International Journal on Data Science and Technology
2026; 15(4): 123-132
http://www.sciencepublishinggroup.com/j/ijdst
doi: 10.11648/j.acm.20261504.11

Comparative Analysis of Finite Difference and Crank-nicolson Schemes in Simulating Air Pollution Dispersion

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To cite this article:

Jimrise Ochwach, Julius Njiru Nyaga, Mark Okongo. (2026). Comparative Analysis of Finite Difference and Crank-nicolson Schemes in Simulating Air Pollution Dispersion. *International Journal on Data Science and Technology, 15*(4), 123-132.
https://doi.org/10.11648/j.acm.20261504.11

Received: 5 October 2025; **Accepted:** 18 October 2025 **Published:** 11 August 2026

Abstract: Accurate prediction of atmospheric pollutant transport is essential for air quality assessment and environmental management. Classical advection-diffusion models often neglect the combined effects of temperature and humidity, despite their significant influence on pollutant transport and dispersion within the atmospheric boundary layer. This study develops a two-dimensional meteorology-dependent advection-diffusion-reaction model that incorporates temperature-dependent thermodiffusion through the Soret effect and humidity-dependent modification of advective transport. The governing equation is solved numerically using the Explicit Finite Difference (FD) and Crank-Nicolson (CN) schemes to evaluate their accuracy, stability, and computational performance. Von Neumann stability analysis is employed to establish the stability conditions of both numerical methods. The analysis shows that the FD scheme is conditionally stable and requires restrictive time-step selection to satisfy the Courant-Friedrichs-Lewy condition, whereas the CN scheme remains unconditionally stable for the diffusion component and demonstrates superior numerical robustness under practical simulation conditions. Numerical experiments implemented in MATLAB reveal that the CN scheme produces smoother concentration profiles, reduced numerical diffusion, and improved solution accuracy, particularly for long simulation periods. The simulations further indicate that increased wind velocity enhances pollutant transport, higher relative humidity suppresses dispersion and increases pollutant residence time, and elevated temperatures promote stronger atmospheric mixing through thermally induced diffusion. These findings demonstrate that incorporating meteorological variables substantially improves the physical realism of atmospheric dispersion models. The study concludes that the Crank-Nicolson method provides a more reliable and efficient numerical framework for simulating pollutant transport under varying environmental conditions and offers a practical tool for urban air quality assessment, environmental planning, and evidence-based pollution control strategies.

Keywords: Advection-diffusion Equation, Atmospheric Pollutants, Boundary Layer, Finite Difference Method, Numerical Simulation

1. Introduction

Air pollution remains one of the most pressing environmental and public health issues globally. The growing rate of industrialization, urbanization, and energy consumption has led to increased emissions of particulate matter, greenhouse gases, and other toxic pollutants. These emissions degrade air quality, alter atmospheric chemistry, and cause respiratory and cardiovascular illnesses among exposed populations [1]. Effective control of pollution requires accurate prediction of pollutant behavior under different atmospheric and meteorological conditions. Mathematical and numerical models have become essential tools for describing, predicting, and managing air pollution dynamics.

Mathematical modeling provides a quantitative framework

for studying pollutant transport and transformation in the atmosphere. Through simplified representations of physical processes, such as advection, diffusion, and chemical reactions, models allow researchers to simulate pollutant dispersion over time and space [4, 10]. The advection-diffusion equation has been widely used to represent the combined effects of wind-driven transport and turbulent mixing on pollutant concentration. In real atmospheric conditions, however, factors such as temperature, humidity, and wind velocity introduce nonlinearity into dispersion behavior. These parameters significantly affect the rate at which pollutants spread, dilute, or accumulate within the atmospheric boundary layer [5, 6].

Several global assessments have underscored the scale of air pollution challenges. The World Health Organization reported that exposure to fine particulate matter $(PM_{2.5})$ above the annual limit of 10 $\mu g/m^3$ contributes to millions of premature deaths each year [2]. Many developing countries experience pollutant levels several times higher than these recommended limits. Poor ventilation, unregulated industrial emissions, and the burning of low-quality fuels exacerbate local air quality deterioration. In addition to human health effects, atmospheric pollutants interact with solar radiation and cloud microphysics, influencing regional climate processes [4].

The study of pollutant dispersion is closely linked to fluid dynamics and heat transfer. Diffusion coefficients, wind profiles, and temperature gradients govern the motion and transformation of pollutants in the boundary layer. The classical Fickian diffusion theory describes pollutant movement from regions of high to low concentration, while Soret diffusion explains transport induced by temperature gradients [8, 11]. Variations in humidity alter air density and molecular diffusivity, thereby modifying the effectiveness of both advective and diffusive transport mechanisms. When relative humidity increases, pollutant particles often absorb moisture and grow in size, leading to slower dispersion and longer atmospheric residence times [5]. These interactions demonstrate the importance of incorporating meteorological variables into numerical dispersion models.

Modeling pollutant transport under realistic meteorological conditions requires reliable numerical schemes that can handle spatial and temporal variations without introducing excessive numerical diffusion or instability. Finite difference and Crank-nicolson methods are two widely used numerical approaches for solving parabolic partial differential equations, including the advection-diffusion type. The finite difference scheme provides a straightforward discretization of derivatives but may exhibit conditional stability, depending on time step and grid size. The Crank-nicolson method, on the other hand, offers second-order accuracy in both space and time and is unconditionally stable for linear problems [7, 10]. Comparing their performance in pollutant dispersion simulation is crucial for identifying efficient and stable techniques suitable for large-scale atmospheric modeling.

