ANALYTICAL MODEL OF ATMOSPHERIC POLLUTANT DISPERSION RELEASED FROM LINE SOURCE

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Abstract. *Many models of passive pollutant dispersion in the atmosphere are based on the advection diffusion equations. Moreover, models that incorporate line sources are used to investigate the vehicular pollution, that occurs in auto-roads, assuming themselves a uniform distribution of vehicles. The use of analytical solutions still remains the easiest way to model the diffusion and advection in Planetary Boundary Layer (PBL). Thus, the objective of this work is to present a three-dimensional solution of the advection-diffusion equation, considering a line source, and eddy diffusivities depending on source distance. The solution will be arrived using the Generalized Integral Transform Technique (GITT).*

Keywords*: line source, dispersion model, analytical model, planetary boundary layer*

1. Introduction

Pollutants dispersion in the atmosphere is a significant problem nowadays. The increasing number of vehicles has generated problems to public health. On the other hand, some other problems raised up such as pesticides and ammonia dispersion in farmlands. Also it has been reported analysis of pollutants dispersion from power plants. Almost all countries have rules and regulation about the pollution. The environmental agencies have supported studies to create models to preview and control the impacts in environment (Nagendra and Khare, 2002).

In vehicular pollutants, there are issues of great interest. Some of them are:

- The evaluation of source strength.
- The inventory of sources.
- The source modeling.
- Some models do not work well when the wind direction is nearly parallel to highways or the wind speed is low.
- The models are very sensitive to the geometry nearby the roads, like traffic junctions or city canyons.
- Theoretical models to turbulent diffusion in atmosphere.

In the literature, several works dealing with analytical models, can be found. Among them the works of Vilhena, 1998 and Moreira, 2005 and others are indicated for point sources. But articles about line source analytical models are more sparing. Some authors have pointed out that analytical models furnish better results under some circumstances and have low computational costs. So it seems to be a very promising study (Lin and Hildemann, 1995; Kastner-Klein and Fedorovich, 2002).

2. Line Source Model Review

Air pollution has been increased substantially in these last twenty years. One of the most important reason is that the road traffic have grown, causing more pollutants in atmosphere (vehicular exhausts); Goyal and Krishna (1999) have pointed out that the NO_2 concentrations observed in New Delhi is 3 to 6 times that of safety limits prescribed by World Health Organization (WHO). The most common pollutants in atmosphere due to vehicular exhausts are CO and NO_x (NO and NO_2).

The dispersion of pollutants in roadways is described by Line Source Models (LSM) by the majority of approaches in literature. The LSM can be classified as deterministic and/or statistical (Nagendra and Khare, 2002). The deterministic models are a set of differential equations relating pollutant concentration to average wind and turbulent diffusion. It is based on description of physical/chemical process.

Statistical models do diagnosis and prediction of air quality by means of interpolation and extrapolation. Theses models do not distinguish the physical causes of dispersion phenomena. All possible uncertainties are taken into account by “noise” variable with assigned statistical properties (Nagendra and Khare, 2002).

The LSM have been widely applied for a great range of purposes, mainly to previous pollutants concentration near roadways. For example, these works can be cited:

- Hao et al. (2000) – Beijing (China)
- Khare and Sharma (1999) – New Delhi (India)

- Goyal and Krishna (1999) – New Delhi (India)
- Marmur and Maname (2003) – Jerusalem (Israel)

The LSM can also be Gaussian, numerical and analytical. The Gaussian LSM assumptions are: The sum or concentrations from all infinitesimal sources make up a line source; The mechanism of diffusion from each point source is assumed to be independent of the presence of other point sources; The emission from a point source spreading in atmosphere in the form of plume whose concentration profile is generally gaussian in both horizontal and vertical directions.

The numerical techniques can be applied to solve the differential equations of diffusion phenomena, using gaussian LSM, to preview the receptor concentration, spatially and temporarily distributed. Some numerical softwares have been developed based on these assumptions for example HIWAY-2, CALINE-4 and ROADWAY-2.

Some theoretical approaches about LSM have been treated recently, like:

- Oettl et al. (2001) analyzed the pollutant dispersion under low wind speed.
- Held et al. (2003) have proposed that the dispersion solution can be estimated by Huang dispersion (UCD 2001 model).
- Kumar et al. (2004) have modeled a composite receptor to take into account gaseous components (NO_2 and SO_2) and suspended particulated matter, applied to Mumbai (India).
- Jacobson and Seinfeld (2004) have studied the modifications in distribution of particles emitted from point and line sources.

Analytical models have been proposed and have promising perspective. These solutions are computationally much more economic than numerical solutions. According to Lin and Hildemann (1995), analytical models:

- Clearly show the influence of parameter because they are explicit expressed in mathematical closed form. The effect of the individual parameter on model results can therefore be easily investigated.
- Are useful for examining the accuracy and performance of numerical methods.
- Allow insights regarding the behavior of a system.

