NOx Emission Modelling and Simulation Using Point Source Dispersion Model

by

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CERTIFICATION OF APPROVAL

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Chemical Engineering Programme
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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.

NUR FARHANA BINTI DZULKAFLI

ABSTRACT

Process industry is a leading industrial sector in Malaysia and a vital part of the national economy. However, emissions of gases are unavoidable events during activities in process industry which will cause air pollution. The objective of this project is mainly to develop a computer simulation program of point source dispersion using Visual Basic software. The purpose of this software is to estimate the NOx concentration after the gas is released from the industrial stacks. This software is also used to estimate the percentage of people affected as a result from the exposure to NOx at certain concentration. The application is called Point Source Dispersion Software (PSDS) and it is specifically developed for emission of pollutant gases released from industrial stacks. Pasquill equation which modified by Gifford is used in this software. The model consider the atmospheric conditions, stack parameters and distance as the inputs of the simulation program. The simulation program is complex and this is the reason why the computer simulation is necessary in order to derive the reliable results. The results of PSDS show the concentration of respective pollutant gases over the distance as well as the percentage of people affected as a result from the exposure to the pollutant at certain concentration. The results from this software are validated with data from case studies and SCREEN3 (US EPA air pollution modelling software) to identify any error occur during writing the program.

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INTRODUCTION

1.1 BACKGROUND

Industrial activities are one of the major contributors to air pollution due to the emission of various pollutant gases such as nitrogen oxides (NOx), particulate matter (PM), carbon monoxide (CO), sulful dioxide (SO_2), and lead. These pollutants can affect human, animal, vegetation health or even can erode structures if present in large quantities.

In order to predict the air quality impacts from the industrial activities, air quality models are used. Air quality models are valuable tools in air quality management. Models are mathematical descriptions of pollution transport, dispersion and related processes in the atmosphere (DEQ, 2000). For point source dispersion, an air quality model is used to estimate the air pollutant concentration over downwind distance.

The air quality model provides a cost effective way to analyze impacts over a wide spatial area where factors such as meteorology, topography and emissions from nearby sources could be important (DEQ, 2000). It is important to predict the ground level concentrations of the pollutants that have released from industrial stack to the environment.

1.2 PROBLEM STATEMENT

Process industry is a leading industrial sector in Malaysia and a vital part of the national economy. However, emissions of gases are unavoidable events during activities in process industry which will cause air pollution. Burning of fuels in furnaces and some operations will produce emissions of pollutant gases and particulates from the stacks. The released of pollutant gases and particulates at certain concentration could harm human health, the environment, and cause property damage. Nitrogen oxides (NOx) are one of the pollutant gases released from the stacks which formed due to hydrocarbon burning. Computer simulation software for point source dispersion model has been developed to estimate the pollutant concentrations which released from the stacks.

1.3 SIGNIFICANT OF THE PROJECT

The significance of the project is that once the development of this software is completed, companies and industries can utilize this software to assess the air quality and predict the impacts to the environment and health. This software also could assists in controlling air pollution, in reducing harmful air pollutant exposure to environment as well as to predict future air pollutant concentration.

1.4 OBJECTIVES

The main objectives of this project are:

- To develop a computer simulation program using point source dispersion model. This software is able to estimate NOx concentration after the gas is released from the industrial stacks.
- To estimate the percentage of people affected as a result from the exposure to NOx at certain concentration.
- To validate and verify the results with established software and also with data from case study.

1.5 SCOPE OF STUDY

An air pollution modelling software is developed through this project which is capable in solving the mathematical equations of point source dispersion. The model used in the software is the point source dispersion model developed by Pasquill and modified by Gifford which is existing model that is developed outside of this project. Point Source Dispersion Software (PSDS) is developed using Visual Basic language which will simulate and solve the mathematical equations based on the input that keyed in by the user. The results from PSDS simulation will be validated and verified with other established dispersion modelling and also compared with results from established data.

The scopes of study for this project are:

- Selection the most suitable model for point source dispersion which to be used in the software.
- Familiarization with Visual Basic 6.
- Developing a computer simulation program for point source dispersion using Visual Basic 6.
- Verify and validate the result from the simulation using other established dispersion modelling software and established data.

CHAPTER 2

LITERATURE REVIEW

2.1 AIR POLLUTION

Air pollution has been defined as the presence of substances in the ambient atmosphere, resulting from the activity of man or from natural processes, causing adverse effects to man and the environment (Weber, 1982). Pollution is actually comes from a Latin word which is pollutus. Pollutus means unclean or dirty. Thus, air pollution is usually defined as an atmospheric condition in which substances are present at concentrations higher than their normal ambient (clean atmospheric) levels to produce significant effects on humans, animals, vegetation, or materials (Seinfeld, 1986).

The air pollution could be caused by natural or man made chemical elements whether in form of gaseous, liquid, or solid. Those pollutants could harm human health, the environment, and cause property damage. Human activities have caused air pollution ever since our ancestors began building fires. But it became a serious problem only during the last 200 years when growing population and industrialization produced vast quantities of contaminants. The total worldwide emissions of these pollutants are around 2 billion metric tons per year (Arya, 1999).

World Health Organization (WHO) is the directing and coordinating authority for health within the United Nations system. It is responsible for providing leadership on global health matters, shaping the health research agenda, setting norms and standards, articulating evidence-based policy options, providing technical support to countries and monitoring and assessing health trends. The WHO states that air pollution is a major environmental risk to health and is estimated to cause approximately 2 million premature deaths worldwide per year. Exposure to air pollutants is largely beyond the control of individuals and requires action by public authorities at the national, regional and even international levels (WHO, 2008).

2.2 SOURCE OF AIR POLLUTION

Air pollutant sources can be categorized according to the type of source, their number and spatial distribution, and the type of emissions. Categorization by type includes natural and anthropogenic sources (Liu and Lipták, 2000). Natural air pollutant sources include (Liu and Lipták, 2000):

- Dust from natural sources.
- Methane, emitted by the digestion of food by animals.
- Radon gas from radioactive decay within the Earth's crust.
- Smoke and carbon monoxide from wildfires and volcanic activity, which produce sulfur, chlorine, and ash particulates.

Anthropogenic sources include (Liu and Lipták, 2000):

- Stationary sources, such as smoke stacks of power plants, manufacturing facilities, municipal waste incinerators.
- Mobile sources, such as motor vehicles, aircraft.
- Marine vessels, such as container ships or cruise ships, and related port air pollution.
- Burning wood, fireplaces, stoves, furnaces and incinerators.
- Oil refining, and industrial activity.
- Chemicals, dust and controlled burn practices in agriculture and forestry management.
- Fumes from paint, hair spray, varnish, aerosol sprays and other solvents.
- Waste deposition in landfills, which generate methane.
- Military, such as nuclear weapons, toxic gases, germ warfare and rocketry.

Table 2.1 summarizes the sources and sinks of the majority of pollutants.

Table 2.1: Natural and anthropogenic sources of a selection of trace gases (Cox and Derwent 1981).

Compound	Natural sources	Anthropogenic sources
	Carbon-containing compounds	
Carbon dioxide (CO_2)	Respiration; oxidation of natural CO; destruction of forests.	Combustion of oil, gas, coal and wood; limestone burning.
Methane (CH_4)	Enteric fermentation in wild animals; emissions from swamps, bogs etc., natural wet land areas; oceans.	Enteric fermentation in domesticated ruminants; emissions from paddy fields; natural gas leakage; sewerage gas; colliery gas; combustion sources.
Carbon monoxide (CO)	Forest fires; atmospheric oxidation of natural hydrocarbons and methane.	Incomplete combustion of fossil fuels and wood, in particular motor vehicles, oxidation of hydrocarbons; industrial processes; blast furnaces
Light paraffins, C_2–C_6	Aerobic biological source.	Natural gas leakage; motor vehicle evaporative emissions; refinery emissions
Olefins, C_2–C_6	Photochemical degradation of dissolved oceanic organic material.	Motor vehicle exhaust; diesel engine exhaust.
Aromatic hydrocarbons	Insignificant	Motor vehicle exhaust; evaporative emissions; paints, gasoline, solvents.
Terpenes ($C_{10}H_{16}$)	Trees (broadleaf and coniferous); plants.	Refrigerants; blowing agents; propellants.
CFCs & HFCs	None	
	Nitrogen-containing trace gases	
Nitric oxide (NO)	Forest fires; anaerobic processes in soil; electric storms.	Combustion of oil, gas, and coal.
Nitrogen dioxide (NO_2)	Forest fires; electric storms.	Combustion of oil, gas, and coal; atmospheric transformation of NO.
Nitrous oxide (N_2O)	Emissions from denitrifying bacteria in soil; oceans.	Combustion of oil and coal.
Ammonia (NH_3)	Aerobic biological source in soil Breakdown of amino acids in organic waste material.	Coal and fuel oil combustion; waste treatment
	Sulfur-containing trace gases	
Dimethyl sulfide (DMS)	Phytoplankton.	Landfill gas.
Sulfur dioxide (SO_2)	Oxidation of H_2S; volcanic activity.	Combustion of oil and coal; roasting sulfide ores.
	Other minor trace gases	
Hydrogen	Oceans, soils; methane oxidation, isoprene and terpenes via HCHO.	Motor vehicle exhaust; oxidation of methane via formaldehyde (HCHO).
Ozone	In the stratosphere; natural NO–NO_2 conversion.	Man-made NO–NO_2 conversion; supersonic aircraft.
Water (H_2O)	Evaporation from oceans.	Insignificant.

2.3 AIR QUALITY IN MALAYSIA

The industries in Peninsular Malaysia are rubber and oil palm processing and manufacturing, light manufacturing industry, electronics, tin mining and smelting, and logging and processing timber. Sabah has logging and petroleum production while Sarawak has agriculture processing, petroleum production and refining, and logging. Oil and gas industry as well as petrochemical industry are among the major industries in the country that affecting air quality (ADB, 2006).

Malaysia's economic growth is mainly based on its manufacturing (especially electronics), chemical and rubber industries. Higher production rates also lead to higher emissions of organic and inorganic gases, chemicals and dust. Different industries emit different pollutants. For example, the chemical industry releases emissions that contain many nitrogen and sulphur compounds while refineries discharge sulphur dioxide and hydrocarbons. The metal working industry is partially responsible for the emissions of sulphur dioxide and large amounts of toxic dust. Human activities have resulted in harmful substances and polluting emissions being released into the air. They endanger our health and our natural ecosystem, and lead to an additional greenhouse effect (DOE, 2006). Figure 2.1 shows the estimation of air pollutant emission load from all sources in Malaysia in year 2005 and 2006. NOx has second highest emission load in year 2005 and 2006 after CO and followed by SO_2, and particulate matter (PM).

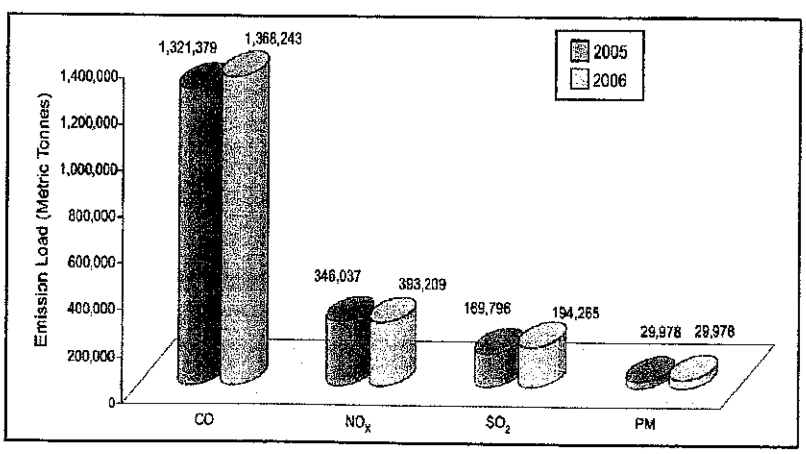

Figure 2.1: Air Pollutant Emission Load from All Sources, 2005 – 2006 (DOE, 2006)

A study from the Department of Environment (DOE) in 2005 to 2006 as in Figure 2.2 showed that motor vehicles contributed 70% to NOx emission. Other sources contributing to air pollution were 24% from industries and 6% from power stations (DOE, 2006).