Pollutant dispersion studies also depend on accurate parameter estimation. Constants such as the gas constant, diffusion coefficients, and the heat of transport influence the accuracy of computed concentrations [9]. Earlier modeling efforts by [3] highlighted how soil porosity affects nitrate transport using advection-dispersion equations. The same conceptual framework can be extended to atmospheric environments, where pollutant particles undergo similar advection and diffusion processes. Integrating meteorological dependencies into this framework enhances predictive power and ensures closer alignment between model output and observed air quality data.

The present study builds upon these foundations to develop a meteorology-sensitive pollutant dispersion model and evaluate the comparative performance of finite difference and Crank-nicolson schemes. By coupling temperature- and humidity-dependent terms into the governing equations, the study aims to provide a more realistic representation of atmospheric dispersion. This approach supports improved understanding of air pollution dynamics and contributes to better-informed decisions in environmental management and public health policy.

2. Model Development

To accurately simulate the transport and dispersion of atmospheric pollutants, a mathemtical model based on the advection diffusion equation is employed.This approach captures two primary physical processes influencing pollutant behaviour in the atmosphere.Advection which represents transport of pollutants by wind flow and diffusion which accounts for the spread due to turbulence. The advection-diffusion model is used to simulate air pollutant distribution. The advection-diffusion equation of air pollutants in one dimension is in the form of equation 1.

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} - D_x\frac{\partial^2 C}{\partial x^2} = 0 \tag{1}$$

Where: the first term describes the concentration gradient, the second term describes the advection term and the third term describes the diffusion term.

Equation 1 can be rewritten in three dimensions as shown in equation 2:

$$\begin{aligned}\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = \frac{\partial}{\partial x}\left(K_x\frac{\partial C}{\partial x}\right) \\ + \frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right) + \lambda C\end{aligned} \tag{2}$$

Where: $C(x, y, z, t)$ is the pollutant concentration at any location (x, y, z) at time t, u, v, w are the wind components in the x, y, z directions respectively, K_x, K_y, K_z are eddy diffusivity in downwind (x), crosswind (y), and vertical (z) directions respectively and λ is the source or sink term of air pollutants.

In physical processes, advection carries the pollutants in the x-direction and diffusion takes place alongside advection due to turbulence (Ulfah *et al*., 2018). Assuming that the mean

concentration of pollutants is constant along the y-direction, equation 2 reduces to two dimensions as shown in equation 3 :

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + w\frac{\partial C}{\partial z} = \frac{\partial}{\partial x}\left(K_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial C}{\partial z}\right) + \lambda C \tag{3}$$

Where λ is the removal mechanism.

Boundary and Initial Conditions

Assume: No flux across domain boundaries: $\frac{\partial C}{\partial n} = 0$, Initial condition: $C(x, y, 0) = 0$, Source: localized in a region (x_s, y_s)

3. Modification of Advection-diffusion Equation

In this work, the study is two-dimensional. The dispersion of pollutants is in the x-direction and z-direction. Therefore, the advection-diffusion equation 3 in two dimensions is modified and used in simulation. The rate of air transport by mechanical dispersion is generalized by the form of Fick's law of diffusion[3].

3.1. Fick's Diffusion

It relates the diffusive flux to the concentration gradient. The flux moves from the regions of high concentration to low concentration. The governing equation in one dimension is given by equation 4:

$$\frac{\partial C}{\partial t} + \frac{\partial Q}{\partial x} = 0 \tag{4}$$

Where: C is the concentration of the diffusing gas and Q is the diffusion flux.

3.2. Soret Diffusion

Soret diffusion is described with the same equation as Fick's diffusion, where Q is given by equation 5:

$$Q = -D\frac{Q^* C}{RT^2}\frac{\partial T}{\partial x} \tag{5}$$

Where: D is the Fick's diffusion coefficient, R is the ideal gas constant. , T is temperature and Q^* is the heat of transport. If $Q^* > 0$, the diffusion gas moves towards the cooler end. If $Q^* < 0$ the diffusion gas moves towards the hotter end. Substituting equation 5 into equation 4 yields:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{Q^* C}{RT^2}\frac{\partial T}{\partial x}\right) \tag{6}$$

Since humidity affects the velocity of air pollutants, the advection of the general form of the advection-diffusion equation can be modeled. By letting the humidity content be ϕ, where $0 < \phi < 1$, and introducing $1 - \phi$ in the advection terms yields expression 7:

$$u(1-\phi)\frac{\partial C}{\partial x} + w(1-\phi)\frac{\partial C}{\partial z} \tag{7}$$

