AIR POLLUTION MODELLING – A REVIEW

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ABSTRACT

Air pollution modelling is a set of mathematical equation which simulates the natural atmospheric conditions. The present study aims to evaluate the current status of the mathematical modelling of air pollutant dispersion, transport and transformation, with emphasis on types of modelling techniques which may be readily applied in support of environmental decision making.

Keywords: Air Quality Modelling

I. INTRODUCTION

Air pollution in recent decades has increased massively with increase in industrial, transportation and other anthropogenic activities. Government and other regulato.dry agencies throughout the world (including India) have taken numerous of efforts in recent decades to reduce air pollution and improve air quality. Despite this, air quality issues such as photochemical smog and visibility degradation etc. are persistent. Estimates are that, worldwide, nearly one billion people in urban environments are continuously being exposed to health hazards from air pollutants (Smit et al., 2008).

Effective air pollution control is extremely challenging to both researcher and administrators around the world, due to heterogeneous and dynamic nature of natural environment. To reduce the impact of air pollution and improve the air quality, constant efforts are required 1) to build extensive inventories of pollutant emissions, 2) to determine the source, substance and dispersion rates of these emissions, 3) to develop computer-based numerical models based on mass conservation flows, 4) to assess the levels of concentration and exposure to air pollution at every location over a particular urban area (Liu et al., 2007). Thus, in order to form various air pollution control policies and strategies, air pollution modelling plays an important role. Air pollution dispersion models are used to effectively and efficiently plan the management (environment management plan) of air pollution on particular area/ road corridor, along with monitoring of air pollutants. They not only aid in determining the presently influenced area but also help in identifying the future scenarios under different emission/source and meteorological conditions made by these models.

1.1 REQUIREMENTS OF AIR POLLUTION MODELLING

Now days air pollution problem is not bound to an area and it becomes global problem (Global warming, ozone depletion etc). It is very difficult to control air pollution on global scale. To control the air pollution at local or regional scale, air pollution modelling is the most important component in air pollution control policy making. Air pollution modelling required for two major goal 1) increase domain knowledge and 2) Reliable forecasting of pollutant concentration (Karatzas et. al., 2007).

Air quality models use mathematical and numerical techniques to simulate the physical and chemical processes that affect air pollutants as they disperse and react in the atmosphere. Based on inputs of meteorological data and source information like emission rates and stack height, these models are designed to characterize primary pollutants that are emitted directly into the atmosphere and, in some cases, secondary pollutants that are formed as a result of complex chemical reactions within the atmosphere. These models are important to our air quality management system because they are widely used by agencies tasked with controlling air pollution to both identify source contributions to air quality problems and assist in the design of effective strategies to reduce harmful air pollutants. Air quality model is one of the most important components of air quality management. Air quality models are used to predict concentration of one or more species in space and time.

Modelling provides the ability to assess the current and future air quality in order to enable "informed" policy decisions to be made. This will help the regulatory agencies to assess the extent and type of the air pollution control management strategies (Afshar and Delavar, 2007). Air pollution models are routinely used in environmental impact assessments, risk analysis and emergency planning, and source apportionment studies (*Macdonald R.*, 2003). Air quality model also support in attainment/maintenance of all National Ambient Air Quality Standards (NAAQS). Thus, air quality modelling play an important role in providing sufficient information for air quality management planning.

II. AIR QUALITY MODELLING

A mathematical model is an assembly of concepts or phenomena in the form of one or more mathematical equations, which approximate the behavior of a natural system or phenomena. They are usually employed to predict the impacts or concentration of parameters under different types of current or future scenarios, using readily available or measured input data. Mathematical models can be used to determine the environmental impacts of the existing or developing projects which combine the effects of source strength and meteorology to describe the resulting ambient air concentrations.

