Modelling and Simulation of CO emission using Point Source Model

by

Nur Farahana bt Ghazali

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Universiti Teknologi PETRONAS
Bandar Seri Iskandar
31750 Tronoh
Perak Darul Ridzuan

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CERTIFICATION OF APPROVAL

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Approved by,

DR. MOHANAD EL-HARBAWI
Lecturer
Chemical Engineering Department
Universiti Teknologi PETRONAS
Bandar Seri Iskandar, 31750 Tronoh.
Perak Darul Ridzuan, MALAYSIA

(Dr Mohanad M.A.A El-Harbawi)

UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

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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 FARAHANA BT GHAZALI

ABSTRACT

The framework for developing computerized software for air dispersion is presented in this project. The software is called Plume Dispersion Modelling Software (PluDMS) which focuses on carbon monoxide dispersion from a point source. PluDMS is developed using Visual Basic (VB) programming language to specifically predict carbon monoxide concentrations over distance. Atmospheric conditions and emission parameters are the required inputs for the software. The output is the concentration of gas over the distance and the fatality predicted for that concentration dispersed. The software is validated using other established air dispersion software; SCREEN3. Existing models are utilized to predict the dispersion scenarios and their impact to the environment and humans. The model used in the software is a Pasquill-Gifford Gaussian point source model.

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CHAPTER 1

INTRODUCTION

1.1 Problem Statement

The industrial activities such as the oil and gas industry produce pollutant gases such as nitrogen oxides (NOx), Sulphur Oxides (Sox), and carbon monoxide (CO) and these pollutants are released from the stacks into the environment. CO, for instance, is a product of incomplete combustion that affects the oxygen transport in the blood stream. These pollutant gases, if released at a high enough concentration could be hazardous to humans, environment and even properties. The impact of the gases emission to the environment could be predicted using the air pollution model. A computer simulation can be developed based on the mathematical model to predict the ground level concentration of the dispersed pollutants at a certain distance. The computer simulation is also able to estimate the impact of the pollutants to humans using the probit model.

1.2 Objectives

The main objectives of this project are:

- To develop an application that is capable to simulate the point source dispersion using Visual Basic to study the dispersion of CO
- To estimate the percentage of people affected as a result of exposure to CO at a certain concentration in a period of time.
- To compare the result of simulation with the results obtained from other established softwares

1.3 Scopes of Study

An air pollution modelling system software is developed through this study. The software is capable of solving mathematical equation of light pollutant gases. The model used in the software is a point source model developed by Pasquill and modified by Gifford. The software, Plume Dispersion Modelling Software (PluDMS) which is developed using the Visual basic language, will be able to simulate and solve the mathematical equations based on the inputs by the user. The results obtained will be validated with other established dispersion modelling software to determine the accuracy.

The scopes of study for this project are:

- Selection of the most suitable mathematical model to be used in the software
- Familiarization of Visual Basic
- Developing the software using Visual Basic
- Validation and verification of the software using other established software

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

According to the Columbia Encyclopedia, 2006, air pollution is defined as contamination of the air by noxious gases and minute particles of solid and liquid matter (particulates) in concentrations that endanger health. Air pollution is the presence of undesirable material in air, in quantities large enough to produce harmful effects (Nevers, 2000). The major sources of air pollution are transportation engines, power and heat generation, industrial processes, and the burning of solid waste. (Columbia Encyclopedia, 2006)

2.2 Sources of Air Pollution

The combustion of gasoline and other hydrocarbon fuels in automobiles, trucks, and jet airplanes produces several primary pollutants: nitrogen oxides, gaseous hydrocarbons, and carbon monoxide, as well as large quantities of particulates, chiefly lead. In the presence of sunlight, nitrogen oxides combine with hydrocarbons to form a secondary class of pollutants, the photochemical oxidants, among them ozone and the eye-stinging peroxyacetylnitrate (PAN). Nitrogen oxides also react with oxygen in the air to form nitrogen dioxide, a foul-smelling brown gas. In urban areas like Los Angeles where transportation is the main cause of air pollution, nitrogen dioxide tints the air, blending with other contaminants and the atmospheric water vapor to produce brown smog. Although the use of catalytic converters has reduced smog-producing compounds in motor vehicle exhaust emissions, recent studies have shown that in so doing the converters produce nitrous oxide, which contributes substantially to global warming.(Columbia Encyclopedia, 2006)

In cities, air may be severely polluted not only by transportation but also by the burning of fossil fuels (oil and coal) in generating stations, factories, office buildings, and homes and by the incineration of garbage. The massive combustion produces tons of ash, soot, and other particulates responsible for the gray smog of cities like New York and Chicago, along with enormous quantities of sulfur oxides. These oxides rust iron, damage building stone, decompose nylon, tarnish silver, and kill plants. Air pollution from cities also affects rural areas for many miles downwind. (Columbia Encyclopedia, 2006)

Every industrial process exhibits its own pattern of air pollution. Petroleum refineries are responsible for extensive hydrocarbon and particulate pollution. Iron and steel mills, metal smelters, pulp and paper mills, chemical plants, cement and asphalt plants–all discharge vast amounts of various particulates. Uninsulated high-voltage power lines ionize the adjacent air, forming ozone and other hazardous pollutants. Airborne pollutants from other sources include insecticides, herbicides, radioactive fallout, and dust from fertilizers, mining operations, and livestock feedlots.(Columbia Encyclopedia, 2006)

2.3 Air Pollution Modeling

An air pollution model is defined as a mathematical simulation of the physics and chemistry governing the transport, dispersion and transformation of pollutants in the atmosphere. Modeling mathematically simulates atmospheric conditions and behavior. It calculates spatial and temporal fields of concentrations and particle or gas deposition. Usually, the modeling is in the form of graphs or tables or just on paper. Presently, it is most commonly found in the form of computer programs (Lim, 2008).

2.3.1 Air dispersion modelling

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. Mathematical models can be; deterministic models, based on fundamental mathematical descriptions of atmospheric processes, in which effects (i.e., air pollution) are generated by causes (i.e., emissions) and statistical models, based upon semiempirical statistical relations among available data and measurements (Zannetii, 1993). The deterministic models are the most important and better for prediction the spatial concentration distributions within urban areas. The factors that affect the transport, dilution, and dispersion of air pollutants can be grouped into (AIR-EIA, 2000):

- Emission or source characteristics
- The nature of the pollutant material
- Meteorological characteristics
- The effects of terrain and anthropogenic structures.

