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An Analytical Approach for Predicting Atmospheric Concentration of Air Pollutants

A. M. Jibrin, R. O. Olayiwola*, A. T. Cole and M. D. Shehu

Abstract

Many forms of atmospheric pollution affect human health and the environment at levels from local to global. These contaminants are emitted from diverse sources, and some of them react together to form new compounds in the air. This paper presents a three-dimensional transient equation describing the pollutant transport in the atmosphere. We assume the atmosphere is subjected to pollutant due to the time-dependent source concentration. We use the parameter-expanding method and seek direct eigenfunctions expansion technique to obtain analytical solution of the model. The results are presented graphically and discussed. It is discovered from the results obtained that increase in reaction rate and decrease in wind speed change significantly the atmospheric concentration of air pollutant.

1. Introduction

Air pollution occurs within the atmospheric planetary boundary layer under the combined effects of meteorological factors, earth surface topographic features and releases air pollutants from various sources. Meteorological factors such as

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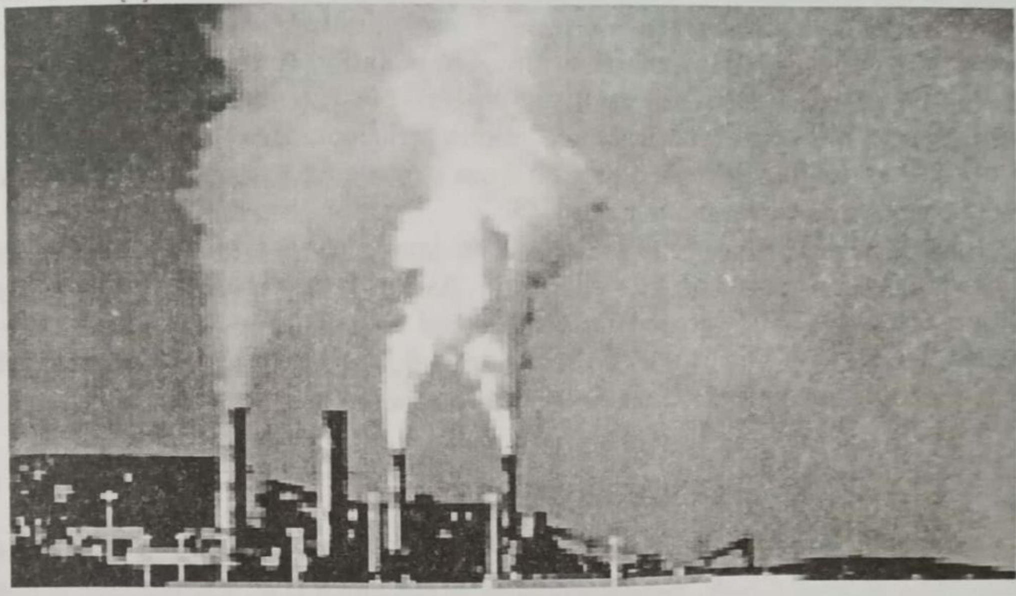
Department of Mathematics, Federal University of Technology, Minna, Nigeria.
e-mail: olayiwola.rasaq@futminna.edu.ng

wind velocity, wind direction, temperature, and relative humidity together with earth surface roughness are effective agents for mixture of air pollutants. The most important role of meteorology is in the dispersion, transformation and removal of air pollutants from atmosphere. The wind speeds determine the amount of dispersion of pollutants in the atmosphere. The temperature contributes transformation of pollutants in the atmosphere [2]. The topography and solar heating of region surrounding a particular pollution source affects the concentration. High pollution levels can be expected during fair weather conditions resulting local wind system and strong temperature inversions in cities situated in mountainous region [2].

Air pollution may be classified into two types according to the nature of formation: primary pollutants which are emitted from their sources directly to the atmosphere such as industry, traffic, domestic heating in winter season and secondary pollutants which results from the chemical reaction between the primary pollutants [2].



Air pollution. Source: National Park Service

Over the past half-century, scientists have learned much more about the causes and impacts of atmospheric pollution. Many nations have greatly reduced their emissions, but the problem is far from solved. In addition to threatening human health, air pollutants damage ecosystems, weaken Earth's stratospheric ozone shield, and contribute to global climate change [7]. Industrialized nations have made important progress toward controlling some pollutants in recent decades, but air quality is much worse in many developing countries, and global circulation patterns can transport some types of pollution rapidly around the world [7].

