MODELLING AND SIMULATION OF AIR POLLUTION EMISSION USING LINE SOURCE DISPERSION MODEL

By

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FINAL YEAR PROJECT REPORT

Submitted to the Chemical Engineering Programme in Partial Fulfillment of the Requirements for the Degree Bachelor of Engineering (Hons) (Chemical Engineering)

> Universiti Teknologi Petronas Bandar Seri Iskandar 31750 Tronoh Perak Darul Ridzuan

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by

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CERTIFICATION OF APPROVAL

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A project dissertation submitted to the Chemical Engineering Programme Universiti Teknologi PETRONAS in partial fulfilment of the requirement for the Bachelor of Engineering (Hons) (Chemical Engineering)

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CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

Mai Nazura Meor Kamarul Zaman

ABSTRACT

Road traffic represents one of the major sources of air pollution in urban areas, and substantial effort is devoted the development of technological and transport policy measures to reduce its impacts. To determine whether ambient air quality standards are exceeded, a variety of atmospheric dispersion models are employed to predict vehicular pollution effects. The purpose of this project is mainly to develop an atmospheric dispersion application to predict the impacts of air pollution hazard. Equations and algorithms representing atmospheric processes are incorporated into various dispersion models. In this case, source model of air pollution is identified from line source emission specifically roadway emission. The basic concept of the roadway air dispersion model is to calculate air pollutant levels in the vicinity of an urban street canyon. The main attraction of this model lies in the simplicity of its application. Measured traffic and meteorological data were used as the input parameters in the model. Producing the calculations is complex that a computer model is necessary to arrive at reliable results. The results will show the concentration at specific area on the road and the concentration of pollutant at certain distance. These calculations are produced and simulated in Microsoft Visual Basic 6.0. The results obtained are then compared with actual value to from case study. The software proves to be reliable when the error produced is very low.

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CHAPTER 1 INTRODUCTION

1.1 Background

Currently, traffic congestion is a major problem in developing country. This problem induces others sub-problems. One of them is environmental problems of which currently air pollution has been receiving the highest attention. Since most vehicles consume fossil fuel, so they emit many types of toxic gasses. Pollutants from internal combustion process consist of Carbon Monoxide, Sulphur Dioxide, Nitrogen Dioxide, Hydrocarbons, and particulates.

The main sources of additional particulates are motor vehicle exhaust and some industrial activities. Therefore, an important pollutant is PM10 where its concentration is difficult to measure in practice due to the lack of measuring equipments, permanent measuring stations inappropriately located or not covering entire areas of interest, etc. The measurements are also time consuming and costly and cannot be used to predict future problems.

The predicting of ambient PM10 by applying mathematical models can solve these inconveniences. Thus, an air pollution model can be developed using mathematical simulation of the physics and chemistry governing the transport, dispersion and transformation of pollutants in the atmosphere. This model is important in order to simulate the atmospheric conditions and behaviour. Throughout the years, this model had contributed in estimating the concentration of a specific area under certain specifications.

As a result, an atmospheric dispersion model for estimating the ambient concentration of PM10 will be developed by performing the correct actions and specifying the right parameters.

1.2 Problem Statement

Nowadays our atmosphere is contaminated with chemicals, particulate matter, or biological materials that can cause harm to living organisms and damages the environment. Particulates such as PM₁₀ mainly produced from automobile emissions may contribute to the greenhouse effect and global warming. During recent years the concerns about health effects of particles have increased considerably. This is partly due to results from epidemiological surveys showing that there is a correlation between the mass concentration of particles, and mortality and hospitalisation. (K unzli et al., 2000). Urban pollution plays an important role due to a high concentration of particle sources and a large population exposed to elevated particle concentrations. Air pollution can be identified from many sources such as point source, area source, line source and volume source. For line source, it is important to assess pollutant impacts near transportation facilities given that PM₁₀ is produced from the partial combustion of carbon-containing compounds, notably in internalcombustion engines. Therefore, an atmospheric dispersion model for line source should be developed in order to characterize pollutant dispersion over the roadway besides predicts air concentrations of PM₁₀ near roadways.

1.3 Objective

The objectives of this project are mainly:

- 1. To develop an atmospheric dispersion application that is reliable and cost-
- saving for line source air dispersion using Microsoft Visual Basic 6.0
- 2. To compare the results obtain with the actual value from a different air dispersion models and software.

1.4 Scope of Study

The scope of study for this project is as stated below.

- Develop the dispersion model using Microsoft Visual Basic 6.0
- Identifying and selecting the most practical atmospheric dispersion modelling

CHAPTER 2 LITERATURE REVIEW

2.1 Air Pollution Due to Traffic

Air pollution due to high level of traffic is caused mainly by the burning of fossil fuels, primarily oil in the form of petrol and diesel. The most prevalent pollutants from traffic are carbon monoxide, nitrogen oxides, volatile organic compounds, and particulates. For these emissions, transport sources in advanced countries constitute between 30 and 90 per cent of emissions from all sources. There are also lead compounds, and a smaller amount of sulphur dioxide and hydrogen sulphide. Asbestos may be released into the atmosphere when braking.

Most concern about traffic pollution has been expressed in relation to busy inner-city areas, where high vehicle flows and large numbers of pedestrians share the same streets. A number of countries now monitor the pollution levels in these areas, to ensure that internationally agreed standards are not exceeded. The worst conditions are experienced when there is a combination of high traffic and hot weather without winds; hospitals experience an increase in the number of asthma emergencies. especially of children. Concentrations are highest in or very close to the road, and reduce quite rapidly at even short distances away from the road, especially if there is any wind. However, apart from the direct health effects on people who breathe in traffic fumes, the chemicals interact to produce low-level ozone, which also contributes to global warming, and to produce "acid rain", which has damaging effects on plant life, in some cases in distant countries.