A dispersion model is a mathematical description of the meteorological transport and dispersion processes, using source and meteorological parameters, for a specific period in time. The model calculations result in estimates of pollutant concentration for specific locations and times. The study of the dispersion is not a new (El-Harbawi, 2008). Early work on the subject atmospheric dispersion began with Taylor (1915) whose study the examination of the redistribution of heat in a current over relatively cold sea. Later on, he also developed the famous Taylor-theory of turbulent diffusion (Taylor, 1921). Taylor (1927) also provided the first direct measurements of the turbulent velocities in the horizontal by using the widths of the traces produced by conventional wind speed and direction recorders. Afterwards Scrase (1930) and Best (1935) extended Taylor's study, their research reveal the marked dependence on the thermal stratification of the air and also the existence of a very wide spectrum of frequencies in the generally irregular fluctuation. The paper by Builtjes, (2001) is cited several authors who done a research in dispersion modelling. For instance, the study of the dispersion from low and high level point source done by Smith (1957), Gifford (1957 a,b), Hay and Pasquill (1957) and Haugen (1959. There are five types of air pollution dispersion models, as well as some hybrids of the five types (Colls, 2002):

i. Gaussian model: The Gaussian model is perhaps the oldest (circa 1936) and perhaps the most accepted computational approach to calculating the concentration of a pollutant at a certain point. Gaussian models are most often used for predicting the dispersion of continuous, buoyant air pollution plumes originating from ground-level or elevated sources. Gaussian models may also be used for predicting the dispersion of non-continuous air pollution plumes (called puff models). A Gaussian model also assumes that one of the seven stability categories, together with wind speed, can be used to represent any atmospheric condition when it comes to calculating dispersion. There are several versions of the Gaussian plume model. A classic equation is the Pasquill-Gifford model (El-Harbawi, 2008). 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.

ii. Lagrangian model: a Lagrangian dispersion model mathematically follows pollution plume parcels (also called particles) as the parcels move in the atmosphere and they model the motion of the parcels as a random walk process. Lagrangian modelling well described by number of studies by Rohde (1972, 1974), Fisher (1975), Eliassen (1978), Hanna, (1981), Eliassen et al., (1982) and Robert et al., (1985). Langrangian modelling is often used to cover longer time periods, up to years (Builtjes, 2001).

iii. 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

iv. 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).

v. 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, 2008).

The Gaussian model is chosen as the model for this software as it is the most suitable.

The Gaussian models are based on the following simplifying assumptions (Seinfild, Pandis, 2006).

a) The mass flow of the emission is essentially continuous over time.
b) No material is removed from the plume by chemical reaction, all the mass emitted from the source remains in the atmosphere.
c) There are no gravitational effects on the material emitted.
d) The meteorological conditions are essentially constant over time during the period of transport from source to receptor.
e) The ground roughness is uniform in the dispersion area. There are no obstacles such as mountains or buildings and the ground is horizontal.
f) The cloud is transported by the wind. The time- averaged concentration profiles in the crosswind direction, both horizontal and vertical (perpendicular to the transport direction), can be represented by a Gaussian or normal distribution.

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

- Gaussian theory is basic
- Inputs are relatively simple
- Results are reasonable
- Cost effective

There are a number of limitations of Gaussian plume models [13].

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.

2.3.2 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 four 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.

b) Area sources

Area source is usually understood as an agglomeration of numerous small point sources not treated individually. Typical examples are residential heating or industrial parks with numerous stacks. Area sources are also important in the modelling of particulates where they contribute particles due to wind induced entrainment.

c) Line sources

Line source is typical for the analysis of traffic generated pollutants

d) Volume sources

This source is used for example in the analysis of air craft emissions.

2.4 Carbon Monoxide

Carbon monoxide (CO) is a colourless, odourless gas that can be poisonous to humans. It is a product of the incomplete combustion of carbon-containing fuels and is also produced by natural processes or by biotransformation of halomethanes within the human body. With external exposure to additional carbon monoxide, subtle effects can begin to occur, and exposure to higher levels can result in death. The health effects of carbon monoxide are largely the result of the formation of carboxyhaemoglobin (COHb), which impairs the oxygen carrying capacity of the blood. (WHO, 1999)

Carbon monoxide is produced by both natural and anthropogenic processes. About half of the carbon monoxide is released at the Earth's surface, and the rest is produced in the atmosphere. Many papers on the global sources of carbon monoxide have been published over the last 20 years; whether most of the carbon monoxide in the atmosphere is from human activities or from natural processes has been debated for nearly as long (WHO, 1999).

The recent budgets that take into account previously published data suggest that human activities are responsible for about 60% of the carbon monoxide in the non-urban troposphere, and natural processes account for the remaining 40%. It also appears that combustion processes directly produce about 40% of the annual emissions of carbon monoxide (Jaffe, 1968, 1973; Robinson & Robbins, 1969, 1970; Swinnerton et al., 1971), and oxidation of hydrocarbons makes up most of the remainder (about 50%) (Went, 1960, 1966; Rasmussen & Went, 1965; Zimmerman et al., 1978; Hanst et al., 1980; Greenberg et al., 1985), along with other sources such as the oceans (Swinnerton et al., 1969; Seiler & Junge, 1970; Lamontagne et al., 1971; Linnenbom et al., 1973; Liss & Slater, 1974; Seiler, 1974; Seiler & Schmidt, 1974; Swinnerton & Lamontagne, 1974; NRC, 1977; Bauer et al., 1980; Logan et al., 1981; DeMore et al., 1985) and vegetation (Krall & Tolbert, 1957; Wilks, 1959; Siegel et al., 1962; Seiler & Junge, 1970; Bidwell & Fraser, 1972; Seiler, 1974; NRC, 1977; Seiler & Giehl, 1977; Seiler et al., 1978; Bauer et al., 1980; Logan et al., 1981; DeMore et al., 1985). Some of the hydrocarbons that eventually end up as carbon monoxide are also produced by combustion processes, constituting an indirect source of carbon monoxide from combustion. These conclusions are summarized in Figure 1.1 which is adapted from the 1981 budget of Logan et al., in which most of the previous work was incorporated (Logan et al., 1981; WMO, 1986). The total emissions of carbon monoxide are about 2600 million tonnes per year. Other budgets by Volz et al. (1981) and by Seiler & Conrad (1987) have been reviewed by Warneck (1988). Global emissions between 2000 and 3000 million tonnes per year are consistent with these budgets. (WHO, 1999)

Sources of Carbon Monoxide in the Environment

Table 3. Sources of carbon monoxide[a]

	Carbon monoxide production (million tonnes per year)[b]			
	Anthropogenic	Natural	Global	Range
Directly from combustion				
Fossil fuels	500	—	500	400–1000
Forest clearing	400	—	400	200–800
Savanna burning	200	—	200	100–400
Wood burning	50	—	50	25–150
Forest fires	—	30	30	10–50
Oxidation of hydrocarbons				
Methane[c]	300	300	600	400–1000
Non-methane hydrocarbons	90	600	690	300–1400
Other sources				
Plants	—	100	100	50–200
Oceans	—	40	40	20–80
Totals (rounded)	1500	1100	2600	2000–3000

[a] Adapted from Logan et al. (1981) and revisions reported by the WMO (1986).

Figure 1: Sources of carbon monoxide in USA
Source: (WHO, 1999)

The important producers of CO are industrial processes, heating equipment, accidental fire, cigarettes, and the internal combustion engine. Blast furnace gas contains 25% CO, and coal gas, which was used as a fuel in Europe up until North Sea (natural) gas became plentiful, contains 16% [15]. CO poisoning is the most common cause of fatal gassing and is the cause of death in about 90% of fire victims. Domestic gas supplies still lead to CO poisoning, but now due to leakage of products of combustion from a damaged flue or poorly maintained equipment, rather than the fuel itself, since natural gas is CO free. In the mining industry CO contaminates the atmosphere during and after fires or explosions. The 'afterdamp' occurring in such situations is a mixture of carbon dioxide (CO_2) and CO [15].