The science of air pollution centres on measuring, tracking, and predicting concentrations of key chemicals in the atmosphere. Osalu et al. [9] developed a two dimensional atmospheric dispersion model for computation of the ambient air concentration of reactive pollutants emitted from ground level sources. The result showed that atmospheric chemical reactions are the most complicated and stiff part of pollutants dispersion equations. Arkhipov et al. [1] studied numerically the model of pollutant dispersion and oil spreading using stochastic discrete particles method and concluded that the comparison of numerical and analytical results demonstrates a good fit. Mihaiella et al. [5] performed a case study on pollution prediction through atmospheric dispersion modelling and found that the exposure to ambient air pollution is associated with a series of adverse health effects. Indra et al. [4] considered the classification of air pollution dispersion models and found that dispersion and emission of pollutants into the air is controlled by the prevailing meteorological conditions like wind, temperature and stability of the atmosphere. They further showed that air pollution models are based on the theories of atmospheric physics and thermodynamics. Habingabwa [3], used a two dimensional convection diffusion equation to model air pollution. He found that the pollution dispersion is influenced by the model parameters like diffusion coefficient, drift motion and reaction coefficient. He concluded that the drift velocity of air moves the pollutants from one region to another at the rate which is proportional to its magnitude.

The objective of this paper is to obtain an analytical solution for predicting atmospheric concentration of air pollutants. As in [8], we assume that initially the atmosphere is not clean and it is subjected to pollutant due to the time-dependent source concentration. To simulate the flow analytically, we assumed there is no pollutant flux at the end of other boundaries.

2. Model Formulation

We consider the transport of pollutant in the atmosphere. It is assumed that initially (i.e., at time $t = 0$), the atmosphere is not clean (i.e., the domain is not pollutant free). Let C_i be the initial pollutant concentration in the atmosphere described the distribution of the pollutant at all point of the flow domain. The time dependent source concentration is assumed at the origin (i.e.,$x = 0, \ y = 0, \ z = 0.$) of the domain. At the end of other boundaries (i.e., $x = L, \ y = M, \ z = H$), we assumed there is no pollutant flux. Let $C(x, y, z, t)$ be the pollutant concentration in the atmosphere at position x, y, z and time t. Then, a three-dimensional transient equation describing pollutant concentration in the atmosphere is given as:

$$(1) \quad \frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}+w\frac{\partial C}{\partial z}=\frac{\partial}{\partial x}\left(k_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(k_y\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial z}\left(k_z\frac{\partial C}{\partial x}\right)+S,$$

where C is the concentration of pollutant in the atmospheric air, u is the wind speed along the x- direction, v is the wind speed along the y- direction, w is wind speed along the z-direction, S is the sources and sinks of pollutant in the atmosphere i.e. its emission, removal from the atmosphere by dry and wet deposition, chemical reactions, k_x is the eddy diffusivity along x- direction, k_y is the eddy diffusivity along y- direction, k_z is the eddy diffusivity along z- direction.

In this research work, we assume the following:

(1) A vertical velocity component is neglected.
(2) x-axis is oriented in the direction of mean wind i.e. $(u = U, v = 0)$
(3) No settling or deposition. (i.e., $w=0$)
(4) Downwind diffusion is neglected in comparison to transport due to mean wind (see [10]) i.e. $\left|U\frac{\partial C}{\partial x}\right| >> \left|\frac{\partial}{\partial x}\left(k_x\frac{\partial C}{\partial x}\right)\right|$
(5) Emission source term with pollutant reaction of the constant reaction rate.

Based on the above assumptions equation (??) reduces to

(2) $$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = k_y\frac{\partial^2 C}{\partial y^2} + k_z\frac{\partial^2 C}{\partial z^2} + nC$$

with initial and boundary conditions:

(3) $$\left.\begin{array}{lllll} C(x,y,z,t) = C_1, & x \geq 0, & y \geq 0, & z \geq 0, & t = 0 \\ C(x,y,z,t) = C_0(2-qt), & x = 0 & y = 0, & z = 0, & t > 0 \\ \frac{\partial C}{\partial x} = 0, \quad \frac{\partial C}{\partial y} = 0, \quad \frac{\partial C}{\partial y} = 0, & x = L, & y = M, & z = H, & t \geq 0 \end{array}\right\}$$

