounting for advection, molecular diffusion, and turbulence via Reynolds-averaged techniques. By incorporating eddy diffusivity into the classical advection-diffusion framework, an analytical solution was achieved for simplified conditions, serving as a foundational reference for evaluating numerical approaches. To simulate more realistic transport scenarios, numerical methods including Finite Difference and Crank-Nicolson schemes were employed. The Crank-Nicolson method demonstrated superior performance, especially in diffusion-dominated cases, due to its unconditional stability and enhanced temporal accuracy. Furthermore, analysis of 2D and 3D visualizations showed a consistent decline in pollutant concentration with increasing eddy diffusivity and time. Overall, this combination of analytical and numerical modeling establishes a robust and adaptable approach to studying contaminant dispersion in turbulent atmospheric environments. The outcomes offer practical tools and insights for environmental assessment, monitoring, and the development of effective air quality control strategies.

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