NUMERICAL MODEL OF AIR POLLUTANTS WITH CHEMICAL RESPONSE AND GRAVITATIONAL SETTLING VELOCITY

SURESHA C M, LAKSHMINARAYANACHARI & SUDHEERPAI K L

Associate Professor & Head of the Department of Mathematics, RNSIT, Bangalore, India

Professor & Head of the Department of Mathematics, SVIT, Bangalore, India

Principal, RNS First Grade College, Bangalore, India

ABSTRACT

Right now, study the two dimensional Model of air pollutants produced from a region wellspring of Primary (C_p) and Secondary Pollutants (C_s) through Chemical response and Gravitational Settling Speed. The overseeing fractional (Partial) differential conditions are understood by utilizing Crank-Nicolson implicit finite difference tool. The grouping of pollutants has been examined for different removal mechanisms in both steady (stable) and impartial (neutral) atmospheric circumstances.

KEYWORDS: Air Pollution Model, Gaseous Toxin, Chemical Response, Variable Wind Speed, Crank-Nicolson Certain Limited Contrast Procedure

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1. INTRODUCTION

Quick industrial development and suburbanization have represented a genuine danger to the human lifespan and its condition as of late. Nonstop emanation of air contaminations like CO , NO , SO_2 by the burning of hydrocarbon powers in neighborhood, vehicular debilitates because of traffic stream and a few other main or negligible sources dirty a section or else entire region of activity situation. Contamination from a territory source not just influence individuals and condition inside this zone, yet in addition the individuals remaining in neighboring country non-dirtied zone, as poisons are diffused and adverted downwind.

A two dimensional analytical model for tempestuous scattering of toxins in steady air layer with a quadratic conversation co-efficient and straight speed profile is introduced [1]. Be that as it may, it bombs light on any expulsion system. A numerical model for scattering with chemical response and dry deposition from territory source, which is consistent state in nature, is introduced [2]. All these zone source models manage just primary inert air pollutants. In this way, introduced a time-dependent numerical model for Both essential and optional toxins so as to get time subordinate forms of poison fixation in urban region [3]. This model has been unraveled by utilizing partial advance strategy considering the predefined practical type of vertical eddy diffusivity ($K_z = z$) and velocity profiles $U(z) = z^{0.5}$. A period subordinate territory source scientific model of synthetically receptive air toxins and their side-effect in a secured zone over the source layer with rainout/waste of time and settling [4]. Yet, the flat homogeneity of toxins and steady eddy diffusivity are accepted right now. Corrosive precipitation can happen when particles and gases are expelled from the environment by both wet statement and dry affidavit. So as to legitimize controls on emanations of corrosive forerunners, the connection between a source and the affidavit

design that it delivers should be comprehended [5]-[7]. A period subordinate two dimensional air toxin model for both essential contamination (time subordinate emanation) and the optional poison with quick (dry testimony) and postponed (synthetic change, rainout/waste of time and settling) evacuations [8]. Notwithstanding, this model being expository, manages the uniform speed and swirl diffusivity profiles. A shift in weather conditions dispersion numerical model is introduced for air contaminations with compound response and dry statement [9]. Anyway this model doesn't assess secondary pollutant.

Analytical methodology for air contamination transmitted from line source with chemical reaction and wet deposition [10]. This model doesn't consider the impact of gravitational settling velocity for the line source. Numerical model of air contaminant produced from a zone wellspring of primary contaminant with chemical response [11]. Right now, of gravitational settling velocity for the line source not considered.

Thus, in the current paper we build up a scientific model of area source for both essential (consistent emanation) & auxiliary toxins through progressively reasonable variable wind speed and eddy- diffusivity profiles. Right now, most satisfactory general supposition that is made, "the auxiliary poisons (secondary Pollutants) are shaped by methods first order chemical conversion of primary pollutant ". Both essential & auxiliary toxins are expelled from environment by Gravitational Settling Velocity. Upwind contrast plot is utilized to discretize the shift in weather conditions term of the administering condition and is explained by utilizing Crank-Nicolson certain limited contrast procedure. Concentration contours are plotted and consequences are broke down for the essential just as optional toxins in steady and neutral atmospheric circumstances for different meteorological constraints, territory classes and expulsion & change forms.