We introduce a new space variable as

(4) $$\eta = y + z\sqrt{\frac{k_z}{k_y}}$$

Then equations (??) and (??) reduce to

(5) $$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial \eta^2} + nC$$

and

(6) $$\left.\begin{array}{llll} C(x,\eta,t) = C_1, & x \geq 0, & \eta \geq 0, & t = 0 \\ C(x,\eta,t) = C_0(2-qt), & x = 0 & \eta = 0, & t > 0 \\ \frac{\partial C}{\partial x} = 0, \quad \frac{\partial C}{\partial \eta} = 0, & x = L, & \eta = M + H\sqrt{\frac{K_z}{K_y}} = h, & t \geq 0 \end{array}\right\}$$

where

$$D = K_y\left(1 + \frac{K_z^2}{K_y^2}\right)$$

3. Method of Solution

3.1 Non-dimensionalization

Here, we let $h = L$ and non-dimensionalized equations (??) and (??), using the following dimensionless variables:

$$x' = \frac{x}{L}, \quad \eta' = \frac{\eta}{L}, \quad t' = \frac{Dt}{L^2}, \quad C' = \frac{C}{C_0} \tag{7}$$

and we obtain

$$\frac{\partial C}{\partial t} + u_0 \frac{\partial C}{\partial x} = \frac{\partial^2 C}{\partial \eta^2} + \alpha_0 C \tag{8}$$

together with initial and boundary conditions:

$$\left.\begin{array}{llll} C(x,\eta,t) = \frac{C_i}{C_0}, & x \geq 0, & \eta \geq 0, & t = 0 \\ C(x,\eta,t) = C_0(2 - qt), & x = 0 & \eta = 0, & t > 0 \\ \frac{\partial C}{\partial x} = 0, \quad \frac{\partial C}{\partial \eta} = 0, & x = 1, & \eta = 1, & t \geq 0 \end{array}\right\} \tag{9}$$

where

$u_0 = \frac{UL}{D}$ = Wind speed, $\alpha_0 = \frac{kL^2}{D}$ = reaction rate

Let us introduce another new space variable as

$$\varepsilon = x + \eta \tag{10}$$

Then equations (??) and (??) reduce to:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial \varepsilon}\left(\frac{\partial C}{\partial \varepsilon} - u_0 C\right) + \alpha_0 C \tag{11}$$

$$\left.\begin{array}{lll} C(\varepsilon,t) = \frac{C_i}{C_0}, & \varepsilon \geq 0, & t = 0 \\ C(\varepsilon,t) = 2 - qt, & \varepsilon = 0, & t > 0 \\ \frac{\partial C}{\partial \varepsilon} = 0, & \varepsilon = 2 & t \geq 0 \end{array}\right\} \tag{12}$$

3.2 Solution by Direct Eigenfunctions Expansion Method

This is a non-homogenous boundary value problem. To solve (??) subject to (??) we have to transform the equations to homogeneous boundary. We let

$$w(\varepsilon,t) = a(t) + \varepsilon b(t) = 2 - qt + \varepsilon \cdot 0 \tag{13}$$

and

$$C(\varepsilon,t) = v(\varepsilon,t) + w(\varepsilon,t) \tag{14}$$

Then equations (??) and (??) transformed into

$$\frac{\partial v}{\partial t} = \frac{\partial^2 v}{\partial \varepsilon^2} - u_0 \frac{\partial v}{\partial \varepsilon} + \alpha_0 v - \alpha_0 qt + (2\alpha_0 + q) \tag{15}$$

$$v(\varepsilon,0) = \frac{C_i}{C_0} + qt - 2, \qquad v(0,t) = 0, \qquad v_\varepsilon(2,t) = 0 \tag{16}$$

Suppose the solution $v(x,t)$ can be express as

(17) $$v(x,t) = v_0(x,t) + \epsilon v_1(x,t) + h.o.t$$

where h.o.t stand 'higher order terms in ϵ'. In our analysis we are interested only in the first two terms. Substituting (??) into (??) and (??) and processing, we obtain

(18) $$\frac{\partial v_0}{\partial t} = \frac{\partial^2 v_0}{\partial x^2} + \alpha_0 v_0 + (2\alpha_0 + q - \alpha_0 q t)$$