Air pollution modelling, also known as air pollution dispersion modelling, is the mathematical simulation of how air pollutants disperse in the ambient atmosphere. It is performed with computer programs, called dispersion models, that solve the mathematical equations and algorithms which simulate the pollutant dispersion. The dispersion models are used to estimate or to predict the downwind concentration of air pollutants emitted from emission sources such as industrial plants and vehicular traffic. Such models are important to governmental agencies tasked with protecting and managing the ambient air quality. The models also serve to assist in the design of effective control strategies to reduce emissions of harmful air pollutants (Sharma et al., 2005). A dispersion model is a computer simulation that uses mathematical equations to predict air pollution concentrations based on weather, topography, and emissions data. Any model depends on the following inputs (Fig 1):

- Emission parameter: Type of source, emission rate, location, height, temperature etc.
- Topography: Rural or Urban area, terrain elevation, height and width of any obstruction, receptor location (height, distance from source) etc.

- Meteorological Condition: Wind speed and direction, Atmospheric temperature, Atmospheric stability, Cloud cover, solar radiation etc.

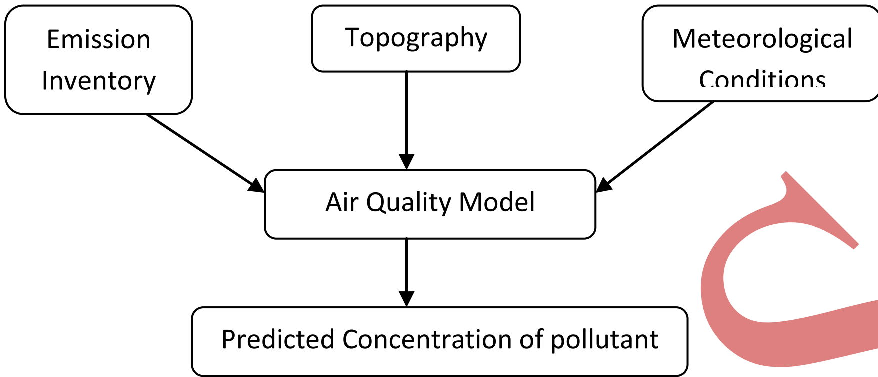

Figure 1: Basic Process of Air Quality Modelling

Major Atmospheric processes simulated in air quality models are (EEA, 1996) as shown in fig 2:

- Chemical Transformation (Gas & aqueous Phase and Heterogeneous chemistry)
- Advection (Horizontal & Vertical)
- Diffusion (Horizontal & Vertical)
- Removal Processes (Dry & Wet Deposition)

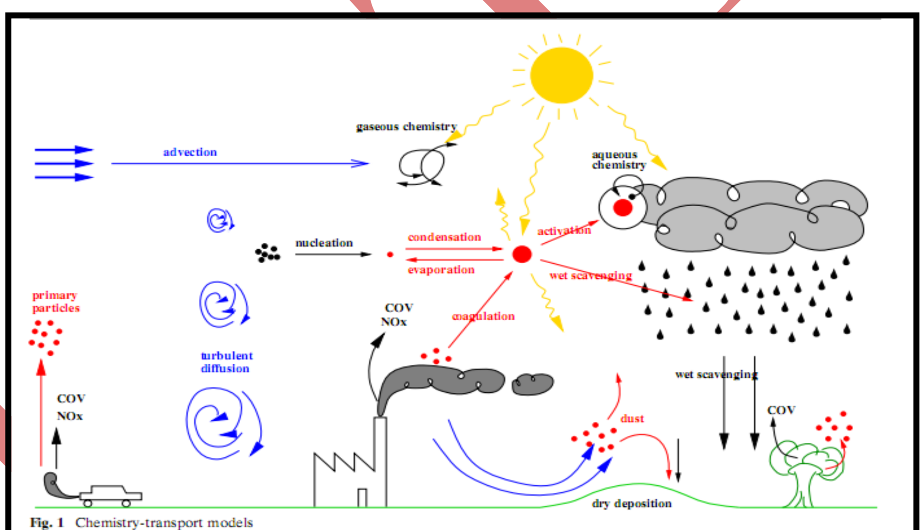

Figure 2: Atmospheric Processes Simulated in Air Quality Models (Sportisse, 2007)

