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SIMULATION OF VERTICALLY POLLUTANT DISTRIBUTION AND DEPOSITION IN ATMOSPHERE: A FINITE ELEMENT APPROACH

Prem Gurung[1], Hem Raj Pandey[2*]

[1,2] School of Engineering, Faculty of Science and Technology, Pokhara University, Nepal
Corresponding Author : hpandey@pu.edu.np (H.R. Pandey)

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ABSTRACT

Nowadays, even in densely populated and industrialized regions, air pollution is a common problem. Air pollution in urban areas has reached crisis proportions, necessitating continuous information on pollution levels. In the present work, we study a one-dimensional unsteady-state model for the distribution of atmospheric pollutants in a vertical direction in the troposphere emitted from a point source; the point source is assumed to be on the lower boundary of the troposphere. We assume that the chemical reaction and diffusivity of pollutants vary with vertical height. So, for simulation purposes, the troposphere is divided into six layers. Hence, the finite element method and the Crank-Nicolson method are used to simulate the model results. The model also includes a study of the effects of dry deposition and gravitational settling velocity in the first layer of the troposphere, measured to the earth's surface. The results of this study provide insights into the vertical behavior of pollutants and the influence of atmospheric processes near the ground level. This model can be further used to inform policy decisions and optimize pollution mitigation strategies in urban environments

Key Words: *Dry deposition; Gravitational settling velocity; Eddy-diffusivity; Finite element method; Crank-Nicolson method.*

1. Introduction

Air pollution has become ubiquitous these days in urban and industrial areas. The continuous development and increase of the population in urban areas, a series of environmental problems such as deforestation, the release of toxic materials, the disposal of solid waste, the air pollution and many more, have attracted much more attention than ever before (Kushwah, Saxena and Kushwah, 2009). The problem of air pollution in cities has become so severe that timely information is needed on changes in pollution level. The dispersion of air pollution is a complex problem

(Ghorani-Azam, Riahi-Zanjani and Balali-Mood, 2016). It deals with the transport and diffusion of pollutants in the atmosphere. The dispersion of pollutants in the atmosphere is determined by pollutant characteristics, meteorological conditions, emissions, and terrain conditions (Stockie, 2011). Physical and mathematical models are developed to describe the dispersion of air pollution. Physical models are small-scale representations of the atmospheric flow carried out in wind tunnels (Dobbins, 1979) . In recent years, the dispersion of atmospheric contaminants has become a global problem due to rapid industrialization and urbanization. The toxic gases and small particles could accumulate in large amounts in urban areas under certain meteorological conditions (Rudraiah, Venkatachalappa and Khan, 1997; Jacobson, 2012). This is one of the serious health hazards in many cities around the world. Industries, automobiles, and indoor pollutants in homes(Christophe and Andre, 2025). The life cycle of pollutants includes the emission, dispersion, and removal by dry deposition on the Earth's surface (Zhang *et al.*, 2023). Mathematical modeling is one of the most effective ways to assess the impact of various pollutants on the environment of a particular area equations and express conservation laws of mass, momentum, and energy (Suresha *et al.*, 2012). Air is considered one of the most vital and precious natural resources. Controlling air pollution is currently one of the most difficult tasks (McMahon, Denison and Fleming, 1976). The diffusion process in the atmosphere from a source in the point area has been studied in various contexts, such as air pollution and the diffusion of pheromones from biological organisms in the atmosphere(Crank, 1975; Hu and Yoshie, 2020; Giri *et al.*, 2023). During dispersion in the atmosphere, the primary species is sometimes converted to secondary species, and both primary and secondary species may be removed by rainout/washout (Zhang *et al.*, 2023; Kumar *et al.*, 2024). Alam and Seinfeld (Seinfeld, 1983) studied the dispersion of sulfur dioxide and sulfate in the atmosphere by solving steady state three-dimensional diffusion equations and discussed the effects of conversion and removal processes by considering them first-order processes. The present research aims to develop a one-dimensional unsteady-state model for the vertical distribution of atmospheric pollutants in the troposphere emitted from a point source and the Finite Element Method (FEM) model is presented for vertically atmospheric pollutants. The article is organized as follows: Section 2 presents the formulation of the problem, while Section 3 outlines the assumptions and boundary conditions. Sections 4 and 5 describe the numerical scheme, simulation results, and discussion. Finally, the conclusions are provided in the last section.