3.3. Humidity Parameterization

Humidity exerts a significant influence on air density, viscosity, and pollutant mobility. To represent this effect, we define a dimensionless humidity factor

$$\phi = \frac{e}{e_s(T)},$$

where e is the partial pressure of water vapor and $e_s(T)$ is the saturation vapor pressure at temperature T. The term $(1 - \phi)$ therefore denotes the effective dry-air fraction within the atmospheric mixture. As relative humidity increases ($\phi \to 1$), the available fraction of dry air decreases and both advection and turbulent diffusion are reduced due to increased air moisture and particle hygroscopic growth. Following empirical treatments in atmospheric transport modeling [4, 5], we scale the advective and diffusive fluxes by $(1 - \phi)$ to account for humidity-induced suppression of pollutant dispersion. Therefore, equation 6 becomes 8

$$\frac{\partial C}{\partial t} = (1-\phi)\frac{\partial}{\partial x}\left(D\frac{Q^* C}{RT^2}\frac{\partial T}{\partial x}\right) \tag{8}$$

Writing equation 8 in two dimensions gives:

$$\frac{\partial C}{\partial t} = (1-\phi)\frac{\partial}{\partial x}\left(D\frac{Q^* C}{RT^2}\frac{\partial T}{\partial x}\right) + (1-\phi)\frac{\partial}{\partial z}\left(D\frac{Q^* C}{RT^2}\frac{\partial T}{\partial z}\right) \tag{9}$$

3.4. Reaction and Source Parameterization

We model chemical or effective removal using first-order decay:

$$S_{\text{rxn}}(x, z, t) = -\lambda(x, z, t)\, c(x, z, t), \tag{10}$$

where c is concentration and λ has units s^{-1}. First-order loss is a standard closure for low to moderate concentrations and small Damköhler number, and it also serves as a lumped representation of multiple microphysical sinks (e.g., oxidation, coagulation linearized about a background state, or unresolved removal). See [4, 5].

Constant Decay Rate In the baseline simulations we set $\lambda(x, z, t) = \lambda_0$ with $\lambda_0 > 0$ (s^{-1}). We report λ_0 and its range in Table 1 and include a sensitivity sweep on λ_0. This choice isolates numerical behavior and allows clean comparison of FTCS and Crank-nicolson schemes.

Photochemical Modulation We write

$$\lambda(x, z, t) = \lambda_0 + \alpha_J\, J(t), \tag{11}$$

where $J(t)$ is a normalized photolysis proxy (0 at night, 1 at noon) derived from solar zenith angle or measured actinic flux, and α_J has units s^{-1}.

Meteorology-coupled Sink We use

$$\lambda(x, z, t) = \lambda_0 + \alpha_u\, |u(x, z, t)| + \alpha_\phi\, \phi(x, z, t), \tag{12}$$

where u is wind speed and ϕ is relative humidity. Coefficients α_u and α_ϕ are calibrated from literature ranges or data.

Dry Deposition If the goal is to represent dry deposition, a boundary flux at $z = 0$ is more physical:

$$-K_z \left.\frac{\partial c}{\partial z}\right|_{z=0} = V_d\, c(x, 0, t), \tag{13}$$

where V_d is deposition velocity ($\mathrm{m\,s^{-1}}$). In this work we treat small unresolved near-surface losses within λ for simplicity; the deposition boundary can replace this approximation when data for V_d are available.

Units and Signs The full tendency is

$$\frac{\partial c}{\partial t} = \cdots - \lambda(x, z, t)\, c + \Lambda(x, z, t), \tag{14}$$

with Λ a nonnegative source term (e.g., emission; units identical to c/s). We provide λ ranges, H_λ, and any modulation coefficients in Table 1 and the code list. Solver tolerances and iteration limits are reported in the Numerical Setup section.

Combining equations 7 and 9 yields:

$$\begin{aligned}\frac{\partial C}{\partial t} &= (1-\phi)\frac{\partial}{\partial x}\left(D\frac{Q^*C}{RT^2}\frac{\partial T}{\partial x}\right)\\ &\quad + (1-\phi)\frac{\partial}{\partial z}\left(D\frac{Q^*C}{RT^2}\frac{\partial T}{\partial z}\right) + u(1-\phi)\frac{\partial C}{\partial x} + w(1-\phi)\frac{\partial C}{\partial z} + \lambda C\end{aligned} \tag{15}$$

Equation 15 is the modified advection-diffusion equation that is used to simulate the dispersion of air pollutants in the atmospheric boundary layer. The concentration values of pollutants at different points are evaluated from the numerical solution described by Equation (2) over a finite domain $0 \leq x \leq 1$, along the longitudinal direction. Units of distance and time are taken as meters (m) and seconds (s), respectively. The initial pollutant concentration C is assumed to be $1.0\ \mathrm{g/m^3}$. The parameter values listed in Table 1 are considered constant throughout the simulations.