(19) $$v_0(x,0) = \frac{C_i}{C_0} + qt - 2, \qquad v_0(0,t) = 0, \qquad v_{0x}(2,t) = 0$$

(20) $$\frac{\partial v_1}{\partial t} = \frac{\partial^2 v_1}{\partial x^2} - \frac{\partial v_0}{\partial x} + \alpha_0 v_1$$

(21) $$v_1(x,0) = 0, \qquad v_1(0,t) = 0, \qquad v_{1x}(2,t) = 0$$

Using eigenfunctions expansion method (see [6] for details), we obtain the solution of (??) - (??) as:

(22)

$$v_0(x,t) = \sum_{n=1}^{\infty} \frac{4}{(2n-1)\pi} \begin{pmatrix} (2\alpha_0 + q)\left(\frac{e^{At}-1}{A}\right) - \alpha_0 q\left(\frac{e^{At}-At-1}{A^2}\right) + \\ \left(\frac{C_i}{C_0} + qt - 2\right) e^{At} \end{pmatrix} \sin\left(\frac{2n-1}{4}\right)\pi x$$

and

(23)

$$v_1(x,t) = \sum_{n=1}^{\infty} -\frac{2(-1)^{2n}}{(2n-1)\pi} \begin{pmatrix} (2\alpha_0 + q)\left(\frac{Ate^{At}-e^{At}+1}{A^2}\right) - \\ \alpha_0 q\left(\frac{Ate^{At}-2e^{At}+At+2}{A^3}\right) + \\ \left(\frac{C_i}{C_0} + \frac{qt}{2} - 2\right) te^{At} \end{pmatrix} \sin\left(\frac{2n-1}{4}\right)\pi x$$

where

$$A = \left(\alpha_0 - \left(\frac{2n-1}{4}\right)^2\right)$$

Then, we obtain

(24) $$v(x,t) = v_0(x,t) + \epsilon v_1(x,t)$$

and

(25) $$C(x,t) = v(x,t) + 2 - qt$$

The computations were done using computer symbolic package MAPLE.

4. Results and Discussion

A three-dimensional transient equation describing pollutant concentration in the atmosphere is solved analytically using parameter-expanding method and eigen-functions expansion technique. Analytical solutions of equations (??) and (??) are computed for the values of $C_1 = 200$, $C_0 = 1.0$, $q = 0.2$ $(/day)$, $u_0 =$ $0.1, 0.2, 0.4$ (km/day), $v_0 = 0.3, 0.5, 0.7$,
$k_y = 0.15$, $k_z = 1.5$. The pollutant concentration values are depicted graphically in Figures 1 - 8.

From figure 1, we can conclude that pollutant concentration decreases as time increases and along the x- direction and decreases along the temporal and spatial directions as wind speed(u_0) increases.

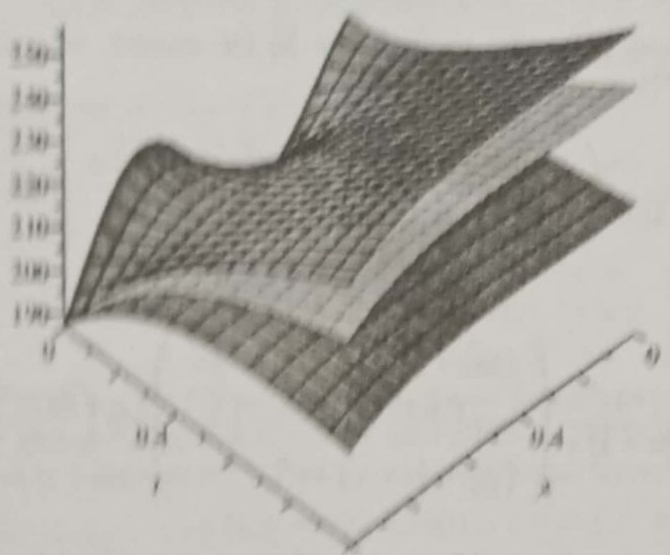


Figure 1: Variation of Pollutant Concentration $C(x, y, z, t)$ against x and t for different values of Wind Speed u_0

From figure 2, we can conclude that pollutant concentration decreases as time increases and along the y- direction and decreases along the temporal and spatial directions as wind speed(u_0) increases.

