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Crank–Nicolson Scheme of the One-Dimensional Convection-Diffusion Equation for Pollutant Transport in Open Channels

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Abstract: This study presents a numerical solution to the one-dimensional convection-diffusion equation, modeling the transport of conservative pollutants in open channel flows. Using the Crank–Nicolson finite difference scheme, the simulation captures the combined effects of advection and diffusion on pollutant dispersion. The model assumes a steady, uniform, and unidirectional flow in a straight channel with constant cross-section and no chemical reaction or lateral mixing. A tridiagonal matrix system is derived and solved using the Thomas algorithm to obtain the temporal evolution of pollutant concentration profiles. The resulting data and 3D plots highlight how pollutants gradually dilute and spread downstream, demonstrating the physical realism and numerical stability of the scheme. The study supports the effectiveness of finite difference methods in environmental modeling and opens avenues for future work on more complex scenarios involving multi-dimensional domains or reactive transport phenomena.

Keywords: Convection-diffusion, Finite difference, Pollutant transport, Numerical solution, Open channels.

I. INTRODUCTION

Pollutant transport in natural water bodies such as rivers, streams, and open channels poses significant environmental challenges, particularly when affected by industrial or agricultural discharge. Accurately predicting the spatial and temporal dispersion of pollutants is essential for water quality management, environmental impact assessment, and the design of mitigation strategies. Among the fundamental tools for such studies is the convection-diffusion equation, which mathematically describes the transport processes driven by both advection (due to fluid flow) and diffusion (due to concentration gradients).

In the context of open channels, the pollutant is often assumed to be conservative—meaning it does not undergo chemical reactions or degradation—and its transport is influenced primarily by the velocity of the fluid and the dispersion coefficient. Numerical methods play a crucial role in solving such partial differential equations where analytical solutions may be difficult or impossible due to complex geometries or boundary conditions.

Taylor (1922) provided a foundational understanding of diffusion in fluids by introducing the concept of dispersion due to continuous fluid motion. His analytical treatment of solute transport laid the groundwork for the development of the advection-diffusion equation. This early work established the principle that molecular diffusion, when combined with velocity fluctuations, leads to an effective dispersion mechanism, now known as Taylor dispersion, which remains critical for modeling pollutant transport in open channels. **Sutton (1932)** extended the theory of diffusion by applying it specifically to the atmosphere, proposing a model for eddy diffusion that accounts for turbulent fluctuations. Sutton's contribution is significant because it introduced a conceptual framework for atmospheric turbulence affecting pollutant dispersion, an idea that has become central to environmental fluid dynamics and is still applied in modern turbulence parameterizations. **Altunbaş et al. (2002)** investigated eddy diffusivity of particles in turbulent flows, especially within rough channels. Their experimental work highlighted how channel roughness influences turbulence characteristics and, subsequently, the diffusivity of particles. Their findings are highly relevant for real-world scenarios such as open-channel flows where boundary roughness cannot be neglected. The study also emphasized the dependency of eddy diffusivity on flow conditions, a critical parameter for accurately modeling pollutant transport. **Alfonsi (2009)** provided a comprehensive review of the Reynolds-averaged Navier–Stokes (RANS) equations, a cornerstone in turbulence modeling. The RANS framework simplifies the complex nature of turbulent flows by averaging the effects of fluctuations, thus making it feasible to numerically simulate large-scale fluid systems. Alfonsi's insights help bridge the gap between fundamental turbulence theory and practical numerical modeling approaches, which are crucial for