Table 1. *Parameter values for pollutant dispersion in the atmosphere.*

Symbol	Parameter	Value	Source
D	Diffusion coefficient	$1\ \mathrm{m^2/s} \leq D \leq 100\ \mathrm{m^2/s}$	[4]
C	Pollutant concentration	Variable	–
u	Wind velocity along x-axis	$2\ \mathrm{m/s} \leq u \leq 10\ \mathrm{m/s}$	[6]
R	Ideal gas constant	$8.314\ \mathrm{J/(mol \cdot K)}$	[7]
Q^*	Soret diffusion flux	$1 < Q^* < 100 J/mole$	[9]
ϕ	Humidity content	$0 < \phi < 1$	[5]
Λ	Source strength	$1 < \Lambda < 30\ \mathrm{g/km}$	[9]
T	Temperature	$0^\circ\mathrm{C} < T < 47^\circ\mathrm{C}$	[5]
t	Time	Variable	–

4. Stability Analysis of the Model

The stability analysis of the modified transport equation 15 is tested by Von Neumann stability condition after introducing the following dimensionless variables such that:

$$\begin{aligned}\varphi &= \frac{(1-\phi)DQ^*C}{RT^2}\\ \omega &= u(1-\phi)\\ \sigma &= w(1-\phi)\end{aligned} \tag{16}$$

Therefore, equation 15 can be written as shown in equation 17:

$$\begin{aligned}\frac{\partial C}{\partial t} &= \varphi\frac{\partial^2 T}{\partial x^2} + \varphi\frac{\partial^2 T}{\partial z^2}\\ &\quad +\omega\frac{\partial C}{\partial x} + \sigma\frac{\partial C}{\partial z} + \lambda C\end{aligned} \tag{17}$$

4.1. Boundary and Initial Conditions

Let the domain of equation 17 be defined as shown in equation 18:

$$x \in [0, L_x], \quad z \in [0, L_z], \quad t \geq 0 \tag{18}$$

with initial conditions as shown in equations 19:

$$C(x, z, 0) = \begin{cases} C_s, & \text{if } (x, z) \text{ near source location} \\ 0, & \text{otherwise} \end{cases} \tag{19}$$

The boundary conditions of equation 17 is defined at the inlet, outlet,ground level and at the top and it is defined by equations 20, 21,22 and 23 such that: At the inlet when $(x = 0)$ the boundary condition is given by equation 20:

$$C(0, z, t) = C_s \tag{20}$$

At the outlet when $(x = L_x)$ the boundary condition is

given by equation 21:

$$\frac{\partial C}{\partial x}(L_x, z, t) = 0 \tag{21}$$

At the ground when $(z = 0)$ the boundary condition is given by equation 22:

$$\frac{\partial C}{\partial z}(x, 0, t) = 0 \tag{22}$$

While At the top when $(z = L_z)$ the boundary condition is given by equation 23:

$$C(x, L_z, t) = 0 \quad \text{or} \quad \frac{\partial C}{\partial z}(x, L_z, t) = 0 \tag{23}$$

4.2. Finite Difference Scheme

The finite difference scheme is one of the several techniques for obtaining numerical solutions to partial differential equation. Discritizing equation 17 using a finite difference scheme the following steps are followed:
Time derivative of equation 17 yeilds 24

$$\frac{\partial C}{\partial t} = \frac{C_{ij}^{n+1} - C_{ij}^{n}}{\Delta t} \tag{24}$$

Second derivative in x,z (central) yeilds equation 25

$$\frac{C_{i,j}^{n+1} - C_{i,j}^{n}}{\Delta t} = \varphi\left(\frac{C_{i+1,j}^{n} - 2C_{i,j}^{n} + C_{i-1,j}^{n}}{\Delta x^2} + \frac{C_{i,j+1}^{n} - 2C_{i,j}^{n} + C_{i,j-1}^{n}}{\Delta z^2}\right) \tag{25}$$

First derivative in x,z using upwind for stability yeilds equation 26

$$D_x C_{i,j}^{n} = \begin{cases} \dfrac{C_{i,j}^{n} - C_{i-1,j}^{n}}{\Delta x}, & \omega > 0, \\ \dfrac{C_{i+1,j}^{n} - C_{i,j}^{n}}{\Delta x}, & \omega < 0, \end{cases}$$
$$D_z C_{i,j}^{n} = \begin{cases} \dfrac{C_{i,j}^{n} - C_{i,j-1}^{n}}{\Delta z}, & \sigma > 0, \\ \dfrac{C_{i,j+1}^{n} - C_{i,j}^{n}}{\Delta z}, & \sigma < 0. \end{cases} \tag{26}$$

Combining the results with $\omega > 0$ and $\sigma > 0$, the finite difference scheme of equation 17 becomes

$$C_{i,j}^{n+1} = C_{i,j}^{n} + \Delta t\left[\varphi\,\frac{T_{i+1,j}^{n} - 2T_{i,j}^{n} + T_{i-1,j}^{n}}{\Delta x^2} + \varphi\,\frac{T_{i,j+1}^{n} - 2T_{i,j}^{n} + T_{i,j-1}^{n}}{\Delta z^2} + \omega\, D_x C_{i,j}^{n} + \sigma\, D_z C_{i,j}^{n} + \lambda\, C_{i,j}^{n}\right]. \tag{27}$$

4.3. Von Neumann Stability Analysis on Finite Difference Scheme

The stability of PDE can be investigated by performing Von Neumann stability analysis since it ignores the boundary conditions [14]. To investigate the stability of equation 17 using Von Neumann stability analysis, substitute the trial solution of equation 28.

$$C_{i,j}^{n} = G^{n} e^{\mathrm{i}(k_x i\Delta x + k_z j\Delta z)}. \tag{28}$$

Where, G is the amplification factor, and k_x, k_z are the wave numbers in x and z directions respectively. To discrete Operators in Fourier Space, substitute (28) into the finite differences equation 27 term by term : Linearize to find the amplification factor G:

$$G = 1 + 2\varphi\Delta t\Big[\frac{\cos(k_x\Delta x) - 1}{\Delta x^2} + \frac{\cos(k_z\Delta z) - 1}{\Delta z^2}\Big] + \mathrm{i}\,\omega\Delta t\,\frac{\sin(k_x\Delta x)}{\Delta x} + \mathrm{i}\,\sigma\Delta t\,\frac{\sin(k_z\Delta z)}{\Delta z} + \lambda\Delta t. \tag{29}$$

For stability of the system $|G| \leq 1$ for all (k_x, k_z).