Large-scale American studies show that the mortality of persons rises, if they are exposed to fine particles over a longer period of time. There are also indications showing that living close to busy roads increases this risk significantly. Living on busy roads and chronic exposure to PM10 and NO2 are risk factors for diseases of

the respiratory system and reduced pulmonary function. In addition, mortality of diseases of the cardiovascular system and the respiratory system may be increased among exposed persons. From a German case study conducted by GSF Research Centre for Environment and Health in several regions of North Rhine-Westphalia from 2002 to 2005, 8 % of the women died, 3 % of them died of cardiopulmonary causes, i.e. diseases of the cardiovascular system or the respiratory system. Associations were found between cardiopulmonary mortality and living within a 50 m distance from busy roads, where the mortality was 70 % higher.

Birmingham University reported thousands of people in England have died from pneumonia caused by pollution. According to the study, published in the Journal of Epidemiology and Community Health, there is a "strong correlation" between deaths, engine exhaust fumes and other transport-related substances. Professor George Knox, from University of Birmingham, looked at details of atmospheric emissions, published causes of death and expected causes of death from 1996 to 2004. The data, gathered from 352 local authority areas in England, was used to calculate the impact of pollution on death rates. Result showed total of 386,374 people died from pneumonia in England during the eight-year period. This showed that correlations with pneumonia deaths were exceptional. High mortality rates were observed in areas with elevated ambient pollution levels. The strongest single effect was an increase in pneumonia deaths. He also said that road transport was the chief source of the emissions responsible although it was not possible to discriminate between the different chemical components. Calculations revealed that pneumonia, peptic ulcers, coronary and rheumatic heart diseases, lung and stomach cancers and other diseases were associated with a range of combustion emissions.

2.2 Particulate Matter (PM₁₀)

Particulate matter is the term for solid or liquid particles found in the air. Some particles are large or dark enough to be seen as soot or smoke. Others are so small they can be detected only with an electron microscope. Because particles originate from a variety of mobile and stationary sources (diesel trucks, woodstoves, power plants, etc.), their chemical and physical compositions vary widely. Particulate

matter can be directly emitted or can be formed in the atmosphere when gaseous pollutants such as SO₂ and NOx react to form fine particles.

The size of particles is directly linked to their potential for causing health problems. United States Environmental Protection Agency (EPA) is concerned about particles that are 10 micrometers in diameter or smaller because those are the particles that generally pass through the throat and nose and enter the lungs. Once inhaled, these particles can affect the heart and lungs and cause serious health effects. EPA groups particle pollution into two categories:

- "Inhalable coarse particles," such as those found near roadways and dusty industries, are larger than 2.5 micrometers and smaller than 10 micrometers in diameter.
- "Fine particles," such as those found in smoke and haze, are 2.5 micrometers in diameter and smaller. These particles can be directly emitted from sources such as forest fires, or they can form when gases emitted from power plants, industries and automobiles react in the air.

2.2.1 Sources of Particulate Matter

Particulate matter is composed of a wide range of materials arising from a variety of sources. These have been classified into three predominant source types:

- i. Primary particles arising from combustion sources (mainly road traffic);
- ii. Secondary particles mainly sulphate and nitrate formed by chemical reactions in the atmosphere; and
- iii. Coarse particles such as suspended soils and dusts, sea-salt, biological particles and particles from construction work.

It has been estimated by East Lindsey District Council that each of these three sources make up approximately one-third of total long-term average PM_{10} concentrations at urban background locations. The relevant contribution of

each source type varies from day to day according to meteorological conditions and quantities of emissions from mobile and static sources.

Particulate emissions can travel long distances. It has been estimated that around 20% of the primary fraction of annual mean PM_{10} arises from emissions from mainland Europe. Emissions from mainland Europe also contribute to around 50% of secondary particles (15% of total PM_{10}) in the UK, with much higher concentrations during years with more frequent easterly winds.

UK emissions of PM_{10} have declined from a level of 0.49 million tonnes in 1970 to 0.16 million tonnes in 1998. This reflects a trend away from the use of coal, particularly by domestic users. However, more recently road transport emissions of PM_{10} have been on the increase, particularly as the proportion of diesel vehicles has increased. This increase has offset some of the decline in emissions from other sources. Coal use and road transport contributed to 51% of UK emissions of PM_{10} in 1998. Although road traffic contributes to around 25% of national PM_{10} emissions, in city centres this proportion typically increases to 30 - 40%.

2.2.2 Particulate matter standard

National Ambient Air Quality Standards for Particle Pollution				
Pollutant	Primary Stds.	Averaging Times	Secondary Stds.	
Particulate Matter (PMua)	Revoked ⁽¹⁾	Annual ⁽¹⁾ (Arithmatic Mean)		
(11110)	150 μg/m ³	24-hour ⁽²⁾	· · · · · · · · · · · · · · · · · · ·	
Particulate Matter	15.0 μg/m ³	Annual ⁽³⁾ (Arithmatic Mean)	Same as Primary	
(* ***2.3)	35 μg/m ³	24-hour ⁽⁴⁾		

 Table 2. 1 Particulate Matter Standards (Source : EPA)

Units of measure for the standards are micrograms per cubic meter of air $(\mu g/m^3)$.

Footnotes:

(1) - Due to a lack of evidence linking health problems to long-term exposure to coarse particle pollution, the agency revoked the annual PM_{10} standard in 2006 (effective December 17, 2006).

(2) - Not to be exceeded more than once per year on average over 3 years.

(3) - To attain this standard, the 3-year average of the weighted annual mean $PM_{2,5}$ concentrations from single or multiple community-oriented monitors must not exceed 15.0 μ g/m³.

