Air Quality Monitoring Using Model: A Review

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Abstract: ***Air pollution is a global environmental challenge that has continued to receive worldwide attention despite the recent decline in concentration of atmospheric pollutants following stringent environmental protection regulations. The major source of this pollution remains fossil fuels; hence the urgent need for cleaner energy sources. This study presents a review of the models applied in monitoring ambient air quality. The primary aim of air pollution modeling is to identify and quantitatively characterize pollutant emission at its source and subsequent dispersion through the atmosphere, subject to meteorological conditions, physical and chemical transformations. The common models and model assumptions for modeling air pollution and quality were critically reviewed and analyzed in this work for application in both forecasting and estimation of air pollutants on the basis of considered causes and in air quality assessment and air pollution control.***

Keywords: Pollutants, Gaussian, Dispersion, Models

1. Introduction

Substances altering physical or chemical properties of the air, added in sufficient concentration to produce a measurable effect on man or vegetation, are considered as pollutants. Many studies have emphasized that localized critical concentrations of pollutants can seriously affect air quality. As a consequence, the relationship between observed concentrations of air pollutants and human receptors is searched for.

The evidence of air pollution effects on man, animals and vegetation has suggested the need for better understanding of the involved phenomena. On account of its effect on human life, air pollution in urban and industrial areas has become a major problem. Its characteristics have not changed significantly in recent times, but the atmospheric process knowledge and the control technology has greatly improved. The quality of air in an atmosphere depends on the number of sources of pollutants, the rate at which pollutants are sent into the atmosphere and the ability of the atmosphere to disperse these pollutants, which is largely controlled by weather patterns.

Mobile sources which includes a variety of vehicles, road is the largest source of air pollution, with emission varying from one type of vehicle to another, type of driving, vehicle age, pollution control equipment, degree of maintenance and other factors [1].

Air pollution model is the mathematical or statistical description of the meteorological transport and dispersion processes using source and meteorological parameters for a specific period of time. Model calculations result in estimates of pollutant concentration for specific locations and time. Air pollution models can be used to perform both forecasting and estimation of air pollutant on the basis of considered causes, thus they are applied in air quality assessment and air pollution control. Monitoring air quality helps in better understanding the sources, movements and effects of various pollutants in the atmosphere. It also helps to ensure that facilities which are releasing pollutants into the air are within the limits established by national standards and guidelines.

The data collected helps to control sources of air pollution within an area, and to negotiate with governments in other jurisdictions for controls on air pollution that crosses borders. The more information available on air pollution, the more effectively air quality and the environment can be enhanced and protected.

Although stringent regulations on engine performance and fuel formulation have brought about a decline in the amount of air pollution produced by individual vehicles bringing down the overall amount of air pollution caused by mobile sources, there is still cause for concern because the number of vehicles on the roads and highways have increased considerably over the years and hence more pollutants are being released into the atmosphere. This work is a review of researches on air pollution and air quality monitoring models.

2. Review of Previous Works

Aronica [2] applied Eulerian model (equation 1) to estimate the quantity of gas produced and released into the atmosphere from a landfill.

$$\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial y}+w\frac{\partial c}{\partial x}=-\frac{\partial}{\partial x}(u'c')-\frac{\partial}{\partial y}(v'c')-\frac{\partial}{\partial z}w'c' \quad (1)$$

$u', v' and w'$ are fluctuations of the speed components along x, y, and z axes respectively, and c' is the pollutant concentration. The solution of eq. (1) is given by Gaussian model (eq. (2))

$$c = \frac{Q}{2\pi u \sigma_y \sigma_z} e^{\frac{y^2}{2\sigma^2_y}} \left[e^{\frac{z^2}{2\sigma^2_z}} \right] \quad (2)$$

Q = flow rate of the emitted pollutant, given by:

$$Q = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} c(x,y,z)u\,dy\,dz = \text{Constant} \quad (3)$$

And the quantities σ_y and σ_z are representative of the side dimensions of the medium profile of the concentration and the Gaussian standard deviations on the planes (x, y) and (y, z). They estimated the monthly biogas emission from the landfill into the atmosphere to be about 60% of the total biogas produced by the landfill. Modeling of the same landfill using LandGEM software gave the gas emitted as

50% of the total produced by the landfill. A more sophisticated dispersion model may be required to validate their work.