Air pollution modelling involves four stage approach (Leksmono et al., 2006):

1. Raw data collection (like emission rate, background concentration, source type, source characteristics etc.)
2. Assessment of screening model (model for emission rate determination, Meteorological data model etc.)
3. Running the complex model (prediction of concentration of pollutant)
4. Analysis/ assessment of model output in order to verify findings.

2.1 CLASSIFICATION

There are several ways of classifying the variety of existing models according to their specific attributes (Sharma, 2004). The most important criteria being:

(i) **Source – receptor relationship:** source – oriented (point, area, line, volume) and receptor – oriented (street canyon, intersection model etc.)

(ii) **Basic model structure:** deterministic or non-deterministic, steady state or time dependent

(iii) **Frame of reference:** Eulerian or Lagrangian

(iv) **Dimensionality of computational domain:** one dimensional, two dimensional, three dimensional or multi dimensional

(v) **Scale (space and time):** microscale (1m, sec-min), mesoscale (5-10 km, hour), small synoptic (100 km, hour-day), large synoptic (100 – 1000 km, days) and planetary (>1000 km, weeks)

(vi) **Model structure and the approach:** used for the closure of the turbulent diffusion equation (closed- form, analytical and numerical, statistical and physical)

(vii) **The terrain/area:** to which they are applicable (rural flat terrain, urban flat terrain, complex terrain, coastal areas)

(viii) **Level of sophistication:** level1 (screening models) and level 2 (refined models)

Whatever may be the classification criteria adopted for classifying the models, the characteristics of the system being studied

(i) Size (local, regional, national, global)

(ii) Time horizon (hour, day, month, year)

(iii) Pollutant of concern (SO_2, NOx, CO, SPM, photochemical oxidant etc.)

are equally important. However, the most important and popular way of classifying air pollution models is based on the model structure and the approach used for the closure of the turbulent diffusion equation which is widely used in urban air pollution modelling also (Sharma et al., 2004). Air pollution model can be classified as:

1. Dispersion Model
2. Statistical Model
3. Physical Model

2.1.1 DISPERSION MODEL

The deterministic mathematical models (DMM) calculate the pollutant concentrations from emission inventory and meteorological variables according to the solutions of various equations that represent the relevant physical processes (Daly and Zannetti, 2007). In other words, differential equation is developed by relating the rate of change of pollutant concentration to average wind and turbulent diffusion which, in turn, is derived from the mass conservation principle. The common Gaussian Model is based on the superposition principle, namely concentration at a receptor, which is the sum of concentrations from all the infinitesimal point sources making up a line/ area source. This mechanism of diffusion from each point source is assumed to be independent of the presence of other point sources. The other assumption considered in DMM is the emission from a point source spreading in the atmosphere in the form of plume, whose concentration profile is generally Gaussian in both horizontal and vertical directions. Deterministic model includes analytical model and numerical model. Both analytical and numerical models are based on mathematical abstraction of fluid dynamics processes (Nagendra and Khare, 2002; Sharma, 2004). Example: AERMOD, CALINE 4 etc.

