

Air Pollution Modelling, Simulation and Computational Methods: A Review

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ABSTRACT

The air pollution problem has received more attention during the last decades whereby there has been a significant increase in public awareness of the potential dangers caused by chemical pollutants and their effects on both human beings and the environment. The purpose of this paper is to present an overview of the existing literature about air pollution assessment and evaluation for earlier and current methods. These methods include; mathematical models, simulation modelling, and simulation software. The basic technology for predicting the impact of air pollution is through the use of a variety of mathematical models. Even though these mathematical models have many advantages, they are not easy to use and difficult for non-experienced users to perform calculations on these complex models. Obviously, to evaluate the impact from air pollution using complex models, the best way is by simulating the mathematical models through computer techniques. Furthermore, the integration of Geographic Information Systems (GIS) and simulation models, combined with suitable databases and expert systems within a common and interactive Graphical User Interface (GUI) should make for more powerful and easy to use - and understand - risk information systems.

Keywords: Air pollution; Mathematical modelling, Simulation software, GIS

1.0 INTRODUCTION

Air pollution is the presence of undesirable material in air, in quantities large enough to produce harmful effects (Nevers, 2000). The World Health Organisation (WHO) estimates that 500,000 people die prematurely each year because of exposure to ambient concentrations of airborne particulate matter (Colls, 2002). Air pollution is definitely not a new problem but dates back to the middle ages when the use of coal in cities such as London began to escalate. The problems of poor urban air quality even as early as the end of the 16th century are well documented. Hundreds of years later, in 1952, a five-day temperature inversion in London trapped fog laden with pollutants created by burning coal. More than 4000 deaths were attributed to this deadly "black fog." Similar incidents claimed 1000 lives in 1956 and 700 lives in 1962 (Bouhel *et al.*, 1994). However, during the 1980s the number of motor vehicles in urban areas steadily increased and air quality problems associated with motor vehicles became more prevalent. In the early 1980s, the main interest was the effects of lead pollution on human health, but by the late 1980s and early 1990s, the effects of other motor vehicle pollutants became a major concern. Between September 1997 and November 1997 in Indonesia, there were 527 haze-related deaths, 298,125 cases of asthma, 58,095 cases of bronchitis, and 1,446,120 cases of acute respiratory infection reported (Amagai *et al.*, 2002).

The most common disaster of air pollution the one accrued because release of hydrogen sulphide at Poza Rica, Mexico in 1950 (McCabe and Clayton, 1952) and the other example is toxic release at Bhopal, India. Table 2 summarized the air pollution disasters between years 1930 and 1991 (Bosanquet, and Pearson, 1936; Amagai *et al.*, 2002).

Worldwide air pollution is responsible for a large number of deaths and cases of respiratory disease. While major stationary sources are often identified with air pollution, the greatest source of emissions is actually mobile sources, mainly automobiles. Gases such as carbon dioxide, which contribute to global warming, have recently gained recognition as pollutants by climate scientists, while they also recognize that carbon dioxide is essential for plant life through photosynthesis. Motor vehicle emissions are one of the leading causes of air pollution (Transport Canada, 2001; Buchanan and Horwitz, 2005). China, United States, Russia, Mexico, and Japan are the world leaders in air pollution emissions. Principal stationary pollution sources include chemical plants, coal-fired power plants, oil refineries (Beychok, 1967), petrochemical plants, nuclear waste disposal activity, incinerators, large livestock farms (dairy cows, pigs, poultry, etc.), PVC factories, metals production factories, plastics factories, and other heavy industry.

2.0 AIR POLLUTION MODELLING AND SIMULATION

A model is a simplified picture of reality. It doesn't contain all the features of the real system but contains the features of interest for the management issue or scientific problem we wish to solve by its use. Models are widely used in science to make predictions and/or to solve problems, and are often used to identify the best solutions for the management of specific environmental problems. Models may be (Ministry for the Environment, 2004):

- Physical: a scaled-down representation of reality
- Mathematical: a description of the system using mathematical relationships and equations.