Zhao and Wu [3] developed a model which they called Particle filter group model, for modeling particle fate in ventilation system. The model can be used to predict particle fate in an entire ventilation system by calculating the concentration and quantity of particle deposited in each part of the system. The model may also be used to calculate the particle distribution within the system. Equations (4) and (5) show Particle filter group model

$$C_{in,sp} = \frac{Q_{fresh} C_o P_{fd}}{Q_s - Q_{r,return} P_{sd} \mathrm{P}_{room,s} \mathrm{P}_{rd}} \quad (4)$$

$$C_{in,sp} = \frac{Q_{r,return} / Q_s \sum_i^B (S_{pi} \mathrm{P}_{room,sp,i} \mathrm{P}_{rd})}{Q_s - Q_{r,return} P_{sd} \mathrm{P}_{room,s} \mathrm{P}_{rd}} \quad (5)$$

Where $Q_{r,return}$ is the recycled air flow rate, Q_s is the supply air flow rate, P_{rd} is the penetration coefficient of return duct and S_{pi} is the generating rate of the ith particle source. Q_{fresh} is the fresh flow rate and C_o is the particle concentration of the outdoor air. They validated the model experimentally. Hence particle concentration and deposition quantity at each part of a ventilation system can be calculated easily, which can help in the control of indoor particle concentration.

Mok et al [4] used a modified Gaussian plume model to simulate the dispersion of a non-reactive air pollutant (SO_2) released into the atmosphere under a non-homogenous wind condition through a multi-puff approach. They applied the equations (6) and (7) below to a specific urban case study and the result obtained were compared to measured air quality data. Optimal interpolation technique, which is based on correlation functions determined from historical air concentration data was added to the developed model which improved their result.

$$c(x_1, x_2, 0, t) = \frac{q}{(2\pi)^{3/2} \sigma_2^2 \sigma_3} \exp\left[-\frac{R^2}{2\sigma_2^2}\right] X \left\{2\exp\left[\frac{h_e^2}{2\sigma_3^2}\right] + E_T\right\} \quad (6)$$

$$E_T \left\{ {}^0 \; \Sigma_{n=1}^4 2\exp\left[\frac{(h_e + 2nH)^2}{2\sigma_3^2}\right] + 2\exp\left[\frac{(h_{e-2nH})^2}{2\sigma_3^2}\right] \right. \quad (7)$$

Where $\sigma_2^2 \, and \, \sigma_3^2$ = variances of the Gaussian concentration distributions

$$R^2 = (x_1 - Ut)^2 + X_2^2 \quad (8)$$

U = average velocity in the horizontal x_1
X_2= horizontal direction normal to x_1
n = number of reflections

Sabapathy [5] studied air quality outcomes of fuel quality and vehicular technology in an Indian city, where fuel quality and vehicular technology measures were implemented. The air quality was monitored using high volume gravimetric samples at different locations within the city. Monthly average concentrations for the four pollutants – SO_2, NOx, SPM and RSPM were collated for four different time periods for a longitudinal assessment of whether there have been any air quality improvements resulting from the vehicle technology and fuel quality policies implemented in the city. A one-way single-factor analysis of variance was carried out using the monthly average concentrations for the four pollutants in each time period to test the hypothesis that pollution levels in each time period are lower than the preceding time periods. Exceedance above the annual standards was also analyzed. Results from the study showed substantial improvement in air quality (Mean monthly average $S0_2$ concentration reduced from 43.2 μgm^{-3} to 7.5 μgm^{-3}) over the city in spite of a 50% increased traffic loads.

Tirabassi [6] studied operational models that use solutions of the advection-diffusion equation based on the assumptions of homogeneous wind and eddy diffusivity coefficients (equation 9). He introduced a new parameterization for the model using a solution that accepts wind and eddy diffusivity profiles described by power functions of height. The performance of the model with the new parameterization was assessed using experimental data.

$$C(x, y, z) = \frac{c_y}{\sqrt{2\pi\sigma_y}} \exp\left[-\frac{y^2}{2\sigma_y^2}\right] \quad (9)$$

C_y = cross-wind integrated concentrations, y = cross-wind distance

σ_y = lateral diffusion parameter.