Limitation of deterministic model:

(i) Inadequate dispersion parameters

(ii) Inadequate treatment of dispersion upwind

(iii) Gaussian based plume models perform poorly when wind speeds are less than 1m/s

Gaussian Dispersion Model: Most of the air pollution models are depends on Gaussian Dispersion model. These Gaussian models despite several limitations and assumptions have found favour with the scientific community, as they are very simple and include the solution to the simple Gaussian equation. In addition to their user-friendly nature and simplicity, these models are conceptually appealing as they are consistent with the random nature of the turbulence of the atmosphere. Further the development of Gaussian type dispersion equations/ models has reached a level of sophistication such that they are routinely used as assessment tools by various regulatory agencies (USEPA, 2000). The concentration of pollutants (C) at location (x, y, z) (Fig 3) from a continuous elevated point source with an effective height of H is given by following Gaussian dispersion equation (Gilbert, 1997; Macdonald, 2003)

$$C(x, y, z, H) = \frac{Q}{2\pi\sigma_y\sigma_z U}\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\left[\exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]+\exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right]\right] \quad ....(1)$$

Where, σ_y and σ_z are horizontal and vertical dispersion parameters, determined as a function of stability class and distance from the source. U is the mean wind speed, Q is the uniform rate of release of pollutants and H is the effective plume height. For a continuously emitting infinite line source at ground level when wind direction is normal to the line source, the equation (1) reduces to

$$C(x,z) = \frac{Q}{\sqrt{2\pi}U\sigma_z}\left\{\exp\left[-\frac{1}{2}\left(\frac{z+h_o}{\sigma_z}\right)^2\right]+\exp\left[-\frac{1}{2}\left(\frac{z-h_o}{\sigma_z}\right)^2\right]\right\} \quad ....(2)$$

For ground level sources H = h_0 (plume rise).

Most of the air dispersion models used for the preliminary estimation for screening purpose retained the basic Gaussian dispersion approach but used modified vertical and horizontal dispersion curves to account for the effects of surface roughness, averaging time and vehicle induced turbulence (Gilbert, 1997).

2.1.2 STATISTICAL MODEL

In contrast to deterministic modelling, the statistical models calculate concentrations by statistical methods from meteorological and traffic parameters after an appropriate statistical relationship has been obtained empirically from measured concentrations. Regression, multiple regression and time-series technique are some key methods in statistical modelling. The time-series analysis techniques [Box–Jenkins models] have been widely used to describe the dispersion of Vehicular Exhaust Emissions at traffic intersection and at busy roads. Various studies involving statistical techniques have been used to forecast real-time, Short-term as well as long-term pollutant concentrations

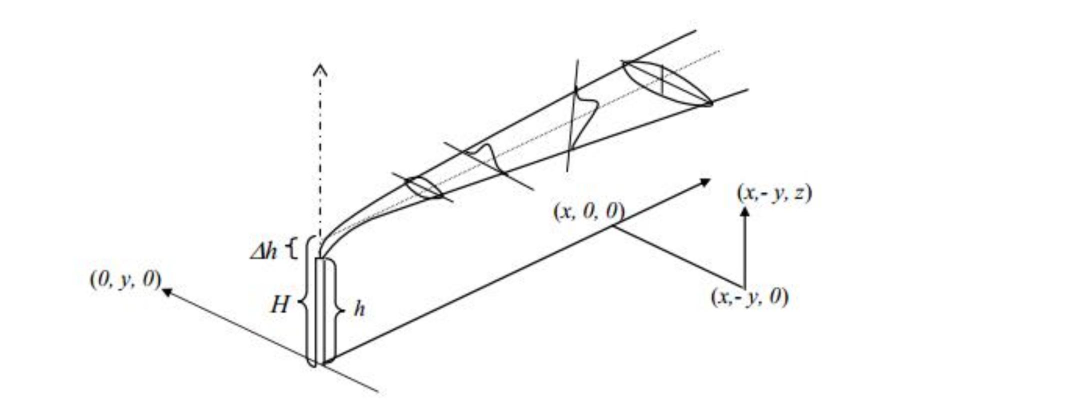

Fig. 3 Plume dispersion coordinate system, showing Gaussian distributions in the horizontal and vertical directions

Figure 3: Plume Dispersion Coordinate System, Showing Gaussian Distributions in the Horizontal and Vertical Direction (Ferdous and Ali, 2005).

and for their trend analysis. This has been done by mostly using long-term (some time short also) emission, meteorology and pollution concentration data. This modelling technique has been employed to find concentrations of primary as well as highly complex secondary pollutants like ozone (Nagendra and Khare, 2002; Sharma, 2004). Example: Artificial Neural Network (ANN) etc.