2.1 Mathematical Modelling

Eykhoff (1974) defined a mathematical model as a representation of the essential aspects of an existing system (or a system to be constructed) which presents knowledge of that system in usable form.

Air dispersion modelling has been evolving since before the 1930s (Beychok, 2005). Air quality modelling is an essential tool for most air pollution studies. Models can be divided into; physical models and mathematical models. The mathematical models will be only discussed in this article. Mathematical models can be; deterministic models, based on fundamental mathematical descriptions of atmospheric processes, in which effects (i.e., air pollution) are generated by causes (i.e., emissions) and statistical models, based upon semiempirical statistical relations among available data and measurements (Zannetti, 1993). The deterministic models are the most important and better for prediction the spatial concentration distributions within urban areas.

The factors that affect the transport, dilution, and dispersion of air pollutants can be grouped into (AIR-EIA, 2000):

- emission or source characteristics
- the nature of the pollutant material
- meteorological characteristics
- the effects of terrain and anthropogenic structures.

2.1.1 Air Pollution Dispersion

Air dispersion terminology describes the words and technical terms that have a special meaning to those who work in the field of air pollution dispersion modelling (Beychok, 2005). Emission and vaporization are followed by dispersion of vapour to form a vapour cloud (Lees, 1996). The paper will only discuss the dispersion factor.

Air pollution dispersion terminology describes the words and technical terms that have a special meaning to those who work in the field of air pollution dispersion modelling. A dispersion model is a mathematical description of the meteorological transport and dispersion processes, using source and meteorological

parameters, for a specific period in time. The model calculations result in estimates of pollutant concentration for specific locations and times.

The study of the dispersion is not a new. Early work on the subject atmospheric dispersion began with Taylor (1915) whose study the examination of the redistribution of heat in a current over relatively cold sea. Later on, he also developed the famous Taylor-theory of turbulent diffusion (Taylor, 1921). Taylor (1927) also provided the first direct measurements of the turbulent velocities in the horizontal by using the widths of the traces produced by conventional wind speed and direction recorders. Afterwards Scrase (1930) and Best (1935) extended Taylor's study, their research reveal the marked dependence on the thermal stratification of the air and also the existence of a very wide spectrum of frequencies in the generally irregular fluctuation. The paper by Builtjes, (2001) is cited several authors who done a research in dispersion modelling. For instance, the study of the dispersion from low and high level point source done by Smith (1957), Gifford (1957 a,b), Hay and Pasquill (1957) and Haugen (1959). Other research for Prairie grass experiment done by Stewart *et al.*, (1958), Monin (1959), Ogura (1959). Accounts of gas dispersion include those given in Micrometeorology (Sutton, 1953), atmospheric diffusion (Pasquill, 1962, 1974), an evaluation of dispersion formulas (Anderson, 1969), workbook of atmospheric dispersion estimates (Turner, 1970), turbulent diffusion in the environment (Csanady, 1973) and handbook on atmospheric diffusion (Hanna *et al.*, 1982) and those given by Pasquill and Smith (1983).

The qualitative aspect of dispersion theory is to describe the fate of an emission to atmosphere from a point, area or line source. There are five types of air pollution dispersion models, as well as some hybrids of the five types (Colls, 2002):