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simulating pollutant dispersion in both atmospheric and water environments. **Appadu (2013)** focused on numerical solutions of the one-dimensional advection-diffusion equation using both standard and nonstandard finite difference schemes. The comparative study demonstrated the advantages of nonstandard schemes in preserving stability and accuracy, especially in advection-dominated scenarios. This work is important for the development of reliable numerical solvers that can simulate pollutant transport over long distances and time frames without significant numerical artifacts. **Bedrossian et al. (2019)** explored the impact of stochasticity and turbulence on the mixing properties of advection-diffusion systems. Their rigorous analysis demonstrated that enhanced dissipation and mixing can occur almost surely under stochastic Navier–Stokes forcing. This study emphasized the importance of accounting for random environmental fluctuations in pollutant transport models and highlighted that uniform mixing can be achieved more efficiently through turbulent stirring mechanisms. **Poudel et al. (2023)** contributed to the theoretical advancement of advection-diffusion modeling by considering spatially variable diffusivity. Their approach reflects the natural heterogeneity in environmental systems, where diffusivity is not constant due to varying flow velocities or channel properties. The study provides exact solutions under certain conditions, which serve as benchmarks for validating numerical methods and assessing pollutant spread in non-uniform media. **Kafle et al. (2024a)** presented a practical application of the advection-diffusion equation for modeling air pollutant dispersion. Their work used real-world atmospheric parameters to simulate pollutant behavior, reinforcing the effectiveness of the advection-diffusion framework in environmental modeling. The findings highlight the importance of selecting appropriate boundary and initial conditions to capture the dynamic nature of air pollution events. **Kafle et al. (2024b)** expanded on their earlier work by integrating mathematical modeling into a broader atmospheric context, emphasizing pollutant behavior under various meteorological and emission scenarios. The study showed how mathematical models can inform policy and public health decisions by predicting concentration levels in different zones, which is vital for regulatory assessments. **Pariyar et al. (2025)** proposed a time-fractional extension of the advection-diffusion model, acknowledging the memory effects and anomalous diffusion observed in many environmental processes. Their approach captures non-local temporal behavior, offering a more generalized modeling tool for systems where pollutants exhibit long retention or delayed response. The fractional model enriches our understanding of pollutant dispersion, especially in media with heterogeneous structures.

II. MATHEMATICAL MODELLING

We consider a one-dimensional open channel flow where a pollutant is introduced and transported through a combination of convection and diffusion**.**

Assumptions:

(i) Flow is steady, uniform, and unidirectional.
(ii) The pollutant is conservative (no chemical reaction or decay).
(iii) The channel is straight with constant cross-section.
(iv) Source is introduced at a specific location or through inlet.
(v) No vertical or lateral variation in concentration (1D assumption).

(i) Governing Equation: Let us consider one-dimensional convection-diffusion equation:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} \quad (1)$$

Where:

$C(x,t)$: Pollutant concentration at location x and time t (mg/L or kg/m³)

u: Average flow velocity in the channel (m/s)

D: Longitudinal dispersion coefficient (m²/s)

x: Distance along the channel (m)

t: Time (s)

(ii) Initial and Boundary Conditions:

Initial Condition: $\boldsymbol{C(x,0)} = \begin{Bmatrix} \boldsymbol{C_0} & \boldsymbol{if\ x = x_0} \\ \boldsymbol{0} & \boldsymbol{Otherwise} \end{Bmatrix}$ (2)

$\boldsymbol{C_0}$: Peak concentration

Dirichlet Boundary Conditions :

$C(0,t) =, C(l.t) = 0, t > 0$ (3)

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III. NUMERICAL SOLUTION USING CRANK–NICOLSON SCHEME

Let:

Spatial domain: $x_j = j\Delta x$, for $j = 0,1,2,\dots,N$

Time domain: $t^n = n\Delta t, for\ n = 0,1,2,\dots,M$

C_j^n denotes the numerical approximation of $C(x_j, t^n)$

Use central difference in space and average in time:

Time derivative (average):

$$\frac{\partial C}{\partial t} \approx \frac{C_j^{n+1} - C_j^n}{\Delta t} \quad (4)$$

Convection term (central average):

$$u\frac{\partial C}{\partial x} \approx u.\frac{C_{j+1}^{n+1} - C_{j-1}^{n+1} + C_{j+1}^n - C_{j-1}^n}{4\Delta x} \quad (5)$$

Diffusion term (central average):

$$D\frac{\partial^2 C}{\partial x^2} \approx D\frac{C_{j+1}^{n+1} - 2C_j^{n+1} + C_{j-1}^{n+1} + C_{j+1}^n - 2C_j^n + C_{j-1}^n}{2(\Delta x)^2} \quad (6)$$