A model for air pollutants with profiles of realistic meteorological parameters is presented in this paper. The ramification of removal mechanisms such as chemical response and washout is studied for primary pollutant. Also, for secondary pollutant the effect of gravitational Settling velocity is considered. For the study of grid-independence, we have computed absorption for 40×156 , 80×312 , 160×624 and 240×1248 grids and examined. The result reveals that absorption level of both the pollutants for 40×156 and 80×312 grids vary considerably versus those on 160×624 grids. Further, there is no perceivable change of values obtaining on 240×1248 grids from that of 160×624 grids. It is therefore justifiable to presume that the solution occurred on 160×624 grids is a contingent solution. The above calculation cycle is then reiterated for each of the next time levels and consistent state solution is obtained when the following convergence convention for the residual defined as

$$\left| \frac{C_{ij}^{n+1} - C_{ij}^n}{C_{ij}^{n+1}} \right| < \varepsilon$$

Is gratified. Here, C is the concentration, n indicates time, i and j indicates to the space coordinates.

2. FORMULATION OF MODEL

Figure 1: Physical Format of the Model.

For C_p , the Governing condition (equation) is:

$$\frac{\partial C_p}{\partial t} + U(z) \frac{\partial C_p}{\partial x} = \frac{\partial}{\partial z} \left(K_z(z) \frac{\partial C_p}{\partial z} \right) - kC_p \quad (1)$$

The underlying (initial) and limit conditions (Boundary) under the fitting suppositions are, given by,

$$C_p = 0 \text{ at } t = 0, 0 \leq x \leq X_0 \text{ and } 0 \leq z \leq H, \quad (2)$$

$$C_p = 0 \text{ at } x = 0, 0 \leq z \leq H \text{ and } \forall t > 0. \quad (3)$$

$$K_z \frac{\partial C_p}{\partial z} = \begin{cases} -Q, & \text{at } z = 0, 0 < x \leq l \\ 0, & \text{at } z = 0, l < x \leq X_0 \end{cases} \quad \forall t > 0, \quad (4)$$

$$K_z \frac{\partial C_p}{\partial z} = 0 \text{ at } z = H, x > 0, \forall t. \quad (5)$$

For C_s , the Governing equation is

$$\frac{\partial C_s}{\partial t} + U(z) \frac{\partial C_s}{\partial x} = \frac{\partial}{\partial z} \left(K_z(z) \frac{\partial C_s}{\partial z} \right) + W_s \frac{\partial C_s}{\partial z} + V k C_s, \quad (6)$$

The underlying and limit conditions are given by,

$$C_s = 0 \text{ at } t = 0, \text{ for } 0 \leq x \leq X_0 \text{ and } 0 \leq z \leq H. \quad (7)$$

$$C_s = 0 \text{ at } x = 0, \text{ for } 0 \leq z \leq H \text{ and } \forall t > 0. \quad (8)$$

$$K_z \frac{\partial C_s}{\partial z} + W_s C_s = 0 \text{ at } z = 0, 0 \leq x \leq X_0 \text{ and } \forall t > 0. \quad (9)$$

$$K_z \frac{\partial C_s}{\partial z} + W_s C_s = 0 \text{ at } z = H, 0 \leq x \leq X_0 \text{ and } \forall t > 0, \quad (10)$$

3. METEOROLOGICAL PARAMETER

According to Shir [12], the eddy diffusivity profiles for neutral condition, is

4794 $K_z = 0.4u_*ze^{\frac{-4z}{H}}$ and

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For stable condition, as per Ku *et al.*, [13] is $K_z = \frac{\kappa u_* z}{0.74 + 4.7 \frac{z}{L}} e^{-b\eta}$, where $b = 0$, $\eta = \frac{z}{L\sqrt{\mu}} \mu = \frac{u_*}{|fL|}$ (12)

The wind speed profiles for neutral and stable cases are due to Ragland [14],

Table 1

Neutral stability	$z < 0.1 \kappa \frac{u_*}{f}$	$U = \frac{u_*}{\kappa} \log \left(\frac{z + z_0}{z_0} \right)$
Stable case	$0 < \frac{z}{L} < 1$	$U = \frac{u_*}{\kappa} \log \left(\frac{z + z_0}{z_0} \right) + \frac{\alpha}{L} z$
	$1 < \frac{z}{L} < 6$	$U = \frac{u_*}{\kappa} \log \left(\frac{z + z_0}{z_0} \right) + 5.2$

In planetary limit layer, over the outward layer, power rulesystem is utilized.

$$U = u_{sl} + \left(\frac{z - z_{sl}}{H - z_{sl}} \right)^p (u_g - u_{sl}), \quad (13)$$

Where

Table 2

p=0.2	Neutral condition
p=0.35	Slightly stable flow
p=0.5	Stable flow

Suggested by Jones *et al.*, [15].

