DEVELOPMENT OF AN ATMOSPHERIC DISPERSION MODEL FOR AIR QUALITY ASSESSMENT

Manju Mohan[1] and T. A. Siddiqui[2]
[1]Centre for Atmospheric Sciences, Indian Institute of Tehnology,
Hauz Khas, New Delhi-110016,INDIA
[2]Environment Department, Engineers India Limited,
Bhikaji Gama Place, New Delhi, INDIA

INTRODUCTION

A new mathematical model (IIT Air Quality Model or IITAQM) is developed to retain all the desired features of a Gaussian model while at the same time overcoming most of the disadvantages associated with the Gaussian model. The IITAQM is numerical box model which incorporate improved parameterisations of physical processes in the atmospheric boundary layer and at the same time avoiding the disadvantages of 3-D numerical models with detailed physics. It is a multi-box model based on the numerical solution of steady state advection-diffusion equation for elevated/ground level point source. The main input parameters such as wind and eddy-diffusivity profiles and dispersion coefficient values are estimated at each grid point for all atmospheric stability conditions based on recent formulations on turbulence characteristics in the boundary layer. The earlier work done (Ragland,1975; Manju Kumari and Sharma,1988) with regard to the multiple box models with above features included the estimation of crosswind integrated concentration (CIC) only and hence lacked validation with observed data in effective manner. IITAQM estimated hourly ground level concentrations are compared with 154 hours of data from SF_6 tracer diffusion experiments conducted by the Electric Power Research Institute (EPRI) in Central Illinois, USA, at the Kincaid Power Plant.

MAIN FEATURES OF IITAQM

In the IITAQM, the vertical extent of the domain up to the mixing height is divided into several boxes and input parameters like wind speed and eddy diffusivity profiles are estimated at each grid point. The pollutants in the vertical column of multiple boxes are transported in the horizontal over a finite grid distance interval with the estimation of advection and diffusion processes in and out of each box based on conservation of mass. The assumption of horizontal homogeneity is considered for the meteorological fields.

Two dimensional steady state advection-diffusion equation is considered assuming that the transport of pollutants is along the x-axis and the pollutant transport due to wind in the x direction is very large compared to the downwind diffusion. Considering crosswind integrated concentration as C', the mass conservation equation is represented in the following form.

$$\partial C'/\partial t + u\partial C'/\partial x = \partial/\partial z\left(K_z \partial C'/\partial z\right) \tag{1}$$

Here u is the mean wind speed in x-direction at height z, K_z is the vertical eddy-diffusivity for pollutants and z is the vertical axis.

Model equation (1) is solved numerically with the following boundary conditions and using Keller's (1971) 'box method'.

At x = 0, C=B (2)

At z = 0, $-\partial C' / \partial z \, K_z = Q$ (3)

At $z=Z_i$, $-K_z \, \partial C' / cz = 0$ (4)

C' = C' (x, z) is the crosswind integrated ambient air concentration of the pollutant species.
K_z = K_z (z) is the turbulent eddy-diffusivity.
B = B (z) is the background concentration of the pollutant species.
Q = Q (x) is the emission rate of the pollutant species.

An implicit finite difference scheme is used to solve equation (1). The detailed mathematical procedure for solving the equation is described in Ragland (1973) and Manju Kumari and Sharma (1988).

The concentration calculated by this technique C_t (x,z) is the total concentration integrated through the plume across wind. In order to obtain a 3-D distribution of concentrations from C_t (x, z), a Gaussian profile of concentration distribution is assumed in terms of σ_y *and* σ_z so as to provide ground level concentration. Hence the concentration C(x, y, z) in terms of CIC is given as follows:

$$C(x, y, z) = 1/\sqrt{2\pi}\,\sigma_y \exp\left(-y^2/2\sigma_y^2\right) C_t(x, z) \quad (5)$$

EVALUATION OF INPUT PARAMETERS

The basic meteorological parameters required for the evaluation of pollutant dispersal from equation (5) include mixed layer height (Z_i), wind speed (u) profile, eddy-diffusivity profile, dispersion coefficients and effective stack height and plume penetration estimation on hourly basis. The background concentration is considered zero as the field experiments involve release of SF_6 tracer which is non existent in the atmosphere. Hourly variation of mixed layer height is taken from the observed values.

Monin-Obukhov (M-O) similarity theory is used during daytime conditions to estimate-u profile by extension of this to the whole PBL (Smith and Blackall, 1979). As M-O theory cannot effectively be used during stable conditions power law profile is considered (Wark and Warner, 1981).

K_z profile is estimated using Wippermann (1972) formulation as it provides reasonable estimates of K_z and ground level concentrations. Schayes (1982) demonstrated a satisfactory comparison between the K_z profiles obtained from Wipperman's formulation and a one-dimensional turbulent kinetic energy (TKE) - closure PBL model for all stability conditions using Wangara data. The dispersion coefficients in IITAQ model are estimated from sophisticated methods based on Taylor theory and detailed estimation of these parameters from different methods is included in Mohan and Siddiqui (1997). The detailed methodology for the estimation of turbulence parameters needed in this study is described in Mohan and Siddiqui (1998).