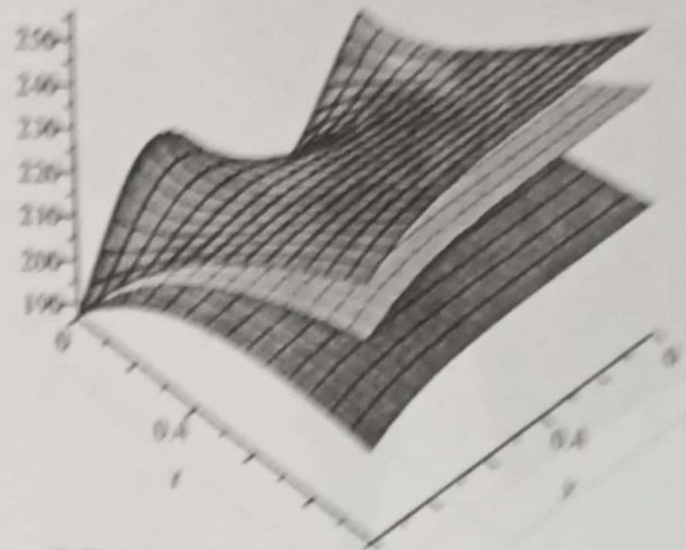


Figure 2: Variation of Pollutant Concentration $C(x, y, z, t)$ against y and t for different values of Wind Speed u_0

From figure 3, we can conclude that pollutant concentration decreases and along the z- direction and decreases along the spatial direction as wind speed(u_0) increases.

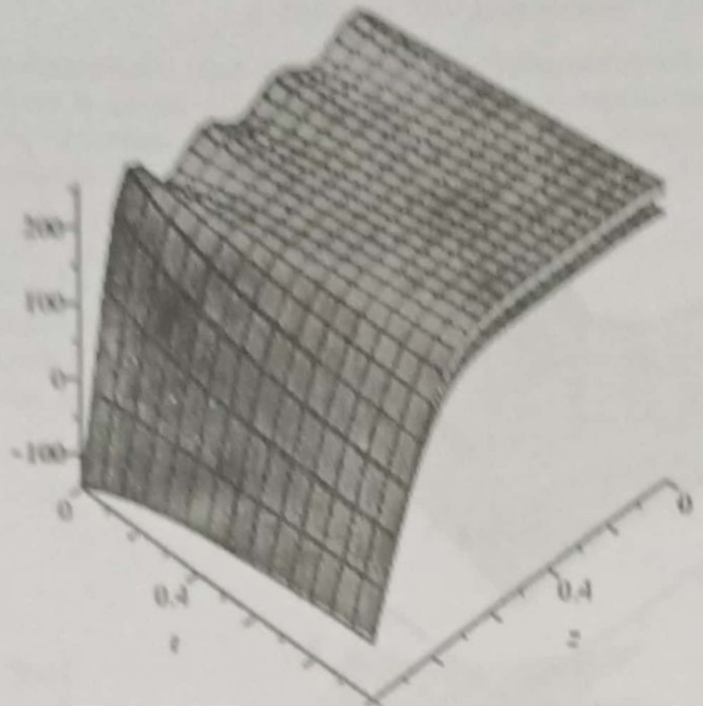


Figure 3: Variation of Pollutant Concentration $C(x, y, z, t)$ against z and t for different values of Wind Speed u_0

From figure 4, we can conclude that pollutant concentration decreases along the x and y -directions and decreases along the spatial directions as wind speed(u_0) increases.