Lin and Hildemann (1995) have proposed an analytical solution based on the superposition of Green's function, enabling the possibilities to estimate ambient concentrations from single point, multiple points, line or area releases.

Kastner-Klein and Fedorovich (2002) compared data obtained in wind tunnel. The shape of normalized concentration profile agreed well with analytical predictions from Pasquill and Smith (1983), and Seinfeld (1986).

3. The solution

The equation of the atmospheric diffusion, taking into consideration an incompressible fluid and the theory of the gradient transport (K-Theory), for a Cartesian coordinates system has the following format:

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}+w\frac{\partial C}{\partial z}=\frac{\partial}{\partial x}\left(K_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right)+S+R \tag{1}$$

Where c is a pollutant average concentration; *S* and *R* are source and removal terms respectively; *u, v, w* and K_x, ,K_y, K_z are the mean wind speeds and eddy diffusivities terms in the *x, y* and *z* directions respectively.

Considering steady state conditions, vertical speed lesser than the horizontal, mean wind speed in the *x* direction, and removal component negligible, the equation above reduces to:

$$U\frac{\partial c}{\partial x}=\frac{\partial}{\partial x}\left(K_x\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial c}{\partial z}\right)+S \tag{2}$$

This equation forms the base of the majority air quality models (Sharan et al.; 1996). The nature of the solution of this equation depends on the specification of the mean wind speed *U*, eddy diffusivities *K* and the source *S*. Normally *U* is considered constant (Nieuwstadt, 1980), or more realistic, as a height depending power law function (Pasquill and Smith, 1983). In the same way, eddy diffusivities *K* are also assumed constant (Sharan et al.; 1996 a,b), power functions of height *z* or taken with functions of space coordinates (Tirabassi 1987).

In this work, we considered *U* a constant and the eddy diffusivities are taken as source distance functions (Degrazia, 1989). Neglecting the longitudinal diffusion with respect to wind advection ($U >> u'$) and considering a vertical and longitudinal eddy diffusivities described by a large eddy length and a velocity scale, and depending on the downwind distance from source:

$$U\frac{\partial c(x,y,z)}{\partial x}=K_Z(x)\frac{\partial^2 c(x,y,z)}{\partial z^2}+K_Y(x)\frac{\partial^2 c(x,y,z)}{\partial y^2} \tag{3}$$

Where *c(x,y,z)* c is a pollutant average concentration; *U e* K_y *(x)* , K_z *(x)* are the component of the speed of the average wind and the eddies diffusivities in the cartesian directions *y, z* respectively. Note that the source term will be considered in the boundary conditions.

This problem is subject to the following boundary condition:

1) Zero flux at the ground and Planetary Boundary Layer top.

$$\frac{\partial c(x,y,z)}{\partial z}=0 \qquad z=0, z_i. \tag{4}$$

2) The emission rate at height *zf* is described by:

$$\frac{c(x,y,z)}{Q}=\delta(y-y_0) \qquad x=0 \tag{5}$$

Here δ is the generalized Dirac delta function.

3) Zero concentration at great source distances $\pm b$ a:

$$c(x,y,z)=0 \qquad y=\pm b. \tag{6}$$

Following the idea of spectral method (Cotta and Mikhailov, 1997), the solution of this problem is assumed to be written as:

$$c(x,y,z)=\sum_m\sum_n \phi_{n,m}\left(x,\varphi_{n,m}\right)\cdot Yn(\gamma_n,y)\cdot Zm(\beta_m,z) \tag{7}$$

Where the eigenfunctions Yn (γ_n, y) e *Zm* (β_m, z) are obtained of the referred Sturm-Liouville problems. Thus, the eigenfunction *Zm* (β_m, z) is the solution of the problem:

$$\frac{\partial^2 Zm(\beta_{m,}z)}{\partial z^2}+\beta_m^2 Zm(\beta_m,z)=0 \tag{8}$$

with boundary conditions:

$$\frac{\partial Zm(z)}{\partial z}=0 \qquad z=0 \ and \ z_i \tag{9}$$

Here, the eigenvalue $ß_m$ and the eigenfunctions $Z_m(ß_m, z)$ are well known, and taken from Özisik, (1980):

$$Z_m(\beta_m,z)=\cos(\beta_m,z) \tag{10}$$

Where β_m are the positive roots of $\sin(\beta_m,z)=0$.