4. NUMERICAL SOLUTION

We utilize the Crank-Nicolson plan to discretize the eq.(1).

$$\frac{\partial C_p}{\partial t} \Big|_{ij}^{n+\frac{1}{2}} + 0.5 \left[U(z) \frac{\partial C_p}{\partial x} \Big|_{ij}^n + U(z) \frac{\partial C_p}{\partial x} \Big|_{ij}^{n+1} \right] = 0.5 \left[\frac{\partial}{\partial z} \left(K(z) \frac{\partial C_p}{\partial z} \right) \Big|_{ij}^n + \frac{\partial}{\partial z} \left(K(z) \frac{\partial C_p}{\partial z} \right) \Big|_{ij}^{n+1} \right] - \frac{k}{2} (C^n + C^{n+1}), \quad (14)$$

for $i = 1, 2, \dots, j = 1, 2, \dots$

where

$$\frac{\partial C_p}{\partial t} \Big|_{ij}^{n+\frac{1}{2}} = \frac{C_p^{n+1} - C_p^n}{\Delta t} \quad (15)$$

$$U(z) \frac{\partial C_p}{\partial x} \Big|_{ij}^n = U_j \left[\frac{C_p^n - C_p^{n-1}}{\Delta x} \right], \quad (16)$$

$$U(z) \frac{\partial C_p}{\partial x} \Big|_{ij}^{n+1} = U_j \left[\frac{C_p^{n+1} - C_p^n}{\Delta x} \right]. \quad (17)$$

$$\frac{\partial}{\partial z} \left(K(z) \frac{\partial C_p}{\partial z} \right) \Big|_{ij}^n = \frac{K_z \left(\frac{\partial C_p}{\partial z} \right)_{ij+0.5}^n - K_z \left(\frac{\partial C_p}{\partial z} \right)_{ij-0.5}^n}{1 \cdot K + K}$$

ij

Δz

$C^{n+1} - C^n$

$\frac{1}{K} \frac{K}{C} +$

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$$= \frac{1}{\Delta z} \left(\frac{j}{2} \right) \left(\frac{p_{i,j+1}}{\Delta z} - \frac{p_{i,j}}{\Delta z} \right) - \frac{1}{\Delta z} \left(\frac{j-1}{2} \right) \left(\frac{p_{i,j}}{\Delta z} - \frac{p_{i,j-1}}{\Delta z} \right).$$

Hence,

$$\frac{\partial}{\partial z} \left(K_z \frac{\partial C_p}{\partial z} \right) \Big|_j^n = \frac{1}{2(\Delta z)^2} [(K_{j+1} + K_j)(C_{pij+1} - C_{pij}) - (K_j + K_{j-1})(C_{pij} - C_{pij-1})] \quad (18)$$

Similarly,

$$\frac{\partial}{\partial z} \left(K_z \frac{\partial \bar{C}_p}{\partial z} \right) \Big|_j^{n+1} = \frac{1}{2(\Delta z)^2} [(K_{j+1} + K_j)(C_{pij+1} - C_{pij}) - (K_j + K_{j-1})(C_{pij} - C_{pij-1})] \quad (19)$$