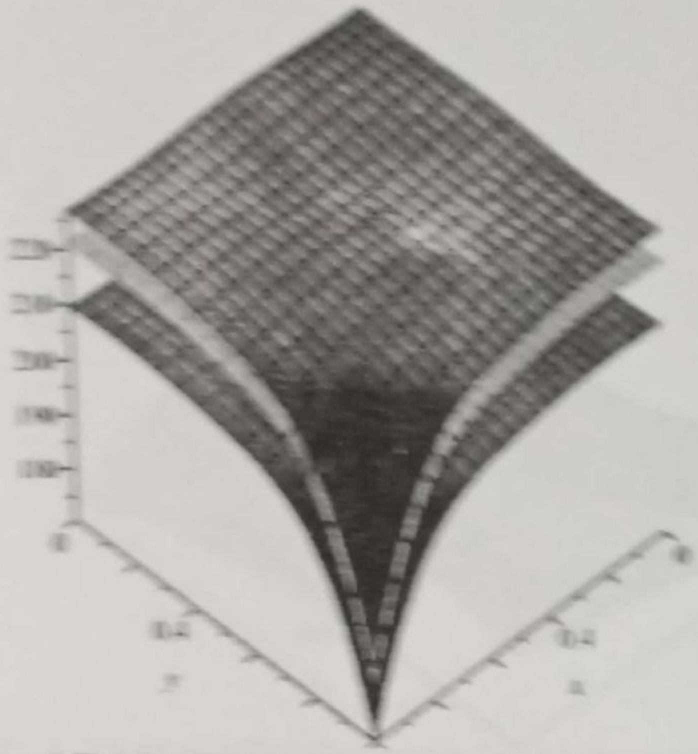


Figure 4: Variation of Pollutant Concentration $C(x, y, z, t)$ against x and y for different values of Wind Speed u_0

From figure 5, we can conclude that pollutant concentration increases as time increases and along the z– direction and increases along the temporal and spatial directions as reaction rate(α_0) increases.

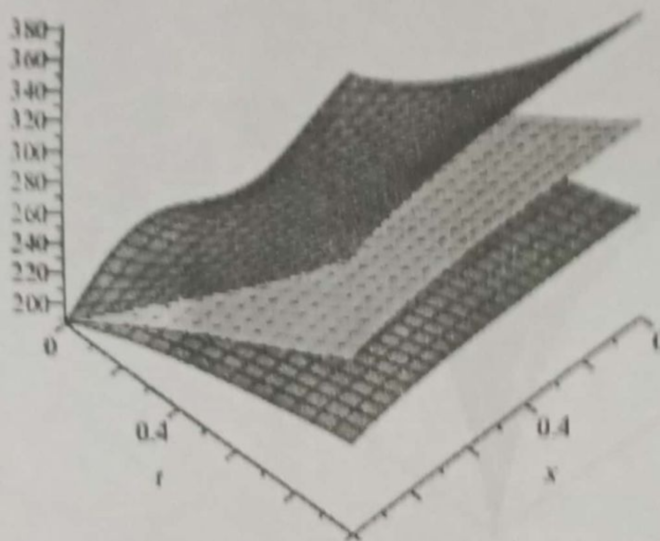


Figure 5: Variation of Pollutant Concentration $C(x, y, z, t)$ against x and t for different values of Reaction Rate α_0

From figure 6, we can conclude that pollutant concentration increases as time increases and along the y- direction and increases along the temporal and spatial directions as reaction rate(α_0) increases.

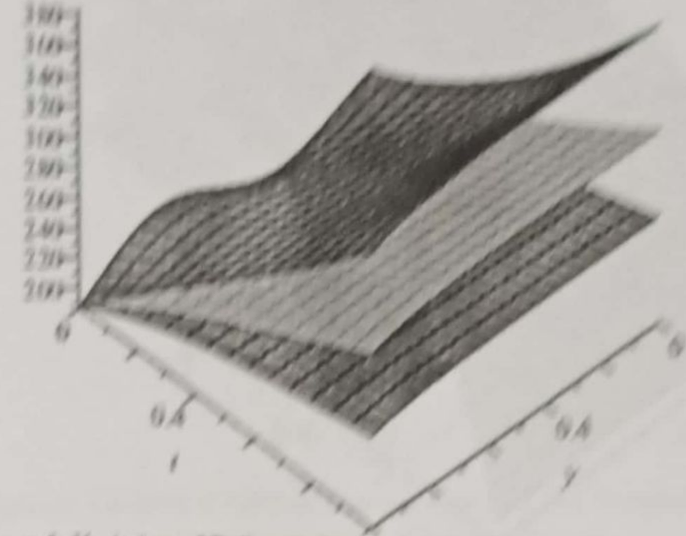


Figure 6: Variation of Pollutant Concentration $C(x, y, z, t)$ against y and t for different values of Reaction Rate α_0

From figure 7, we can conclude that pollutant concentration increases along the y-direction and increases along the spatial direction as reaction rate(α_0) increases.