- **Gaussian model:** The Gaussian model is perhaps the oldest (circa 1936) and perhaps the most accepted computational approach to calculating the concentration of a pollutant at a certain point. Gaussian models are most often used for predicting the dispersion of continuous, buoyant air pollution plumes originating from ground-level or elevated sources. Gaussian models may also be used for predicting the dispersion of non-continuous air pollution plumes (called *puff models*). A Gaussian model also assumes that one of the seven stability categories, together with wind speed, can be used to represent any atmospheric condition when it comes to calculating dispersion. There are several versions of the Gaussian plume model. A classic equation is the Pasquill-Gifford model. Pasquill (1961) suggested that to estimate dispersion one should measure the horizontal and vertical fluctuation of the wind. Pasquill categorized the atmospheric turbulence into six stability classes named A, B, C, D, E and F with class A being the most unstable or most turbulent class, and class F the most stable or least turbulent class.
- **Lagrangian model:** a Lagrangian dispersion model mathematically follows pollution plume parcels (also called particles) as the parcels move in the atmosphere and they model the motion of the parcels as a random walk process. Lagrangian modelling well described by number of studies by Rohde (1972, 1974), Fisher (1975), Eliassen (1978), Hanna, (1981), Eliassen *et al.*, (1982) and Robert *et al.*, (1985). Lagrangian modelling is often used to cover longer time periods, up to years (Builtjes, 2001).
- **Box model:** Box models are the simplest ones in use. As the name implies, the principle is to identify an area of the ground, usually rectangular, as the lower face of a cuboid which extends upward into the atmosphere (Colls, 2002). Box models which assume uniform mixing throughout the volume of a three dimensional box are useful for estimating concentrations, especially for first approximations (Boubel *et al.*, 1994). Box model is well discusses by; Derwent *et al.*, (1995), Middleton (1995, 1998).
- **Eulerian model:** Eulerian dispersions model is similar to a Lagrangian model in that it also tracks the movement of a large number of pollution plume parcels as they move from their initial location. The most important difference between the two models is that the Eulerian model uses a fixed three-dimensional Cartesian grid.
- **Dense gas model:** Dense gas models simulate the dispersion of dense gas plumes (i.e., pollution plumes that are heavier than air). The most common used dense gas models are (Beychok, 2005):

the DEGADIS model developed by Dr. Jerry Havens and Dr. Tom Spicer at the University of Arkansas under commission by the US Coast Guard and the US Environmental Protection Agency. The SLAB model developed by the Lawrence Livermore National Laboratory funded by the US Department of Energy, the US Air Force and the American Petroleum Institute. The HEGADAS model developed by Shell Oil's research division.

Potential air pollution impact is usually estimated through the use of air quality simulation models. A wide variety of models is available. The model requires two types of data inputs: information on the sources including pollutant emission rate, and meteorological data such as wind velocity and turbulence. The model then simulates mathematically the pollutant's transport and dispersion, and perhaps its chemical and physical transformations and removal processes. The model output is air pollution concentration for a particular time period, usually at specific receptor location (Boubel *et al.*, 1994).

2.1.1.1 Factors Affecting Dispersion

There are a number of factors that will affect how emissions disperse once released to atmosphere. These factors are (Lees, 1996):

- Fluid buoyancy (neutral buoyancy, positive buoyancy, negative buoyancy)
- Momentum (low momentum, high momentum)
- Source geometry (point source, line source, area source)
- Source duration (instantaneous, continuous, intermediate)
- Source elevation (ground level source, elevated source)
- Meteorology (wind, stability)
- Topography (surface roughness, near building and obstructions, over urban areas, over coastal zones and sea, over complex terrain)

Meteorology is the most important factor. Meteorological parameters used in dispersion models include wind direction, wind speed, ambient temperature, atmosphere mixing height, and various stability parameters. These parameter are described and discussed in details by number of authors (Turner, 1970; Pasquill, 1974; Hanna, *et al.*, 1982; Lees, 1996 and Builtjes, 2001).

2.2 Simulation

Simulation can be used to predict the effect of changing conditions to optimized operation quickly and safely and it can be used to provide in-depth knowledge about complete system behaviour, to improve and facilitate cost calculation and planning of operation. Simulation methods comes in two types viz Digital and analogue simulation. Of these two types, digital simulation which involves the use of code and programme are more in use since they can be implemented on modern computer with exceptional speed and accuracy, (Koutitas, 1988; Alhassan and Jimoh, 2006).