Substituting (15) to (19) in equation (14), then

$$A_j C_{pi-1j}^{n+1} + B_j C_{pij-1}^{n+1} + D_j C_{pij}^{n+1} + E_j C_{pij+1}^{n+1} = F_j C_{pi-1j}^n + G_j C_{pij-1}^n + M_j C_{pij}^n + N_j C_{pij+1}^n \quad (20)$$

for each $i = 2, 3, 4, \dots, imaxl \dots imaxX_0$, for each $j = 2, 3, 4, \dots, jmax - 1$ and $n = 0, 1, 2, 3, \dots$

$$\text{where, } A_j = U_j \frac{\Delta t}{2\Delta x}, F_j = -A_j, B_j = \frac{\Delta t}{4(\Delta z)^2} (K_j + K_{j-1}),$$

$$G_j = -B_j E_j = -\frac{\Delta t}{4(\Delta z)^2} (K_j + K_{j+1}), N_j = -E_j,$$

$$D_j = 1 + U_j \frac{\Delta t}{2\Delta x} + \frac{\Delta t}{4(\Delta z)^2} (K_{j-1} + K_j + K_{j+1}) + \frac{\Delta t}{2} k,$$

$$M_j = 1 - U_j \frac{\Delta t}{2\Delta x} - \frac{\Delta t}{4(\Delta z)^2} (K_{j+1} + K_j + K_{j-1}) - \frac{\Delta t}{2} k,$$

$i = imaxl$ and $imaxX_0$ are the i values at $x = l$ and X_0 respectively and $jmax$ is the value of j at $z = H$.

The discretization of equations (2) to (5) are as follows

$$C_{pij}^0 = 0, j = 1, 2, \dots, jmax, i = 1, 2, \dots, imaxl \dots imaxX_0$$

$$C_{pij}^{n+1} = 0, j = 1, 2, \dots, jmax, n = 0, 1, 2, \dots$$

$$C_{pij}^{n+1} - C_{pij+1}^{n+1} = -\frac{Q\Delta z}{K_j} \quad (21)$$

for $j = 1, i = 2, 3, 4, \dots, imaxl$ and $n = 0, 1, 2, 3 \dots$

$$C_{pij}^{n+1} - C_{pij+1}^{n+1} = 0, \quad (22)$$

for $j = 1, i = imaxl + 1, \dots, imaxX_0$ and $n = 0, 1, 2, 3 \dots$

$$C_{pijmax-1}^{n+1} - C_{pijmax}^{n+1} = 0, \quad (23)$$

for $j = jmax, i = 2, 3, 4, \dots, imaxl \dots imaxX_0$

In the same way, finite difference equations for C_s can be composed as

$$A_j C_{si-1j}^{n+1} + B_j C_{sij-1}^{n+1} + D_j C_{sij}^{n+1} + E_j C_{sij+1}^{n+1} = F_j C_{si-1j}^n + G_j C_{sij-1}^n + M_j C_{sij}^n + N_j C_{sij+1}^n + V_g k C_{sij}^n, \quad (24)$$

for $i = 2, 3, 4 \dots imaxl, \dots imaxX_0, j = 2, 3, 4, \dots jmax - 1$

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The initial and border conditions C_s are

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$C_{sij}^0 = 0, i = 1, 2, \dots imaxl \dots imaxX_0, j = 1, 2, \dots jmax,$

$$C_{s1j}^{n+1} = 0, j = 1, 2, \dots, j_{\max}, n = 0, 1, 2, \dots$$

$$(1 - (W_s \Delta z) \frac{\Delta t}{K_j}) C_{sij}^{n+1} - C_{sij+1}^{n+1} = 0, \text{ for } j = 1, i = 2, 3, \dots, i_{\max}, \dots, i_{\max} X \quad (25)$$

$$C_{sij-1}^{n+1} + (\frac{W_s \Delta z}{K_j} - 1) C_{sij}^{n+1} = 0, \text{ for } j = j_{\max}, i = 2, 3, 4, \dots, i_{\max}, \dots, i_{\max} X \quad (26)$$

$$\text{where, } A = U \frac{\Delta t}{2\Delta x}, F = -A B = -\frac{\Delta t}{4(\Delta z)^2} (K_j + K_{j-1}) + \frac{W_s \Delta t}{2\Delta z}$$

$$G_j = \frac{\Delta t}{4(\Delta z)^2} (K_j + K_{j-1}) - W_s \frac{\Delta t}{2\Delta z}, E_j = -\frac{\Delta t}{4(\Delta z)^2} (K_j + K_{j+1}),$$

$$N_j = \frac{\Delta t}{4(\Delta z)^2} (K_j + K_{j+1}), D_j = 1 + U \frac{\Delta t}{2\Delta x} + \frac{\Delta t}{4(\Delta z)^2} (2K_j + K_{j+1} + K_{j-1}) - W_s \frac{\Delta t}{2\Delta z}$$

$$M_j = 1 - U \frac{\Delta t}{2\Delta x} - \frac{\Delta t}{4(\Delta z)^2} (K_{j+1} + K_{j-1} + 2K_j) + W_s \frac{\Delta t}{2\Delta z}$$

Equations from (20) to (23) and from (24) to (26) are solved using Thomas algorithm.