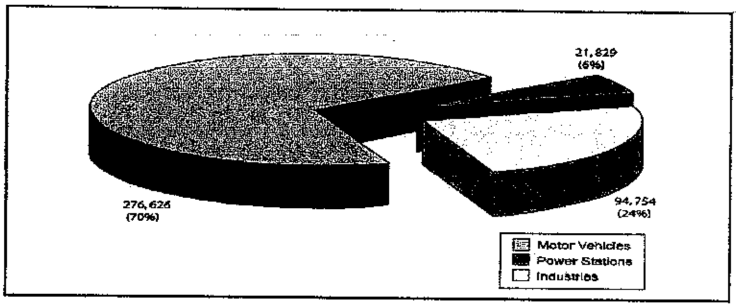

Figure 2.2: NOx Emission by Sources (Metric Tonnes), 2005 – 2006 (DOE, 2006)

2.4 MALAYSIA AIR POLLUTION STANDARDS

In 1989, Department of Environment (DOE) in Malaysia formulated a set of air quality guidelines called the Recommended Malaysian Air Quality Guidelines (RMG) (see Table 2.2). Based on RMG, DoE subsequently developed the Malaysian Air Quality Index (MAQI) in 1993 (ADB, 2006). The limits given are the basis for assessing atmospheric load in Malaysia. The figure is corresponding to international guidelines for assessment.

Table 2.2: Malaysia and WHO 2005 Ambient Air Quality Guidelines (Yahya and Ishak, 2006)

Pollutant	Averaging Time	Malaysian Air Quality Guidelines		WHO (2005)[1]
		ppm	μg/m³	
Sulfur dioxide (SO_2)	1 hr	0.13	350	
	24 hrs	0.04	105	20
PM_{10}	24 hrs		150	50
	1 year		50	20
TSP	24 hrs		260	—
Nitrogen dioxide (NO_2)	1 hr	0.17	320	200
	24 hrs			—
	1 year	0.04	90	40
Carbon monoxide (CO)	1 hr	30.00	35 mg/m³	
	8 hrs	9.00	10 mg/m³	
Ozone (O_3)	1 hr	0.10	200	—
	8 hrs	0.06	120	100
Lead (Pb)	3 months		1.5	1.5

2.5 NITROGEN OXIDES (NOx)

Nitrogen oxides or NOx is the generic term for a group of highly reactive gases, all of which contain nitrogen and oxygen in varying amounts. Many of the nitrogen oxides are colorless and odorless. Nitrogen oxides form when fuel is burned at high temperatures, as in a combustion process. The primary sources of NOx are motor vehicles, electric utilities, and other industrial, commercial, and residential sources that burn fuels. Since 1970, EPA has tracked emissions of the six principal air pollutants which are carbon monoxide, lead, nitrogen oxides, particulate matter, sulfur dioxide, and volatile organic compounds. Emissions of all of these pollutants have decreased significantly except for nitrogen oxides which have increased approximately 10 percent over this period (US EPA, 1998).

2.5.1 NOx Production

The two principal oxides of nitrogen are nitric oxide (NO) and nitrogen dioxide (NO_2). The sum of these two is known as NOx. Despite their quite different physical properties, chemical affinities and environmental impacts, they are often lumped together. Around 90% of the emissions from combustion sources are of NO rather than NO_2; however, since the NO can all potentially be converted to NO_2, it is usual to express all the NOx as NO_2 when making mass emission estimates. NO is a colorless gas that rapidly combines with O_2 in the atmosphere to form NO_2 (Colls, 2002).

2.5.2 Health and Environmental Impact of NOx

NOx causes a wide variety of health and environmental impacts. According to US EPA (1998), there impacts of NOx to the health and environments are:

a) Ground-level Ozone (Smog)

   Smog is formed when NOx and volatile organic compounds (VOCs) react in the presence of sunlight. Children, people with lung diseases such as asthma, and people who work or exercise outside are susceptible to adverse effects such as damage to lung tissue and reduction in lung function. Ozone can be transported by wind currents and cause health impacts far from original sources. Other impacts from ozone include damaged vegetation and reduced crop yields.

b) Acid Rain

NOx and sulfur dioxide react with other substances in the air to form acids which fall to earth as rain, fog, snow or dry particles. Some may be carried by wind for hundreds of miles. Acid rain damages; causes deterioration of cars, buildings and historical monuments; and causes lakes and streams to become acidic and unsuitable for many fish.

c) Particles

NOx reacts with ammonia, moisture, and other compounds to form nitric acid and related particles. Human health concerns include effects on breathing and the respiratory system, damage to lung tissue, and premature death. Small particles penetrate deeply into sensitive parts of the lungs and can cause or worsen respiratory disease such as emphysema and bronchitis, and aggravate existing heart disease.

d) Water Quality Deterioration

NOx could increased nitrogen loading in water bodies, particularly coastal estuaries, upsets the chemical balance of nutrients used by aquatic plants and animals. Additional nitrogen accelerates "eutrophication," which leads to oxygen depletion and reduces fish and shellfish populations.

e) Climate Change

NOx will accumulate in the atmosphere with other greenhouse gasses causing a gradual rise in the earth's temperature. This will lead to increased risks to human health, a rise in the sea level, and other adverse changes to plant and animal habitat.

f) Toxic Chemicals

In the air, NOx reacts readily with common organic chemicals and even ozone, to form a wide variety of toxic products, some of which may cause biological mutations.

g) Visibility Impairment

Nitrate particles and nitrogen dioxide can block the transmission of light, reducing visibility in urban areas and on a regional scale.

2.6 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 (El-Harbawi *et al.*, 2008). 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. Physical model is a scaled down representation of reality while mathematical model is a description of the system using mathematical relationships and equations (El-Harbawi *et al.*, 2008).

2.6.1 Air Pollution Dispersion Models

Dispersion models are vital tool for environmental impact assessment in any area and for air quality impacts. The models provide capability to predict the effects of any emission source to the environment. There are various types of dispersion models that have been developed for different sources, meteorology, downwind distances and other parameters that could affect the atmospheric dispersion (Lim, 2008).

However, all of these models require two types of data which are the information about the source of the dispersion, including emission information and information about the dispersing characteristics of the meteorology surrounding the source, such as wind speed and wind direction. The models use this information to mathematically simulate the pollutant's downwind dispersion in order to estimate the concentration at a specified location. Model comes in many styles, depending on the intended purpose but also the available data (Lim, 2008).

The study of the dispersion is not a new subject. Early work on the subject atmospheric dispersion began with Taylor (1915) who studied 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 (El-Harbawi *et al.*, 2008).

The paper by Builtjes, (2001) is cited several authors who have conducted research in dispersion modelling. For instance, the study of 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, 1961, 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) (El-Harbawi *et al.*, 2008).

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 four types of air pollution dispersion models, as well as some hybrids of the four types (Colls, 2002):

a) 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 (El-Harbawi *et al.*, 2008). 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.

b) Lagrangian model

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 (El-Harbawi *et al.*, 2008). Lagrangian modelling well described by number of studies by Rohde (1972, 1974), Eliassen (1978), Hanna, (1981), Eliassen *et al.*, (1982) and Robert *et al.*, (1985). Langrangian modelling is often used to cover longer time periods, up to years (Builtjes, 2001).

c) 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).

d) 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 (El-Harbawi *et al.*, 2008).

The advantages of the Gaussian based dispersion models are (Lim, 2008):

a) Gaussian theory is basic
b) Inputs are relatively simple
c) Results are reasonable
d) Cost effective

There are a number of limitations of Gaussian plume models (McElroy, 1969).

a) It is only applicable for open and flat terrain.
b) It does not take into account the influence of obstacles.
c) It assumes uniform meteorological and terrain conditions over the distance it is applied.
d) It should only be used for gases having a density of the same orders as that of air.
e) It should only to be used with wind speeds greater than 1 m/s.
f) Predictions near to the source may be inaccurate.

2.6.2 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 characteristic (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 (El-Harbawi *et al.*, 2008). These parameters are described and discussed in details by number of authors (Turner, 1970; Pasquill, 1974; Hanna, *et al.*, 1982; Lees, 1996 and Builtjes, 2001).

2.6.2.1 Source Characteristic

Source characteristic is for a given set of source discharge conditions which include the emission rate, exit velocity, exit temperature and release height. The ground level concentration is proportional to the mass flux (the amount emitted per unit time or emission rate). Increasing emission rates will therefore lead to a proportional increase in ambient concentrations (Lim, 2008). Source in modelling are divided in three broad types (Lim, 2008):

a) Point sources

   Point source is the most common type representing industrial stacks. This includes a description of plume rise due to momentum and thermal buoyancy. Point source of dispersion is chosen for this project. The point source problem is the best understood, since it involves simpler mathematics and has been studied for a long period of time, dating back to about the year 1900. It uses a Gaussian dispersion model for buoyant pollution plumes to forecast the air pollution isopleths, with consideration given to wind velocity, stack height, emission rate and stability class (Turner, 1994; Beychok, 2005) This model has been extensively validated and calibrated with experimental data for all sorts of atmospheric conditions.

b) Area sources

Area source is usually understood as an agglomeration of numerous small point sources not treated individually. Area sources are also important in the modelling of particulates where they contribute particles due to wind induced entrainment. Area source models were developed in 1971 through 1974 by the Environmental Research and Technology (ERT) and ESL groups, but addressed a smaller fraction of total air pollution emissions, so that their use and need was not as widespread as the line source model, which enjoyed hundreds of different applications as early as the 1970s. Similarly photochemical models were developed primarily in the 1960s and 1970s, but their use was more specialized and for regional needs, such as understanding smog formation in Los Angeles, California. Area sources is a cluster of point or line sources (e.g. a large number of vehicles in a parking lot) may be treated as an area source. Similarly, a large city may be split into a number of grid squares (each with both traffic and industrial emissions), and the emissions from each square treated as an array of area sources. Roads and industrial chimneys are by far the most commonly modelled sources of air pollution. The type of model that is used is dependent upon the pollutant released, and the appropriate period over which concentrations will be considered (El-Harbawi *et al.*, 2008).

c) Line sources

Line source is typical for the analysis of traffic generated pollutants. The line source model was developed starting in the late 1950s and early 1960s in response to requirements of the National Environmental Policy Act and the U.S. Department of Transportation (then known as the Federal Highway Administration) to understand impacts of proposed new highways upon air quality, especially in urban areas. Several research groups were active in this model development, among which were: the Environmental Research and Technology (ERT) group in Lexington, Massachusetts, the ESL Inc. group in Sunnyvale, California and the California Air Resources Board group in Sacramento, California. The research of the ESL group received a boost with a contract award from the United States Environmental Protection Agency to validate a line source model using sulfur hexafluoride as a tracer gas. This program was successful in validating the line source model developed by ESL inc. Some of the earliest uses of the model were in court cases involving highway air pollution, the Arlington, Virginia portion of Interstate 66 and the New Jersey Turnpike widening project through East Brunswick, New Jersey (El-Harbawi *et al.*, 2008).

2.6.2.2 Distance

The greater the distance from the discharge point, the greater the volume of air available for dilution. However for stacks, since the plume starts above the ground and needs some time to reach the ground, there is no concentration observable in the immediate vicinity of the stack, then an increase can be observe for some distance as the plume approaches the ground. After that, the ground level concentration will decrease with increasing distance from emission source (Lim, 2008).

2.6.2.3 Wind Speed and Wind Direction

Wind direction will determine the direction in which the pollutants will move across local terrain (Lim, 2008). It is conventionally specified as the direction from which the wind is blowing, because what the wind has collected before it reaches the terrain is more important than in where it will go afterwards. The magnitudes of both horizontal and vertical variations for the wind direction are influenced by the atmospheric stability, which in turn depends on the balance between the adiabatic lapse rate and the environmental lapse rate (Colls, 2002).

Wind speed affects the plume rise from stacks, and will increase the rate of dilution. The effects of wind speed work in two opposite directions (Lim, 2008):

- Increasing wind speed will decrease plume rise, thus increase ground level concentrations.
- Increasing wind speed will increase mixing, thus decreasing ground level concentrations.