(4) - To attain this standard, the 3-year average of the 98th percentile of 24hour concentrations at each population-oriented monitor within an area must not exceed 35 μ g/m³ (effective December 17, 2006).

2.2.3 Highest PM10 contributor

According to the chart below, the highest source of contributing PM10 is from roadways followed by miscellaneous and fires.



National PM10 Emissions by Source Sector in 2002



2.2.4 PM10 Health Effect

In the year 2000, WHO had conducted studies relating to PM10 and its health effect.

Effects on experimental animals

The complexity of particulate matter, both physical and chemical, makes it very difficult to conduct animal bioassays that will reliably predict what will happen to humans when they are exposed to airborne particles in various settings. Differences in particle deposition and clearance from the lung between different experimental animal species and humans, briefly discussed above, only add to the complexity. Much work has been devoted to elucidating the effects of acid aerosols on animals; these studies are reviewed in the next section. In this section, some examples will be given of experimental studies aimed at understanding the role of airborne particles (other than acid aerosols) in the causation of adverse effects in the human lung.

Effects on humans

The data regarding controlled human exposure to particulate matter has been limited to sulphuric acid and acid sulphates in normal and asthmatic subjects. There are, however, a number of complicating factors that lead to differences in exposure which can produce inconsistent findings. These include technical difficulties in controlling both particle size and concentration adequately, and the hygroscopic properties of the particles. Fine hygroscopic particles can penetrate deeply into the respiratory tract but they grow in size and become dilute in the process.

Larger particles having diameters from a few micrometres upwards are more likely to affect the upper respiratory tract. Neutralization and buffering of sulphuric acid are liable to occur on inhalation depending on a number of factors including gaseous ammonia released by ammonia producing bacteria in the mouth and endogenous ammonia sources, the buffering capacity of airway mucus and the partitioning of airflow between the nose and the mouth.

Besides, studies suggest that air pollution exposure may be associated with adverse birth outcomes (Gray, 2007). Innovative geospatial methods were used to link NC Detailed Birth Records for 2000–2003 to USEPA PM_{10} and $PM_{2.5}$ monitoring data for pregnant women residing within 20km of a monitor. Maternal exposure to PM_{10} and $PM_{2.5}$ in the second trimester and during the entire pregnancy was negatively associated with birthweight (BWT). Compared to women living in areas with average PM levels, women living in areas with 10^{th} percentile levels of PM_{10} (PM_{2.5}) showed an 8 (7) g increase in BWT and those living in areas with 90^{th} percentile levels of PM_{10} (PM_{2.5}) showed a 9 (8) g decrease in BWT. Tobacco use was associated with 150g lower BWT in both PM models.

2.3 Atmospheric Dispersion Modelling

Atmospheric dispersion modelling is an essential step in the air quality assessment process as it is the only way to evaluate the impact of future changes in air pollutant emission sources. It is the mathematical simulation of how air pollutants disperse in the ambient atmosphere. Dispersion modelling is used to predict atmospheric concentrations of pollutants at specific locations. The process involves using a computer model to mimic the way pollutants are emitted from sources, and how the atmosphere disperses them. The model takes emissions from a source, estimates how high into the atmosphere they will go how widely they will spread and how far they will travel based on hourly meteorological data. The model then outputs the concentrations that will occur at the selected receptors. 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 pollutant.

For line source case, the determination of air pollution within urban streets is based on several factors such as the local (fixed and mobile) sources, the local dispersion (transport and pollutants by wind, dispersion by turbulence, chemical transformations) and the local emissions (from the neighbourhood streets). The numerous parameters that influence the dispersion of pollutants within the street

make the analysis of the developing airflow often complex. In particular, traffic increases the concentration of pollutants within the street, but at the same time the motion of the vehicles generates additional turbulence that modifies the concentration fields in the street and possibly enhances their dispersion (Kastner-Klein et al., 1998, DePaul and Sheih, 1986). Wind speed and direction also affect the dispersion of pollutants. It has been observed that one or more vortices may develop in the street depending on the wind speed and wind direction (Berkowicz et al. 1996, Dabberdt et al. 1973) as well as on the geometry of the street e.g. its aspect ration Height/Width, H/W (Oke, 1988). Radiation may cause photochemical reactions of the primary pollutants emitted by the vehicles (Harrison et al., 1999). It also changes the fields of temperature and the flow regimes in the street (Berkowicz et al., 1997, Sini et al., 1996).

2.3.1 Data Inputs

This section outlines various data inputs required for a dispersion modelling run. These include characteristics of each emission source, meteorological parameters such as wind speed and direction.

a) Emission Sources

Dispersion models require several pieces of information about each emission source being included in the model, including:

- Source type.
- Emissions of each pollutant for each time period being investigated.

Depending on the source type, some additional information about the sources is likely to be required to model dispersion of pollutant emissions. These additional information requirements include:

- Source layout, including location and height.
- For stack emissions, parameters including stack gas temperature, exit velocity, and inside stack diameter.
- For mobile sources, surface roughness length of surrounding area.