The penetration scheme used in this study is based on the work of Briggs (1984), Weil and Brower (1982), Turner (1985), and Rao (1985) and plume rise is estimated from Carson and Moses(1969) formulation.

RESULTS AND DISCUSSION

The observed hourly maximum ground level concentrations at different downwind distances varying form 0.5 km to 15 km were compared with the model predicted plume centerline ground level maximum concentrations covering all types of atmospheric stability.

Model performance measures viz; Fractional Bias (FB), Normalised Mean Square Error (NMSE), Correlation Coefficient (COR), Fraction within a factor of two (FAC_2) and ratio of Unsystematic Mean Square Error (UMSE) and Mean Square Error (MSE) are used for model validation. A brief description on these parameters is included in Hanna, Strimaitis and Chang, 1991. The values for FB, NMSE, COR, FAC2 and UMSE/MSE are -.42, 1.55, 0.28, 0.31 and 0.71 respectively. This includes 153 hours of observations at about 632 points covering various downwind distances. The ideal values for FB, NMSE, COR, FAC2 and UMSE/MSE are 0.0, 0.0, 1.0, 1.0 and 1. FB shows a tendency to over-predict and the value is also not very high. 31% observations are within a factor of two and correlation coefficient is 0.28. UMSE/MSE ratio ideally should be one but in this case it is 0.71. Though model has scope of further improvement, the results are promising for the approach and formulation adopted in this study

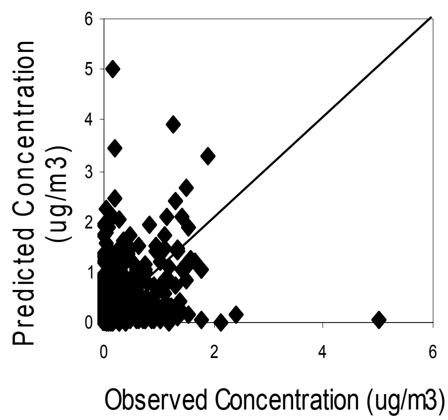

Fig 1. Scatter plot of observed & predicted concentration

Figure 1 shows a scatter plot of observed and model estimated concentrations. The scatter plot shows that the scatter is on both sides of the diagonal line and many of the points lie close to this line indicating a reasonable performance of this model

CONCLUSIONS

A numerical multi-box model and Gaussian model is used in combination to accommodate desired features of both model types. Input parameters derived are from the more recent parameterizations of turbulence characteristics in the atmospheric boundary layer. A preliminary attempt is made for model validation with Kincaid data and results are promising suggesting a step in the right direction.

REFERENCES

Briggs, G.A., 1984: Plume rise and buoyancy effects in atmospheric Science and Power production. D. Randerson (Ed.) DOE/IL 27601, Technical Information Center, Oak Ridge, TN, Chapter 8, 327-366.

Carson, J.E., and H. Moses, 1969: The validity of several plume rise formulae. *J. Air Pollu. Control Assoc.*, **26,** 11, 862-866.

Hanna, S.R., D.G. Strimaitis, and J.C.Chang 1991: Hazard response modelling uncertainty (A quantitative method), Vol. I: User's guide for software for evaluating hazardous gas dispersion models, sigma Research Corporation, Westford, USA.

Keller, H.B., 1971: A New Diffeerence Scheme for Parabolic Problems in Numerical Solutions of Partial Differential Equations *(*Edited by Hubbart,B.)**Vol.2**. Academic Press, New York.

Kumari Manju, and O.P. Sharma, 1988: A model for ambient air quality analysis using routine meteorological observations. *Atmos. Environ*., **22,** 651-661.

Mohan, Manju, and T.A siddiqui, 1997: An evaluation of dispersion coefficients for use in air quality models*. Boundaryu Layer Meteorology***, 84**, 177-206.

Mohan, Manju, and T.A. Siddiqui, 1998: Applied modelling of surface fluxes under different stability regimes, *J.Appl. Meteorol*., **37**, 98-125.

Ragland, K.W., 1973: Multiple box model for dispersion of air pollutants from area sources. *Atmos. Environ***.,7**, 1017-1031.

Rao, K.S., 1985: User's Guide for PEM-2. NOAA Tech. Memo. ERL ARL-137.

Schayes, G., 1982: Direct determination of diddusivity profiles from synoptic reports. *Atmos.Environ*., **27**, 1122-1137.

Smith, F.B., and Blackall, 1979: Application of data from field programmes to estimation of K-profiles and vertical dispersion. Mathematical modelling of turbulent diffusion in the environment, editor: C.J. Harris Academic Press (ISBN 0-12-328350-7)

Turner, D.B., 1985: Proposed pragmatic methods for estimating plume rise and plume penetration through atmospheric layers *Atmos. Environ*, **19**, 1215-1218.

Wark, K., and C.F. warner, 1981: Air Pollution : Its origin and Control., Harpar and Row, Publisher Inc., Newyork, Second edition, pp526.

Wippermann, F., 1972: Universal profiles in the barotropic boundary layer. *Contr.Atmos.Phy.,* **25,** 148-163.