2.6.2.4 Atmospheric Stability

Stability is related to both the change of temperature with height and wind speed. Stability classes are defined for different meteorological situations, characterized by wind speed and solar radiation during the day and cloud cover during the night (Lim, 2008). There are six stability categories named A, B, C, D, E, and F. Class A is most unstable, class D is neutral class and class F is the most stable class (Turner, 1970). Comparison of adiabatic lapse rates with ambient air temperature gradients can be used to define stability classes which categorize and quantify turbulence (Beychok, 2005).

a) Super adiabatic

   Any rising air parcel (expanding adiabatically) will cool more slowly than the surrounding ambient air. At any given altitude, the rising air parcel will still be warmer than the surrounding ambient air and will continue to rise. Likewise, descending air (compressing adiabatically) will heat more slowly than the surrounding ambient air and will continue to sink, because at any given altitude, it will be colder than the surround ambient air. Therefore, any negative ambient air temperature gradients with larger absolute value than 5.5°F/1000 feet will enhance turbulent motion and result in unstable air condition. Such ambient air gradients are called super adiabatic (more than adiabatic) (Beychok, 2005).

b) Sub adiabatic

Any air parcel in vertical motion (expanding or compressing adiabatically) will change temperature more rapidly than the surrounding ambient air. At any given altitude, a rising air parcel will cool faster the surrounding air and tend to reverse its motion by sinking. Likewise, a sinking air parcel will warm faster than the surrounding air and tend to reverse its motion by rising. Thus negative ambient air temperature gradients with lower absolute values than 3°F/1000 feet will suppress turbulence and promote stable air conditions. Such ambient air gradients are called sub-adiabatic (less than adiabatic) (Beychok, 2005).

c) Inversion

A positive ambient air temperature gradient is referred to as an inversion since the ambient air temperature increases with altitude. The difference between the positive ambient air gradient and either the wet or dry adiabatic lapse rate is so large that vertical motion is almost completely suppressed. Hence air conditions within an inversion are very stable (Beychok, 2005).

d) Neutral

If the ambient air temperature gradient is essentially the same as the adiabatic lapse rate, then rising or sinking air parcels will cool or heat at the same rate as the surrounding ambient air. Thus vertical air motion will neither be enhanced nor suppressed. Such ambient air gradients are called "neutral" (neither more or less than adiabatic) (Beychok, 2005).

2.6.2.5 Mixing Height

Mixing height is the distance above the ground to which relatively unrestricted vertical mixing occurs in the atmosphere. When the mixing height is low but still above plume height, ambient ground level concentrations will be relatively high because the pollutants are prevented from dispersing upward. It is also defined as the base of a surface inversion layer (Lim, 2008).

2.6.2.6 *Ground Conditions*

Ground conditions affect the mechanical mixing at the surface and wind profile with height. Trees and buildings increase mixing, whereas lakes and open areas decrease it. Figure 2.3 shows the change in wind speed versus height for a variety of surface conditions (Crowl and Louvar, 2002).

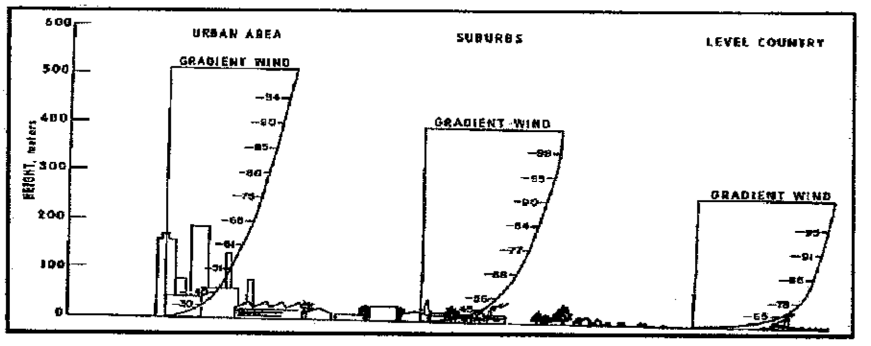

Figure 2.3: Effect of ground conditions on vertical wind gradient (Turner, 1970).

2.6.2.7 *Buoyancy and Momentum*

The buoyancy and momentum of the material released change the effective height of the release. The momentum of a high-velocity jet will carry the gas higher than the point of release, resulting in a much higher effective release height. If the gas has a density greater than air, then the released gas will initially be negatively buoyant and will slump toward the ground. The temperature and molecular weight of the released gas determine the gas density relative to that of air. For all gases, as the gas travels downwind and is mixed with fresh air, a point will eventually be reached where the gas has been diluted adequately to be considered neutrally buoyant. At this point the dispersion is dominated by ambient turbulence (Crowl and Louvar, 2002).

2.6.3 Computer Programs for Dispersion Modelling

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 modellers 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. These models 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 (Boubel *et al.*, 1994).

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 into a variety of formats; visually and statistically (Kinsman *et. al.*, 1994).

Example of codes and software that already established; Breeze is one of them whereby it is an air quality modelling system used to assess the impact of air emissions from a variety of industrial sources. ADMS (Atmospheric Dispersion Modelling) software was developed by Cambridge Environmental Research Consultants (CERC). The application is used for air quality management and assessment studies of complex situations in towns, cities, motorways, counties and large industrial areas. ISC-AERMOD View is a complete and powerful Windows air dispersion modelling system. ISC-AERMOD View provides a comprehensive air quality analysis, which includes; graphical interface, 3D visualization, rapid model comparisons and Report-ready output (El-Harbawi *et al.*, 2008).

CALPUFF View software is a comprehensive modelling tool that includes meteorological and geophysical data processors, a meteorological model, a puff-based dispersion model, and post-processing modules. DISPER is software designed for air pollution dispersion analysis. This program calculates the pollutant concentration at each point of the air considering each one of the pollutant sources and the conditions of the atmosphere. The program is based on Microsoft Windows operating system whereby one is able to work intensively with the use of the mouse and graphic windows. However, in Malaysia no such software has been developed as yet for air pollution modelling, therefore, the inspirational idea to create, design and develop this software of such a specific nature and exclusive functionality emerged (El-Harbawi *et al.*, 2008).

CHAPTER 3

METHODOLOGY

3.1 INTRODUCTION

This chapter will focus more on modelling and development of simulation for the point source dispersion software using Microsoft Visual Basic 6. Emissions of gases are unavoidable events during activities in petroleum industry which will cause air pollution. Burning of fuels in furnaces and some operations will produce emissions of pollutant gases including NOx from the stacks. The purpose of this project is to develop simulation software using Visual Basic 6 in order to estimate NOx concentration using point source model. Refer the project milestone to Table A.2 in appendix.

3.2 DISPERSION MODEL

As mentioned in chapter 2, there are five types of air pollution dispersion models which are Gaussian model, Lagrangian model, Box model and Eulerian model. The models are depending on the intended purpose as well as the available data, but in principle they all are of a general form (Lim, 2008):

$$C(x,y,z,t) = f(Q,M) \tag{3-1}$$

Where C is the ambient concentration at the location (x, y, z) and time (t), which is a function of the emissions (Q) and the meteorology (M).

Gaussian model is perhaps the oldest and perhaps the most commonly used model type. It assumes that the air pollutant dispersion has a Gaussian distribution, meaning that the pollutant distribution has a normal probability distribution. Gaussian models are most often used for predicting the dispersion of continuous, buoyant air pollution plumes originating from ground-level or elevated sources (Beychok, 2006). The model allows estimating the pollutant concentration at any location through its plume. Gaussian plume model needs specific information about each source located through the workspace, this implies additional and constant efforts to keep updated information that other models don't need (El-Harbawi *et al.*, 2008). Therefore Gaussian model is the selected dispersion model for this project that includes source related factors and a methodological factor to estimates pollutant concentration from continuous sources such as industry stacks.

3.2.1 Gaussian Plume Model

This model is characterized by the behaviour of the pollutants through the atmosphere. This model describes the pollutant concentration as a horizontal and vertical function of a Gaussian Bell. The model allows estimating the pollutant concentration at any location through its plume. Gaussian plume model needs specific information about each source located through the workspace, this implies additional and constant efforts to keep updated information that other models do not need (El-Harbawi *et. al.*, 2007).

A Gaussian model 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 (Eq 3-2) (El-Harbawi *et. al.*, 2007). Most of the equation uses today to calculate the steady state concentration of an air contaminant in the ambient air resulting from a point source are based on the following general equation (Eq 3-2) which was suggested by Pasquill (Pasquill, 1961) and modified by Gifford (Gifford, 1961) (Crowl and Louvar, 2002):

$$C(x,y,z)=\frac{Q}{2\pi u\sigma_y\sigma_z}\left\{\exp\left(\frac{-(z-H)^2}{2\sigma_z^2}\right)+\exp\left(\frac{-(z+H)^2}{2\sigma_z^2}\right)\right\}\left\{\exp\left(\frac{-(y)^2}{2\sigma_y^2}\right)\right\} \quad (3\text{-}2)$$

The ground-level concentration is found by setting z=0 (Crowl and Louvar, 2002):

$$C(x,y,0)=\frac{Q}{\pi\sigma_y\sigma_z u}\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2-\frac{1}{2}\left(\frac{H}{\sigma_z}\right)^2\right] \quad (3\text{-}3)$$

The ground-level centerline concentrations are found by setting y=z=0 (Crowl and Louvar, 2002):

$$C(x,0,0)=\frac{Q}{\pi\sigma_y\sigma_z u}\exp\left[-\frac{1}{2}\left(\frac{H}{\sigma_z}\right)^2\right] \quad (3\text{-}4)$$

The maximum ground-level concentration along the x axis C_{max} is found using (Crowl and Louvar, 2002):

$$C_{\max}=\frac{2Q}{e\pi uH^2}\left(\frac{\sigma_z}{\sigma_y}\right) \quad (3\text{-}5)$$

From the models:

C(x,y,z) : mean concentration of diffusing substance at a point (x,y,z) [μg/m^3]

x : downwind distance [m]

y : crosswind distance [m]

z : vertical distance above ground [m]

Q : contaminant emission rate [μg/s]

σ_y : lateral dispersion coefficient function [m]

σ_z : vertical dispersion coefficient function [m]

U : mean wind velocity in downwind direction [m/s]

H : stack height ($H = \Delta h + h$), where Δh is plume rise and h is physical stack height.

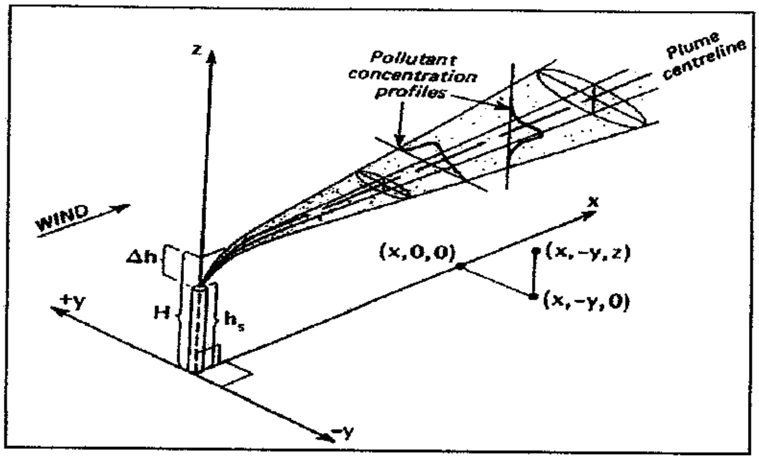

Figure 3.1: Schematic diagram of plume dispersion after pollutants are released from a stack (Gaussian distribution)

There are two main groups of input data for the Gaussian plume models which are the emission and stack parameters as well as the meteorological situation. The emission and stack parameters are (Lim, 2008):

- Emission rate
- Stack height
- Stack diameter
- Flue gas exit velocity
- Flue gas temperature

While the meteorological data needed are (Lim, 2008):

- Wind direction
- Wind speed
- Atmospheric stability, usually expressed as (Pasquill) stability classes which used to select diffusion coefficients
- Mixing height
- Ext temperature

Stability is related to both the change of temperature with height and wind speed. Stability classes are defined for different meteorological situations, characterized by wind speed and solar radiation during the day and cloud cover during the night (Lim, 2008). A Gaussian model 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 as shown in Table 3.1 (Turner, 1970).

Table 3.1: Atmospheric stability classes and categories (Turner, 1970)

Wind speed (m/s)	Day (radiation intensity)			Night (cloud cover)	
	Strong	Medium	Slight	Cloudy	Calm &clear
<2	A	A-B	B	E	F
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
>6	C	D	D	D	D

3.2.1.1 Assumptions of the Gaussian Model

The assumptions of the Gaussian Model are (Colls, 2002):

- Release and sampling times are long compared to the travel time from source to receptor. This means that the release is effectively steady state and that diffusion along the mean wind direction is negligible compared to advection (movement with the mean wind). Measurement time scales of hours rather than minutes are implied.
- The material is chemically stable and is not deposited to the ground. This means that gases must be unreactive, and particles must be < 20 μm in diameter so that

they do not sediment out. The equation of continuity will then apply the integral of the concentration over all space at any time is equal to the total mass of material emitted. In practice, most gases are deposited to some extent; this can be allowed for by, for example, an additional exponential decay factor in the concentration with distance from the source.