The data requirements and likely sources of information are listed below.

i. Source Type

Dispersion models for complex sites such as urban area provide categories for each of the source types likely to be found on the site. These categories are necessary because of the differences in the way that the sources are represented in the dispersion model. For example, stacks are modelled as stationary point sources with a rising plume whereas roadways may be modelled as a line source with no plume rise but with consideration of the effect of surface roughness on dispersion. Therefore, specification of the source category type tells the computer how to model a given source and which additional pieces of information are required.

ii. Emissions of Each Pollutant

The main goal of the source inventory is to estimate the emissions of pollutants from each source. The pollutants of concern at roadways are generally CO, NO_x , SO_2 , PM10, and HC. For some sources such as vehicle engines, emission factors are available for all of these. Other sources emit only one pollutant. For example, particulate matter is the only air pollution problem associated with sand or salt piles. The emissions inventory typically provides an average rate of emissions of each pollutant for each source.

iii. Location and Height of Emission Sources

The physical layout of the emission sources is required by a dispersion model because the goal is to provide a pollutant concentration in air that varies with location. To this end, all sources should be located on a master grid that is used for the dispersion model. The height of the emission point is also required for each source, as it is used in the Gaussian equation to calculate ground-level concentrations downwind.

iv. Stack Characteristics

Stack emissions, which make up a very small percentage of the overall emissions at airports, require an estimate of plume rise before the Gaussian approximation may be applied. Plume rise is a result of thermal buoyancy of the stack gas and the vertical momentum of the gas as it leaves the stack. Three parameters are required to calculate plume rise that are not otherwise collected in the emissions inventory: stack gas temperature, vertical velocity of the gas exiting the stack, and the inside diameter of the stack. These may be obtained by direct sampling of the stack.

v. Surface Roughness Length

The surface roughness length of the area surrounding the roadway is often a required input parameter in the dispersion modelling of emissions from mobile source. The surface roughness length, in meters or centimetres, is a measure of the near-surface wind resistance. Table 2.1 provides typical surface roughness lengths for a variety of land uses.

Surface Type	Surface Roughness Length (cm)
Smooth desert	0.03
Grass (4 cm)	0.14
Grass (5-6 cm)	0.75
Alfalfa (15.2 cm)	2.72
Grass (60-70 cm)	11,4
Wheat (60 cm)	22.00
Corn (220 cm)	74.00
Citrus Orchard	198.00
Fir Forest	283.00
City Land Use:	
- Apartment residential	370.00
- Central business district	321.00
- Office	175.00
- Park	127.00
- Single family residential	108.00

Table 2. 2 Surface	Roughness	Lengths f	or Various [Land Uses	(Source:	EPA)
	<u> </u>	<u> </u>			•	· · · · ·

b) Meteorology

Dispersion of pollutants in the atmosphere is largely dependent upon meteorological conditions, especially the following:

- Wind speed and direction
- Atmospheric stability
- Mixing depth

2.4 Meteorological Factors Influencing Dispersion

According to Durbin, P.A. and Pettersson Reif, (2001), some of the most important parameters that play a leading role in the dispersion of pollutants in the atmosphere are wind velocity, atmospheric turbulence, stability, temperature, humidity, etc. The pollutants get transported along the direction of wind. But it is the atmospheric turbulence that determines the lateral and vertical spread of the pollutants. Stability assumes a critical role in determining the amount of turbulence in the atmosphere and thus directly affects the level of dispersion.

2.4.1 Turbulence

Turbulence is a phenomenon associated with fluid flows. Fluid motion is governed by the *Navier Stokes* equations. They comprise a set of coupled, non-linear partial differential equations. They are the momentum equations (one each for the three components of velocity) and the continuity equation that conserves total mass. Furthermore, there is one equation each for temperature and any additional species to predict their transport. The inherent non-linearity in the equations gives rise to extremely complicated behaviour of the flow solution that is known as turbulence. There are no known analytical solutions to the *Navier Stokes* equations except for a few simplified cases. One has to resort to numerical techniques to make some progress.

Turbulent flows are characterized by vertical motions and high rates of dissipation. The vertical motion causes increased dispersion and strong rates of mixing. High dissipation rates contribute to substantial increase in pressure drop across flows in internal channels and also result in high drag across obstacles in flows. The turbulence in the atmosphere is the reason behind the dispersion of pollutants. If there were no turbulence, the pollutants would have just followed the streamlines of mean wind velocities, so point sources of pollutants would have given rise to long lines of pollutant transport with minimal mixing (due to molecular viscosity) in the lateral directions.

2.4.2 Modelling and Simulation of Turbulent Flows

The *Navier Stokes* are the governing equations of fluid mechanics. A complete solution of these equations with the correct initial and boundary conditions would exactly predict the flow field including the turbulence. This approach, known as the *Direct Numerical Simulation* (DNS) has been followed by many fluid dynamicists but huge computational resources are required. Still, DNS remains a very popular tool for detailed understanding of simple flows of academic interest. But it is not feasible to perform these massive computations for practical and industrial problems. Some level of turbulence modelling has to be introduced to alleviate this problem. In general, the higher the level of modelling involved, the greater is the possibility of generating erroneous results, but with skilful use of cleverly developed and carefully calibrated turbulence models, it is possible to obtain engineering results of a wide variety of problems within reasonable accuracy.

Large Eddy Simulation (LES) is a technique that is being increasingly used nowadays both in industry and in academia. Here, the large scales in the flow field are fully resolved numerically while the smaller scales are modelled. The rationale behind modelling the smaller scales (known as *sub-grid scale* (SGS) modelling) is that they are more universal and do not depend too much on the exact nature of the mean flow; this makes them more amenable to modelling. Some of the more popular SGS models are the *Smagorinsky* and the dynamic models.