Figure 1.2 presents the national carbon monoxide emissions by source factor in the United States while Figure 1.3 and 1.4 show the amount of CO emission in Malaysia and other Asian countries in the year 1995 and 2000, respectively.

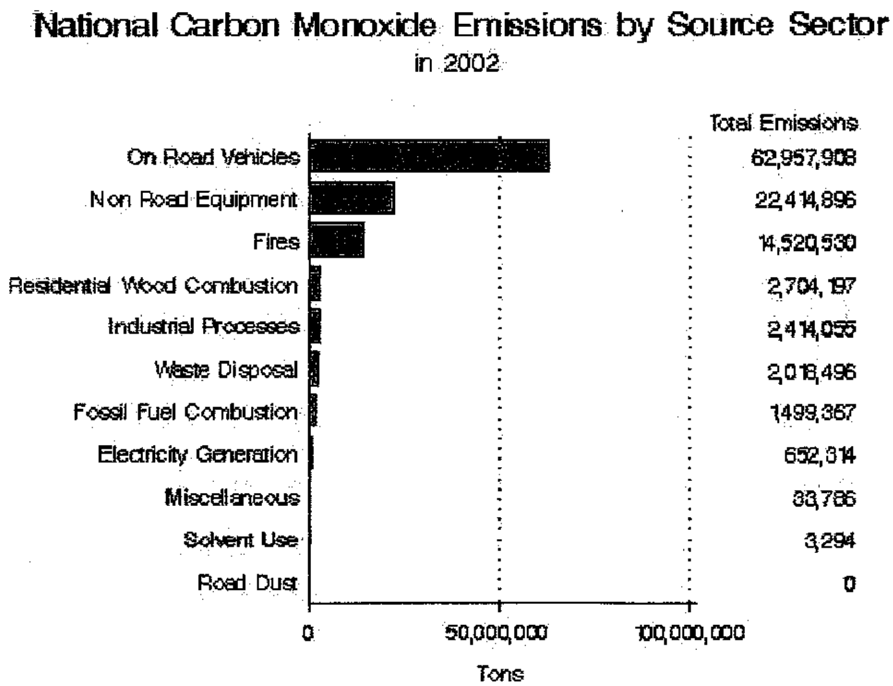


Figure 2: National Carbon Monoxide Emissions by Source Sector in US
Source: (US EPA, 2008)

Atmosphere and Climate– Malaysia

Non-CO2 Air Pollution, thousand metric tons	Malaysia	Asia (excl. Middle East)	World
Sulfur dioxide emissions, 1995	430	55,129	141,875
Nitrogen oxide emissions, 1995	532	28,962	99,271
Carbon monoxide emissions, 1995	10,334	258,325	852,415
Non-methane VOC emissions (f), 1995	1,938	42,036	159,634

Figure 3: Non-CO2 air pollution in Malaysia, Asia (excl. Middle East) and the world in 1995. (Source: EarthTrends, 2003)

Climate and Atmosphere — Air Pollution: Carbon monoxide emissions
Units: Thousand metric tons

		2000
Region/Classification		
Asia (excluding Middle East)		302,687.8
Country		
Korea, Rep	KOR	6,288.5
Kyrgyzstan	KGZ	131.7
Lao People's Dem Rep	LAO	5,842.9
Macau	MAC	19.5
Malaysia	MYS	8,730.3

Figure 4: Carbon Monoxide emissions in various countries, including Malaysia (Source: The Emission Database for Global Atmospheric Research (EDGAR))

2.4.1 Health effects of exposure to CO

The health significance of carbon monoxide in ambient air is largely due to the fact that it forms a strong bond with thehaemoglobin molecule, forming carboxyhaemoglobin, which impairs the oxygen carrying capacity of the blood. The dissociation of oxyhaemoglobinin the tissues is also altered by the presence of carboxyhaemoglobin,so that delivery of oxygen to tissues is reduced further. The affinity of human haemoglobin for carbon monoxide is roughly 240 times that for oxygen, and the proportions of carboxyhaemoglobinand oxyhaemoglobin formed in blood are dependent largely on the partial pressures of carbon monoxide and oxygen. (WHO,1999)

Concerns about the potential health effects of exposure to carbon monoxide have been addressed in extensive studies with both humans and various animal species. Under varied experimental protocols, considerable information has been obtained on the toxicity of carbon monoxide, its direct effects on the blood and other tissues, and the manifestations of these effects in the form of changes in organ function. Many of the animal studies, however, have been conducted at extremely high levels of carbon monoxide (i.e., levels not found in ambient air). Although severe effects from exposure to these high levels of carbon monoxide are not directly germane to the problems resulting from exposure to current ambient levels of carbon monoxide, they can provide valuable information about potential effects of accidental exposure to carbon monoxide, particularly those exposures occurring indoors. Some of the health effects CO has on humans are (WHO, 1999):

- Cardiovascular effects
- Acute pulmonary effects
- Cerebrovascular and behavioural effects
- Developmental toxicity

2.4.2 Recommended WHO guidelines

Air quality guidelines for carbon monoxide are designed to protect against actual and potential human exposures in ambient air that would cause adverse health effects. The World Health Organization's guidelines for carbon monoxide exposure (WHO, 1987) are expressed at four averaging times, as follows:

- 100 mg/m3 (87 ppm) for 15 min
- 60 mg/m3 (52 ppm) for 30 min
- 30 mg/m3 (26 ppm) for 1 h
- 10 mg/m3 (9 ppm) for 8 h

The following guideline values (ppm values rounded) and periods of time-weighted average exposures have been determined in such a way that the carboxyhaemoglobin level of 2.5% is not exceeded, even when a normal subject engages in light or moderate exercise (WHO, 1999).

2.5 Meteorology of air pollution

Meteorology is the most important factor affecting dispersion of emitted gases. The other factors include fluid buoyancy, momentum, source geometry, source duration, source elevation, and topography. Meteorological parameters used in dispersion models include wind direction, wind speed, ambient temperature, atmosphere mixing height, and various stability parameters (Lees, 1996). 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).

The important aspects of air pollution meteorology are atmospheric turbulence, scales of atmospheric turbulent motion, plume behavior, planetary boundary layer (PBL), effects on dispersion and applications. The atmospheric turbulence is responsible for the dispersion or transport of the pollutants. The parameters of the atmospheric movement are randomly fluctuating such as the velocity, temperature and scalar concentration. If the turbulence velocity increases, so does the dispersion of the pollutants. Dispersion is affected by the atmospheric turbulence in a way that when turbulence increases, so does the dispersion of air pollutants. Dispersion is also affected by the wind speed and direction, temperature, stability and mixing height. (Lim, 2008)

The planetary boundary layer is the layer in the atmosphere extending upward from the surface to a height that ranges anywhere from 10 to 3000 meter. The presence of the earths surfaces through mechanical and thermal forcing influence the boundary layer. Each of the forcings generates turbulence. It the planetary boundary layer (PBL) is below the stack top, there would be little to no concentrations of pollutants at the surface. If the PBL is well above stack top, there would be decreased concentrations of pollutants at the surface. Another scenario is if the PBL is just above the stack top, there is an increased concentration of pollutants at the surface. (Lim, 2008)

2.5.1 Atmospheric Stability

As mentioned before, dispersion is also affected by stability. For stack pollution dispersion, unstable stability conditions lead to greater dispersion of pollutants while stable conditions lead to less dispersion of pollutants. Stability is important as it affects the plume rise, dispersion and appearance of plumes being emitted from stacks. Plume rise can be calculated using information about the stack gases and meteorology (Lim, 2008). Stability is divided into six classes. Table 1.1 shows the six classes of stability.