- The lateral and vertical variations of the material concentration can both be described by Gaussian distributions, which are functions of x only.
- The windspeed is constant with height. This is never true in practice, as has already been seen. Windspeed variation with height can often be described by a logarithmic profile. More advanced versions of the Gaussian formulation divide the atmosphere up into layers, each layer having a specified set of characteristics such as windspeed and stability.
- The wind direction is constant with height. Again, this is rarely true. The most common form of the variation is the Ekman spiral, in which the direction tends towards the geostrophic (parallel with the isobars) as height increases, over the first few hundred meters.

3.3 CONCENTRATION ESTIMATION

The ground-level centreline concentration can be estimated using Eq (3-4) (Crowl and Louvar, 2002).

$$C(x,0,0) = \frac{Q}{\pi \sigma_y \sigma_z u} \exp\left[-\frac{1}{2}\left(\frac{H}{\sigma_z}\right)^2 \right] \qquad (3\text{-}4)$$

It is important to realise that σ_y and σ_z describe the width of the concentration distribution, not of the plume itself. The dispersion coefficients are function of the atmospheric stability class and the downwind distance x from the air pollutant emission source. Martin (1976) has developed the following equation where constants *a, c, d,* and *f* are defined in Table 3.2. Equation 3-6 and 3-7 were developed to yield σ_y and σ_z in meters for downwind distance x in kilometres (Davis and Masten, 2004).

$$\sigma_y = ax^{0.894} \quad (3\text{-}6)$$

$$\sigma_z = cx^d + f \quad (3\text{-}7)$$

Table 3.2: Values of *a, c, d,* and *f* for calculating σ_y and σ_z (Davis, 2004)

Stability Class	*a*	$x < 1$ km			$x > 1$ km		
		c	*d*	*f*	*c*	*d*	*f*
A	213	440.8	1.941	9.27	459.7	2.094	-9.6
B	156	106.6	1.149	3.3	108.2	1.098	2.0
C	104	61.0	0.911	0	61.0	0.911	0
D	68	33.2	0.725	-1.7	44.5	0.516	-13.0
E	50.5	22.8	0.678	-1.3	55.4	0.305	-34.0
F	34	14.35	0.740	-0.35	62.6	0.180	-48.6

3.4 PLUME RISE

In order to establish the effective emission height, the plume rise must be accounted. Upon leaving the stacks, the plume usually encounters a crosswind which causes the plume to bend over. After that the plume will cease rising, and the plume rise is added to the actual stack height to determine the effective emission height. Holland's equation is usually used to find the plume rise. For neutral conditions, the formula is as follows (Schnelle, 2000):

$$\Delta h = \frac{v_s d_s}{u}\left[1.5 + (2.68\, x10^{-3})\, P_a \left[\frac{T_s - T_a}{T_s}\right] d_s\right] \quad (3\text{-}8)$$

Where:

Δh is the rise of the plume above the stack (*m*)

u is the wind speed at stack height (*m/s*)

v_s is the stack gas velocity (*m/s*)

d_s is the inside stack diameter (m)

P_a is the atmospheric pressure (mb)

T_s is the stack gas temperature (K)

T_a is the atmospheric temperature (K)

For non-neutral conditions, multiply Δh by the following correction factor, CF, where St is the stability factor (Schnelle, 2000):

$$CF = \left(\frac{St}{10}\right) + 0.70 \quad (3\text{-}9)$$

Table 3.3: Stability correction factors for Holland plume rise equation (Schnelle, 2000)

Stability	St	CF
A	5.0	1.20
B	4.0	1.10
C	3.5	1.05
D	3.0	1.00
E	2.0	0.90
F	1.0	0.80

3.5 WIND SPEED AT STACK HEIGHT

In order to calculate the plume rise, the wind speed at the stack height need to be estimated by extrapolating from the wind speed measured by the anemometer (often located at a standard height of 10 meters) (VicEPA, 1985). The wind speed is assumed to increase with height according to the power law (Panagiotou and Michalakopoulos, 2000). Equation (3-10) can be simplified further to a power law relation (Table 3.4) if the wind speed is compared to a wind speed at a fixed height (Hanna *et al.*, 1982):

$$U_z = U_{ref}\left(\frac{Z}{Z_{ref}}\right)^p \quad (3\text{-}10)$$

Where:

U_z is the wind speed at height Z above the ground (m/s)

U_{ref} is the wind speed measured at 10 m height (m/s)

Z is the height (m)

p is the power law that varies with atmospheric stability (dimensionless)

Table 3.4: Wind profile exponent (Panagiotou and Michalakopoulos, 2000)

Pasquill-Gifford Stability class	Power law atmospheric coefficient, p	
	Urban	Rural
A	0.15	0.07
B	0.15	0.07
C	0.20	0.10
D	0.25	0.15
E	0.40	0.35
F	0.60	0.55

3.6 EFFECTS OF CHEMICAL HAZARDS ON HUMANS

In order to estimate the consequences of an accident on people and the damage caused by the accident, the best method is probit analysis. The idea of probit analysis was originally published in Science by Chester Ittner Bliss in 1934 (Vicent, 2009). Usually, the method used is the probit analysis, which relates the probit (probability unit) variable to the probability. The estimation of the number of people affected by a given accident is achieved through the conversion from the probit variable to the percentage of people affected, by means of tables and figures. This is a significant problem when the calculations are done by means of a computer program or by a hand calculator (Vilchez *et. al.*, 2000).

The probit variable Y, is a measure of the percentage of a population submitted to effect with a given intensity (V) which will undergo certain damage (Vilchez *et. al.*, 2000).

This variable follows a normal distribution, with an average value of 5 and a normal deviation of 1. The relationship between the probit variable (Y) and the probability (P_r) is the following (Finney, 1971):

$$P_r = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{5} \exp\left(-\frac{V^2}{2}\right) dV \tag{3-11}$$

Equation (3-11) provides a relationship between the probability P_r and the probit variable Y. For spreadsheet computations a more useful expression for performing the conversion from probits to percentage is given by (Crowl and Louvar, 2002):

$$P_r = 50\left[1 + \frac{Y-5}{|Y-5|} erf\left(\frac{|Y-5|}{\sqrt{2}}\right)\right] \tag{3-12}$$

Where *erf* is the error function. Abramowitz and Stegun (1964) have given a rational approximation for digital computation:

$$erf(x) \approx 1 - \left(a_1\phi + a_2\phi^2 + a_3\phi^3\right)\exp\left(-x^2\right) + \varepsilon \tag{3-13}$$

Where:

$\phi = \frac{1}{(1+\alpha x)}$; $\alpha = 0.47047$; $a_1 = 0.34802$;

$a_2 = -0.09587$; $a_3 = 0.74785$ and $\varepsilon \leq 2.5 \times 10^{-5}$

Most of the previous works about probit analysis have been given by Finney, (1971), Eisenberg *et. al.*, (1975), TNO, (1990), and Vílchez, *et. al.*, (2000). The following expression is normally used to calculate the value of Y:

$$Y = a + b \ln V \tag{3-14}$$

Where Y is the probit variable, a and b are constants which are experimentally determined from the information on accidents, or, in some cases, from experimentation with animals. V is a measure of intensity of the damaging effect; it can be just one parameter or a combination of various parameters (for example, the concentration and time in toxic gas release) (Vilchez *et. al.*, 2000).

For about 20 commonly a used substance (Table A.1), there is some information on dose-response relationships that can be applied to a probit function to quantify the number of fatalities that are likely to occur with a given exposure. The probit method is a statistical curve fitting method. Furthermore, the results are often extrapolated beyond the experimental data range. This project only focuses on concentration of gases and use probit equation constants for lethal toxicity (Schubach, 1995):

$$Y = a + b \ln C^n t \qquad (3\text{-}15)$$

Where:

Y = The probit variable

a, b, n = constants

C = The concentration in ppm by volume

t = The exposure time in minutes

The effects are calculated by using Equation (3-15) is transformed to percentages by using Table A.1.

3.7 AIR POLLUTION MODELLING PROCEDURES

There are three procedures involved in air pollution modelling which are data input, data processing and data analysis (El- Harbawi et al., 2008).

Stage 1: Data Input

Data is collected to be used as inputs for the software or atmospheric dispersion model. The data must include the meteorological conditions, the emission source and other related information. All data will be processed during the second stage to predict the ground level concentrations of pollutants.

Stage 2: Data Processing

Data processing is done in the second stage when all the data collected is key-in into the software. The results obtained will represent the ground level concentration of the pollutants being studied.

Stage 3: Output Analysis

In the final stage, the pollutants concentration and percentage of fatality which is represented by result data list and graph is analyzed to know the potential environmental and health effects.

3.8 PSDS DEVELOPMENT STAGES

The information about the meteorology, dispersion model, and data gathering for input parameters are done by literature review. Research is done through several case studies and books which are mostly about air pollution, meteorology and atmospheric dispersion modelling. From the research done, the most suitable model to be used for the point source dispersion modelling is found. The meteorological and emission data that is found from case studies could also be used as the input parameters to the selected model. The data could also be assumed based on the literature review. Table 3.5 summarize the Point Source Dispersion Software (PSDS) development stages.

Table 3.5: PSDS Development Stages (El- Harbawi et al., 2008)

Stage	Development	Description
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. VB 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. Several interfaces will be used for different types of hazard calculations, whereby each GUI will be logically connected. VB 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 Microsoft Visual Basic 6.0 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 VB program (code).
Stage 4	Software validation and verification	The validation and verification must be performed after the successful development of the software using results from the development software and comparing them to those from published literature and other experimental data.

3.9 SIMULATION TOOL

The simulation tool used in this project is Visual Basic 6. As its name implies, Visual basic is more visually oriented than most other programming languages. It was designed to be simple as well as easy to learn and use. Graphical User Interface (GUI) technology made it easier for users to communicate with computers and the language allows programmers to create simple user interface applications, as well as to develop complex applications. In order to estimate the concentration downwind dispersion of a plume release from the point source, the behaviour of the gas emission must be the input to the simulation program created. The input data are parameters such as stack height, stack diameter, emission rate, and so on. The result from the simulation will be compared to the actual values in order to determine the accuracy of the program created. The computation of the mathematical models for concentration of the gaseous emission from the stack and the fatality has been written in VB program and Figure 3.2 shows the logic diagram for the calculation of Point Source Dispersion Software (PSDS) using a Gaussian dispersion model.