Currently, the most widely used turbulence modelling technique in the industry is the *Reynolds Averaged Navier Stokes* (RANS) approach. In this method, the *Navier Stokes* equations are *ensemble*-averaged and the resulting RANS equations are solved numerically. However, due to the averaging, these equations contain additional unknown terms known as the *Reynolds Stress* terms that have to be modelled. The exact equations of these Reynolds stresses can be derived but they

contain even more additional unknown terms and this is the well known *turbulence closure* problem. Closure of these terms can be done at different levels of complexity giving rise to a complete hierarchy of turbulence models. The simplest ones construct constitutive relations for the Reynolds stress terms by means of *turbulent viscosity*. Closure of this turbulence viscosity can be done in different ways of varying complexity starting from pure algebraic *zero-equation* models to *oneequation* (*e.g.* Spalart-Almaras model) and *two-equation* (e.g. k- ε , k- ω *etc.*) models that require one and two partial differential equations respectively. More sophisticated models are the *second moment closure* (SMC) models that solve separate partial differential equations for each of the Reynolds Stresses. Reynolds scalar fluxes and variance in most cases.

2.4.3 Atmospheric Stability

Atmospheric stability is related to the vertical profile of density in the atmosphere. Spatial variation of temperature and specific humidity leads to a corresponding variation of density, which is known as density stratification. If cooler (and hence heavier) parcels of air reside above hotter (and hence lighter) parcels, then there is always a tendency of the heavier parcels to move down and the lighter parcels to move up. This kind of stratification is unstable and the associated turbulence is also higher. Stable stratification is a result of lighter parcels residing on top of heavier parcels and is characterized by low turbulence. Uniform density of air results in neutral stratification. Stability plays a direct role in the amount of turbulence present in the atmosphere and therefore significantly affects atmospheric dispersion.

2.4.4 Modelling Turbulent Dispersion

Modelling turbulent dispersion in the atmosphere is extremely challenging because of the complicated physics mentioned above. Broadly, there are two different modelling approaches – the *Eulerian* and the *Lagrangian* techniques. The fluid motion is mostly defined by equations in the *Eulerian* frame where the fundamental parameters like velocity, pressure and density of the fluid are considered at fixed points in space. The alternate route is the *Lagrangian* technique where these parameters are considered at each individual fluid particle as it moves along its trajectory. In general, the *Eulerian* approach will give rise to partial differential equations as the variation of the flow quantities occur in both space and time, while the *Lagrangian* route will result in ordinary differential equations as the parameters will vary only in time. In dispersion modelling, the flow-field is assumed to be known and the concentration field is required to be computed.

The pollutant source is specified as an input in most pollutant dispersion problems. In general, there may be a large number of sources that may vary in size and shape (e.g. point, line, area and volume sources). However, a source of any shape and size can be modelled as a collection of suitably chosen points. Moreover, the principle of superposition is usually invoked which essentially means that computations can be carried out for each source individually and subsequently the results can be added to get the concentration field for the combined effect of all the sources. Therefore, the point can be regarded as the most fundamental form and a lot of research has focussed on this form of source. However, if the concentration field due to the different sources interact with each other (as in chemical reactions), the assumption of superposition can no longer be valid.

2.5 Analytical Models of Dispersion

There are some analytical models that are widely used especially for regulatory purposes mainly because of their simplicity. Most of these belong to the category of *Gaussian Plume* diffusion models. The concentration field predicted by these models show Gaussian distribution. It has a theoretical basis in the sense that both Eulerian and Lagrangian forms of the governing equations in extremely simplified cases give solutions of this form. The solutions are valid for instantaneous point sources and continuous point and line sources. The main assumptions associated with these models are uniform, steady flow with homogeneous turbulence. In general, these are not met in actual atmospheric flows and hence more sophisticated models are required.

2.5.1 Eulerian Approach Towards Describing Turbulent Dispersion

In this approach, the exact governing equation is a transport equation of a scalar (pollutant concentration in this case). Any level of modelling for turbulence will give rise to unknown terms due to *Reynolds scalar fluxes*. It is these terms that result in

high rates of dispersion for the scalar. Investigators in the atmospheric sciences community have widely used gradient transport theories to close the scalar fluxes. These theories, also known as K theories, advocate the use of turbulent diffusivities to address the turbulent scalar diffusion. Further simplifications can be introduced to make the diffusivity isotropic and constant. Analytical solutions exist for these cases making the approach very attractive. Anistropic and some simple, prescribed onedimensional (in the vertical direction) forms of diffusivities can also give rise to analytical solutions and fairly accurate predictions in some cases. However, in order to get meaningful solutions in complex flows, more complicated forms of diffusivities have to be incorporated in the scalar transport equation, thereby necessitating the use of numerical techniques to solve the equations. Often, when one resorts to numerical simulation, the fluid flow equations along with the associated turbulence models are also solved. The two equation and other lower forms of turbulence models generate eddy viscosities for momentum. Scalar diffusivities are then evaluated by adding a constant value of turbulent Prandtl number as a factor. The more sophisticated and expensive second moment closure models solve separate equations for the *Reynolds stresses* and the *Reynolds scalar fluxes*. The unsteady, three-dimensional large-eddy-simulation (LES) currently remains the most expensive and accurate technique for predicting dispersion in atmospheric flows and generally requires the use of large supercomputers.

2.5.2 Lagrangian Approach Towards Describing Turbulent Dispersion

This approach is generally regarded as more fundamental. Numerical modelling by this technique in most cases assumes the particles that are released at sources to be exactly the same in size, shape and chemical composition as any other fluid particle in the flow field. However, these particles coming out from the sources are viewed as *tagged* and the study of how they move in the atmosphere comprises the dispersion modelling effort. There are two broad ways of doing the simulation. One is to do a complete and detailed numerical computation by the Eulerian approach like the LES to obtain both the mean and the turbulent velocities in the entire flow field and use these values to compute the Lagrangian trajectories of the *tagged* particles. This technique, due to its higher accuracy, has been followed by some researchers but it is prohibitively expensive, entailing the use of very powerful workstations and

supercomputers. The other, more popular method needs only some mean values as input and calculates the turbulent, fluctuating values by use of a *Lagrangian Stochastic Model* (LSM). In general, the LSM is actually a set of *stochastic differential equations* (SDE's), defining the turbulent velocities and in some cases the turbulent temperature. The mean values that are required as input can be obtained from simple experimental observations, empirical relations or some relatively inexpensive Eulerian RANS models. The LSM is the heart of the Lagrangian technique and in most cases the accuracy of the predictions depends wholly on the sophistication of the LSM. These models have progressively developed over the years from the simple models for homogeneous, isotropic turbulence to more complicated ones that take turbulence anisotropy, inhomogeneity and stratification into account. Recently, there have been attempts to obtain direct mathematical relationships with the sophisticated turbulence models like the SMC, resulting in enhanced physics-capturing capabilities and sophistication of the LSM's.