Table 1: The six stability classes

Stability Class	Definition
A	Very unstable
B	Unstable
C	Slightly unstable
D	Neutral
E	Stable
F	Very stable

Class A denotes as the most unstable or most turbulent conditions and class F denotes the most stable or least turbulent conditions (Beychok, 2005).

Atmospheric air turbulence is created by many factors, such as: wind flow over rough terrain, trees or buildings; migrating high and low pressure air masses and "fronts" which cause winds; thermal turbulence from rising warm air; and many others (Beychok,2005)

Comparison of adiabatic lapse rates with ambient air temperature gradients can be used to define stability classes which categorize and quantify turbulence (Beychok, 2005):

- 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)

- 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)

- 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)

- 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 nor less than adiabatic). (Beychok, 2005)

2.5.2 Wind speed and direction

In terms of wind speed and direction, the direction will determine the direction in which the pollutants will move across terrain. 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 increasing ground level concentrations
- Increasing wind speed will increase mixing thus decreasing ground level concentration

The wind speed profile for neutral, stable and unstable stability class is shown in figure (5):

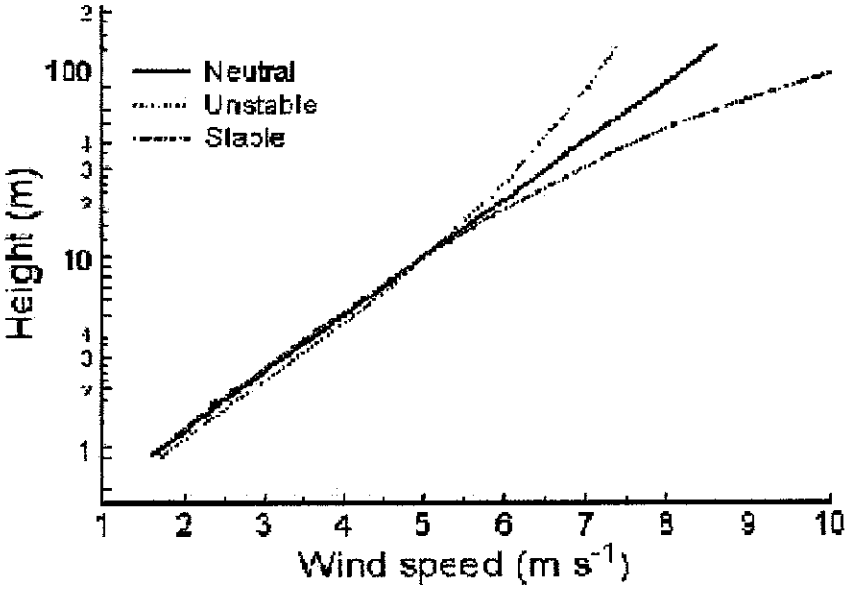


Figure 5: Wind speed profile for neutral, stable and unstable stability class

2.5.3 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).

2.5.4 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 1.5 shows the change in wind speed versus height for a variety of surface conditions (Crowl and Louvar, 2002).Figure (6) shows the effect of ground conditions on vertical wind gradient.

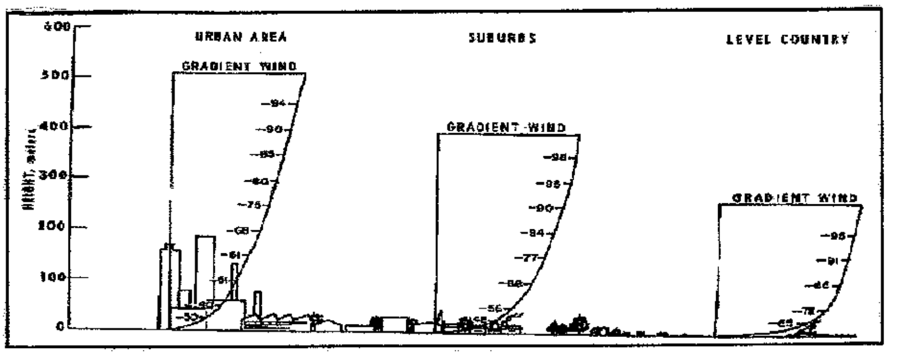


Figure 6: Effect of ground conditions on vertical wind gradient (Turner, 1970).

2.5.5 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).

The fluid may have neutral, positive or negative buoyancy. Neutral density is generally the default assumption and applies where the density of the gas- air mixture is close to that of air and the concentration of the gas is low. Gases with positive buoyancy include those with low molecular weight and hot gases (El-Harbawi et al., 2008).

2.6 Input Parameters

2.6.1 Receptor location

The receptor is the point at which an emission concentration is calculated. It is located by its height above ground level (z_r), and by its crosswind distance (y) from the plume's vertical centerline plane (Beychok, 2005).

Although, the downwind distance from the emission source to the receptor (x) does not appear in the Gaussian dispersion equation, it is one of the factors in determining the plume rise as well as the dispersion coefficients values. Thus it is a required input parameter or specification. The receptor location in terms of x, y and z_r require no further elaboration beyond recognition that is an input parameter or specification (Beychok, 2005).

2.6.2 Dispersion coefficients, σ_z and σ_y

The derivation of the Gaussian dispersion equation requires that σ_z and σ_y constants throughout the vertical z-dimension and the horizontal y-dimension. (Beychok, 2005)

There are two types of terrain for the dispersion coefficients; rural and urban.

2.6.2.1 Rural versus urban Dispersion coefficient

Dispersing plumes encounter more turbulence in urban areas than in rural areas due to the buildings as well as the somewhat warmer temperature on urban areas. Higher turbulence also occurs in the industrial plants densely populated with buildings or other structures. The additional turbulence created by an urban or industrial area is enough to alter the localized atmospheric stability to a less stable class than indicated by the prevailing meteorological conditions. In other words, if the prevailing meteorological conditions in an urban or industrial area indicate class B stability, the increased turbulence would actually disperse a plume as if class A stability conditions prevailed. Thus for any given set of meteorological conditions, the urban plume dispersion coefficients should be larger than the rural plume dispersion coefficients (Beychok, 2005). Experimental data obtained by many investigators, notably McElroy and Pooler [10, 11] among others have confirmed that urban areas have higher dispersion coefficients. (Beychok, 2005)

2.7 Probit analysis

Probit Analysis is a methodology which transforms the complex percentage affected versus dose response into a linear relation of probit versus dose response. The probits can then be translated into percentages. The method is useful because of the typical curve shape found in the dose response curve. The method is clearly approximate but it does allow quantification of consequence due to exposure (Howat, 1998)

CHAPTER 3

METHODOLOGY

3.1 Introduction

The tool used in this project to develop the PluDMS software is Visual Basic 6. Visual basic 6 not only allows the user to create simple Graphic User Interface (GUI), but also develop complex applications. In the PluDMS, the user has to key in several inputs to obtain the output. Such inputs include the meteorological conditions (atmospheric temperature, pressure, surface wind velocity, stability class, and type of terrain) and the emission parameters (stack gas flow, stack exit temperature, exit height, and stack diameter). The outputs are the concentration over the distance and the user has the option to predict the fatality of the concentration dispersed to humans. The model used in the software is Gaussian Dispersion Model for Point Source plume that has been modified by Pasquill Gifford. (The project milestone is attached in the appendices section of the report in **A.2:Project Gantt Chart**)

3.2 Gaussian Air Pollutant Dispersion Equation

The technical literature on air pollution dispersion is quite extensive and dates back to the 1930's and earlier (Bosanquet, Pearson, 1936). One of the early air pollutant plume dispersion equations was derived by Bosanquet and Pearson (Bosanquet, Pearson, 1936). Their equation did not assume Gaussian distribution nor did it include the effect of ground reflection of the pollutant plume. Figure 6 shows the visualization of a buoyant Gaussian air pollution plume.