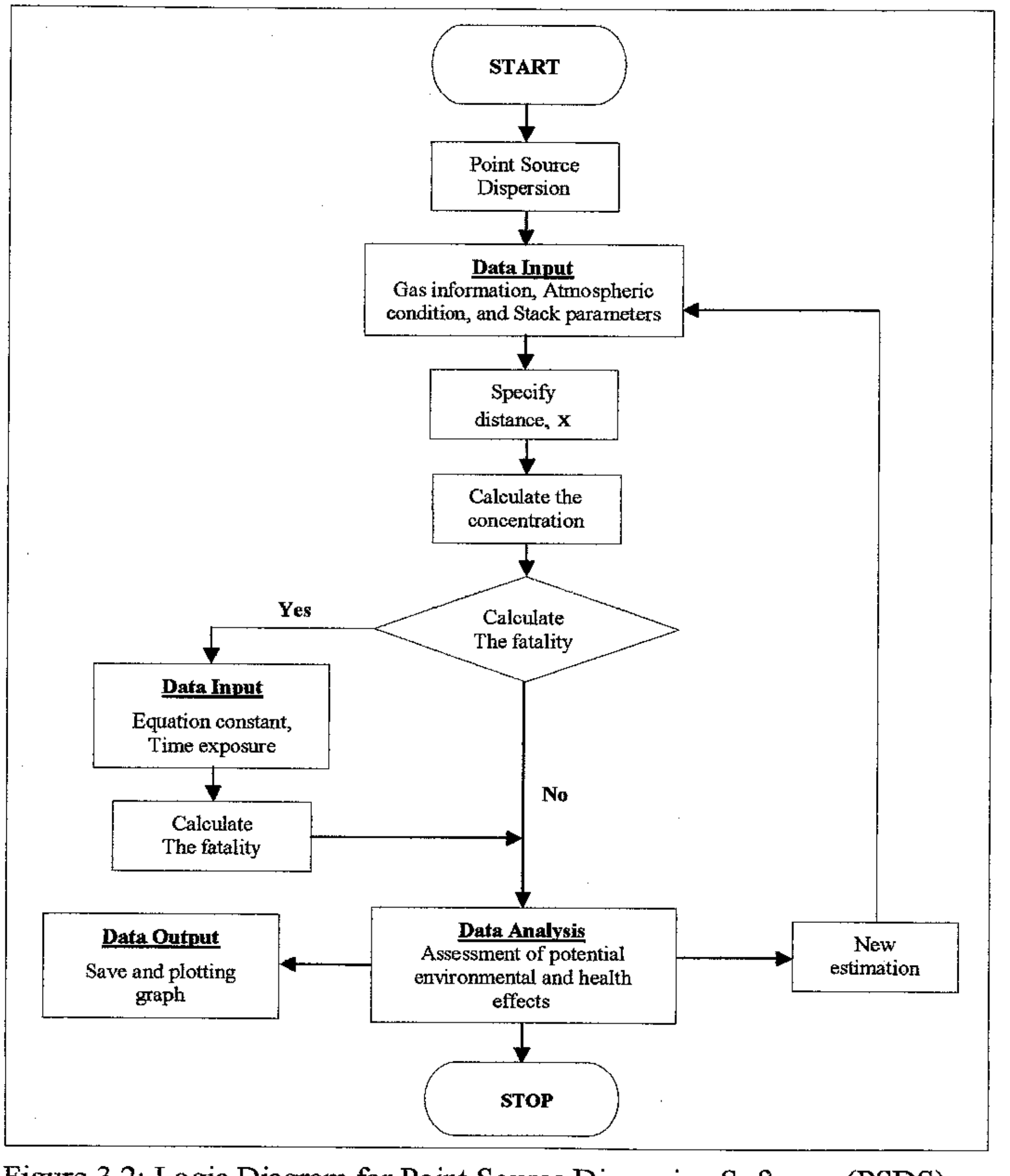

Figure 3.2: Logic Diagram for Point Source Dispersion Software (PSDS)

CHAPTER 4

RESULT AND DISCUSSION

4.1 INTRODUCTION

The PSDS software has been successfully developed and implemented in an interactive Visual Basic (VB) environment. The software is designed to be user-friendly to simulate different atmospheric stability and release condition (rural and urban). The possibility of making mistakes in manual calculation is greatly reduced. In this chapter, the developed PSDS interface using VB will be explain in detail. The results obtained from the current research also will be explained and discussed in the context with the findings of earlier studies.

4.2 POINT SOURCE DISPERSION SOFTWARE (PSDS) INTERFACE

The developed PSDS software interface consists of four sections in order to allow users to view the results of the simulation and to estimate the concentration of emission gas from the stack. Figure 4.1 shows the main interface for PSDS software. "Pollutants Information" is the first section of the software which the users have to key in the name of the pollutant and the molecular weight. For the "Atmospheric Conditions" section, users have to key in the wind speed (u), select the type of terrain (rural or urban) from release condition's combo list and the user also need to select the atmospheric stability class form the atmospheric stability class's combo list. The third section is the "Stack parameters". In this section the users have to enter the stack height (h), stack diameter (d), gas exit temperature (Ts), ambient temperature (Ta), atmospheric pressure (p), gas emission rate (Q) as well as the gas exit velocity (Vs). In the fourth section which is the

"Distance" section, the users have to choose the distance either less than 1 km or more than 1 km as well as the concern distance.

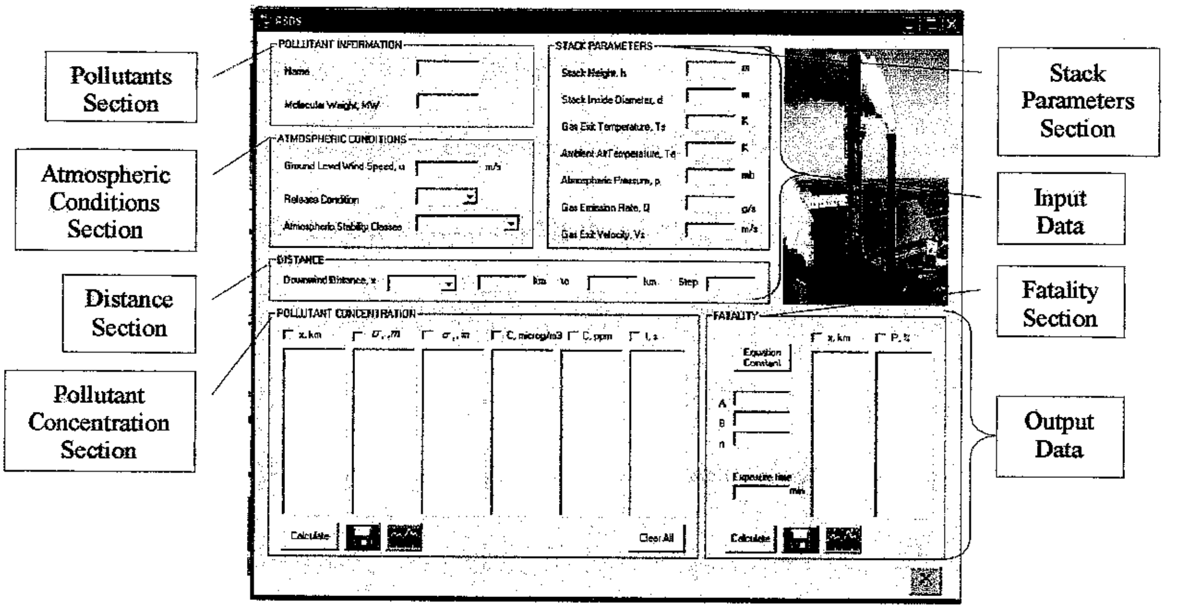

Figure 4.1: PSDS Graphical User Interface (GUI)

After the users filled up all the input sections, they can perform the concentration calculation by clicking on the "Calculate" button in pollutant concentration section. This software is also designed to alert the users if the value entered is not valid or the user failed to enter any of the required variables. The error message will appear after the user click the calculate button (Refer Figure 4.2).

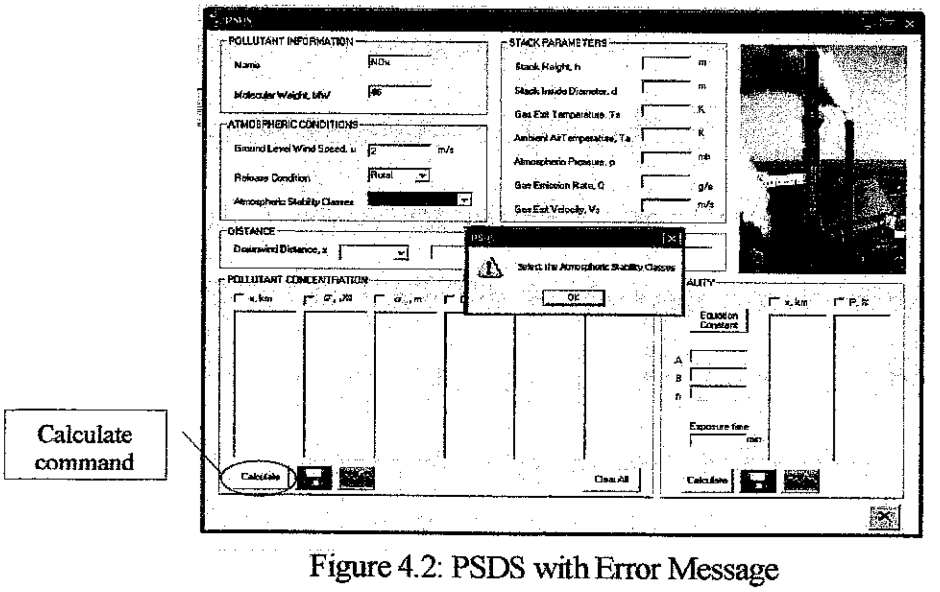

Figure 4.2: PSDS with Error Message

When all the data are adequate, the result will be shown in the "Pollutant Concentration" section as shown in Figure 4.3. The figure illustrates the calculation of Nitrogen Oxides (NOx) that released from a stack. Besides the predicted concentration and distance lists, the pollutant concentration section also consists of lists of the calculated dispersion coefficients, σ_z and σ_y as well as the time of dispersion. If the users would like to make start a new estimation, the users have to click on "Clear All" button as shown in Figure 4.3.

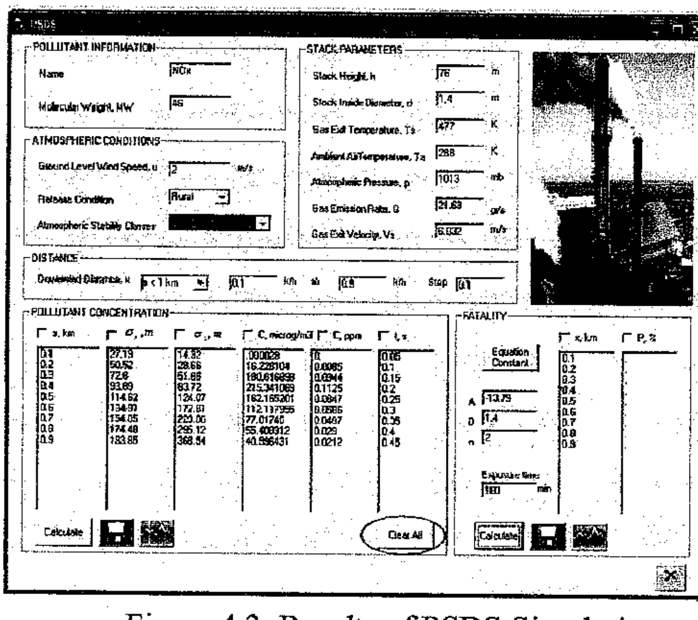

Figure 4.3: Results of PSDS Simulation

The codes behind this software will retrieve the information from the input data that user key in, then the software will process the input data, and finally display the results which can be saved as text file or word file by clicking on save button as shown in Figure 4.4. Figure 4.5 shows the result in saved in text and word file. PSDS also designed to plot graph either via Visual Basic (VB) or Microsoft Excel by checking the check boxes of the desired x-axis and y-axis. The check boxes are shown in Figure 4.6. The user then may plot the graph by clicking the graph button as shown in Figure 4.4. Figure 4.7 and Figure 4.8 shows the graphs plotted using VB and Microsoft Excel.