2. Formulation of the problem

Mathematical models are important tools and can play a crucial role in the methodology developed to predict the distribution of pollutants (Kushwah, Saxena and Kushwah, 2009). Sometimes the pollutant appears in the form of larger particles, on which the effect of gravitational acceleration cannot be neglected. In this case, the pollutant will come down to the surface with a gravitational settling velocity. Particles less than 20 μm in diameter are treated as gases, and effects due to their fall velocity are generally ignored (Lakshminarayanachari *et al.*, 2013). Particles larger than 20 μm in diameter have appreciable settling velocities. The mathematical description of the dispersion of air pollution from an industrial stack considers the following five main physical and chemical processes (Sharan *et al.*, 1996): Horizontal transport (advection) , Horizontal diffusion , Deposition (both dry deposition and wet deposition) , Chemical reactions plus emissions , Vertical transport and diffusion.

Under the above processes, the basic governing equation of the pollutant dispersion is given by

$$\frac{\partial C}{\partial t}+\frac{\partial U_x}{\partial x}+\frac{\partial U_y}{\partial y}+\frac{\partial U_z}{\partial z}=\frac{\partial}{\partial x}\left(D_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(D_z\frac{\partial C}{\partial z}\right)+S+R \qquad (1)$$

Where, C = pollutant concentration in air at any direction in time t, wind velocity in x, y and z-directions respectively, coefficients of eddy diffusivity in D_x, D_y, D_z = x, y and z- direction respectively, S =emission source of pollutants; and R = chemical reaction rate coefficient.

3. Model assumptions

The assumptions made for the present study are as follows:

• Unsteady state condition, $\left(\frac{\partial C}{\partial t}=0\right)$,

• Effects of environmental factors such as wind velocity are not considered in the model $\left(U_x=U_y=U_z=0\right)$,

• Transport of bulk motion in vertical direction, i.e., z-direction exceeds diffusion in the x-direction and y-direction , i.e., $D_x=0$ and $D_y=0$.

By applying the above assumptions, equation (1) reduces to:

$$\frac{\partial C}{\partial t}=\frac{\partial}{\partial z}\left(D_z\frac{\partial C}{\partial z}\right)+S+R \qquad (2)$$

The given description provides in Figure 1, and a mathematical formulation to model the distribution of chemically reactive air pollutants in the troposphere under specific conditions.

Initial Condition:

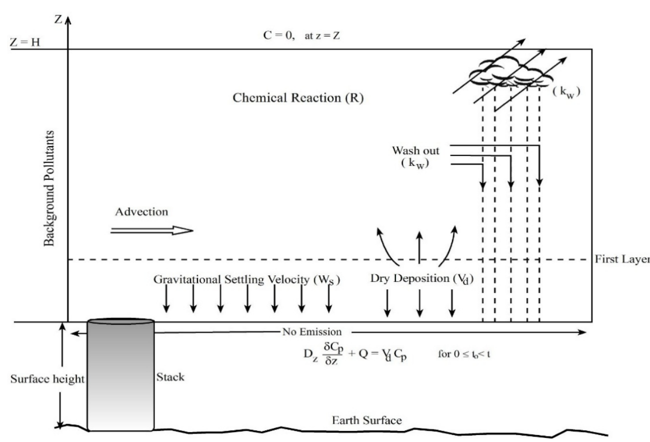

Figure. 1: The schematic physical descriptions of the model.

At the beginning of the emission (t = 0), it is assumed that the region of interest is free of pollutants: C =0 at t=0, where C represents the concentration of the pollutant.

Boundary Conditions:

1. Lower Surface of the Troposphere (z = 0):

Pollutants are emitted at a steady rate , and their distribution is affected by: Diffusion $\left(D_z \frac{\partial C}{\partial z}\right)$ gravitational settling velocity $(W_s C)$, emission rate (Q), and dry deposition velocity (V_d) . The condition z = 0 is expressed as:

$$D_z \frac{\partial C}{\partial z} + W_s C + Q = V_d C$$

at t=0.

2. Top Boundary of the Mixing Layer (z = H):

The pollutants are confined within the mixing height (H), and no pollutant leakage occurs across the top boundary. C =0 at z=H. This sets up models of dispersion of pollutants within the troposphere, considering:

Emission Source: The pollutants are released at the lower boundary.