Limitation of statistical model:

(i) Require long historical data sets and lack of physical interpretation

(ii) Regression modelling often underperforms when used to model non-linear systems

(iii) Time series modelling requires considerable knowledge in time series statistics i.e. autocorrelation function (ACF) and partial auto correlation function (PACF) to identify an appropriate air quality model

(iv) Statistical models are site specific

2.1.3 PHYSICAL MODEL

In physical modelling, a real process is simulated on a smaller scale in the laboratory by a physical experiment, which models the important features of the original processes being studied. Typical experimental devices such as wind tunnels or water tunnels are employed, in which the atmospheric flows, for which boundary layer wind tunnels (wind tunnel modelling) are used. This type of physical modelling carried out in the wind tunnel, in which atmospheric flows have been modelled with air as fluid medium, has also been referred to as fluid modelling by various researchers (Nagendra and Khare, 2002; Shama 2004).

Limitation of Physical model:

(ii) Major limitations of wind tunnel studies are construction and operational cost

(iii) Simulation of real time air pollution dispersion is expensive

(iv) Real time forecast is not possible

(v)

III. SELECTION OF MODEL

A model must include the essential physics of the dispersion process and provide reasonable and reproducible estimates of pollutant concentration (Macdonald R., 2003). There are numbers of model available out of which selection of one model is difficult. Model which require minimum numbers of input variable, suitable for type of source and produce good result should be selected. With increase in numbers of input, uncertainty of model output increases. Quality of model is judge by model consistency and model accuracy (EEA, 1996). Batterman et al. (2010) evaluate the sensitivity analysis of CALINE 4 and Mobile 6.2 to determine the input variables which influence the model result most. So that uncertainty can be minimized while identifying the input variables. Prodanova et al. (2008) evaluates that Community Multi-Scale Air Quality (CMAQ) model approach is capable to reproduce the concentration of sulphur dioxide over Baulgeria, Stara Zagora.

An understanding of fundamental concept of model and their physical process is also necessary before selection of a model. The background knowledge is required to ensure the most sensible choice are made in all aspects of the data input stages, selection of model options and the interpretation of results (Macdonnald R., 2003). Easy availability of model should also be kept in mind while selecting a model.

Accuracy of predicted value of a model depends on (EEA, 1996):

- Input data accuracy and how the latter affects the accuracy of model results.
- Uncertainties in model assumptions and parameterizations.
- Methodologies for judging to what extent model results represent reality.

3.1 APPLICATION OF MODEL

- Regulatory Purposes: Model results are used in issuing emission permits but model accuracy has not been specified in majority of countries.
- Policy Support: support policy by forecasting the effect.
- Public Information: by air quality forecasting and possible occurrence of smog episodes.
- Scientific research; Description of dynamic effects and simulation of complex chemical process involving air pollutants.

3.2 INADEQUACY OF AIR POLLUTION MODELLING

The total uncertainty involved in the air pollution modelling simulation can be considered as the sum of three components: (1) the uncertainty due to the errors in the model physics, (2) the uncertainty due to the input data errors (meteorology and emission-related parameters) and (3) the uncertainty due to stochastic processes (e.g. turbulence) in the atmosphere. It may be possible to reduce the first component of model uncertainty by introducing more physically realistic and computationally efficient algorithms (as done in the new generation of air quality models). It may also be possible to eliminate some of the effects of input data errors once more accurate monitoring instruments are set up at representative locations. However, the stochastic fluctuations are natural characteristics of the atmosphere that cannot be eliminated. Thus, the first two types of uncertainties are reducible uncertainties and the third one due to atmospheric processes is intrinsic uncertainty, which cannot be reduced (Sharma et al., 2004).