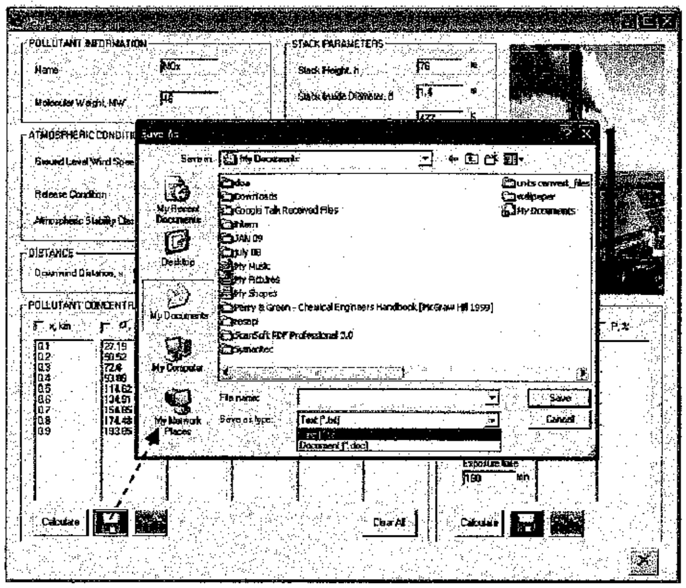

Figure 4.4: Save the Simulation Results

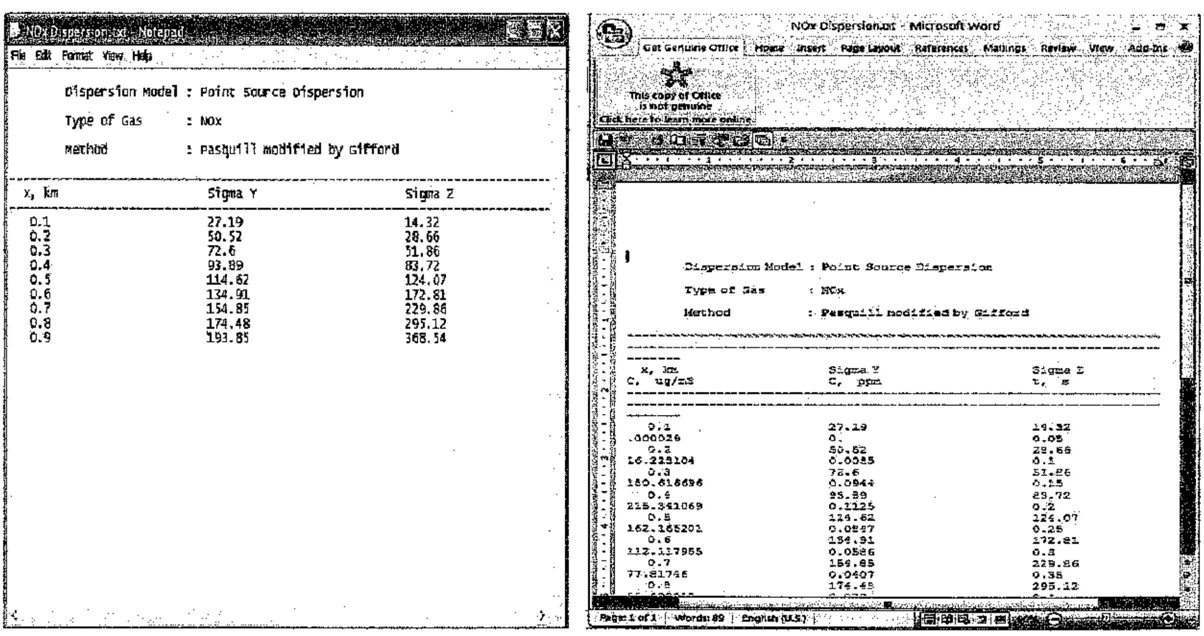

Figure 4.5: Results Saved in Text and Word File

Check boxes for the graph x and y-axis

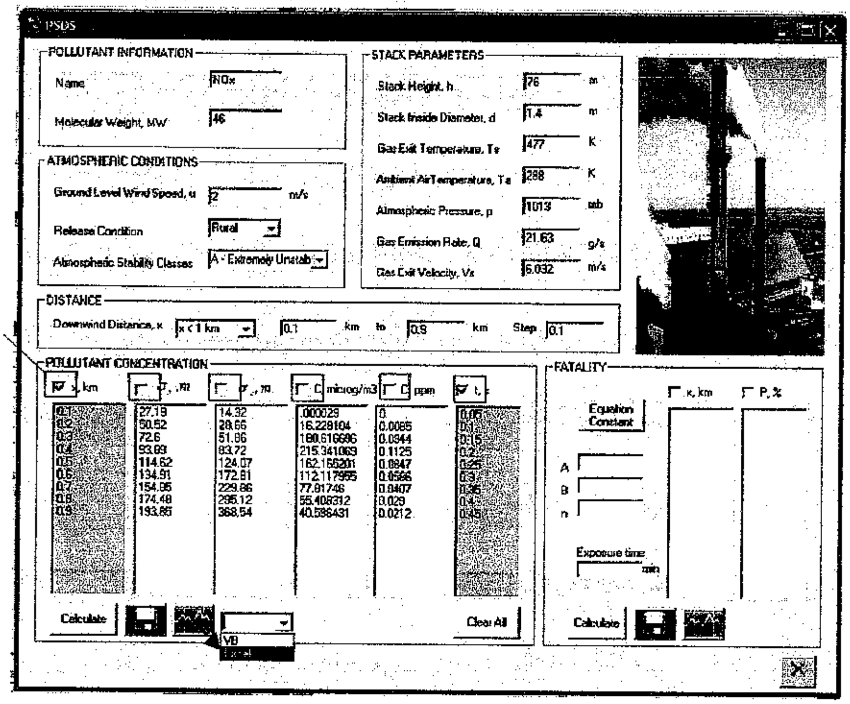

Figure 4.6: Plotting the Graph via VB and Microsoft Excel

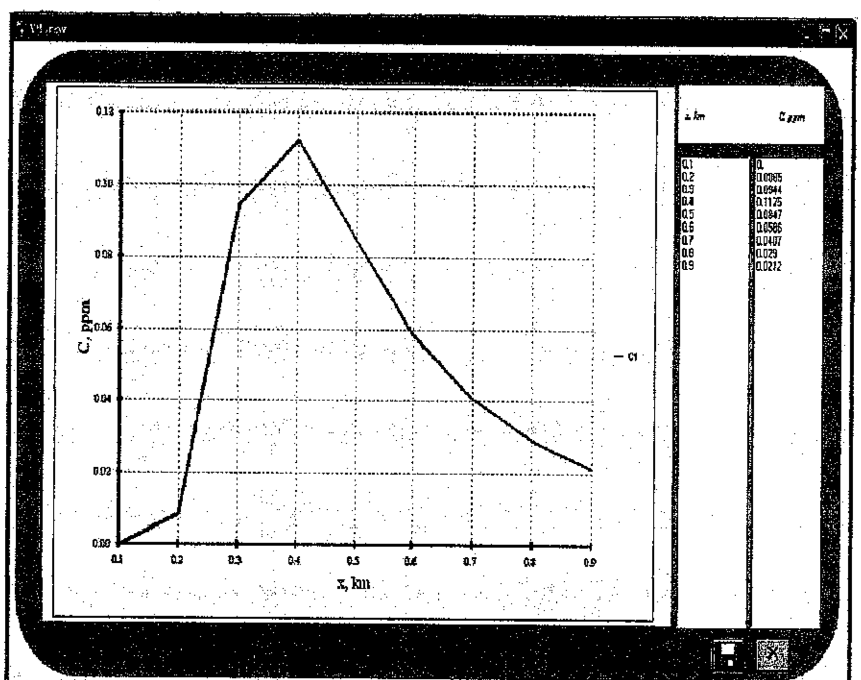

Figure 4.7: Graph of Concentration (ppm) vs Distance, X (km) Plotted Using VB

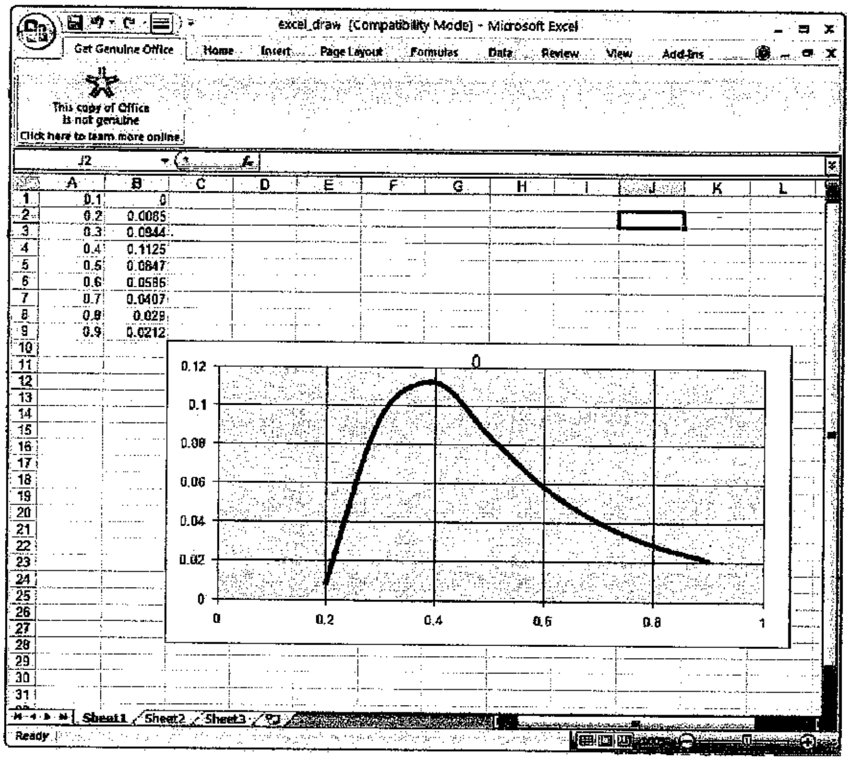

Figure 4.8: Graph of Concentration (ppm) vs Distance, X (km) Plotted Using Microsoft Excel

It should be noted that PSDS is also design to estimate the human fatality (the percentage of people affected). In order to calculate the percentage of people effected, user need to key in the variables in fatality section, (i.e., constant of A, B, n, and time exposure in minutes). The users have to click on the "Equation Constant" command button to view the equation constant table as shown in Figure 4.9. The result of fatality could be determined by clicking "Calculate" button in fatality section. The user may also save the results either in text or word file as well as plot a graph via Visual Basic or Microsoft Excel as shown in Figure 4.10.

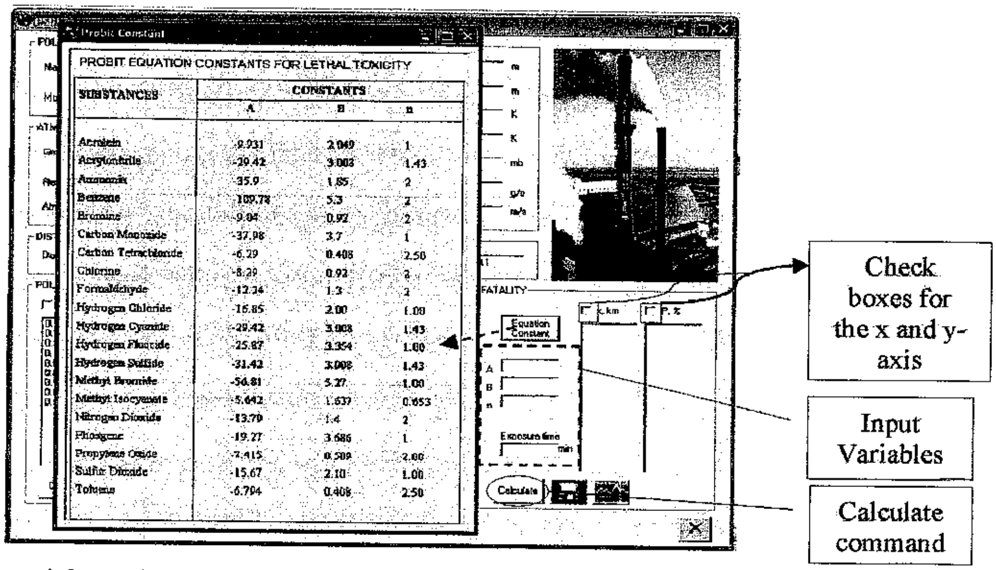

Figure 4.9: Probit Equation Constants Table and Fatality Section

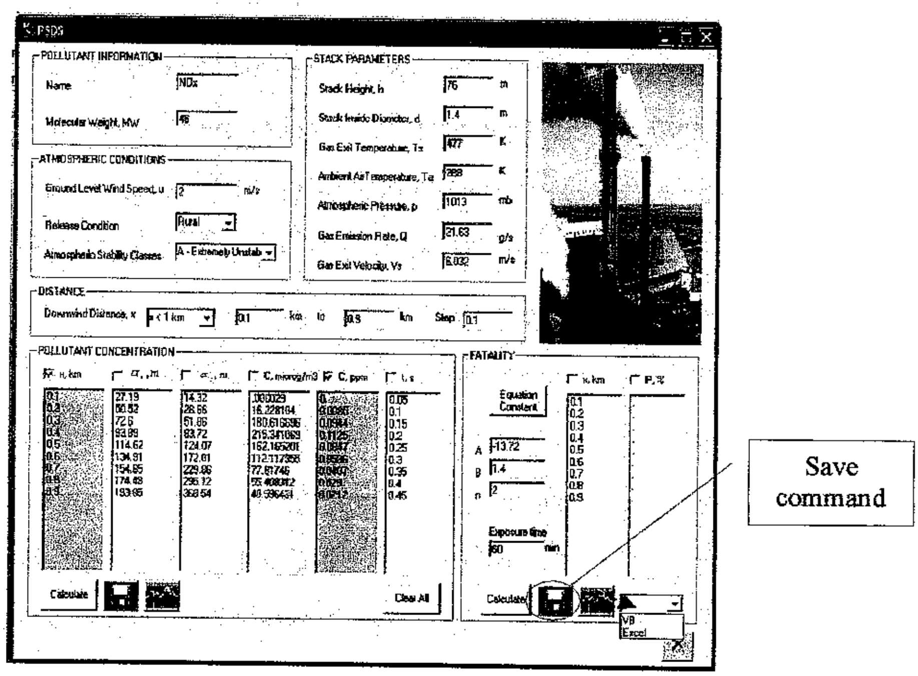

Figure 4.10: Save and Plot Graph Command for Fatality Section

4.3 WRITING THE COMPUTER PROGRAMME

The program is written in standard Microsoft Visual Basic 6 and distributed in object format with the source code (El- Harbawi et. al, 2008). After creating the interface for the PSDS software, it's necessary to write the code that defines the applications behaviour.