Vertical Processes:

- **Dry Deposition** (V_d):Removal of pollutants as they settle onto surfaces.
- **Gravitational Settling** $(W_s C)$: The downward movement of pollutant particles due to gravity.
- **Diffusion Movement** (D_z):of pollutants caused by concentration gradients.

Mixing Height: The upper limit (H) of the atmospheric layer where the pollutants are distributed.

4. Numerical solution

In this section, we take a linear distribution assumption of the pollutant concentration in each layer i, which is assumed to vary linearly. FEM (Hurbner et al., 2001; Reddy, 2019)and Crank-Nicolson numerical method (Suresha et al., 2012; Guo et al., 2022) is implemented for the solution proposed of the given model.

$$C^{(i)} = A_i + B_i z, \text{ for i=1, 2, 3, 4, 5, 6}$$

where,

$$A_i = \frac{C_{(i-1)} z_i - C_i z_{i-1}}{z_i - z_{i-1}}, \text{ and } B_i = \frac{C_i - C_{i-1}}{z_i - z_{i-1}}.$$

Now, to solve the differential equation (1) using finite element method, we derive the equivalent variational formation of the equation (1). The derivation is based on Euler-Lagrange's equation as;

$$\frac{\partial F}{\partial C} - \frac{d}{dt}\left(\frac{\partial F}{\partial C'}\right) = 0 ,$$

The functional I for layer i is derived as

$$I_i = \frac{1}{2}\int_{z_{i-1}}^{z_i} \left[D^{(i)} \left(\frac{\partial C^{(i)}}{\partial z}\right)^2 - 2\left(S^{(i)} + R^{(i)}\right) C^{(i)} + \frac{\partial \left(C^{(i)}\right)^2}{\partial t} \right] dz + \delta_1 \qquad (3)$$

where, $\delta_1 = \frac{V_d}{2} {C_0}^2 - \frac{W_s}{2} {C_0}^2 - QC_0.$

4.1 Evaluation of functional I for each layer:

$$I_1 = {C_1}^2 P_1 + {C_0}^2 P_2 - C_0 C_1 P_1 - C_1 P_4 - C_0 P_5 + \alpha \frac{\partial}{\partial t}({C_1}^2 + {C_0}^2 + C_0 C_1),$$

$$I_2 = {C_2}^2 P_6 + {C_2}^2 P_6 - C_1 C_2 P_7 - C_2 P_8 - C_1 P_8 + \beta \frac{\partial}{\partial t}({C_1}^2 + {C_2}^2 + C_2 C_1),$$

$$I_3 = {C_3}^2 P_9 + {C_2}^2 P_9 - C_3 C_2 P_{10} - C_3 P_{11} - C_2 P_{11} + \gamma \frac{\partial}{\partial t}({C_3}^2 + {C_2}^2 + C_2 C_3),$$

$$I_4 = {C_4}^2 P_{12} + {C_3}^2 P_{12} - C_3 C_4 P_{13} - C_4 P_{14} - C_3 P_{14} + \mu \frac{\partial}{\partial t}({C_3}^2 + {C_4}^2 + C_4 C_3),$$

$$I_5 = {C_5}^2 P_{15} + {C_4}^2 P_{15} - C_5 C_4 P_{16} - C_5 P_{17} - C_4 P_{17} + \eta \frac{\partial}{\partial t}({C_5}^2 + {C_4}^2 + C_4 C_5),$$

$$I_6 = {C_5}^2 P_{18} - {C_5}^2 P_{19} + \lambda \frac{\partial}{\partial t} {C_5}^2,$$

Where, Pk ($1 \le k \le 19$), α , β , γ, μ , η are all constants depending upon the value of physical and physiological parameters.

