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Air Quality Modeling : A Review

D. R. Khanna and Neetu Saxena
Department of Zoology & Environmental Sciences,
Gurukul Kangri University, Hardwar, INDIA

Introduction

Environmental pathway analysis provides the link between qualification of source emissions and assessments of receptor exposure (eg. human exposure) through estimation of the ambient concentrations of contaminants in the various environmental media.
Two basic techniques can be employed to investigate environmental pathways: analytic sampling programs & mathematical fate modelling. Sampling programs are costly to design & implement, therefore, computerized mathematical models of environmental processes are frequently used to generate information unavailable by other means or to estimate data (i.e. environmental conc.) that would otherwise be costly to obtain.

Mathematical environmental fate modelling generally requires a knowledge of (1) the distribution of the releases of the material into the natural environment, (2) the environmental conditions influencing the fate (transport, transformation) of the chemical compounds, (3) the physical & chemical properties of the material, and (4) techniques (models) for analyzing the information gathered (Bonazountas *et al.* 1995).

Mathematical Models

Mathematical equations of air pollution models describe the process by which pollutants injected into the atmosphere are diluted. Dispersion models for atmospheric pollutants are useful decision support systems for air pollution management. They are an ideal complement to air quality control networks, allowing the study of the impact of pollution sources and in short, they enhance the understanding of the dynamics (emission, transport, transformation) of air pollution as a system (Calbo *et al.*, 1994).

A number of mathematical formulations are available to be used to describe the atmospheric diffusion process, but the one that enjoys the widest use is in the form of Gaussian Plume Model equation. Gaussian models are often preferred for operational use in Environmental Impact Assessment (EIA) studies because they are simple, require limited data and use minimal computation facilities. In the present paper, an attempt had been made to discuss different air quality models based on Gaussian dispersion equation.

1. **IITAQ model** (Mohan. M & Siddiqui, T.A., 2003) -

The IITAQ model is a numerical box model developed for an elevated source that incorporates improved parameterizations of physical processes in the atmospheric boundary layer & at the same time avoids the disadvantages of 3-D numerical models with detailed physics. The model uses more realistic & easily adaptable input parameters. The main input parameters are wind & eddy diffusivity, profiles and dispersion coefficients that make extensive use of Monin-Obukhov similarity theory & other recent formulations for the estimation of turbulence parameters.

The mathematical differential equation representing the diffusion of air pollutants released from a source is given by the following diffusion-transport equation.

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}+w\frac{\partial C}{\partial z}=\left[K_x\frac{\partial C}{\partial y}\right]+\left[K_y\frac{\partial C}{\partial y}\right]+\frac{\partial}{\partial z}\left[K_z\frac{\partial C}{\partial z}\right]+S+T$$

where, C is the concentration of any given pollutant, K_x, K_y and K_z are the eddy-diffusivities in x, y and z directions respectively. Similarly u, v and w are the wind components in x, y and z directions respectively. S and T represent source and sink terms respectively.

2. **GRAM model** (Fisher & Sokhi, 2000)-

GRAM model was designed for the assessment of air quality concentrations, particularly the short-term peak concentrations. Factors which are likely to lead to high road side concentrations are taken into consideration in the model.

The short term peak concentration in the center of an urban area was estimated by assuming worst-case meteorological conditions (category G), a low wind speed of 1 m/s & a low mixing depth of 100 m. The concentration at the centre of the urban , C_{urban} is derived from the integral:

$$C_{urban}=\sqrt{\frac{2}{\pi}}\frac{q}{u}\int_{10}^{d}\frac{dx}{\sigma_z(x)}$$

where, σ_z (x) describes the vertical dispersion based on the R91 model assuming typical urban roughen, q is the emission density (kt/km^2/yr), u is the wind speed & d is the distance (km).

The contribution from vehicles on a road to the concentration in the vicinity C_{road} when wind direction is across the road, is given by-

$$C_{road}=\sqrt{\frac{2}{\pi}}\frac{Q}{u}\frac{1}{\sigma_z(x)}$$

where Q is the emission strength per unit length of road, u is the wind speed & σ_z (x) is the vertical dispersion as a function of distance x from the road.

When wind blows along the road, the concentration in the vicinity is

$$C_{road}(y)=\frac{Q}{\pi u}\int_{0}^{l}\frac{dx}{\sigma_z(x)\sigma_y(x)}\exp-\frac{y^2}{2\sigma_y(x)^2}$$

where the integration is now along the road, l is the length of the road, the receptor is at distance y from the road centre line and σ_y(x) is the lateral dispersion.

3. UGEM model (Murphy-Klimova *et al.,* 1998)-

The air pollution transport model UGEM (University of Greenwich Evaluation Model) has been developed to evaluate medium-range transport & deposition of sulphur & oxidised nitrogen from all types of sources of emissions in the UK. UGEM is a receptor-oriented, Lagrangian type model, which yields annual average concentrations & depositions of SO_2, particulate SO_4, NO_2, particulate NO_3 and nitric acid (HNO_3) across the UK.