5. RESULTS AND DISCUSSIONS

Right now, have built up a numerical model for the C_p and C_s in a city region with a progressively practical wind speed and eddy diffusivity profile with expulsion components, for example, gravitational settling (W_s). The concentration circulation is registered in the source area just as source free area till the ideal separation of $X=12\text{KM}$.

In Figure 2 the impact of k_c on C_p and C_s as to remove for stable case is examined. As k_c expands, the concentration of C_p and C_s diminishes. In the event that $k_c=0.0015$, the ground level centralization of C_p increases up to 180 and as k_c expands, the ground level fixation diminishes quickly with downwind separation (distance). The ground level centralization of C_s is high if $k_c=0.0015$ and as k_c builds the ground level focus diminishes with downwind separation for $W_s=0$.

In Figure 3 the impact of k_c on C_p and C_s with respect to the separation for neutral case is examined. As the k_c increase, the centralization of C_p and C_s diminishes. On the off chance that $k_c=0.0015$ the ground level convergence of C_p rises up to 55 and as k_c expands the ground level focus diminishes quickly with downwind separation. Comparative impact is watched for C_s regarding downwind separation. From Figures 2 and 3 it is discovered that the magnitude of the concentration of C_p and C_s contaminants in stable circumstance is higher when equated to the neutral circumstance.

In Figures 4 and 5, the grouping of C_p and C_s for various estimations of k_c with respect to tallness for stable circumstance is contemplated. Comparative impact is seen in neutral circumstance as on account of stable environment yet the convergence of C_p is nil around the height of $z=60$ meters in stable case $z=400$ meters in neutral case and secondary poisons is zero around the height of $z=40$ meters in stable circumstance and $z=200$ meters in neutral circumstance. This shows the neutral climate circumstance upgrades the vertical dissemination of C_p and C_s conveying the toxins to higher heights.

In Figure 6, the ground level concentration of C_s for various estimations of W_s with downwind separation for stable

and neutral case is contemplated. The convergence of C_s diminishes as W_s increments. The extent of secondary contaminations is higher for the situation stable when contrast with neutral case for various estimations of W_s .

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In Figure 7, the ground level centralization of C_s for changed estimations of W_s with respect to height for together

stable and neutral cases is considered, yet the convergence of C_s is zero around the height $z=45$ meters in stable and $z=250$ meters in neutral circumstance. This shows the neutral circumstance improves vertical dispersion of C_s , where as stable case suppresses the vertical diffusion of pollutants which results in more concentrations near the ground surface.

Figure 2: Variety of Ground Level Fixation Regarding Separation of Primary & Secondary Toxins for Stable Circumstance.

Figure 3: Variety of Ground Level Fixation Regarding Distance of Primary & Secondary Toxins for Neutral Circumstance.

Figure 4: Variety of Ground Level Fixation as for Tallness of Primary and Secondary Contaminations for Stable Case.

Figure 5: Variety of Ground Level Fixation as For Height of Primary and Secondary Contaminations for Neutral Case.

Figure 6: Variety of Ground Level Fixation as for Distance of Secondary Contaminations for Steady and Neutral Cases.

Figure 7: Variety of Ground Level Fixation Concerning Height of Secondary Contaminations for Stable and Neutral Case.

6. CONCLUSIONS

From the above outcomes, we inferred that ground level concentration of C_p achieves top an incentive at the downwind finish of the urban area and diminishes quickly to a consistent incentive over the source free region. This is because of the way that there is no discharge past as far as possible and consequently the fixation diminishes asymptotically to a steady worth. The

concentration of C_p and C_s decreases as the removal mechanisms such as K_C rises for stable and neutral cases. The convergence of C_p and C_s arrives at more heights in neutral situation when contrasted with the stable climatic state. This shows neutral air state improves the vertical dissemination conveying the contaminations focus to more prominent heights and hence the fixation is less at the surface area. Therefore, neutral case is attractive to plants and creatures from the air contamination perspective.

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