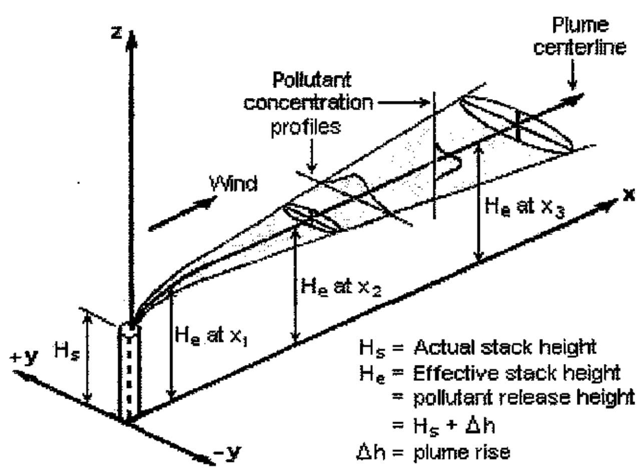


Figure 7: Visualization of a Buoyant Gaussian Air pollution Plume

Sir Graham Sutton (Sutton, 1974) derived an air pollutant plume dispersion equation in 1947 which did include the assumption of Gaussian distribution for the vertical and crosswind dispersion of the plume and also included the effect of ground reflection of the plume. The Complete Equation for Gaussian Dispersion Modeling of Continuous, Buoyant Air Pollution Plumes shown below (Beychok, 2005) (Turner, 1994):

$$C = \frac{Q}{u} + \frac{f}{\sigma_y \sqrt{2\pi}} . \frac{g_1 + g_2 + g_3}{\sigma_z \sqrt{2\pi}} \qquad \text{(Eqn 1)}$$

Where:

f = crosswind dispersion parameter

$= \exp [-y^2 / (2\sigma_y^2)]$

g= vertical dispersion parameter

$= g_1 + g_2 + g_3$

$g_1 = \exp [-(z-H)^2 / (2\sigma_z^2)]$

$g_2 = \exp [-(z+H)^2 / (2\sigma_z^2)]$

$g_3 = \exp\sum \{\exp[-z-H-2mL)^2/(2\sigma_z^2)] + [\exp[-z+H+2mL)^2/(2\sigma_z^2)] + [\exp[-z+H-2mL)^2/(2\sigma_z^2)]\} + \exp [-z-H+2mL)^2 / (2\sigma_z^2)$

C=concentration of emissions in g/m^3 at receptor

Q=source pollutant emission rate in g/s

U=horizontal wind velocity along the plume centerline, m/s

H=height of emission plume centerline above ground level, m

σ_z= vertical standard deviation of the emission distribution, m

σ_y= horizontal standard deviation of the emission distribution, m

L= height from ground level to the bottom of the inversion loft

Exp=exponential function *e* which is equal to approximately 2.71828 and also known as Euler's number

The above equation not only includes upward reflection of the pollution plume from the ground, it also includes downward reflection from the bottom of any temperature inversion lid present in the atmosphere (Chemie.DE). The sum of the four exponential terms in g_3 converges to a final value quite rapidly. For most cases, the summation of the series with $m = 1$, $m = 2$ and $m = 3$ will provide an adequate solution (Chemie.DE).

It should be noted that σ_z and σ_y are functions of the atmospheric stability class (i.e., a measure of the turbulence in the ambient atmosphere) and of the downwind distance to the receptor. The two most important variables affecting the degree of pollutant emission dispersion obtained are the height of the emission source point and the degree of atmospheric turbulence (Chemie.DE). The more turbulence, the better the degree of dispersion.

The resulting calculations for air pollutant concentrations are often expressed as an air pollutant concentration contour map in order to show the spatial variation in contaminant levels over a wide area under study. In this way the contour lines can overlay sensitive receptor locations and reveal the spatial relationship of air pollutants to areas of interest (Chemie.DE).

3.3 Point-Source Gaussian Plume Model

The Gaussian plume model is a relatively simple mathematical model. It is typically applied to point source emitters, such as coal-burning electricity-producing plants. Occasionally, this model will be applied to non-point source emitters, such as exhaust from automobiles in an urban area [18].

3.3.1 Effective height of emission (He)

He is oftem referred to as the effective stack height which should not be confused with the actual height of the emission source. The effective stack height or emissions height is greater the actual source height by the amount that the plume rises after it issues from the source stack or vent (Beychok, 1979).

Plume coming out from the top of the stacks is the source of air pollution. In order to calculate the concentration released, one of the primary calculation involved is the effective stack height which is the stack height plus the plume rise.

The effective stack height is:

$$He = h + \Delta h \qquad \text{(Eqn 2)}$$

Where He=effective stack height

h=stack height

Δh= plume rise

The Holland's equation below (Eqn 3) is used to calculate the plume rise:

$$\Delta h= \frac{v_s d_s}{U}[1.5 + 2.68(10)^{-3}P_a\frac{[T_s-T_a]}{T_s}d_s \qquad \text{(Eqn 3)}$$

Where:

Δh= plume rise, mv_s= velocity of exit gas, m/s

ds= diameter of stack, m

U= wind speed, m/s

Pa= atmospheric temperature, milibar

Ts= temperature of stack gas exit

Ta= atmospheric temperature

Holland (1953) suggests that a value between 1.1 and 1.2 times the Δh from the equation should be used for unstable conditions; a value between 0.8 and 0.9 times the Δh from the equation should be used for stable conditions.(Turner,1970)

Only once the plume has reached the effective stack height will the dispersion begin in 3 dimensions. The model assumes that dispersion in these two dimensions will take the form of a normal Gaussian curve, with the maximum concentration in the center of the plume (Bosanquet and Pearson, 1936)

The equation for Gaussian plume at z=0 (Turner, 1970),

$$C(x,y) = \frac{Q}{\pi u_H \sigma_y \sigma_z} \exp(\frac{-H^2}{2\sigma_y^2}) \exp(\frac{-y^2}{2\sigma_y^2}) \qquad \text{(Eqn 4)}$$

Where:

C(x, y) = concentration at ground-level at the point (x, y), µg/m3

x = distance directly downwind, m

y = horizontal distance from the plume centerline, m

Q = emission rate of pollutants, µg/s

H = effective stack height, m

u_H = average wind speed at the effective height of the stack, m/s

σy = horizontal dispersion coefficient (standard deviation), m
σz = vertical dispersion coefficient (standard deviation), m

3.3.2 Wind speed

The average ground level wind speed is 4.5 m/s and less than 0.5 m/s are defined as calm wind. Wind speed and height are proportional to each other and the ground friction slows lower level wind.