Similarlly, the eigenfunction $Y_n(\gamma_n, y)$, with boundary conditions can be described as:

$$\frac{\partial^2 Yn(y)}{\partial y^2}+\gamma_n^2\cdot Yn(y)=0 \qquad \forall y\in[-b,+b] \tag{11}$$

$$\frac{\partial Yn(y)}{\partial y}=0 \qquad y=0 \tag{12}$$

$$Yn(y)=0 \qquad\qquad y=\pm b \tag{13}$$

At the same way, these eigenfunctions *Yn (* γ_n *, y)*, and the eigenvalues γ_n are taken from Özisik (1980):

$$Yn(\gamma_n, y)=\cos(\gamma_n \cdot y). \tag{14}$$

Here, γ_n are the positive roots of cos (γ_n . b) = 0.

Replacing this auxiliary solutions in Eq.(7) and further in Eq (3) is obtained the following expression to $N_{n,m}(x)$:

$$\frac{\partial \phi_{n,m}(x)}{\partial x}+\frac{\beta_m^2 K_z(x)+\gamma_n^2 K_y(x)}{U}\cdot \phi_{n,m}(x)=0 \tag{15}$$

And its solution:

$$\phi_{n,m}(x)=\varphi_{n,m} e^{-\int_0^x \frac{\beta_m^2 K_2(x)+\gamma_n^2 K_y(x)}{U}dx} \tag{16}$$

At this point, to determine the function $N_{n,m}$ its necessary bearing in mind that the set of eigenfunctions *Zm (z,* β_m) e *Yn* (*y*), constitutes a set of linearly independent functions. With the boundary conditions in *x=0*, and taking the properties of linearly independent functions, the solution of $N_{n,m}$ is obtained.

Now, with all terms known, the solution Eq. (7) can be constructed. Finally, the solution of the problem (Eq. 3) is obtained:

$$c(x,y,z)=\frac{2Q}{z_i^u}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\cos(\beta_m \cdot zf)\cdot\cos(\beta_m . z)\cdot\cos(\gamma_n \cdot y)\cdot e^{-\int_0^x \frac{\beta_m^2 K_z(x)+\gamma_n^2 K_y(x)}{U}}dx+ \frac{Q}{z_i^u}\sum_{n=1}^{\infty}\cos(\gamma_n \cdot y)\cdot e^{-\int_0^x \frac{\gamma_n^2 K_{y(x)}}{U}dx.} \tag{17}$$

It is opportunity to remember that the eddy diffusivities $K_z(x)$ and $K_y(x)$ are functions of the Cartesian coordinate *x*, or constant. Here we can, for example, take the following expressions derived by Degrazia (1989), based on spectral properties and Taylor's statistical diffusion theory, for unstable Planetary Boundary Layer:

$$K_z(x)=0.09.c^{1/2}\psi^{1/3}.w_* z_i\int_0^\infty \frac{sin\left(7.84c^{1/2}\psi^{1/3}Xn'\right)}{(1+n')^{5/3}n'}dn' \tag{18}$$

$$K_y(x)=0.1546.c^{1/2}\psi^{1/3}.w_* z_i\int_0^\infty \frac{sin\left(5.98c^{1/2}\psi^{1/3}Xn'\right)}{(1+n')^{5/3}n'}dn' \tag{20}$$

Where w_* is the convective velocity scale, is the $\psi=(\varepsilon z_i)/w^3$ nondimensional molecular dissipation rate function, *X* is the nondimensional distance, and *n´* is a dimensionless frequency.

These eddy diffusivities are initially zero, increase with *x* at first linearly and then more slowly and tend towards a constant value. Because this they are appropriated for far source dispersion.

The analytical solution (17) can be applied and is valid for homogeneous turbulence when the mean wind speed is uniform everywhere and where the vertical turbulence $K_y\ (x)$ structure can be idealized as nearly homogeneous. Eq (17) is analytical in sense that no approximation is made along its derivation. Since the solution (Eq. 17) is composed by Fourier series, the convergence of this solution is based on the Fourier series convergence study, and thus, must be satisfying the same convergence conditions of this series. The solution above has the advantage that the intrinsic method error can be determined.

4. Conclusion

Line source emission is an important tool in control and management of vehicular exhaust emissions (VEE) in urban environment. The US Environmental Protection Agency and many other research institutes has been developed a number of line source models to describe temporal and spatial distribution of VEE on roadways. Most of these models incorporate an analytical solution on their conceptions.

In this work, a tridimensional solution has obtained from the atmospheric diffusion equation that uses K-theory approximation for the closure of the turbulent diffusion equation. To obtain this solution the GITT method has been used and the solution is analytical in sense that no approximation is made along its derivation.

Because this is a deterministic model it is most suitable to predict long-term average concentration for planning decisions (Benarie, 1980; Juda, 1986; Zaneti (1990).

This model, with the eddy diffusivities from Degrazia (1988), has the advantage of dealing with the physical causes of dispersion phenomena, upon that the turbulent parameters are taking into account in the derivation of eddy diffusivities. In additional, the intrinsic method error (sum truncation) can be determined.

The next step of this study is to validate this solution with experimental data and compare it with other analytical solutions.

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