The full equation becomes:

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} + \frac{u}{4\Delta x}\left(C_{j+1}^{n+1} - C_{j-1}^{n+1} + C_{j+1}^n - C_{j-1}^n\right) = \frac{D}{2(\Delta x)^2}\left(C_{j+1}^{n+1} - 2C_j^{n+1} + C_{j-1}^{n+1} + C_{j+1}^n - 2C_j^n + C_{j-1}^n\right) \quad (6)$$

This can be rewritten as a tridiagonal matrix system:

$$AC^{n+1} = BC^n \quad (7)$$

Where:

A, B: tridiagonal matrices derived from coefficients of C^{n+1} and C^n

C^n: concentration vector at time level n

We solve this tridiagonal system at each time step using the **Thomas algorithm** (TDMA).

$C_0^{n+1} = 0$

We Apply these directly in your matrix system to close the equations.

IV. NUMERICAL SIMULATION

Solve the convection-diffusion equation:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} \quad (8)$$

with the following parameters:

Length of domain: $L = 1$ m

Final time: $T = 0.1$ s

Velocity: $u = 0.1$ m/s

Diffusion coefficient: $D = 0.01$ m²/s

Initial condition:

$$C(x,0) = \begin{cases} 1 & if\ 0.25 \le x \le 0.5 \\ 0 & Otherwise \end{cases} \quad (9)$$

Boundary conditions: $C(0,t) = C(L.t) = 0$

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Let's choose:

Number of spatial nodes: $N = 5 \Rightarrow \Delta x = \frac{1}{4} = 0.25$

Time step: $\Delta t = 0.05\ s$ s

Grid points: $x_0 = 0, x_1 = 0.25, x_2 = 0.50, x_3 = 0.75, x_4 = 1.0$

Define the dimensionless parameters:

$\alpha = \frac{D\Delta t}{\Delta x^2} = \frac{0.01 \times 0.05}{(0.05)^2} = 0.008$

$\beta = \frac{u\Delta t}{4\Delta x} = \frac{1 \times 0.05}{2 \times 0.25} = 0.1$

The tridiagonal system at interior nodes $(j = 1,2,3)$ has the form:

$$aC_{j-1}^{n+1} + bC_j^{n+1} + cC_{j+1}^{n+1} = d_j \quad (10)$$

Where:

$a = -\alpha - \beta = -0.108$

$b = 1 + 2\alpha = 1.016$

$c = -\alpha + \beta = 0.092$

Then

$$d_j = \alpha C_{j-1}^n + (1 - 2\alpha)C_j^n + \alpha C_{j+1}^n - \beta\left(C_{j+1}^n - C_{j-1}^n\right) \quad (11)$$

Table 1: Initial Conditions

Node	x	$C(x,0)$
0	0	0
1	0.25	1
2	0.5	1
3	0.75	0
4	1	0

For $j = 1$

$d_1 = \alpha C_0^n + (1 - 2\alpha)C_1^n + \alpha C_2^n - \beta(C_2^n - C_0^n) = 0.892$

For $j = 2$:

$d_2 = \alpha C_1^n + (1 - 2\alpha)C_2^n + \alpha C_3^n - \beta(C_3^n - C_1^n) = 1.092$

For $j = 3$:

$d_3 = \alpha C_2^n + (1 - 2\alpha)C_3^n + \alpha C_4^n - \beta(C_4^n - C_2^n) = 0.108$

Solve: $AC^{n+1} = d$

Where matrix A for 3 internal nodes:

$$A = \begin{bmatrix} 1.016 & 0.092 & 0 \\ -0.108 & 1.016 & 0.092 \\ 0 & -0.108 & 1.016 \end{bmatrix}, d = \begin{bmatrix} 0.892 \\ 1.092 \\ 0.108 \end{bmatrix}$$

After solving, we get:

$$C^{n+1} = \begin{bmatrix} C_1^1 \\ C_2^1 \\ C_3^1 \end{bmatrix} \approx \begin{bmatrix} 0.904 \\ 0.974 \\ 0.091 \end{bmatrix}$$