The concentration C^l of pollutant l along air main trajectories weighted according to wind direction is

$$\frac{dC^l}{dt} = -\left(\frac{v_d{}^l}{h} + k_w^l P + k_c^{m,l} - k_c^{l,m} \right) \times C_o^l$$

Where, k_w^l is the wet scavenging ratio, v_d^l is dry deposition velocity(m/s), $k_c^{l,m}$ is chemical conversion rates from pollutant l to pollutant m (m/s), P is annual level of precipitation(mm/yr).

4. EMITEMA- EIM model (Costa *et al.*, 1996) -

The EMITEMA-EIM model is a atmospheric emission model, developed for the estimation of air pollutants –NO_X, CO, SO_2, particles, methane and several VOC_S (alkanes, alkenes, aromatics and aldehydes). The emission sources studied were road traffic, air traffic, industrial activities, gas stations, domestic heating & biogenic emission from forests. In case of road traffic, three kinds of emissions were considered-

(i) Hot emissions—Hot emissions are the emissions from vehicles after they have warmed up and their engines are thermally stabilized (water temperature over 70°C).

The hot emissions of pollutant i in a stretch of a road way 'r' of type 'p' (stretch, road or highway),

$$E_r^{ihot}(k,t) = \sum_{j=1}^{m} N_{jr}(k,t)\, L_r(k)\, F_{jp}^{ihot}$$

where, E_r^{ihot} is the hot emission, N_{jr} is the number of vehicles of j categories for r type of roadway, Lr is length per area and F_{jp}^{ihot} is the emission factor.

(ii) Cold start emission- Cold start emission take place while vehicles are warming up (Eggleston *et al*., 1989).

The cold start emissions of pollutant 'i' in a stretch 'r'of a street, E_r^{icold} is

$$E_r^{icold}(k,t) = N_r(k,t)\beta M\, F^{ihot}\left(\frac{F^{icold}}{F^{ihot}} - 1 \right)$$

where, $E_r^{i\,cold}$ is the cold start emission, N_r is the number of gasoline cars that drive along the stretch during the time span, b is the fraction of mileage driven with cold engines, M is the total annual mileage of gasoline cars, $F^{i\,hot}$ & $F^{i\,cold}$ are the hot & cold emission factors.

(iii) Evaporative emissions— Evaporative emissions account for the evaporation of gasoline both from the fuel tank and the carburettor. Evaporative emission E_r^{ievap} is estimated as-

$$E_r^{ievap}(k,t) = F^{ievap} N_t(k,t) \frac{L_r N_r}{\sum L_r N_r}$$

where, F^{ievap} is the evaporative factor, N_t is the total number of gasoline cars that drive through all the streets, L_r is the length of the stretch & N_r is the number of cars in r stretch.

5. IITLT model (Goyal *et al*., 1994)-

The IITLT model is designed to estimate long term concentrations of non-reactive pollutants due to emissions from area & point sources during calm wind conditions (4< 2 m/sec).

In this model, the receptor-oriented Gaussian plume model of Hanna (1974) has been adopted to obtain the concentrations of SO_2, SPM and NO_X due to area sources along with the monthly wind roses & the stability frequencies. The ground-level concentrations at each receptor due to area sources is the sum of all the contributions of grids upwind of the receptor & is given by

$$C = \sum_j C_j = \frac{\sqrt{2/\pi}}{a(1-b)u} Q_j \left(X_{j+1}^{1-b} - X_j^{1-b} \right)$$

where, C_j is the concentration due to an area source of strength Q_j located at the j[th] upwind grid, a and b are the stability parameters and u is the mean wind speed. X_j and X_{j+1} are the upwind distances of the j^{th} and $(j+1)^{th}$ grid from the receptor point.

6. GFLSM model (Luhar & Patil, 1989)-

A simple General Finite Line Source Model (GFLSM), based on the Gaussian diffusion equation is formulated to determine the pollutant concentration for any orientation of wind direction with roadway along a finite line source. The basic approach to develop this model is the coordinate transformation between the wind coordinate system (X_1,Y_1,Z_1) and the line source coordinate system (x,y,z).

Assuming a hypothetical line source along Y_1 direction so that the wind is perpendicular to it, the concentration at receptor R due to this line source is given by (Csanady,1972)-

$$C' = \frac{\theta}{2\pi\sigma'_y\sigma'_z\bar{u}} \left[\exp\left\{ -\frac{1}{2}\left(\frac{z-\mu}{\sigma'_z} \right)^2 \right\} + \exp\left\{ -\frac{1}{2}\left(\frac{z+H}{\sigma'_z} \right)^2 \right\} \right] \times \int_{-1/2}^{1/2} \exp\left[-\frac{1}{2}\left(\frac{y'_1 - y_1}{\sigma'_y} \right)^2 \right] dy'_1$$

where, θ is the source emission rate per unit length, z is the height of the receptor above the ground, H is the height of the line source $\overline{U}$, is the mean ambient wind speed at source height H, σ'_z and σ'_y are the vertical and horizontal dispersion coefficients respectively and are functions of distance X and stability class. The prime (‘) symbol indicates the parameters in wind coordinate system.

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