According to Deacon's power law (Beychok, 2005):

$$u_2 / u_1 = (z_2/z_1)^P \quad \text{(Eqn 5)}$$

Where;
u_1= speed at elevation z_1

u_2 = wind speed at elevation z_2

p= exponent that depends on stability and ground characteristics

The EPA uses the following exponent n values (Table 2), as a function of the Pasquill stability class in their Climatological Dispersion Model and ascribes the values to the work of DeMarrais, 1959. (Beychok, 2005)

Table 2: Exponents for Equation 5 for rural

Stability class	Exponent, n
A	0.10
B	0.15
C	0.20
D	0.25
E	0.25
F	0.30

Turner's Workbook presents data ascribed to Davenport, which yields the following values as the following values of the exponent n, as a function of the surface area roughness, for use in equation (5);

Level country: n=0.14-0.15

Suburbs: n=0.28

Urban areas: n=0.41

High turbulence and mixing (atmospheric stability class A)result in a much smaller indrease of the wind velocity with increasing attitude as compared to low turbulence (atmospheric stability class F) (Beychok,2005)

Level, smooth country areas also relsut in a smaller increase in wind velocity with increasing altitude as compared to urban areas with buildings which induce high surface friction (Beychok, 2005)

However, for urban areas, the EPA uses the following values in table (3) in their PAL model:

Table 3: Exponents for equation (5) (for use in urban areas)

Stability class	Exponent,n
A	0.15
B	0.15
C	0.20
D	0.25
E	0.40
F	0.60

3.3.3 Dispersion coefficients, σ_y and σ_z

There are different equations that have been suggested to calculate the dispersion coefficients, σ_y and σ_z, However, for this software, the Turner's version of the rural Pasquill dispersion coefficients published by McMullen is used as it is deemed as the most faithful representation (Beychok, 2005).The equation is:

$$\sigma=\exp\left[I+J(\ln x)+K(\ln x)^2\right] \qquad \text{(Eqn 6)}$$

Where:

σ= rural dispersion coefficient, m

x=downwind distance, km

Exp[a] =e^a=2.71828^a

Table (4) shows the constants I, J and K which are provided by McMullen for use in equation (6).

Table 4: constants I, J and K for use with equation (6)

Pasquill stability class	For obtaining σ_z			For obtaining σ_y		
	I	J	K	I	J	K
A	6.035	2.1097	0.2770	5.357	0.8828	-0.0076
B	4.694	1.0629	0.0136	5.058	0.9024	-0.0096
C	4.110	0.9201	-0.0020	4.651	0.9181	-0.0076
D	3.414	0.7371	-0.0316	4.230	0.9222	-0.0087
E	3.057	0.6794	-0.0450	3.922	0.9222	-0.0064
F	2.621	0.6564	-0.0540	3.533	0.9191	-0.0070

For urban conditions, Gifford restated Briggs' urban dispersion coefficient and developed the following equation (Beychok, 2005):

$$\sigma = (Lx)\,(1+Mx)^{N} \qquad \text{(Eqn 7)}$$

Where

σ= urban dispersion coefficient, m

x=downwind distance, km

Table X shows the constants L, M and N for use in equation (6):

Table 5: Constants L, M and N for use with equation (7)

Pasquill stability class	For obtaining σ_z			For obtaining σ_y		
	L	M	N	L	M	N
A-B	240	1.00	0.50	320	0.40	-0.50
C	200	0.00	0.00	220	0.40	-0.50
D	140	0.30	-0.50	160	0.40	-0.50
E-F	80	1.00	-0.50	110	0.40	-0.50

Other equations for the Pasquill-Gifford dispersion coefficients for plume dispersion are shown in the table (6).

Table 6: Recommended equations for Pasquill-Gifford dispersion coefficients

Pasquill-Gifford stability class	σy(m)	σz(m)
Rural conditions		
A	$0.22x(1+0.0001x)^{-0.5}$	$0.20x$
B	$0.16x(1+0.0001x)^{-0.5}$	$0.12x$
C	$0.11x(1+0.0001x)^{-0.5}$	$0.08x(1+0.0002x)^{-0.5}$
D	$0.08x(1+0.0001x)^{-0.5}$	$0.06x(1+0.0015x)^{-0.5}$
E	$0.06x(1+0.0001x)^{-0.5}$	$0.03x(1+0.0003x)^{-1}$
F	$0.04x(1+0.0001x)^{-0.5}$	$0.016(1+0.0003x)^{-1}$
Urban conditions		
A-B	$0.32x(1+0.0004x)^{-0.5}$	$0.24x(1+0.0001x)^{0.5}$
C	$0.22x(1+0.0004x)^{-0.5}$	$0.20x$
D	$0.16x(1+0.0004x)^{-0.5}$	$0.14x(1+0.0003x)^{-0.5}$
E-F	$0.11x(1+0.0004x)^{-0.5}$	$0.08x(1+0.0015x)^{-0.5}$

The power law function could also be used to calculate the dispersion coefficients. The power law function equation is:

$$\sigma = ax^b \qquad \text{(Eqn 8)}$$

Where x= downwind distance from emission source

a and b= functions of the atmospheric stability class and downwind distance

3.4 Probit v. ln(dose)

The defining equation for this analysis is (Howat, 1998):

$$Pr = a + b\{\ln(V)\} \qquad \text{(Eqn 9)}$$

where Pr=probit value

V=causative variable

a and b=probit constants based on that particular exposure.

The values for constants a,b and n for equation X can be obtained from Table A.1 in the Appendices section.

3.5 Development of Project

The development of the software is divided into several stages as shown in the Figure (8) below.

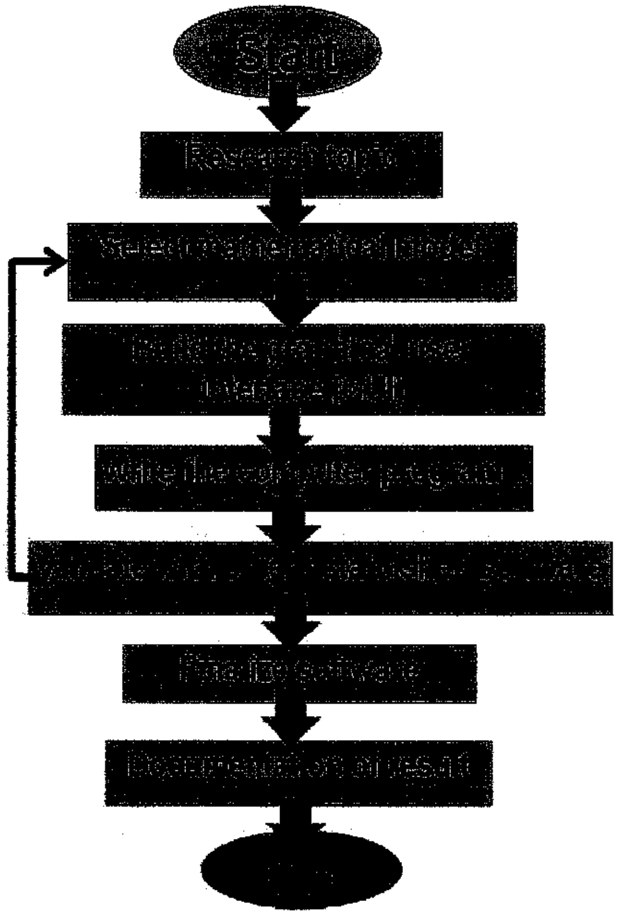


Figure 8: Process flow of the project development

Table (7) summarizes the stage involved in developing the software.