The experience so far has shown that the values of various input parameters to these models are often adopted from other countries without understanding their applicability in Indian context, resulting in inaccurate and unreliable predictions (Sharma et al. 2001). Majumdar et al., (2008) reveals that CALINE 4 with correction factors (0.37) can be applied reasonably well for the prediction of CO in the city of Kolkata. However, in order to make more useful, refinements need to be carried out so as to make it more complete tool for prediction. Every model's accuracy for predicting concentration of pollutant depends on the inputs data. Thus, sensitivity of a model is required to identify the most influential input variables. Sahlodina et al. (2007) used sensitivity analysis of CALINE 4 model to eliminate the less significant input variable.

The Various Gaussian models are routinely used in India for carrying out air pollution predictions generally require various input parameters pertaining to meteorology, traffic, road geometry, land use pattern, besides receptor locations. Besides the basic Gaussian dispersion approach, each dispersion model differs with respect to the treatment of modified wind and turbulence parameters. Adequacies, limitations, reliability and associated uncertainties of these dispersion models have already been discussed by various researchers. Various Gaussian based dispersion models are extensively used in India without properly calibrating them for Indian climatic and traffic conditions. Moreover, various input parameters used in these models are not accurately known leading to incorrect or sometimes even unreliable predictions. Greatest inaccuracy in modelling exercise in India is due to the improper emission factors.

Another source of inaccuracy in these models pertain to non- availability of on-site meteorological data. Most often modellers in India rely on nearest Indian Meteorological Department (IMD) data which does not reflect actual field conditions and adds to inaccurate prediction estimates. Thus, there is a need to upgrade and modernize the facilities so that these IMD stations can better serve in understanding and explaining the dispersion phenomena in urban/city conditions (USEPA, 2000).

3.3 STUDIES ON AIR POLLUTION MODELLING

Due to significance of modelling, a number of studies have been carried out to examine the reliability of predicted concentrations from these models. Models are more reliable for estimating longer time-averaged concentrations than for estimating short-term concentrations at specific locations. These models are reasonably reliable in estimating the magnitude of highest concentrations sometimes occurring within the area (e.g. air pollution episodes). The concentration estimates that occur at a specific time and site are poorly correlated with actually observed concentrations and are less reliable.

Ferdous and Ali (2005) uses CALINE 4 model for different stability class and identify the most suitable dispersion coefficient by using CALINE 4 and Gaussian equation for predicting concentration of carbon monoxide in Dhaka city, Bangladesh. Bhati et al. (2009) uses AERMOD model for comparing percentage source of particulate matter from industrial and traffic emission for Delhi city. They found that model under predict the concentration of particulate matter as compared to observed values and also evaluate that traffic emission contributed 66.4% of particulate matter to Delhi total particulate matter. Sathe Y. V. (2012) compares line source model STREET and STREET Box model for a street canyon in Kolhapur city, Maharashtra, India for particulate matter and sulphur dioxide. He found that STREET Box model is output is closer to observed value than STREET model.

Sportisse (2007) found that air quality modelling and simulation suffer from many uncertainties, for instance, many input data are poorly known, numerical algorithms; also induce uncertainties etc. Therefore, not relevant to view outputs of Chemical Transport Models as deterministic values. Even if the models are "validated" (model-to-data comparisons should performed, when possible), one must keep in mind that there are a large amount of degrees of freedom and only a small number of model outputs can be measured.

IV. CONCLUSION

Air quality has a direct impact on people's health. EPA research has shown that air contaminated with common pollutants like ozone, acidic gases, and toxic components of particulate matter can aggravate asthma symptoms and put stress on cardiovascular systems. There is a need to develop a air dispersion models for Indian condition so that, it would: 1) better represent air movement and reflect the effect of air stagnation conditions of pollutant concentrations and 2) better mimic the dispersion and deposition of pollutant.

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