CHAPTER 3 METHODOLOGY

3.1 Information and Data Collection

Initially, most information is obtained from literature review. Much research is done in order to identify the best model by referring to environmental engineering books, journals and articles. Case studies are conducted to help in the selection of model process. Meteorological data can be estimate with justifications or can be obtained by the Department of Environment (DOE).

3.1.1 Emission Rate

The emission rate per unit length (Q) of the roadway is used as input for the analytical air quality models. The method of vehicle source emission factors is used to calculate it. Vehicle source emission factor is defined as the quantity of a pollutant emitted when a vehicle runs a unit length and depends upon the volume of traffic using a road, its composition and the operating mode of the vehicles. Hence, Q is given by

$$Q = E_f T_v (g_{mh})$$
(3.1)

Where

 E_f = pollutant emission factor in g/m-vehicle T_v = vehicle density in vehicles per hour

Emission factors can be determined by measuring emissions for various types of diesel and petrol cars using proper instrumentation (Luhar and Patil, 1986). Besides, various softwares have also been developed in order to estimate the emission factor of pollutant. In this case, user of the application can either key in the emission rate or emission factor depending on the data available.

3.1.2 Modelling Equation for Line Source Dispersion Model

In this case, the model focuses more on street canyon scenario. Street canyons are a common feature of densely populated urban areas. In these locations, multi-storey residential or office buildings surround relatively narrow streets reducing natural air ventilation. This may result in high concentration of traffic-related pollutants in heavily congested streets. The pollutant dispersion in a street canyon is influenced by several parameters such as wind direction, wind speed, temperature and traffic conditions. The most characteristic feature of the street canyon wind flow is the formation of a wind vortex so that the direction of the wind at street level is opposite to the flow above roof level. Concentrations are calculated as a sum of the direct plume contribution and the recirculating pollution as shown in Figure 3.1.



Figure 3. 1 Schematic illustrations of the basic model principles. (Berkowicz, 1997)

a) Direct Contribution

The selected model is calculated using a simple plume model (Berkowicz, 1997). It is assumed that traffic emission is uniformly distributed across the canyon. The emission field is treated as a number of infinitesimal line sources aligned perpendicular to the wind direction at the street level and with thickness dx. The concentration at a point located at a distance x from the line source is given by

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$$C_{d} = \sqrt{\frac{2}{\pi}} \cdot \frac{Q}{u_{b}} \int_{0}^{t_{max}} \frac{dx}{\sigma_{z}(x)}$$
(3.2)

The dispersion parameter of the plume travelling a distance x is given by

$$\sigma_z(x) = \sigma_w \frac{x}{u_b} + h_o \qquad (3.3)$$

Here h_0 is the initial (immediate) dispersion in the wakes of the vehicles and we assume that $h_0 = 2m$. The vertical dispersion parameter, σ_z , is modelled assuming that the dispersion of the plume is solely governed by the mechanical turbulence. The mechanical turbulence is taken to be generated by two mechanisms: by the wind and by the traffic in the street.

$$\sigma_{w} = \left((\alpha u_{b})^{2} + \sigma_{w_{0}}^{2} \right)^{\frac{1}{2}}$$
(3.4)

where σ_w is the vertical turbulent velocity fluctuation, α is a constant and σ_{wo} is the traffic created turbulence. The proportionality constant, α , is given a value of 0.1, what corresponds to typical levels of mechanically induced turbulence.

Wind Speed at Street Level

The wind speed at street level, u_b , is calculated assuming a logarithmic reduction of the wind speed at roof top towards the bottom of the street. A simplified dependence on the angle between wind and the street axis is also introduced.

$$u_{b} = u_{t} \frac{\ln(h_{a})}{\ln(H)} (1 - 0.2p\sin\phi)$$
(3.5)

where H is the average depth of the canyon, while $p = H_{upwind}/H$ and this ratio is not allowed to exceed 1. h_0 is the initial dispersion height defined in (3.3). In the case of openings between buildings on the upwind side ($H_{upwind} = 0$) the wind speed will be the same as for a parallel flow.

Traffic Induced Turbulence

Traffic-produced turbulence is important for estimation of pollution concentration levels in streets. In urban street canyons there is usually a dense flow of vehicles, and the turbulence field created by them cannot be considered as a simple superposition of non-interacting vehicle wakes. An approach suggested by S. Di Sabatino, 2002 is the same as the simpler approach, which is more suitable for street canyons, which was suggested by Hertel and Berkowicz (1989c). Vehicles in the street are considered as moving flow distortion elements creating additional turbulence in the air.

$$\sigma_{wo} = b \left(\frac{N_{veh} \cdot V \cdot S^2}{W} \right)^{1/2}$$
(3.6)

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where V is the average vehicle speed, N_{veh} is the number of cars passing the street per time unit, S² is the horizontal area occupied by a single car, W is the width of the street and b is an empirical constant related to the aerodynamic drag coefficient. The empirical constant identified to be, b = 0.3.