Atmospheric dispersion modelling is the mathematical simulation of how air pollutants disperse in the ambient atmosphere. It is performed with computer programs that solve the mathematical equations and algorithms which simulate the pollutant dispersion. Computer simulations have become a useful part of mathematical modelling of many natural systems in physics, chemistry and biology, human systems in economics, psychology, and social science and in the process of engineering new technology, to gain insight into the operation of those systems.

Air quality models mathematically simulate the physical and chemical processes that affect air pollutants as they disperse and react in the atmosphere. Meteorological data and source information (e.g. emission rates and stack height) are put into models to characterize pollutants that are emitted directly into the atmosphere. Air quality modelers generally refer to these as primary pollutants. Secondary pollutants, those that form as a result of complex chemical reactions within the atmosphere, can also be modelled.

Models are a key component of air quality management at all scales. They are widely used by local, state and federal agencies charged with addressing air pollution, especially to identify source contributions to air quality problems and to help to design effective strategies aimed at reducing air pollutants (Bouhel *et al.*, 1994).

Most dispersion models are computer-based programs suitable for a desktop PC. All dispersion models need data on the pollutant emission rate. These need not necessarily be exact, as in many cases useful decisions can be made choosing highest likely emissions to represent a worst case (e.g. by assuming that emissions from a chimney are at the limits defined by the regulator, or that traffic on a road is at its peak-hour level. Most models also require details on how the pollutant is being released, and the environment into which the release occurs. It is also necessary to define the locations at which the impact of the emissions will be predicted (Vawda, 2003).

2.2.1 User Interfacing

It is necessary to identify potential hazards caused by air pollutants; this is best conducted through risk assessment. There are several ways to perform air pollution risk assessment; traditionally this is done using mathematical models. Mathematical models are extremely useful tools to simulate the consequences and impact of air pollution, but it is difficult to implement manually. Using computers to perform risk assessment allows estimation of the impact of pollutants on the environment and to sensitive receptors, such as populated areas, using dispersion models with or without various degrees of modification. Development of computer programs or code are able to assess air pollution and enables the consequences of air pollution emissions to be estimated by those who are not specialists in the physical and chemical phenomena associated with such releases (El-Harbawi, 2006). Engineers and other professionals engaged in hazard assessment are no longer satisfied with programs that only accept input from a file or that only produce line printer output, instead they expect the code writer to exploit the full capabilities of modern programming languages and operating environments to provide user-friendly, flexible and increasingly realistic output, which can be presented in a variety of formats; visually and statistically (Kinsman, 1994).

A multitude of computer languages, including C++ and Visual Basic, are available for the development of risk assessment software all of which can be run under Microsoft Windows and can be connected to other computer tools to provide an attractive user-friendly “front-end platform”. New and innovative ideas to evaluate air pollution levels and its potential impact on human health and the environment can easily be included in software development.

Dispersion models are developed to provide accurate pollutant concentration estimates under specified conditions, it rare to find a regulatory model that incorporates a helpful and intuitive user interface or a visual representation of pollutant sources and plume dispersion. For this reason, it has become common for independent companies and other organizations to build GUIs to provide ease of use for model practitioners and, in some cases, add utility to existing models (Jungers *et al.*, 2006).

There are several software have been developed in the past for atmospheric dispersion modelling. For instance, the APPH Module (Air Pollution and Public Health) was developed in Switzerland to draw maps of air pollution emissions from point sources (power plants, industries) and/or area sources (automotive traffic). The three dispersion models used are: a Gaussian model; a Lagrangian model; and a statistic model. The Norwegian Institute for Air Research (NILU) has developed an Air Quality Information System (AirQUIS) having: an emission inventory data base; dispersion models; and a geographical information system (GIS) module. The dispersion models include a source oriented model (EPISODE), a puff-trajectory model, and models for traffic in street canyons and on roads (ROADAIR and CONTILENK). A number of free online calculators for solving various atmospheric dispersion modelling algorithms is developed by AJ Design Software. For accidental releases of neutrally buoyant or heavier-than-air gases, the USA's National Oceanic and Atmospheric Administration (NOAA) was developed ALOHA (The Areal Location of Hazardous Atmospheres model) software. To estimate the impact industrial emissions in complex terrain, French firm of environmental consultants developed an air