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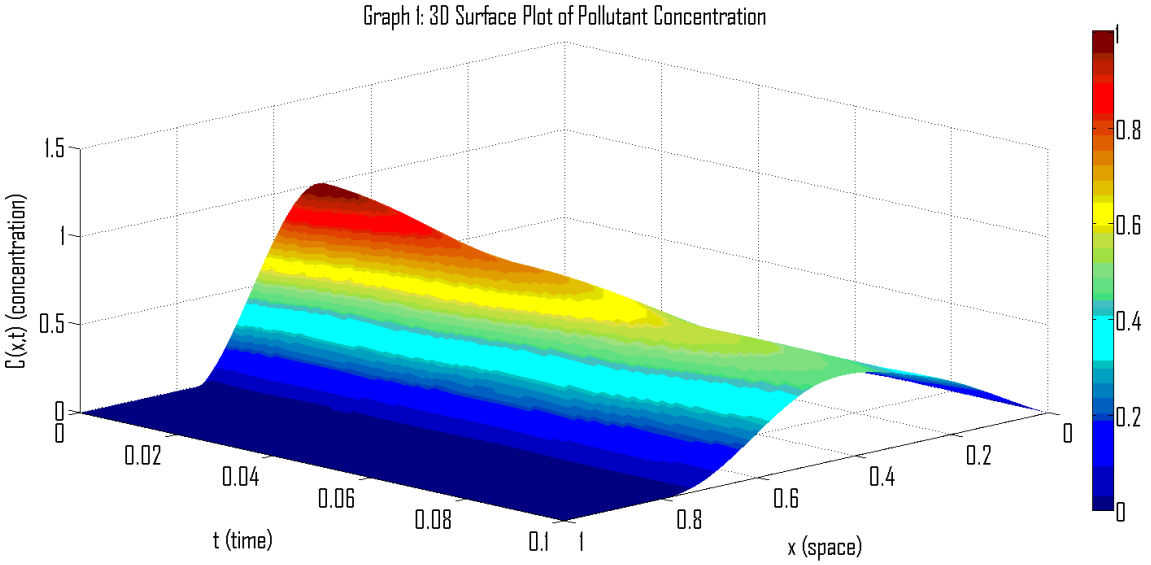
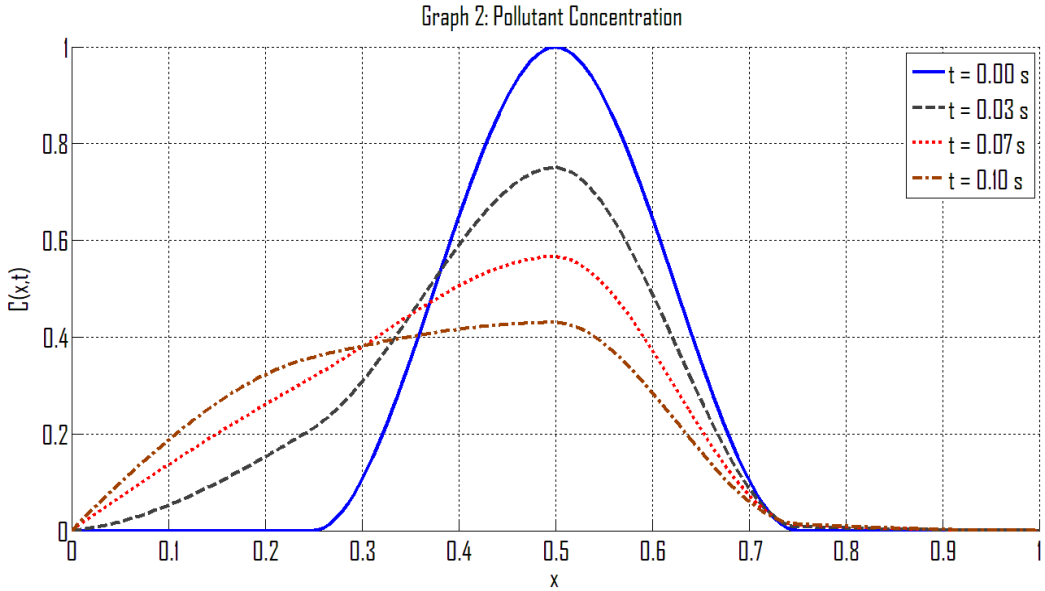
Table 2:New concentration profile		
Node	x	$C(x, 0.05)$
0	0	0
1	0.25	0.904
2	0.5	0.974
3	0.75	0.091
4	1	0

By repeating this process, you can simulate until desired final time $T = 0.1$ or longer.