Table 7: Summary of the stages involved in developing the software

Stage 1	Research topic	The topic needs to be researched thoroughly to ensure all the variables and constants involved in developing the software. The models that would be suitable for the project needs to be compared before selecting one that will be used in the software.
Stage 2	Choose mathematical model	The mathematical model is chosen based on the case the type of dispersion involved which is point source plume dispersion.
Stage 3	Build the Graphical User Interface (GUI), Figure (10)	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 4	Write 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 5	Validation and verification of software	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. If the result is unsatisfactory, the mathematical model could be changed.
Stage 6	Finalize the software	After achieving desired results which are comparable to other softwares and case studies, the software is finalized before proceeding to the next stage
Stage 7	Documentation of result	The results are documented for future references.

The logic diagram of Gaussian Plume dispersion using PluDMS is shown in Figure (9):

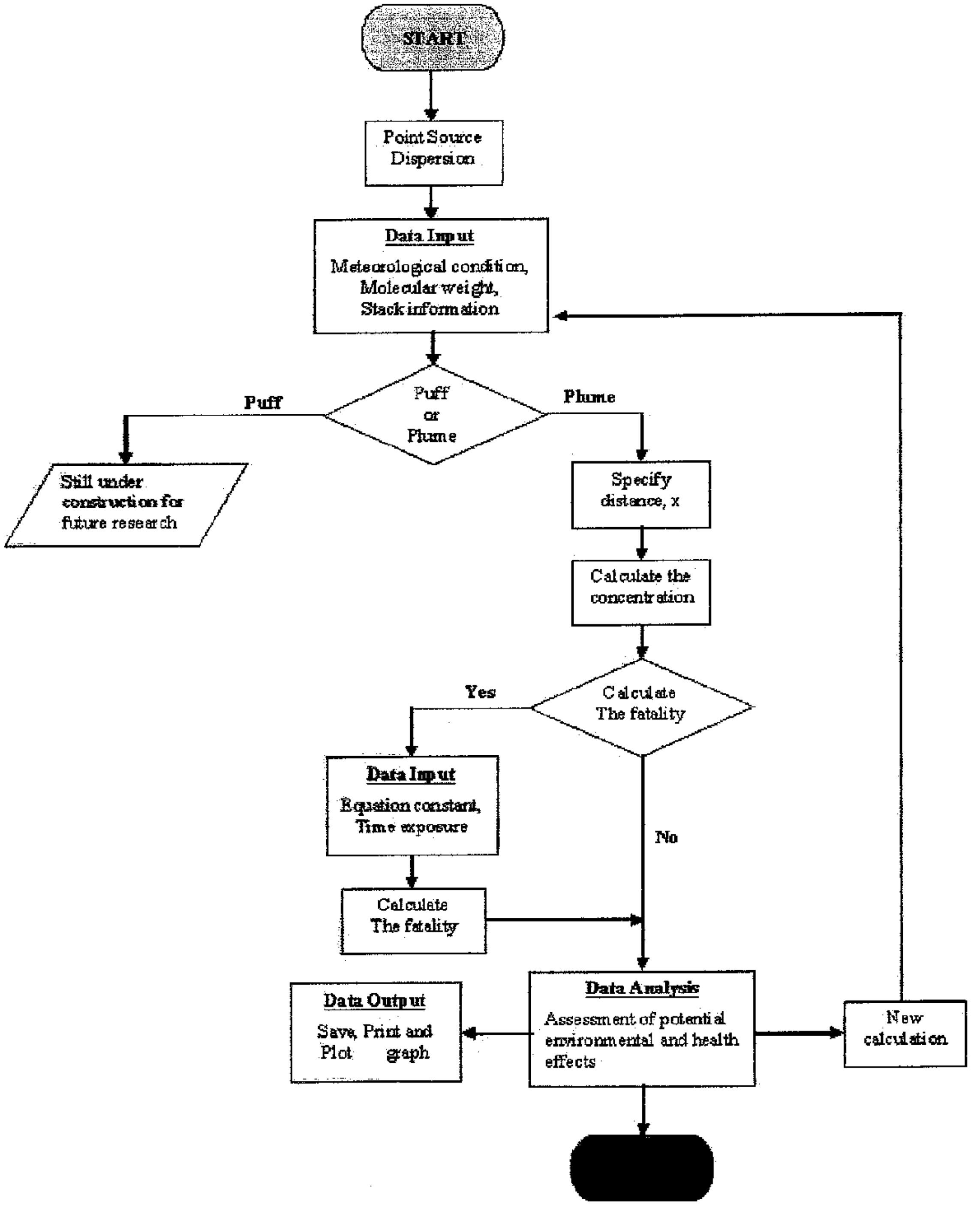


Figure 9: The logic diagram of Gaussian Plume dispersion using PluDMS

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Introduction

The Plume Dispersion Modelling Software is an easy-to-use software that enables users to predict the concentration of the released pollutant gas over a specified distance. The software uses mathematical model to calculate the concentration. The accuracy of the software depends on the accuracy of the inputs from the users.

4.2 Plume Dispersion Modelling Software Interface

The GUI design of the software is affected by several factors such as the use of colours and animations that act as traction to users and thus, their usage is recommended. In all the GUIs, the information flows from the top to bottom and left to right. (El-Harbawi, 2008). The computation of the mathematical models to calculate the concentration of gaseous emissions from the stack and fatality has been written in VB program as illustrated in figure (10).

The software interface consists of two sections which require inputs from the user as shown in figure (10). The first section of the software is the meteorological conditions where the users have to key in the data such as the surface wind speed (u), atmospheric temperature and pressure, atmospheric stability, the type of terrain (rural or urban) and the distance desired. The second section that requires inputs is the emission parameters section. This section is where inputs such as the stack height, stack diameter, stack gas exit velocity and temperature, emission rate and molecular weight of the gas.