4.4 PSDS SOFTWARE VALIDATION AND VERIFICATION

Verification and validation of computational simulations are the primary methods to build confidence and quantify the results. Verification is the assessment of the accuracy of the solution to a computational model. Validation is the assessment of the accuracy of the model used and program developed by comparison with case study or actual data. The validation process will confirm that a good (correct, complete, consistent, operationally and technically feasible, and verifiable) system is being developed. The verification process ensures that the simulation results have met the systems requirement and that the system is ready for use in the operational environment for which it is intended. The PSDS software has been validated and verified with established software which is SCREEN3 (US EPA air pollution modelling software) as well as using data from case study.

4.4.1 Case Studies

It should be pointed out that the use of the PSDS software for predicting the potential consequences of NOx necessitates the investigation of several scenarios. Therefore, results of two case studies are compared with PSDS software and SCREEN3. The descriptions for these studies are as follows:

4.4.1.1 Case study 1

The case study is referred to the *Example Calculation of Dispersion from a Buoyant Plume* in *Atmospheric Dispersion Modelling Compliance Guide by Schnelle and Dey (1999)*. The results of PSDS software are compared to results from this case study and SCREEN3.

A coal-fired power plant with three stacks in line with a source data recorded stack height 91.5 m, diameter stack 3.05 m, stack gas velocity 13.7 m/sec, stack gas temperature 394 K and the emission rate is 375.326 g/sec after multiply multiple stack factor 0.9. The meteorological data is wind speed 5 m/sec, atmospheric temperature 294 K, atmospheric pressure 987 mb and at stability neutral D with a rural area.

4.4.1.2 Case study 2

The case study is from *Fundamental of Stack Gas Dispersion by Milton Beychok (2005)*. This case study is simulated using PSDS software and the results are compared to SCREEN3 results.

Emission of gas is 21.63 g/s. The receptor located at 600 m downwind from a source stack. The given conditions and problem specifics are 2 m/s wind velocity with Pasquill stability class A and rural terrain at ambient temperature of 15 °C. The stack parameters are 1.4 m of stack exit diameter, 76 m of stack exit height and 204 °C of stack exit temperature.

4.4.2 Result and Discussion

This section will discuss about NOx dispersion and the results after simulate by SCREEN3 and the result from Schnelle and Dey (1999) to compare with PSDS software.

4.4.2.1 Result of case study 1

The concentration and dispersion coefficient has been estimated by PSDS software as a function of distance. The results are compared to the results from *Atmospheric Dispersion Modelling Compliance Guide by Schnelle and Dey (1999)* and SCREEN3 as shown in Table 4.1.

Table 4.1: Downwind concentration as function of distance result comparison between the PSDS software with Schnelle and Dey (1999) and SCREEN3 software

Distance, x (km)	Schnelle and Dey (1999)			PSDS			SCREEN3		
	σ_y (m)	σ_z (m)	C (ppm)	σ_y (m)	σ_z (m)	C (ppm)	σ_y (m)	σ_z (m)	C (ppm)
2	130	50	0.0977	126	51	0.1172	130	55	0.0115
3	190	65	0.1730	182	65	0.1708	186	69	0.0350
4	245	77	0.1887	235	78	0.1720	240	81	0.0524
5	300	89	0.1829	287	89	0.1574	293	91	0.0615
8	460	120	0.1348	436	117	0.1102	446	120	0.0627
10	550	137	0.1003	533	133	0.0883	544	137	0.0565
30	1450	255	0.0303	1422	244	0.0232	1435	252	0.0198

Figure 4.11 shows the relationship between the concentrations as a function of distance. The figure shows that there is a fair agreement between the results predicted by PSDS software and the reference book by Schnelle and Dey (1999). However, the result obtained from SCREEN3 is slightly different. The maximum concentration of PSDS software is equal to 0.1720 ppm at a distance of 4 km. From the reference book, the maximum concentration is 0.1887 ppm at 4 km while the maximum concentration from SCREEN3 is 0.0627 ppm at 8 km.

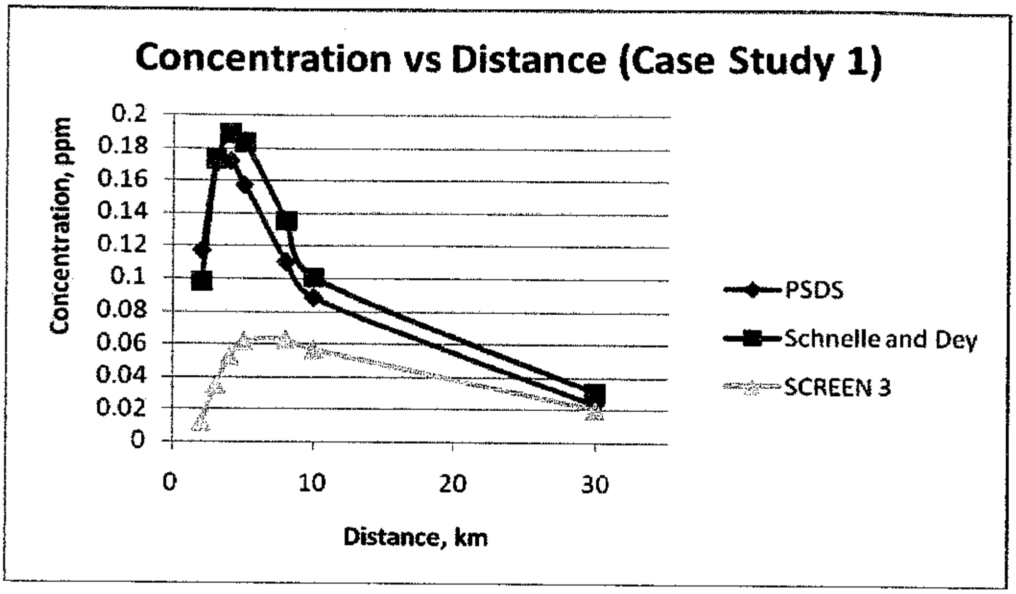

Figure 4.11: Downwind concentration as function of distance result comparison between the PSDS software, Schnelle and Dey (1999) and SCREEN3

The difference in the results could be because of different equation used in both software and also the reference book. The reference book, PSDS software and SCREEN3 are using the same model which is the Pasquill-Gifford dispersion model. However, the difference in equation used to calculate the dispersion coefficients, σ_y and σ_z and the plume rise equation could affects the difference in concentration prediction. In order to find the causes of the difference, the value of σ_y and σ_z from reference book, PSDS software and SCREEN3 are compared as shown in Figure 4.12 and 4.13.

Figure 4.12 and 4.13 shows the relationship between dispersion coefficients for both y and z and distance. The dispersion coefficient will increase when downwind distance increase. Based on both figures, it can be noticed that the dispersion coefficient value predicted by the PSDS software, reference book, and SCREEN3 are similar. This results show that the dispersion coefficient equation used by reference book, PSDS software and SCREEN3 are almost the same.

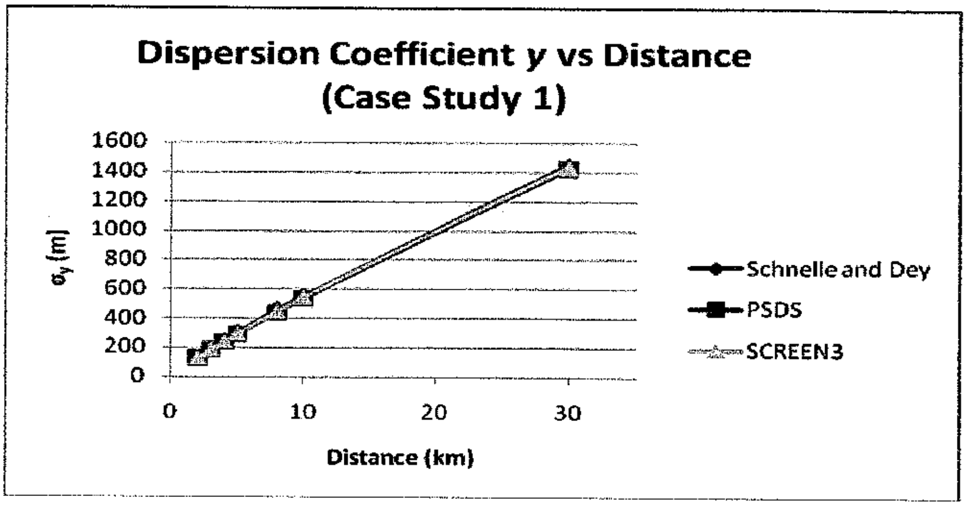

Figure 4.12: Dispersion Coefficient *y* as Function of Distance Comparison between PSDS Software, Schnelle and Dey (1999) and SCREEN3

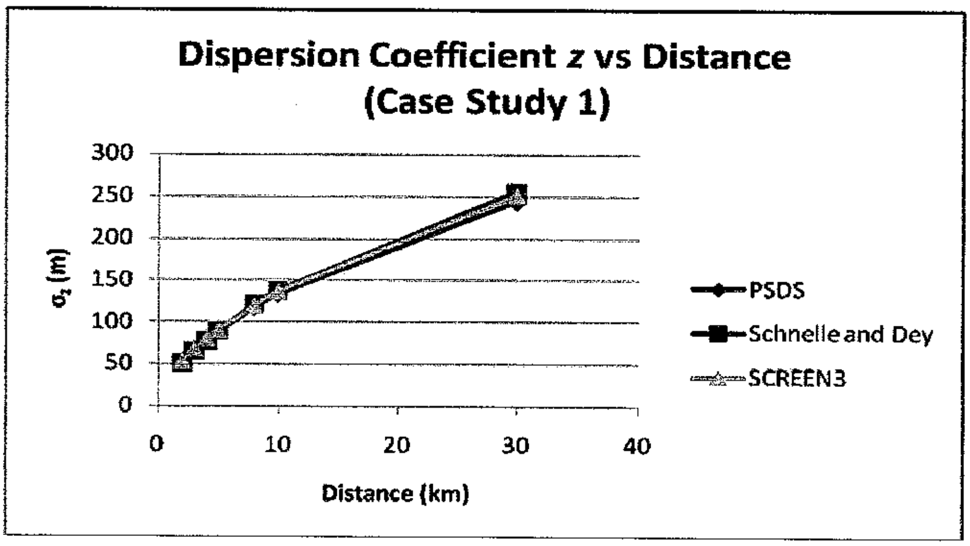

Figure 4.13: Dispersion Coefficient *z* as Function of Distance Comparison between PSDS Software, Schnelle and Dey (1999) and SCREEN3

As mentioned before, the second parameter that might affect the difference between the three results is the plume rise equation. The most common equations used to calculate the plume rise are the Brigg's equation and Holland's equation. The Brigg's equation is more complicated than Holland's equation. According to Schnelle and Dey (1999), the concentration calculated using the Hollands equation will be higher if compared to the Brigg's equation. It should be noted that PSDS software and reference book are using the Holland plume rise equation while the SCREEN3 using the Briggs plume rise equation. This shows that the difference of the concentration values between three results are because of the plume rise equation.

Furthermore based on the condition from the case study, PSDS has simulated the percentage of fatality. From the PSDS software result, it is found that no fatality predicted at the given condition.

4.4.2.2 Result of case study 2

The concentration and dispersion coefficient has been estimated by PSDS software as a function of distance using data from *Fundamental of Stack Gas Dispersion by Milton Beychok (2005)*. The results from PSDS simulation is compared with results from SCREEN3 as shown in Table 4.2.