If variations in the wind velocity (u) and exchange coefficient (Kz) with height (z) are

$$u = u_1 (z / z_1)^\alpha \quad (10)$$
$$K_z = K_1 ((z / z_1)^\beta$$

Z_1 is the height where u_1 and K_1 are evaluated and equation (9) can be written as

$$c_y = \frac{Q(zh)^p z_1^\beta}{\lambda K_1 x} \exp\left[\frac{u_1 z_1^y (z^\lambda + h^\lambda)}{\lambda^2 K_1 x}\right] I_{-v}\left(\frac{2u_1 z_1^y (zh)^q}{\lambda^2 K_1 x}\right) \quad (11)$$

Where x = along-wind direction, Q = source emission, h = source effective height.

$$\lambda = \alpha - \beta + 2, v = (1-\beta)/\lambda, \quad p = (1-\beta)/2, q = \lambda/2$$

Sportisse [7] did a comparative study of the box model and the Eulerian model in his and considered a mono-dimensional Eulerian model by neglecting wind velocity, which is the practical situation for peaks of pollution (no wind, no transport far from source), assuming constant mixing height and diffusive coefficient with time, the equation can be written as:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial z}\left[K(z)\frac{\partial c}{\partial z}\right] + \chi_i(c) \quad (12)$$

With the following boundary conditions:

$K\frac{\partial c}{\partial z} = o$, at z = H, $K\frac{\partial c_i}{\partial z} = v_{dep}^i c_i - E_i(t)$ at z = 0

and a Box model based on the assumption of a perfectly stirred reactor.

$$\frac{dc_i}{dt} = \chi_i(cT(t), t + S_i(t) + \frac{1}{H(t)}(E_i(t) - v_{dep}^i c_i \quad (13)$$

H (t) = mixing height.

He derived an error band for the deviation $e_i(t)$ associated with the species i defined by

$$e_i(t) = c_i(t) - \langle c_i \rangle(t)$$

Where c_i and $\langle c_i \rangle$ denote the solutions of the box model and the average of the Eulerian solution. His analysis showed the dependence of the error induced by the Box model on the fluctuation of concentration. Relative error at a fixed time to compare both models, Eqn. 14

$$ERR(t) = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{\langle c_i \rangle(t) - c_i(t)}{\langle c_i(t) \rangle}\right)^2 \quad (14)$$

Result obtained showed that errors associated with the Box model grew with time and they were much bigger than the usual threshold of 1% advocated in air pollution model. Sivacoumar et al [8] modeled an industrial complex to determine the impact of NOx emission resulting from various air pollution sources within the complex viz industries, vehicles, etc using Gaussian dispersion model, their model considerations included: Production capacities, Raw materials utilized in the industries within the complex, Fuel consumption, Stack emission characteristics, Vehicular count survey and Meteorological data collected using wind monitoring instrument. Model result gave 53% as the industrial contribution of NOx. Model performance evaluated using statistical analysis showed good agreement between the two with 68% accuracy.

Ando [9] proposed a novel black box approach for air pollution modeling. The target of this approach is prediction, on the basis of meteorological forecasts, of the air pollution concentration as a function of the expected causes. The model is expected to forecast as well as estimate air pollutants on the basis of the considered causes so that it can be applied in emission control scheme to determine suitable control measures.

3. Analysis of Important Research Contribution

Several models exist for modeling air pollution and air quality in an atmosphere, but models commonly used, which were also used in the articles being reviewed are: Gaussian plume models; Box models; Eulerian models and Lagrangian models among others.

3.1 Gaussian Plume Models

Gaussian plume models are most often used for predicting the dispersion of continuous, buoyant air pollution plumes originating from ground-level or elevated sources. It assumes that the air pollutant dispersion has a Gaussian distribution, meaning that the pollutant distribution has a normal probability distribution. In the Gaussian plume model, the atmosphere is assumed stagnant and homogeneous, and the downwind concentrations of a pollutant along the vertical and crosswind dimension are assumed to be normally distributed. Also the probability distribution of wind velocity is assumed independent of time and location. The Gaussian plume model shows reasonable results and requires relatively simple input information which include wind speed, wind direction, the dispersion parameters σy, σz , and distance from sources.

The Gaussian-plume models are widely used, well understood, easy to apply, with assumptions, errors and uncertainties that are generally well understood. However it may not always be the best model to apply because of a number of drawbacks, the major one being the linear summation of the model which is the basis of its simplicity, but it is reasonable to assume that a lot of inaccuracies associates with this model is as a result of this assumption, because most processes occurring in the atmospheres during the release and dispersion of pollutant are not linearly related.