Canyon Ventillation Velocity

Canyon velocity ventilation can be determined by equation below.

$$\sigma_{wt} = \left((\lambda u_t)^2 + (0.4\sigma_{wo}^2) \right)^{\frac{1}{2}}$$
(3.7)

where u_t is the wind speed at the top of the canyon and the term with σ_{wo} is added in order to account for the traffic created turbulence. The proportionality constant, λ , is given the same value as α , i.e. 0.1. This is the presently used approach, but contrary to the street level turbulence, some dependence on ambient air stability conditions can not be excluded and further research on this subject is needed.

b) Recirculation Contribution

Considering the simple case when the vortex is totally immersed inside the canyon (this is the case when W/H<1), the recirculation contribution is,

$$C_{rec} = \frac{Q}{\sigma_{wl}W}$$
(3.7)

c) Concentration at Leeward and Windward

The pollution plume from the traffic in the street is known by the wind vortex towards the leeward side, whole on the windward side, the impact is only from the air that has recirculated in the street.

Leeward side,

$$C_{L} = \frac{KQ/3.6}{(u+0.5)\left[(x^{2}+z^{2})^{\frac{1}{2}}+2\right]}$$
(3.8)

Windward side,

$$C_{W} = \frac{KQ/3.6}{W(u+0.5)}$$
(3.9)

where,

C₁ is the concentration (μg/m³);
Q is the emission rate (g/m/s);
u is the wind speed at roof level (m/s);
W is the street width(m);
x and z are horizontal distance and height (both in m) of the receptor point relative to the traffic lane;
K is an empirically determined constant (K=7)

3.2 Air Pollution Modelling Application Procedures

In developing the software, specifically five stages are involved, namely, planning the application, building the Graphical User Interface (GUI), writing the computer program, testing and debugging the application through use of case studies and deploying the project into a distribution package (El-Harbawi, 2008). Table 3.1 summarises the procedures.

Stage 1	Application planning	In order to ensure proper execution of the program, specific information must be identified, which may be user-provided, and/or internally generated-information (data that will be retrieved from a database). Analysis of this information will enable selection of appropriate objects and controls to display this information on the GUIs or to accept user defined input data. Microsoft Visual Basic 6 (VB6) will be used to develop the application.
Stage 2	Building the Graphical User Interface (GUI)	The design of GUIs implements object-oriented programming (OOP) and will use multiple GUIs, which give rise to large amounts of data. VB6 is used to develop the logical application front-end GUI, which provides input for the mathematical models running in the background (programming code). Functionality of the system will include database retrieval, modification and addition.
Stage 3	Writing the computer program	The program will be written in standard VB6 and distributed in object format with the source code. After creating the interface for the application, it is necessary to write the code that defines the applications behaviour. The computation of the mathematical models for air pollution dispersion will be simulated using VB6 program (code).
Stage 4	Stand-alone application developers	In order to provide spatial solutions to users who are not specialised in programming language, developers need the ability to build domain specific, easy-to-use application. VB6 has a debugger integrated into its development environment. This is in many cases a valuable tool when debugging VB code.

Table 3.	. App	lication	deve	lopment	stages
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	Software	The validation and verification must be performed after the
Stage	validation	successful development of the software using results from the
5	and	development software and comparing them to those from
	verification	published literature and other experimental data.

3.2.1 Application Planning

Planning of the application is essential in order to identify various tasks that the application needs to perform (El- Harbawi et. al, 2008). The application is given the name LiSM software. At this stage, the logical relation of these tasks and the objects to which each task will be assigned are identified. The events required to trigger an object into executing it assigned tasks are also classified. Finally a sketch of the graphical user interface is prepared. The application should have the capability to compute the consequences from release hazardous gas from industrial. The application must also be able to save the results in different formats.

The next task is to identify information that is necessary for the proper execution of the program. Research on mathematical models applicable to line source dispersion is conducted by browsing through journals, books and internet. After selecting the most suitable model, data is collected to be used as inputs for the software or atmospheric dispersion model and is classified into user provided information. The data must include the meteorological conditions, the emission source, traffic parameter and other related information. The meteorological data that must be considered in this case is only the wind speed and wind direction. The emission source data is specified as the emission rate which can be obtained by other softwares or models. The traffic parameters consider the traffic density in the area and its average speed. Analysis of this information assisted in the selection of appropriate objects and controls to display this information on the graphical user interface or to accept input data from users.

3.2.2 Building the Graphical User Interface (GUI)

The application designed based on object-oriented programming. It has been designed using multiple Graphical user interfaces (GUIs), which give rise to a large amount of data involved. An interface in Microsoft Visual Basic 6 (VB6) is called a form and has a code window attached to it, where all computer programs (codes) related to the objects in the form are written. However, there is a common code module that can be added to a VB6 application.

All programs written in this module and variables declared there can be . used by any GUI in the application. Each form has specific tasks defined by the functions of the objects placed on it. All the forms are logically connected as showed in Figure 3.2.



Figure 3.2 Air pollution modelling procedures

3.2.3 Writing the computer program

The application is created using some objects which are implemented through VB6, textboxes to enter input data by users, labels to provide identification to other objects in interface and to display output data that the user cannot modify and command buttons that are used for initiating the event procedures for all other objects in the interface. Key factors affecting GUI design include the use of colours and animations act as traction to users and therefore their use is recommended. In all the GUIs, information flows in the top to bottom and left to right fashion. VB6 is used to develop the application as front-end (GUI) and simulate the mathematical models for pollutant in the back-end (codes).

Sketches of the GUIs used for each procedure are made to show the expected structure of all the interfaces.

a) Emission Tab

Estimating the emission is important for line source dispersion model. In this application, user may key in the emission rate. If the emission rate is impossible to be obtained, user may key in the emission factor which LiSM then can calculate the emission rate. Emission factor can be obtained from EPA handbook or other emission related software. Below is an example of LiSM interface when estimating the emission rate.