dispersion modelling software call ARIA. Other software to evaluate the complex terrain modelling was developed by ATM-PRO. This software can be used for realistic 3D atmospheric and dispersion models, accidental pollution and emergency planning and human health risk assessment of air pollution. For air quality modelling software, Trinity Consultants has developed a software call 'BREEZE'. The software offer many solutions for air quality modelling and use to assess the impact of air emissions from a variety of industrial sources. Cambridge environmental research consultants has produced numerous computer models which tackle such issues as air dispersion, planned and emergency releases, air quality management, flow over complex terrain and atmospheric emission data compilation including greenhouse gases. Other air pollution dispersion software is developed by Canarina Algoritmos Numericos. The software call 'DISPER' and it is able to calculates the pollutant concentration in each point of the air considering each one of the pollutant sources and the conditions of the atmosphere.

2.3 Applications of GIS in Air Pollution Modelling

Geographic Information System (GIS) are tools for collecting, storing, retrieving at will, transforming, and displaying spatial data for a particular set of purposes (Burrough and McDonnell, 1998). Given the spatial nature of many environmental impacts, GIS can have a wide application in all EIA stages, acting as an integrative framework for the entire process, from the generation, storage, and display of the thematic information relative to the vulnerability/sensitivity of the affected resources, to impact prediction and finally their evaluation for decision support (Antunes *et al.*, 1996). Various capabilities of GIS may be utilized for air modelling, which may include locating monitoring stations, developing air quality models and development of spatial decision support system. By doing air quality modelling under GIS environment, the output of the pollutant records can be obtained in the form of spatial records. GIS techniques are capable of supporting the development of geospatial air quality models (Agrawa *et al.*, 2003).

In modelling the atmospheric environment, the relationship to geographical data should be self evident. For more complex models that go beyond the classical Gaussian plume models, topographic relief, surface roughness, and surface temperatures are important input parameters. Sources of pollution are spatially distributed, and may be point sources such as large industrial stacks or power plants, line sources such as highways, and area sources, such as urban areas (Fedra, 1994). The prediction of the magnitude of impacts is often undertaken by the application of simulation models (Fedra, 1993). The obtained result will most often be a map of the value of a given environmental descriptor (e.g., concentration of an air pollutant) at any location within the study area. The extension of environmental impacts can therefore be estimated from the spatial distribution of environmental quality values predicted for each alternative.

Many models have been coupled with GIS in the past decade to simulate various environmental processes as described by Longley *et al.*, (2001). Due to the four-dimensional nature of the distribution of atmospheric pollutants, the concept of GIS should be extended to include temporal variations of three-dimensional spatial data. The interpolations, integrations of land cover surface data, and the GIS analyses focused on small scale spatial models carried out in the kilometre grid are discussed by Lee in the book published by Goodchild *et. al.*, (1996) and in the frame of particular studies (Matejicek, 1996, 1998, 1999). In case of large scale air quality modelling, more detailed spatial data are needed to include the impact of buildings and other manmade barriers on the distribution of air pollutants, (Janour *et. al.*, 1999; Civis *et. al.*, 2001). Apart from this approach, the statistical theory is also used to indicate spatio-temporal interactions as described by Briggs (2000).

CONCLUSION

This paper reviewed some of air pollution modelling, simulation and computational Methods. The paper focus on several studies, which is started beginning of previous century and until recent work. Furthermore, this article discussed several parameter related to dispersion modelling and its method of

evaluation. These methods are including traditional mathematical modelling, simulation, software and GIS.

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