Examining the stability of each term of equation 17, The stability of diffusion term occurs when:

$$\Delta t \leq \frac{1}{2\varphi}\left(\tfrac{1}{\Delta x^2} + \tfrac{1}{\Delta z^2}\right)^{-1}. \tag{30}$$

While the stability of advection term and reaction term occur when $|\omega|\,\frac{\Delta t}{\Delta x} \leq 1$, $|\sigma|\,\frac{\Delta t}{\Delta z} \leq 1$. and when $|1 + \lambda\Delta t| \leq 1 \implies -2 \leq \lambda\Delta t \leq 0$. respectively

Combining all the terms, the condition for stability of the system is given by equation 31

$$\Delta t \leq \min\Big\{\frac{1}{2\varphi(\Delta x^{-2} + \Delta z^{-2})}, \frac{\Delta x}{|\omega|}, \frac{\Delta z}{|\sigma|}, \frac{2}{|\lambda|}\Big\}. \tag{31}$$

The scheme is therefore stable if the time step Δt satisfies all three conditions:

Diffusion conditions: This is a second order term which causes the spreading of pollutants.This condition prevents high frequency numerical errors from growing due to diffusion and if violated the solution becomes unstable.This condition is of the form:

$$\Delta t \leq \frac{1}{2\,\varphi}\left(\tfrac{1}{\Delta x^2} + \tfrac{1}{\Delta z^2}\right)^{-1}$$

Advection (CFL) conditions: The terms are of first order derivatives which represent transport with the advection velocities in the x direction and z direction. These are of the form:

$$|\omega|\,\frac{\Delta t}{\Delta x} \leq 1 \quad \text{and} \quad |\sigma|\,\frac{\Delta t}{\Delta z} \leq 1$$

This ensures that the advected waves do not amplify

Reaction conditions: Reaction term can cause exponential growth depending on the reaction rate.This condition ensures no unbounded growth from the reaction.This condition is of the form:

$$-2 \leq \lambda\,\Delta t \leq 0 \quad \implies \quad |1 + \lambda\,\Delta t| \leq 1$$

The combined requirement is

$$\Delta t \leq \min\Big\{\frac{1}{2\varphi(\Delta x^{-2}+\Delta z^{-2})}, \frac{\Delta x}{|\omega|}, \frac{\Delta z}{|\sigma|}, \frac{2}{|\lambda|}\Big\}.$$

If Δt meets this bound, the scheme remains bounded and stable. If any part fails, solutions will exhibit unbounded growth or oscillations.

4.4. Crank Nicolson Scheme

Crank-Nicolson (CN) discretisation of the 2-D advection-diffusion-reaction equation 17 written as:

$$\frac{\partial C}{\partial t} = \varphi\big(\partial_{xx}T + \partial_{zz}T\big) + \omega\,\partial_x C + \sigma\,\partial_z C + \lambda\, C \qquad (32)$$

with $i = 0, \ldots, N_x$ spatial node in x (step Δx), $j = 0, \ldots, N_z$ spatial node in z (step Δz) $n = 0, 1, 2, \ldots$ time level (step Δt)$C^n_{i,j}$ numerical solution $C(x_i, z_j, t_n)$ $i = 0, \ldots, N_x$ spatial node in x (step Δx)$j = 0, \ldots, N_z$ spatial node in z (step Δz)$n = 0, 1, 2, \ldots$ time level (step Δt)$C^n_{i,j}$ numerical solution $C(x_i, z_j, t_n)$ Crank Nicolson discretisation of each term of equation 17 yields equation 33:

$$\begin{aligned}
\delta_{xx}T^n_{i,j} &= \frac{T^n_{i+1,j} - 2T^n_{i,j} + T^n_{i-1,j}}{\Delta x^2},\\
\delta_{zz}T^n_{i,j} &= \frac{T^n_{i,j+1} - 2T^n_{i,j} + T^n_{i,j-1}}{\Delta z^2},\\
\delta_x C^n_{i,j} &= \frac{C^n_{i+1,j} - C^n_{i-1,j}}{2\Delta x},\\
\delta_z C^n_{i,j} &= \frac{C^n_{i,j+1} - C^n_{i,j-1}}{2\Delta z}.
\end{aligned} \qquad (33)$$