Figure 3. 3 Emission tab interface

b) Parameters Tab

For estimation of the concentration of PM10 at leeward and windward side, user is required to key in wind speed, wind direction, building height, street width, and number of traffic lane. Example of the interface is as below.



Figure 3. 4 Parameters tab interface

c) Result Tab

The calculated concentration will be represented in a form of list which will be use to plot a graph. User can choose whether to observe the value in VB6 formatted graph or in Microsoft Excel.



Figure 3. 5 Result tab interface

This software is also designed to alert the users if the value entered is not valid. The error message will appear after the software calculates the input data entered by users and compare it with the valid values programmed in it. All input data will be retrieved by the codes, processed and displayed in the interface. The results can be saved as text file of word file.

3.2.4 Software Validation

Validation is the assessment of the accuracy of a computational simulation by comparison with experimental data. The validation process confirms the right system is being built while verification process ensures that the design solution has met the systems requirement and that the system is ready for use in the operational environment.

CHAPTER 4 RESULTS AND DISCUSSION

4.1 Data Gathering and Analysis

Case study of experimental site was conducted in Jagtvej Street in Copenhagen (M.Ketzel, 2004). The street is identified to be a street canyon and the details are as follow.

Emission rate are estimated by referring to emission factor in specific countries.

Number of vehicles per day	22,000
Width of street (m)	25
Average buildings height (m)	18
Average wind speed (m/s)	4
Distance to receptor, x (m)	10
Height of receptor, z (m)	2
Average vehicle speed (km/hr)	50

Table 4.1 Data available for Jagtvej Street

4.2 Results

4.2.1 Data Processing

Data processing is done in when all the data collected is keyed in into the software. The results obtained will represent the calculated emission rate or level of concentration at the area.



Figure 4. 1 Emission tab interface with display result

Emission	Paramatere	Ŷ	Beaut
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La companya di secondari	·····	Wind Speed	4 m/s
	/ Data output	Wind Direction	90 degree
Reoiroulating	/ · · · · · · · · · · · · · · · · · · ·	Building Height	18 meter
18.6021 _{/E} ///		Street Width	25 meter
		Number of Traffic Lane	2
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Figure 4. 2 Parameters tab display with result



Figure 4. 3 Result tab interface displaying results

4.2.2 Output Analysis

In the final stage, the pollutants concentration which is represented by plotted graph is analyzed to know the potential environmental and health effects.



Figure 4. 4 Graph of Concentration Vs. Distance From Receptor

The graph above describes the level of concentration to the distance from the receptor. The receptor here is assumed to be a person at the side of the road.

Table 4.2 Result of measured and calculated

Measured circulated PM ₁₀ concentration from case study	$17.2 \ \mu g/m^3$
Calculated circulated PM ₁₀ concentration from LiSM Software	18.6 μg/m ³
Error	8%

4.3 Discussion

From the graph shown above, it is known that the trend of line source dispersion is that the highest concentration is at the distance shortest to the receptor. Therefore in every road or street canyon, the highest concentration of pollutant will have effect on the people walking at the side of the road.

Moreover, the error between the case study result and the result calculated from LiSM software was identified to be very low as the concentration was calculated in $\mu g/m^3$. Since μg is a very small value, high level of accuracy is needed. In that case, the mathematical model used for LiSM Software is considered as being quite

accurate and acceptable and can be used compared to the other mathematical models tested.

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CHAPTER 5 CONCLUSION AND RECOMMENDATION

5.1 Conclusion

Assessment of the hazards created by the pollutants emitted from the vehicles can be carried out by the use of mathematical models to calculate the consequences of emissions. The mathematical models are difficult to implement manually for a number of reasons; such as the fact that the calculations involved are difficult and time consuming to perform, a large number of these calculations are required, there are many event outcomes to follow and it is hard to keep track of them. For these reasons, the best estimation can be done by using air pollution software. The framework of developing of air pollution software was described in this paper. The software is called LiSM (Line Source Dispersion Modelling Software) and it was developed using Visual Basic programming language. The software will run under Windows and will be designed to work as a stand alone user-friendly application. The output of the result can be in VB6 graph format or Microsoft Excel format.

For the time being, the model only applies for street canyon condition. It is assumed that the dispersion would result from the atmosphere-induced turbulence and parameters which are evaluated independently. Based on the sensitivity analysis conducted in the literature, the surface roughness and stability class are not required for the model.

LiSM Software is considered to be quite accurate due to a small percentage of error between the average concentration of measured and calculated concentration based on the data from case study. The software is user-friendly and can be understood easily besides being simple and requires minimal input from user. These are important features for any atmospheric dispersion model and can be applied for teaching purposes. LiSM Software is flexible for any modification. Therefore, the model can be developed for future use.

5.2 Recommendation

There are still uncertainties considering the inputs variables and further modification will be done to the model. The sensitivity of the software need to be further identified that is the verification of the boundary of the model. Besides, the software is potential to produce different outputs in addition to distance versus concentration such as wind speed versus concentration, wind direction versus concentration and also the effect on concentration towards different height of building and width of street.

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pendix A: Suggested Milestone for the	• Detail/ Week		Selection of Project Topic	Preliminary Research Work	Submission of Preliminary Report	Seminar 1 (optional)	Project Work	Submission of Progress Report	Seminar 2 (compulsory)	Project work continues	Submission of Interim Report Final Draft	Oral Presentation
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Suggested milestone Process

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Appendix B: Suggested Milestone for the Second Semester of 2-Semester Final Year Project

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Suggested milestone

Process