Also, Gaussian-plume models assume pollutant is transported in a straight line instantly from the source to receptors who may be several hours or more in transport time away from the source, disregarding wind speed. This implies that Gaussian plume models cannot account for causality effects, especially if the receptor is at an appreciable distance away from the source. Gaussian-plume models cannot handle low wind speed or calm conditions effectively due to the inverse wind speed dependence of the steady-state plume equation. Unfortunately worst-case air pollution effects are recorded under these conditions.

Terrain effect was poorly considered in the Gaussian plume model hence in moderate terrain areas, Gaussian models typically overestimate terrain impingement effects during stable conditions. With the steady-state assumption in the Gaussian models, it is assumed that the atmosphere is uniform across the entire airshed, so that transport and dispersion conditions are unchanged for the duration of time it takes the pollutant to reach the receptor. This however hardly occurs in the atmosphere. A lot of atmospheric processes and features produce non-homogeneities in the atmospheric boundary layer that can affect pollutant transport and dispersion.

3.2 Box Models

Box models are widely used in air pollution modeling; they provide simple description of air quality in urban areas, especially where emissions data are only available on a fairly coarse grid, and also produce acceptable results when applied in modeling. Under suitable conditions, the box model offers the possibility of enabling an accurate emissions concentrations relationship to be developed with minimum mathematical complexity. However, as an empirical model, it should be validated before being adopted in a specific area [7]. Also, the box model is so specific that a model developed in one area cannot be implemented on another area without validation. Thus even though the box model is useful especially because of low computer cost, its ability to accurately predict dispersion of air pollutants over an airshed is limited because of its numerous simplifying assumptions.

3.3 Eulerian Model

The Eulerian model, often called the numerical approach, consists of using the continuity equation of mathematical physics to develop a description of the physical and chemical processes that govern the relations between emissions and concentrations. Though the Eulerian approach provides detailed representation of dispersion, it can be extremely complicated, demands a large amount of input data, and is computationally intensive. The Eulerian approach has in principle fundamental advantages especially in the description of physical processes over the Gaussian approach though it cannot readily be implemented in urban areas and is also difficult to apply in complex dispersion geometry. It has also been observed over time that the complex modeling approaches do not provide a substantial improvement in results. This is one of the reasons the Gaussian dispersion model is widely used model.

3.4 Lagrangian Model

The Lagrangian model is based on a probabilistic description of the motion of pollutant particles in the atmosphere to derive expressions for pollutant concentrations. It allows accurate modeling of the spatial variation of turbulent diffusivity. Lagrangian model has the advantage of more accurate calculation of the advection and dispersion from various sources and allow more complete characterization of the impact of turbulence on the transport of air pollutants.

Typical Lagrangian model treat the dispersion of plumes better than Eulerian models but the chemical interactions induced by the mixing of intersecting plumes is ignored. The most serious drawback of Lagrangian model is its excessive demand of computing time even with today's powerful computers, it is still extremely tiresome to use due to the large amount of computing data required, and this makes the model unattractive for many practical applications, such as assessment of air pollution in a long-term. Gualtieri and Tartaglia [10] developed a model to estimate the concentration of NOx in a street canyon, the model which is based on CORINAIR emission inventory software, considered traffic data, meteorological data, site and road topography. The authors did a good job of setting up a simplified street canyon model to account for the behavior of typical reactive pollutant emitted by vehicles, but the model is so simplified that the accuracy is very low. For instance, the model only considered NOx as coming from vehicles alone. A model that considered the concentrations of NOx using a combination of (a plume model) direct contribution from vehicles and (a box model) the recirculating part of the pollutants in the street, would have given a more accurate representation of the actual concentration of NOx in the street because the most characteristic feature of the street canyon wind flow is the formation of wind vortex, such that the direction of the wind at street level is opposite to the flow above. This flow condition usually leads to a situation in which the pollutants emitted from traffic in the street are primarily transported towards the upwind building, while the downwind side is primarily exposed to background pollution and pollution that has recirculated in the street. In general, there is always circulation of wind in the street, which when captured by a model increases the accuracy of the model, even though the model complexity increases.

A major plus to the model is taking into account wind speed conditions, because in traffic induced turbulence, an important feature is the ability to predict pollution concentrations at low wind speed conditions, because most severe pollution episode often occur at such times. Even though NOx formation time is very small, time of exchange with the background air is appreciable and should have been considered in the model; taking into account the residence time of pollutants in the street. Urban background O_3 and NO_2 play important role in NO_2 formation in the street air.