4.2 System of equations

Now, differentiating I with respect to the nodal concentrations Cj ($0 \le j \le 5$) and setting: $\frac{\partial I}{\partial C_j} = 0$,

for ($0 \le j \le 5$) , yields the system of equations in matrix form is,

$$A\dot{C} + BC = W \qquad (4)$$

where,

$$A = \begin{bmatrix} 2\alpha & \alpha & 0 & 0 & 0 & 0 \\ \alpha & 2(\alpha+\beta) & \beta & 0 & 0 & 0 \\ 0 & \beta & 2(\gamma+\beta) & \gamma & 0 & 0 \\ 0 & 0 & \gamma & 2(\gamma+\mu) & \mu & 0 \\ 0 & 0 & 0 & \mu & 2(\mu+\eta) & \eta \\ 0 & 0 & 0 & 0 & \eta & 2(\eta+\lambda) \end{bmatrix}, \quad C = \begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ C_3 \\ C_5 \\ C_6 \end{bmatrix}, \quad W = \begin{bmatrix} P_5 \\ P_4 + P_8 \\ P_{11} + P_8 \\ P_{11} + P_{14} \\ P_{17} + P_{14} \\ P_{17} + P_{19} \end{bmatrix},$$

$$B = \begin{bmatrix} 2P_2 & -P_3 & 0 & 0 & 0 & 0 \\ -P_3 & 2(P_1+P_6) & -P_7 & 0 & 0 & 0 \\ 0 & -P_7 & 2(P_9+P_6) & -P_{10} & 0 & 0 \\ 0 & 0 & -P_{10} & 2(P_9+P_{12}) & -P_{13} & 0 \\ 0 & 0 & 0 & -P_{13} & 2(P_{15}+P_{12}) & -P_{16} \\ 0 & 0 & 0 & 0 & -P_{16} & 2(P_{15}+P_{18}) \end{bmatrix}, \quad \dot{C} = \begin{bmatrix} \frac{\partial C_0}{\partial t} \\ \frac{\partial C_1}{\partial t} \\ \frac{\partial C_2}{\partial t} \\ \frac{\partial C_3}{\partial t} \\ \frac{\partial C_4}{\partial t} \\ \frac{\partial C_5}{\partial t} \end{bmatrix}.$$

To solve the system of ordinary differential equation (4), we use Crank-Nicolson method. According to method the system of equation (4) can be written as:

$$\left(A + \frac{\Delta t}{2} B\right) C^{(i+1)} = \left(A - \frac{\Delta t}{2} B\right) C^{(i)} + \Delta t W \qquad (5)$$

where,

Δt is the time step, and $C^{(i)}, C^{(i+1)}$ are the concentrations at the current and next time steps, respectively.

5. Simulations and discussions

In this section, we study the numerical outcomes of solving equation (3) with the help of CAS (MATLAB)(Acharya, Gurung and Saxena, 2013; C., Gurung and Adhikary, 2013). In order to see how pollutant concentrations, vary with altitude, we use the following parameter values presented in Table 2. Figures 3 - 5 show the findings of the study of how air pollution moves through the troposphere because of dry deposition and gravity-settling speed with Ws = 0 m/hr.

Table 5.1: The values of different parameters

Layers	$D(m^2/hr)$	$S(\mu gm \times m^{-3}/hr)$	$R(\mu gm \times m^{-3}/hr)$	z (meter)
I	180	580	4.32×10^{-8}	2
II	144	450	3.6×10^{-8}	4
III	108	300	2.88×10^{-8}	6
IV	72	250	2.16×10^{-8}	8
V	36	150	1.44×10^{-8}	10
VI	18	0	7.2×10^{-9}	12

The profile of concentration dispersion at the interfaces of the layers is depicted by the graphs in Figure 2. These graphs ignore the effects of Ws and Vd. This trend is pretty consistent with the natural behavior of pollutant dispersion, and the results are compatible with the boundary conditions in which the value of concentration initially starts to rapidly increase with increasing value of time and then eventually becomes constant.