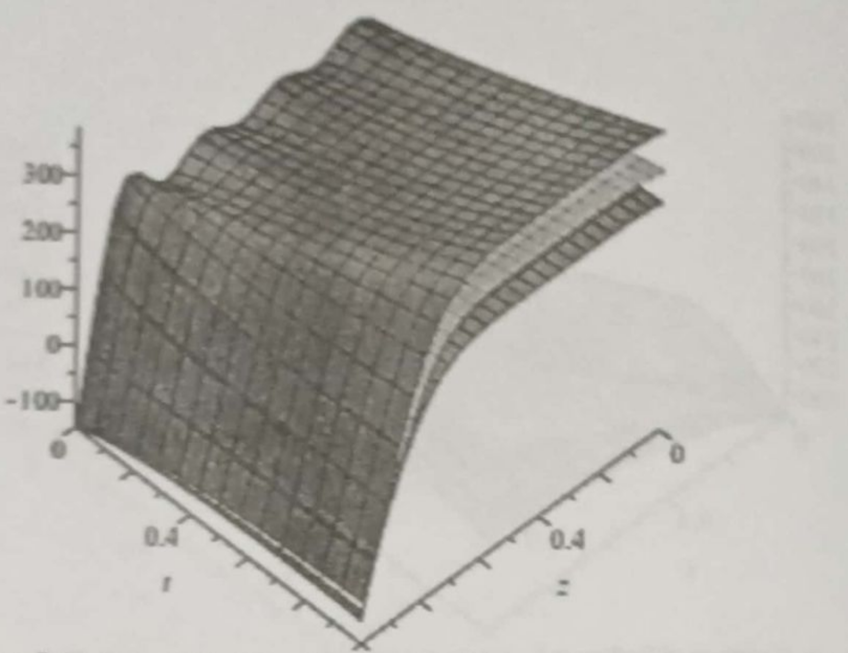


Figure 7: Variation of Pollutant Concentration $C(x, y, z, t)$ against z and t for different values of Reaction Rate α_0

From figure 8, we can conclude that pollutant concentration increases along the x and y-directions and increases along the spatial directions as reaction rate(α_0) increases.

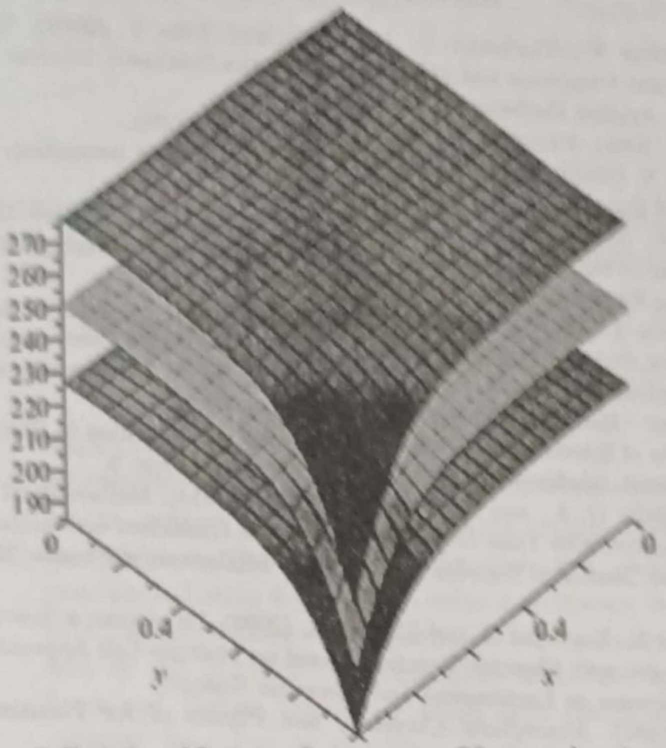


Figure 5: Variation of Pollutant Concentration $C(x, y, z, t)$ against x and y for different values of Reaction Rate α_0

Conclusion

From the studies made on this paper we conclude as under.

(1) Wind speed decreases the pollutant concentration along the temporal and spatial directions.

(2) Reaction rate enhances the pollutant concentration along the temporal and spatial directions.

It is noted that increase in reaction rate and decrease in wind speed change significantly the atmospheric concentration of air pollutant. It shows that the concentration of these chemicals strongly depend on both the mechanisms of formation and the dynamics of transport. This has negative implication on human health. Air pollutants damage ecosystems, weaken Earth's stratospheric ozone shield, and contribute to global climate change. Thus, it is crucial to track concentrations of key chemicals in the atmosphere.

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