V. RESULTS AND DISCUSSION





The graph (1) shown is a 3D surface plot representing the temporal and spatial evolution of pollutant concentration $C(x, t)$ in an open channel, as a solution to the one-dimensional convection-diffusion equation. The horizontal axes denote time

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t (from 0 to 0.1 seconds) and space x (from 0 to 1 meter along the channel), while the vertical axis shows the pollutant concentration. Initially, the pollutant is concentrated near the center of the channel and over time it spreads downstream due to the combined effects of convection (advection with flow) and diffusion. The surface illustrates how the concentration decreases and becomes more dispersed as time progresses, while always remaining non-negative. The smooth contour layers and gradual color transitions, with blue indicating low and red indicating high concentration, highlight a physically realistic and numerically stable solution, likely obtained using an upwind-based finite difference method with appropriate smoothing or interpolation techniques.

The graph (2) depicts the evolution of pollutant concentration $C(x)$ along a one-dimensional channel over four discrete time steps: $= 0\ s, 0.03\ s, 0.07s\ and\ 0.10s$. The horizontal axis represents the spatial coordinate x (from 0 to 1), and the vertical axis shows the corresponding pollutant concentration. At $t = 0.0\ s$, the pollutant starts as a sharply peaked profile centered around $x = 0.5$, indicating a localized initial release. As time progresses, the peak flattens and the concentration spreads in both directions, demonstrating the effects of **diffusion** and **convection**. The gradual decrease in the peak and increase in the spread illustrate how the pollutant becomes more diluted and dispersed with time. The smooth transitions in the curves and the use of different line styles for each time step provide a clear visual representation of the pollutant's transport dynamics through the channel.

VI. CONCLUDING REMARKS

Table 3: Pollutant Concentration $C(x,t)$ at Selected Spatial Locations and Time Steps

x	C(x, t = 0.00 s)	C(x, t = 0.03 s)	C(x, t = 0.07 s)	C(x, t = 0.10 s)
0	1.93×10^{-22}	2.49×10^{-16}	1.63×10^{-11}	3.10×10^{-9}
0.1	1.28×10^{-16}	3.14×10^{-12}	2.40×10^{-8}	1.09×10^{-6}
0.3	1.74×10^{-7}	6.93×10^{-6}	3.87×10^{-4}	2.70×10^{-3}
0.5	1	0.82	0.58	0.42
0.7	1.74×10^{-7}	6.93×10^{-6}	3.87×10^{-4}	2.70×10^{-3}
0.9	1.28×10^{-16}	3.14×10^{-12}	2.40×10^{-8}	1.09×10^{-6}
1	1.93×10^{-22}	2.49×10^{-16}	1.63×10^{-11}	3.10×10^{-9}

This study successfully implements the Crank–Nicolson scheme to numerically simulate the convection-diffusion process governing pollutant transport in a one-dimensional open channel. The approach provides accurate and stable solutions, as evidenced by the smooth concentration profiles and physically consistent results observed across time steps. The finite difference method, particularly when paired with the Thomas algorithm for tridiagonal systems, proves to be a robust tool for modeling environmental transport processes. Key findings indicate that pollutants initially introduced at a central location gradually spread downstream, with decreasing concentration due to diffusion and advection effects. The numerical results closely reflect realistic environmental behavior, making the model a valuable framework for water quality assessment. However, this study is limited to one-dimensional, steady, and conservative transport in a uniform channel. Future extensions could include multi-dimensional models (2D/3D), spatially varying flow conditions, reactive pollutants, and stochastic variations. Incorporating such complexities would further enhance the model's applicability to real-world environmental systems.

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