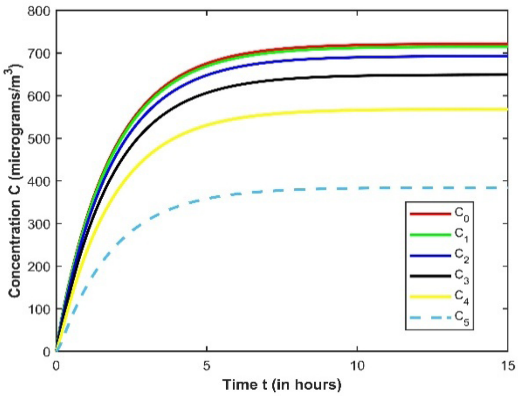

Figure 2 Dispersion of air pollution with Ws = Vd = 0 m/hr

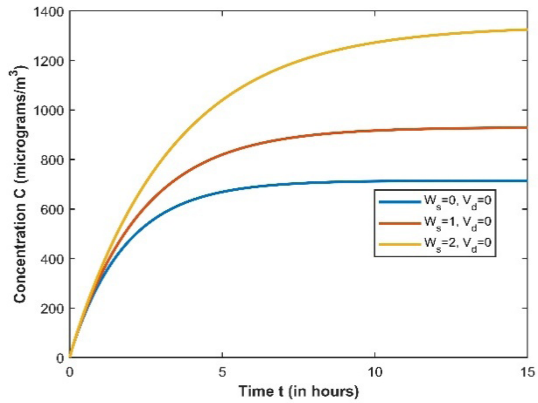

Fig. 3 Effects of gravitational settling velocity at ground level with .

We observed this based on the data presented in Figure 3, which showed that when the settling velocity increases, the ground-level pollutant concentration distribution continues to increase up to a certain extent before becoming stable. This is due to the fact that only the light particles are left extremely high above the ground level, and the gravity force becomes almost useless on these particles. As a result, concentration increases closer to the ground level as the gravitational settling velocity increases.

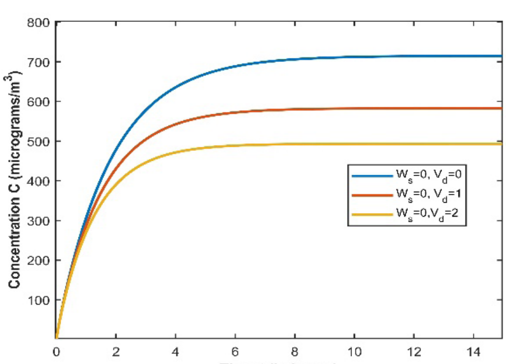

Figure 4 Effects of dry deposition at ground level

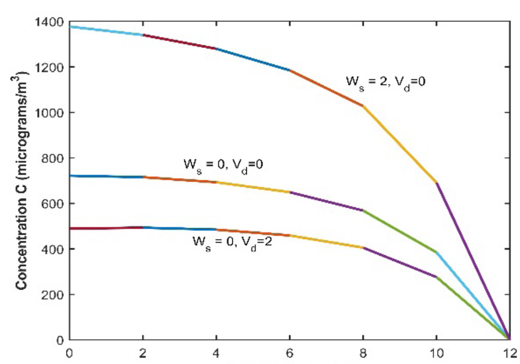

Figure 5 Relation between concentrations

The data presented in Figure 4 that there is a drop in concentration as the values of dry deposition increase. There is a decrease in the concentration of pollutants in the atmosphere as a result of the absorption of pollutants by various organisms such as trees, leaves, plants, and buildings, among other things.

Figure 5, illustrates the relationship between concentration and vertical height when the system is in a steady condition. The figure reveals that the value of concentration is maximum near the ground level, and the value of concentration falls with the increase in vertical height and finally reduces to zero for a big value of z. This illustrates that concentration with local areas of sources is greater and then gradually declines with height.

The study concluded that locations near polluting sources are more affected and the impact decreases with vertical distance from the source. These data are consistent with the expected physical and chemical behavior of pollutants in the environment. So, these trends aid in understanding pollutant behavior under various scenarios, which is important for urban planning, environmental management, and pollution control techniques.

6. Conclusions

A one-dimensional unsteady-state numerical model is developed to study pollutant dispersion, incorporating the effects of chemical reactions, gravitational settling velocity, and dry deposition. The results are presented graphically to demonstrate the influence of gravitational settling and dry deposition on ground-level pollutant concentration. Additionally, the model is analyzed under steady-state conditions to evaluate pollutant concentrations at various heights in the atmosphere (troposphere).

Initially, the pollutant concentration increases rapidly with time and eventually stabilizes. An increase in gravitational settling velocity leads to a rise in ground-level concentration, whereas higher dry deposition rates result in a reduction of ground-level concentration. This reduction is attributed to the role of dry deposition by surfaces such as trees, plants, leaves, and buildings, which effectively lower the pollutant levels at the ground.

Conflict of interest

Declare 'No conflict of interest' if there are none.

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