This model also did not consider advection and convection which are major means of transport in fluids. Taking those into account would have greatly improved the accuracy of the model result. Finally, Parameterization of vehicle conditions in the model either deduced from analysis of experimental data or model tests results would have further improved the model performance. Because it would have represented processes that were not directly captured by the model, but then finding a set of consistent parameterization for models is not always very easy.

3.5 The KAPPAG models

These are non-Gaussian models developed by Tirabassi [6] based on the analytical solutions of the advection-diffusion equation. They can be applied by using as inputs simple ground level meteorological data. Fundamental parameters for the model were all evaluated by ground level-measurement. Included in the model also are parameterization for wind and eddy diffusivity. The model can handle multiples sources and receptors under varying conditions. The model gave good results when compared to the Gaussian model proposed by EPA.

Based on available information about the model properties, its considerations are very narrow which is adequate for specific circumstances, but it's unlikely that it can to handle accurately many of the complexities generally encountered in air pollution modeling. For instance all of its consideration was at ground level, which is only a tiny fraction of air pollution condition. The only major consideration of this model is wind which is also another small fraction of meteorological conditions, when other conditions like atmospheric stability, mixing height etc are taken into consideration; the model will most likely break down.

To improve the use of these models, it will need to take account of what is happening in the vertical structure of the atmosphere and thus should consider a certain height, in addition, more meteorological parameters should be considered because meteorology is a strong determinant of pollutant dispersion, so a good description of meteorology is vital because the effects are cumulative. Emissions from contaminant are a vital requirement in modeling. An emission factor will be a big plus to these models.

4. Improving Air Quality Monitoring Models

Air quality models are needed to determine the effect of pollutants on human health and the environment and to protect people from air pollution by forecasting what may happen to the quality of the air under different potential emissions-control strategies and varying weather conditions.

Dispersion models can take many forms like graphs, tables or formulae. In recent times, dispersion models more commonly take the form of computer programs. The process of air pollution modeling generally contains four stages (data input, dispersion calculations, deriving concentrations and analysis). The accuracy and uncertainty of each stage must be known and evaluated to ensure a reliable assessment of the significance of any potential adverse effects. Currently, the most commonly used dispersion models are steady-state Gaussian-plume models. These are based on mathematical approximation of plume behavior and are the easiest models to use. They incorporate a simple description of the dispersion process, and some fundamental assumptions that do not accurately reflect reality. Hence with these limitations the Gaussian models can only provide reasonable results within the limits of the assumption made even with the most cautious application. An improvement in this area would be the adoption of a more sophisticated and specific approach to describing emission and dispersion using the fundamental properties of the atmosphere rather than relying on general mathematical approximation. This will enable better treatment of difficult situations such as complex terrain and long-distance transport and will produce more realistic results. Since the accuracy of prediction of ground-level concentrations of contaminants from a discharge is based on the accuracy of input data, it is essential that at all time, accurate input parameters be used for modeling. Factors influencing these parameters should be carefully considered.

Models tend to be specific, so that the choice of any particular model should take into consideration the nature of the environment being modeled, because that will determine whether or not an accurate and realistic result will be obtained. Sometimes the sophistication of a model play little role in the output from the model if it is not a good representation of the situation required. Hence results from advanced models should *not* be automatically assumed to be better than those gained from simpler models.

Another important factor in effective dispersion modeling is the choice of an appropriate model to match the scale of impact and the significant potential effects including the sensitivity of the receiving environment. Model validation which ensures that model meet its intended requirement is an essential step in modeling that is often overlooked. Model validation is very essential especially when new models are being tried out. A comparison of the manuals and validation studies of the model being considered with existing ones will provide the modeler with some guidance on the accuracy of his result.

Modeler must recognize that there are limitations to the scope of a model's application and to the accuracy of the predictions from each model; this should always be considered when applying results to real life situations. Finally, regulatory bodies should advance research to develop, evaluate and improve air quality monitoring models for the assessment not just pollutant of interest but also evaluate the interactions of the pollutant with other environmental contaminants.

5. Conclusion

The study of air pollution and air quality monitoring has evolved from simple box model studies to advanced models that can handle different meteorological conditions and complex situations, such that the problem of air pollution even though not yet solved is better understood and can be better controlled.

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