Combining all the terms in 33 yields:

$$\begin{aligned}
\frac{C^{n+1}_{i,j} - C^n_{i,j}}{\Delta t} &= \frac{\varphi}{2}\Big(\frac{T^{n+1}_{i+1,j} - 2T^{n+1}_{i,j} + T^{n+1}_{i-1,j}}{\Delta x^2}\\
&+ \frac{T^{n+1}_{i,j+1} - 2T^{n+1}_{i,j} + T^{n+1}_{i,j-1}}{\Delta z^2}\\
&+ \frac{T^{n}_{i+1,j} - 2T^{n}_{i,j} + T^{n}_{i-1,j}}{\Delta x^2}\\
&+ \frac{T^{n}_{i,j+1} - 2T^{n}_{i,j} + T^{n}_{i,j-1}}{\Delta z^2}\Big)\\
&+ \frac{\omega}{2}\Big(\frac{C^{n+1}_{i+1,j} - C^{n+1}_{i-1,j}}{2\,\Delta x} + \frac{C^{n}_{i+1,j} - C^{n}_{i-1,j}}{2\,\Delta x}\Big)\\
&+ \frac{\sigma}{2}\Big(\frac{C^{n+1}_{i,j+1} - C^{n+1}_{i,j-1}}{2\,\Delta z} + \frac{C^{n}_{i,j+1} - C^{n}_{i,j-1}}{2\,\Delta z}\Big)\\
&+ \frac{\lambda}{2}\big(C^{n+1}_{i,j} + C^n_{i,j}\big).
\end{aligned}$$

4.5. Von Neumann Stability Analysis of the Crank-Nicolson Scheme

We analyze the stability of the Crank-nicolson scheme applied to the following discretized advection-diffusion-reaction equation in 2D:

$$\begin{aligned}
\frac{C^{n+1}_{i,j} - C^n_{i,j}}{\Delta t} &= \frac{\varphi}{2}\left(\frac{T^{n+1}_{i+1,j} - 2T^{n+1}_{i,j} + T^{n+1}_{i-1,j}}{\Delta x^2} + \frac{T^{n+1}_{i,j+1} - 2T^{n+1}_{i,j} + T^{n+1}_{i,j-1}}{\Delta z^2}\right.\\
&\left. + \frac{T^{n}_{i+1,j} - 2T^{n}_{i,j} + T^{n}_{i-1,j}}{\Delta x^2} + \frac{T^{n}_{i,j+1} - 2T^{n}_{i,j} + T^{n}_{i,j-1}}{\Delta z^2}\right)\\
&+ \frac{\omega}{2}\left(\frac{C^{n+1}_{i+1,j} - C^{n+1}_{i-1,j}}{2\,\Delta x} + \frac{C^{n}_{i+1,j} - C^{n}_{i-1,j}}{2\,\Delta x}\right)\\
&+ \frac{\sigma}{2}\left(\frac{C^{n+1}_{i,j+1} - C^{n+1}_{i,j-1}}{2\,\Delta z} + \frac{C^{n}_{i,j+1} - C^{n}_{i,j-1}}{2\,\Delta z}\right)\\
&+ \frac{\lambda}{2}\left(C^{n+1}_{i,j} + C^n_{i,j}\right).
\end{aligned}$$

Assume a trial solution of the form of equation 28, Where, G is the amplification factor, and k_x, k_z are the wave numbers in x and z directions respectively. To discrete Operators in Fourier Space substitute (28) into the finite differences:

$$\begin{aligned}
C^n_{i\pm1,j} &= G^n e^{\mathrm{i}(k_x(i\pm1)\Delta x + k_z j\Delta z)}\\
&= G^n e^{\mathrm{i}(k_x i\Delta x + k_z j\Delta z)} e^{\pm \mathrm{i}k_x\Delta x}\\
&= C^n_{i,j} e^{\pm \mathrm{i}k_x\Delta x}
\end{aligned}$$

Similarly:

$$C^n_{i,j\pm1} = C^n_{i,j} e^{\pm \mathrm{i} k_z \Delta z},$$

$$\begin{aligned}\frac{C^n_{i+1,j} - 2C^n_{i,j} + C^n_{i-1,j}}{\Delta x^2} &= \frac{C^n_{i,j}(e^{\mathrm{i}k_x\Delta x} + e^{-\mathrm{i}k_x\Delta x} - 2)}{\Delta x^2} \\ &= \frac{C^n_{i,j}(2\cos(k_x\Delta x) - 2)}{\Delta x^2} \\ &= -\frac{4\sin^2\left(\frac{k_x\Delta x}{2}\right)}{\Delta x^2} C^n_{i,j}\end{aligned}$$

Define:

$$\mu_x = \frac{4\varphi\Delta t}{\Delta x^2}\sin^2\left(\frac{k_x\Delta x}{2}\right), \quad \mu_z = \frac{4\varphi\Delta t}{\Delta z^2}\sin^2\left(\frac{k_z\Delta z}{2}\right)$$

Advection terms:

$$\begin{aligned}\frac{C^n_{i+1,j} - C^n_{i-1,j}}{2\Delta x} &= \frac{C^n_{i,j}(e^{\mathrm{i}k_x\Delta x} - e^{-\mathrm{i}k_x\Delta x})}{2\Delta x} \\ &= \frac{i\sin(k_x\Delta x)}{\Delta x} C^n_{i,j} \\ \frac{C^n_{i,j+1} - C^n_{i,j-1}}{2\Delta z} &= \frac{i\sin(k_z\Delta z)}{\Delta z} C^n_{i,j}\end{aligned}$$

Let:

$$\alpha = \frac{\omega\Delta t}{\Delta x}\sin(k_x\Delta x), \quad \beta = \frac{\sigma\Delta t}{\Delta z}\sin(k_z\Delta z), \quad \gamma = \lambda\Delta t$$

Collecting all terms, the scheme reduces to:

$$G = \frac{1 - \frac{1}{2}(\mu_x + \mu_z) + \frac{i}{2}(\alpha + \beta) + \frac{\gamma}{2}}{1 + \frac{1}{2}(\mu_x + \mu_z) - \frac{i}{2}(\alpha + \beta) - \frac{\gamma}{2}} \tag{34}$$

Von Neumann stability requires:

$$|G| \le 1 \quad \text{for all } k_x, k_z$$

Since the Crank-nicolson scheme is unconditionally stable for symmetric (diffusion) parts, the condition will hold provided α, β, and γ do not dominate.

