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# Unsteady state mathematical model of chemically reactive pollutants from an instantaneous line source into a stable atmospheric boundary layer

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ABSTRACT

A time dependent atmospheric model represented for chemically reactive primary pollutants emitted from an elevated line source into a stable atmospheric boundary layer over a surface terrain. The model obtained from an analytical solution of the atmospheric diffusion equation with the quadratic diffusion coefficient (exchange coefficient) and the variable wind velocity taken to be of three different types' viz. constant, constant shear and parabolic functions of vertical height. The pollutants considered to be of chemically reactive primary pollutants emitted from a time-dependent line source of Instantaneous type. In order to facilitate the application of the model the results for the general situation that includes chemical reaction rate & time dependent source incorporated in the model.



## 1. Introduction

Recent work in air pollution modeling has begun to focus on the important problems of simulating the concentration of various type of pollutants viz. chemically reactive & non-reactive. Due to rapid industrialization and fast urbanization, air has come under direct attack of various pollutant species emitted in the process. The predictions for air quality based on the various modeling approaches viz. (i) the eddy diffusion model (*k*-theory model), (ii) the Gausian or normal distribution model and (iii) the Gaussian model. The most comprehensive approach to transport theory based on the *eddy diffusion model*, which in turn involves the use of the "mixing length" concept. This is the usual starting point in the development of a dispersion model for the atmosphere. Therefore, "the eddy diffusion model" was choosen. The problem of atmospheric pollution has become a global problem during the last few decades due to the emission of toxic gases into the atmospheric boundary layer under so many meteorological conditions in large quantities over urban areas. Most general and useful mathematical models are essential to asses the impact of pollutants (emits from various sources like industries, highways and urban areas) on the vegetation, buildings and environment of a study area under the influence. During the last few decades, many scientists and mathematicians focused their attention much towards the modeling of air pollution and generated considerable interest in predicting the distribution of concentration of pollutants emitted from various sources. The chemically reactive primary pollutants emitted from the time-dependent line source undergo chemical reactions with existing gases and water vapors present in the atmosphere converted into a particulate matter. Chemical reaction rate depends on the nature of the pollutants and on the stability of atmospheric boundary layer, which has influenced by the heat flux in the Atmospheric Boundary Layer (ABL). Therefore, it is necessary to study the effect of chemical reaction rate on the distribution of pollutants in the atmosphere through the transport equation representing instantaneous and delayed removal. Besides these, the deposition

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velocities of the pollutants in the particulate form at the ground level are also took into consideration. The deposition velocity depends on the factors as the type and size of the pollutant particles, the roughness of the terrain and the type of the ground cover and meteorological conditions.

## 2. Formulation of the model

The model developed for the emission of contaminant in the gaseous state from a time dependent (instantaneous) elevated line source of infinite length into a stable ABL. The instantaneous source or impulse type of source is the type, which occurs by sudden explosion of gaseous container. The Bhopal gas tragedy (1984) is one of the examples for this type of sources. Through which the toxic gaseous pollutants emitted and effect the society, vegetation and buildings. It is essential to study the impact of pollutant injected into the atmospheric boundary layer. The attention focused here on such type of source, has been incorporated in this model, and steadied the impact in the stable atmospheric boundary layer. The degree of stability of the atmospheric boundary layer must be known if we wish to estimate the ability of the atmosphere to disperse it (pollutants) receives from fabricated sources. A stable atmosphere is the one that does not exhibit much vertical mixing or motion (Huang et al. [5]). As a result, pollutants emitted near the earth's surface tend to remain there. The possibility of leakage of pollutants through inversion layer in negligibly less. Therefore, the diffusion coefficient of quadratic in nature considered which is best suited for the stable ABL (Robson [2]) in this model. The height of the atmospheric boundary layer is assumed to be $z = H$, from the surface. The surface terrain is assumed to be of flat, rough and build-up accordingly the wind profile varies from constant, constant shear and parabolic. The contaminants are assumed be chemically reactive. The pollutant transport assumed governed by the atmospheric advection–diffusion equation with delayed removal (Ermak [7], Alam and Seinfield [8]):

$$\partial C/\partial t + u\partial C/\partial x + v\partial C/\partial y + w\partial C/\partial z = \partial/\partial x(K_x\partial C/\partial x) + \partial/\partial y(K_y\partial/\partial y) + \partial/\partial z(K_z\partial/\partial z) - KC + S. \tag{2.1}$$

The model based on the following assumption:

(a) Model is of time dependent & advection dominates over horizontal diffusion

$u\partial C/\partial x \gg \partial/\partial x(K_x\partial C/\partial x).$

(b) It is also assumed that the line source is in the direction of $y$-axis, which leads to the concentration gradient and flux gradient becomes zero along $y$-direction.

$v\partial C/\partial y = 0 \quad \& \quad \partial/\partial y(K_y\partial C/\partial y) = 0.$

(c) The vertical diffusion dominates over advection

$\partial/\partial z(K_z\partial C/\partial z) \gg w\partial C/\partial z.$

(d) The source ($S$) is time dependent line source and is assumed to be

$S = QW(t)\delta(x - x_0)\delta(z - z_0).$

Based on the above assumptions the transport and diffusion Eq. (2.1) becomes:

$$\partial C/\partial t + u\partial C/\partial x = \partial/\partial z(K_z\partial C/\partial z) - K''C + QW(t)\delta(x - x_0)\delta(z - z_0). \tag{2.2}$$

Initial and boundary conditions are:

$$C(x,z,t) = 0 \quad \text{at } t = 0, \quad \forall x,z \in R^+, \tag{2.3a}$$

$$C(x,z,t) = 0 \quad \text{at } x = 0, \quad t = 0, \quad 0 \leqslant z < H, \tag{2.3b}$$

$$K_Z\partial C/\partial z = 0 \quad \text{at } z = 1, \quad \forall x,t \geqslant 0, \tag{2.3c}$$

$$K_Z\partial C/\partial z = v_d C \quad \text{at } z = 0, \quad \forall x,t \geqslant 0, \tag{2.3d}$$

where,

$C(x,y,z)$ = Pollutant concentration (ppm)
$H$ = height of the inversion layer
$z_o$ = height of the source
$(x_o,z_o)$ = the location of the source in $xz$-plane
$K_z$ = Exchange coefficient along vertical direction.
$Q$ = Source strength at $(x_o,z_o)$
$\delta(x)$ = Dirac's delta function
$v_d$ = the deposition velocity
$K''$ = first order delayed removal
$t$ = time in seconds
$W(t)$ = time dependent source of instantaneous or impulse is of the form:
$W(t) = W_o\delta(t)$ (impulsive type).