Table 4.2: Downwind concentration as function of distance result comparison between the PSDS software and SCREEN3 for Case Study 2

Distance, x (km)	**PSDS**			**SCREEN3**		
	σ_y (m)	**σ_z (m)**	**C (ppm)**	**σ_y (m)**	**σ_z (m)**	**C (ppm)**
0.1	27	14	0.000	29	17	0.0000
0.2	51	29	0.0085	52	33	0.0002
0.3	73	52	0.0944	74	50	0.0121
0.4	94	84	0.1125	94	73	0.0422
0.5	115	124	0.0847	114	106	0.0580
0.6	135	173	0.0586	134	155	0.0518
0.7	155	230	0.0407	153	214	0.0391
0.8	174	295	0.0290	172	283	0.0286
0.9	194	369	0.0212	191	364	0.0212
1	213	450	0.016	209	454	0.0165
2	396	1953	0.002	384	1968	0.0080
3	569	4578	0.0006	547	4643	0.0056

Figure 4.14 shows the relationship between the concentrations as a function of distance. The figure shows that the result obtained from PSDS software and SCREEN3 is slightly different. The maximum concentration of PSDS software is equal to 0.1125 ppm at a distance of 0.4 km while the maximum concentration from SCREEN3 is 0.058 ppm at distance of 0.5 km.

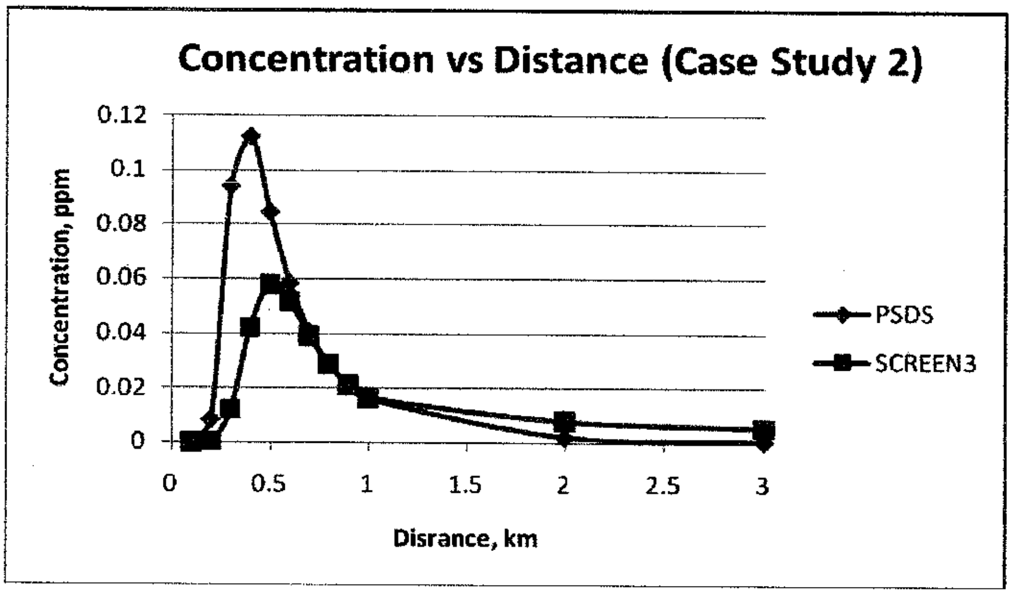

Figure 4.14: Downwind Concentration as Function of Distance Result Comparison between the PSDS software and SCREEN3 for Case Study 2

The difference in the results could be because of different equation used behind both software. PSDS software and SCREEN3 are using the same model which is the Pasquill-Gifford dispersion model. However, the difference in equation used to calculate the dispersion coefficients, σ_y and σ_z and the plume rise equation could affects the difference in concentration prediction. In order to find the causes of the difference, the value of σ_y and σ_z from PSDS software and SCREEN3 are compared as shown in Figure 4.15 and 4.16.

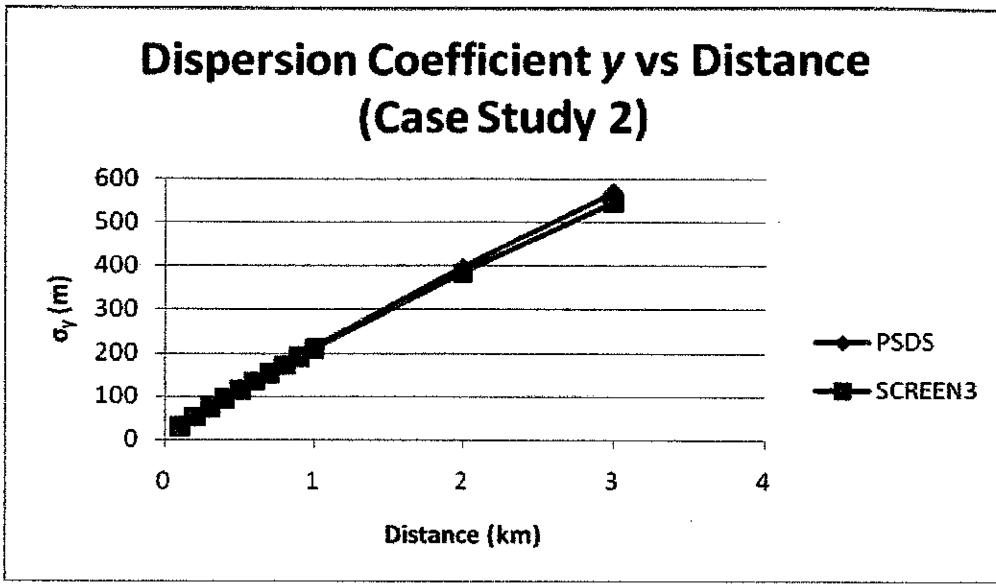

Figure 4.15: Dispersion Coefficient *y* as Function of Distance Comparison between PSDS Software and SCREEN3 for Case Study 2

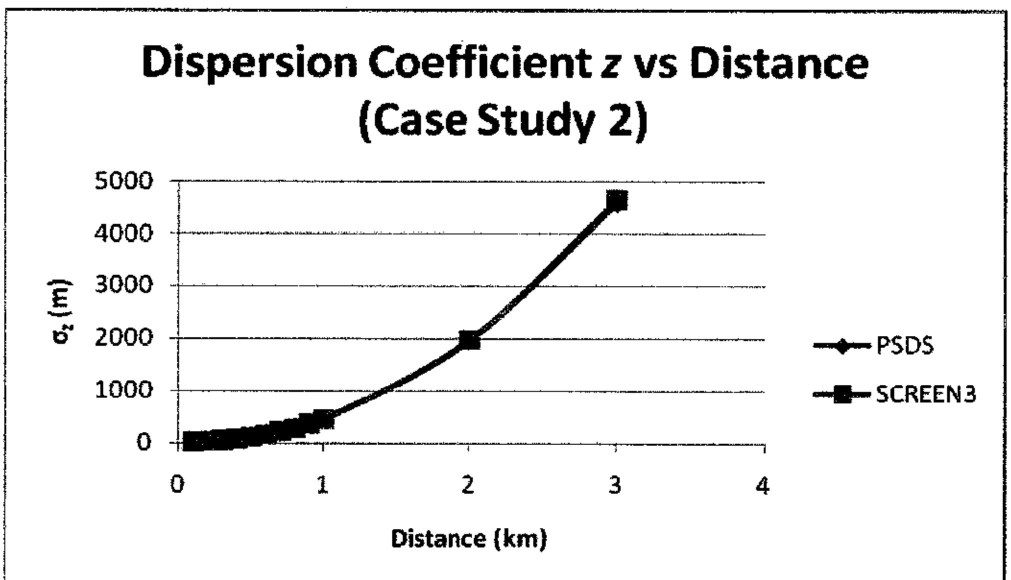

Figure 4.16: Dispersion Coefficient *z* as Function of Distance Comparison between PSDS Software and SCREEN3 for Case Study 2

Figure 4.15 and 4.16 shows the relationship between dispersion coefficients for both y and z and distance. The dispersion coefficient will increase when downwind distance increase. Based on both figures, it can be noticed that the dispersion coefficient value predicted by the PSDS software and SCREEN3 are almost the same. This results show that the dispersion coefficient equation used by PSDS software and SCREEN3 are almost the same.

As mentioned before, the second parameter that might affect the difference between the both results from PSDS software and SCREEN3 is the plume rise equation. The most common equations used to calculate the plume rise are the Brigg's equation and Holland's equation. The Brigg's equation is more complicated than Holland's equation. According to Schnelle and Dey (1999), the concentration calculated using the Hollands equation will be higher if compared to the Brigg's equation. It should be noted that PSDS software is using the Holland plume rise equation while the SCREEN3 is using the Briggs plume rise equation. This shows that the difference of the concentration values between both results are because of the plume rise equation.

Furthermore based on the condition from the case study, PSDS has simulated the percentage of fatality. From the PSDS software result, it is found that no fatality predicted at the given condition.

CHAPTER 5

CONLCUSION AND RECOMMENDATION

5.1 CONCLUSION

Emissions of gases are unavoidable events during activities in process industry which will cause air pollution. Assessment of the hazards posed by the pollutants emitted from the industries can be carried out by the use of mathematical models to calculate the consequences of emissions. The mathematical models are difficult to implement manually because the calculations involved are difficult and time consuming. Usually a large number of these calculations are required. For these reasons, the concentration estimation is best carried out by using air pollution software. The framework to develop air pollution software applications to estimate the concentration of pollutant and also the fatality has been described in this report. The software is called Point Source Dispersion Software (PSDS) and was developed using Visual Basic 6. All the programs have been written and designed within an object-orientated framework. The software was designed to work as user-friendly software.

PSDS has successfully been simulated and the results have been obtained. The validation and verification of the software together with the model used is done using established air pollution modelling software, SCREEN3 and established data. PSDS software produces slightly different values than SCREEN3 but the trends produced by both softwares are similar. The objectives of the project are accomplished.

5.2 RECOMMENDATION

The recommendations for future work are:

- Use a more complicated equation for the plume rise equation to increase the accuracy of the software.
- Evaluate PSDS software using actual data in order to see the error if the software is run using actual data.
- Evaluate PSDS software with other established air pollution dispersion software.

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APPENDIX

Table A.1: Transformation of probits to percentages (Vílchez *et. al.*, 2001)

%	0	2	4	6	8
0	-	2.95	3.25	3.45	3.59
10	3.72	3.82	3.92	4.01	4.08
20	4.16	4.23	4.29	4.36	4.42
30	4.48	4.53	4.59	4.64	4.69
40	4.75	4.80	4.85	4.90	4.95
50	5.00	5.05	5.10	5.15	5.20
60	5.25	5.31	5.36	5.41	5.47
70	5.52	5.58	5.64	5.71	5.77
80	5.84	5.92	5.99	6.08	6.18
90	6.28	6.41	6.55	6.75	7.05
99	7.33	7.41	7.46	7.65	7.88

Table (A.2.1) Project Gantt Chart for semester 1

No	Detail/Week	1	2	3	4	5	6	7	Mid	8	9	10	11	12	13	14
1	Topic selection								Sem							
2	Literature review								Break							
3	Familiarization of tool(VB)															

Table (A.2.2): Project Gantt Chart for Semester 2

No	Detail/Week	1	2	3	4	5	6	7		8	9	10	11	12	13	14
1	Literature review								Mid							
2	Mathematical model selection															
3	GUI Development															
4	Software programming								Sem							
5	Software validation															
6	Documentation								Break							

Table A.3.1: Suggested Milestone for the First Semester of 2-Semester Final Year Project

No.	Detail/ Week	1	2	3	4	5	6	7		8	9	10	11	12	13	14
1	Selection of Project Topic	■	■						Mid-semester break							
2	Preliminary Research Work		■	■	■											
3	Submission of Preliminary Report				●											
4	Seminar 1 (optional)					■	■	■								
5	Project Work					■	■	■								
6	Submission of Progress Report									●						
7	Seminar 2 (compulsory)										■	■	■	■		
8	Project work continues									■	■	■	■	■		
9	Submission of Interim Report Final Draft														●	
10	Oral Presentation															●

● Suggested milestone

■ Process

Table A.3.2: Suggested Milestone for the Second Semester of 2-Semester Final Year Project

No.	Detail/ Week	1	2	3	4	5	6	7		8	9	10	11	12	13	14
1	Project Work Continue	■	■	■					Mid-Semester Break							
2	Submission of Progress Report 1				●											
3	Project Work Continue				■	■	■	■								
4	Submission of Progress Report 2									●						
5	Seminar (compulsory)										■	■	■			
5	Project work continue									■	■	■	■			
6	Poster Exhibition											●				
7	Submission of Dissertation (soft bound)													●		
8	Oral Presentation														●	
9	Submission of Project Dissertation (Hard Bound)															●

● Suggested milestone

■ Process