Therefore, For $\omega, \sigma = 0$, the scheme is unconditionally stable, for advection and reaction present, stability is conditional on:

$$\Delta t \text{ sufficiently small to control } \alpha, \beta, \gamma.$$

To ensure numerical stability, use:

$$\max(\alpha, \beta, \gamma) < 2$$

4.6. Stability Comparison of Crank–nicolson and Explicit FD Schemes

Crank–Nicolson (CN): The Crank-Nicolson stability equation is given by,

$$G = \frac{1 - \frac{1}{2}(\mu_x + \mu_z) + \frac{i}{2}(\alpha + \beta) + \frac{\gamma}{2}}{1 + \frac{1}{2}(\mu_x + \mu_z) - \frac{i}{2}(\alpha + \beta) - \frac{\gamma}{2}}$$

$$|G| \le 1 \quad \text{for all } \Delta t, \Delta x, \Delta z$$

G is the Amplification factor which means how the numerical solution grows or decays from one time step to the next. The magnitude of G is less than one which means Crank-Nicolson scheme is unconditionally stable regardless of the choice of time steps or spatial grid sizes.

Explicit FD (FTCS):The Explicit stability equation is given by

$$G = 1 - \Delta t\left[\lambda + \frac{4\varphi}{\Delta x^2}\sin^2\left(\frac{k_x\Delta x}{2}\right) + \frac{4\varphi}{\Delta z^2}\sin^2\left(\frac{k_z\Delta z}{2}\right)\right]$$

$$|G| \le 1 \Rightarrow \Delta t \le \frac{1}{2\varphi}\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta z^2}\right)^{-1}$$

The equation shows that the explicit difference scheme is conditionally stable which means the choice of the time steps must be done carefully based on the grid size .This limits the size of time steps,if large, the solution becomes unstable.In explicit CF (FTCS) the time steps must be smaller, meaning longer computational time steps.This scheme is first order accurate in time and second order in space which means less accurate in time compared to Crank-Nicolson scheme. The Crank Nicolson scheme is unconditionally stable for diffusion problems no matter how large the time step is and the numerical solution wont blow up.This means CN scheme is more flexible and bigger time steps can be taken without loosing the stability and the simulation is faster.This scheme is second order accurate in time and space meaning it provides a more precise approximations of the solution. [13] compared the explicit finite diference and Crank-Nicolson scheme and compared the two graphically as in Figure 1.

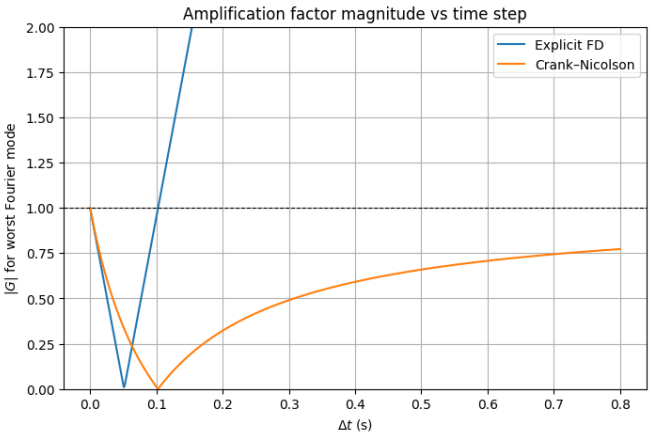

Figure 1. *Amplification factor $|G|$ for the worst Fourier mode versus time step Δt for Explicit Finite Difference and Crank–Nicolson schemes.*

The plot compares the stability behavior of the explicit finite difference (FD) and Crank-nicolson (CN) methods based on the magnitude of the amplification factor $|G|$ over increasing time steps Δt.

Explicit FD Scheme:

The explicit finite difference scheme is conditionally stable, requiring that the amplification factor satisfies $|G| \le 1$. As

shown in the figure, the curve for the explicit scheme exceeds this threshold at larger time steps Δt, indicating numerical instability. This method is accurate only when small time steps are used. Although it is computationally efficient due to its simplicity, its usefulness is limited by strict stability constraints.

The Crank-nicolson scheme maintains unconditional stability, as the amplification factor $|G| \leq 1$ for all time steps Δt. This allows the method to remain stable even when large time steps are used. It is especially suitable for stiff problems and long-duration simulations where stability and efficiency are critical.

While explicit schemes can be simpler to implement, they are restricted by stringent time-step limits. Crank-nicolson offers a robust alternative, allowing for greater efficiency in time without sacrificing stability, especially in diffusion-dominated flows like pollutant transport.

All numerical simulations were implemented in MATLAB R2023b and cross-validated in Python 3.10 under equivalent configurations. For the Crank-nicolson (CN) discretization, the linear system arising from the implicit diffusion-reaction operator was solved using the biconjugate gradient stabilized method (BiCGSTAB) with an incomplete LU preconditioner, ILU(0). The relative tolerance was set to 10^{-8} with a maximum of 500 iterations per time step, and convergence was typically achieved within 100 iterations. For smaller grids, results were confirmed against MATLAB's direct $\backslash$ solver, showing relative differences below 10^{-10}. The explicit finite difference (FTCS) method required no linear solver; updates were computed pointwise using an upwind discretization for advection and central differences for diffusion. Both schemes used identical grid spacing and time-step controls satisfying $\mathrm{CFL} < 1$, ensuring consistent numerical accuracy and reproducibility.

5. Conclusion

This study developed and analyzed a two-dimensional advection-diffusion model that incorporates temperature and humidity as dynamic meteorological variables influencing the transport and dispersion of atmospheric pollutants. The model builds on the classical advection-diffusion formulation described by [4, 5], extending it to include Soret-type thermo-diffusion and humidity-scaled advection. These modifications allow the model to represent the combined effects of wind velocity, thermal gradients, and moisture content on pollutant dispersion within the atmospheric boundary layer.

Numerical analysis was carried out using the finite difference and Crank-nicolson schemes. Stability of the discretized system was verified using the Von Neumann method, confirming that the inclusion of temperature and humidity terms did not compromise numerical reliability. Simulations conducted over realistic atmospheric conditions demonstrated that pollutant concentration decays over time due to advection and diffusion, but the rate of decay depends strongly on relative humidity and air temperature. At low humidity levels, pollutants are transported more efficiently downwind, leading to faster dilution. At high humidity, advection and diffusion are suppressed, resulting in slower dispersion and prolonged pollutant retention near the source. This aligns with findings by [6, 10], who emphasized the role of physical parameters in determining pollutant migration.

Temperature effects were reflected through enhanced diffusivity at higher values and restricted mixing under cooler conditions. Warm air favors greater turbulence and vertical mixing, while stable low-temperature layers confine pollutants near the ground. Such outcomes are consistent with observed behavior reported in atmospheric dispersion literature [4, 5, 12]. The modified model therefore provides a more realistic framework for simulating air pollutant transport in tropical and coastal environments where humidity and temperature gradients vary sharply with time.

By integrating humidity and temperature dependencies, the model improves predictive accuracy of concentration profiles and better supports environmental planning, urban air quality management, and health risk assessment. The approach can be applied to refine existing regulatory dispersion models such as AERMOD and CALPUFF by introducing humidity-scaled advection coefficients and temperature-dependent diffusion parameters. These enhancements can help policymakers evaluate emission scenarios, optimize industrial scheduling, and plan mitigation strategies based on meteorological conditions.

The research confirms that accurate atmospheric modeling requires explicit inclusion of local meteorological effects. Humidity acts as a damping mechanism that limits horizontal and vertical transport, while temperature modulates diffusion through thermal convection and energy gradients. Their combined influence determines pollutant persistence and spatial spread. Hence, meteorology-aware dispersion models such as the one developed in this study can contribute to more effective air quality forecasting, improved environmental monitoring, and evidence-based decision making in both urban and industrial regions.

6. Recommendations

Based on the findings of this study, several recommendations are proposed to enhance both modeling practice and policy application:

1) Incorporate humidity-scaled advection and temperature-dependent diffusion coefficients into standard dispersion models such as AERMOD and CALPUFF to improve prediction accuracy in tropical and coastal regions.
2) Utilize the Crank-Nicolson scheme for air quality simulations where stability and accuracy over long time periods are required, especially in scenarios involving variable meteorological parameters.
3) Integrate meteorological monitoring data-particularly humidity, temperature, and wind speed-into real-time air quality forecasting frameworks to refine environmental management decisions.

4) Conduct further validation of the model using experimental or sensor-based field data to confirm the predicted influence of humidity and temperature on pollutant concentration patterns.
5) Apply the model to support emission-control strategies and industrial scheduling by identifying optimal discharge periods under favorable atmospheric conditions.

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Abbreviations

CN	Crank-Nicolson
FD	Finite Difference
FTCS	Forward Time Central Space
PDE	Partial Differential Equation
CFL	Courant-Friedrichs-Lewy
WHO	World Health Organization
$PM_{2.5}$	Particulate Matter with Aerodynamic Diameter Less Than 2.5 μm
ILU	Incomplete LU Factorization
BiCGSTAB	Biconjugate Gradient Stabilized Method

Acknowledgments

We thank the administrative staff in the department of physical science of Chuka University for their hospitality and assistance in matters related to this work

Author Contributions

Jimrise Ochwach: Conceptualization, Formal Analysis, Investigation, Methodology, Software, Validation, Visualization, Writing – original draft

Julius Njiru Nyaga: Investigation, Methodology, Validation, Writing – review & editing

Mark Okongo: Conceptualization, Project administration, Resources, Supervision, Writing – review & editing

Conflicts of Interest

The authors declare no conflicts of interest.

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