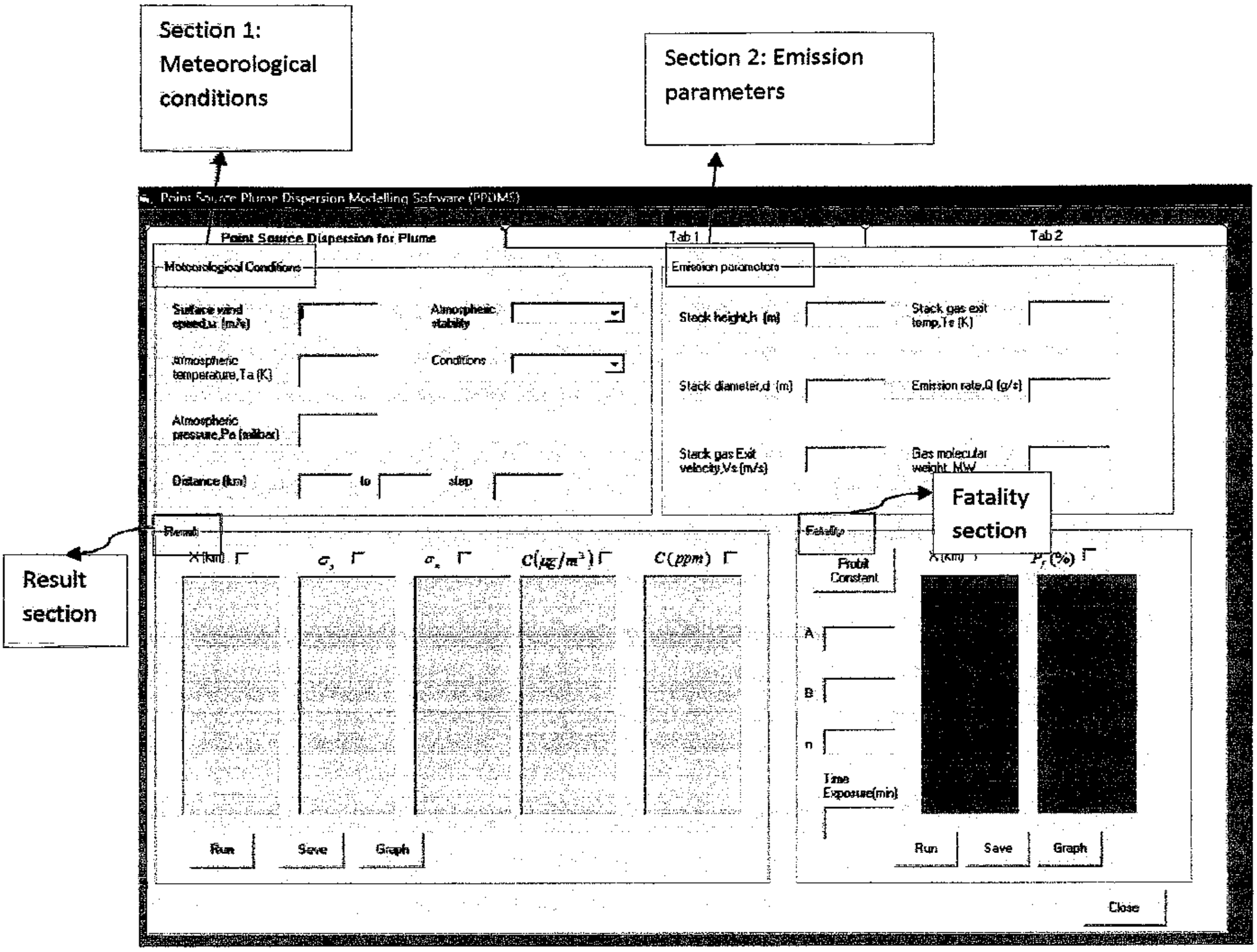


Figure 10: Point source Plume Dispersion Model GUI

After the user has key-in all the data required, the "Run" command has to be clicked by the user to calculate the predicted concentration of the gas (in ppm) over the distance. If the user failed to enter any of the required variables in section one or two, an error message will appear to inform the user of the missing data. An example of this can be seen in figure (11). When all the data are sufficient, the result will be shown in the "Result" section of the interface as labeled in figure (10). Other than the predicted concentration and distance, the result section also consists of values of the dispersion coefficients, σ_z and σ_y calculated. The user is able to plot graphs by clicking the check boxes of the desired x-axis and y-axis. The check boxes are shown in figure (12).The user then may run the "Graph" command before choosing the desired location of the graph, either Visual Basic or Microsoft Excel such as shown in figure (12.1) and (12.2).

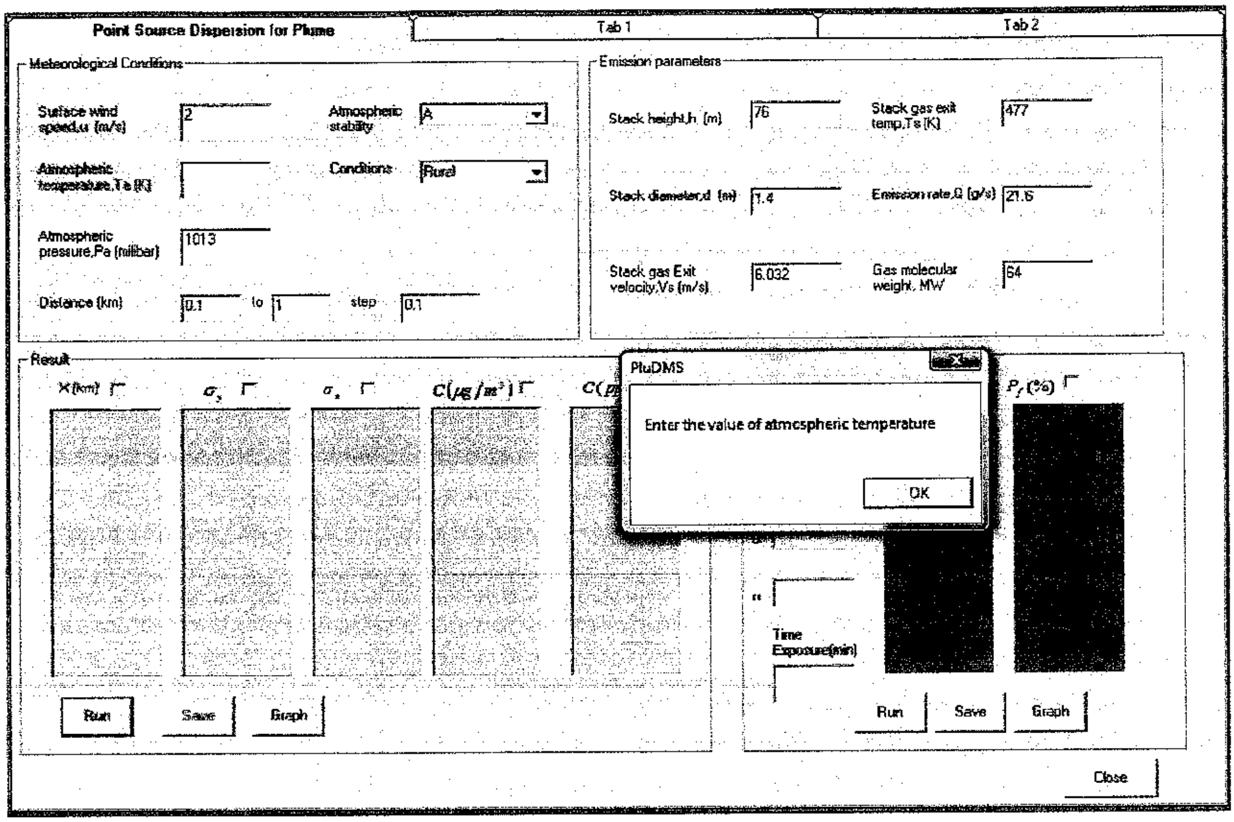


Figure 11: Error message that appears if one of the variables needed is not entered

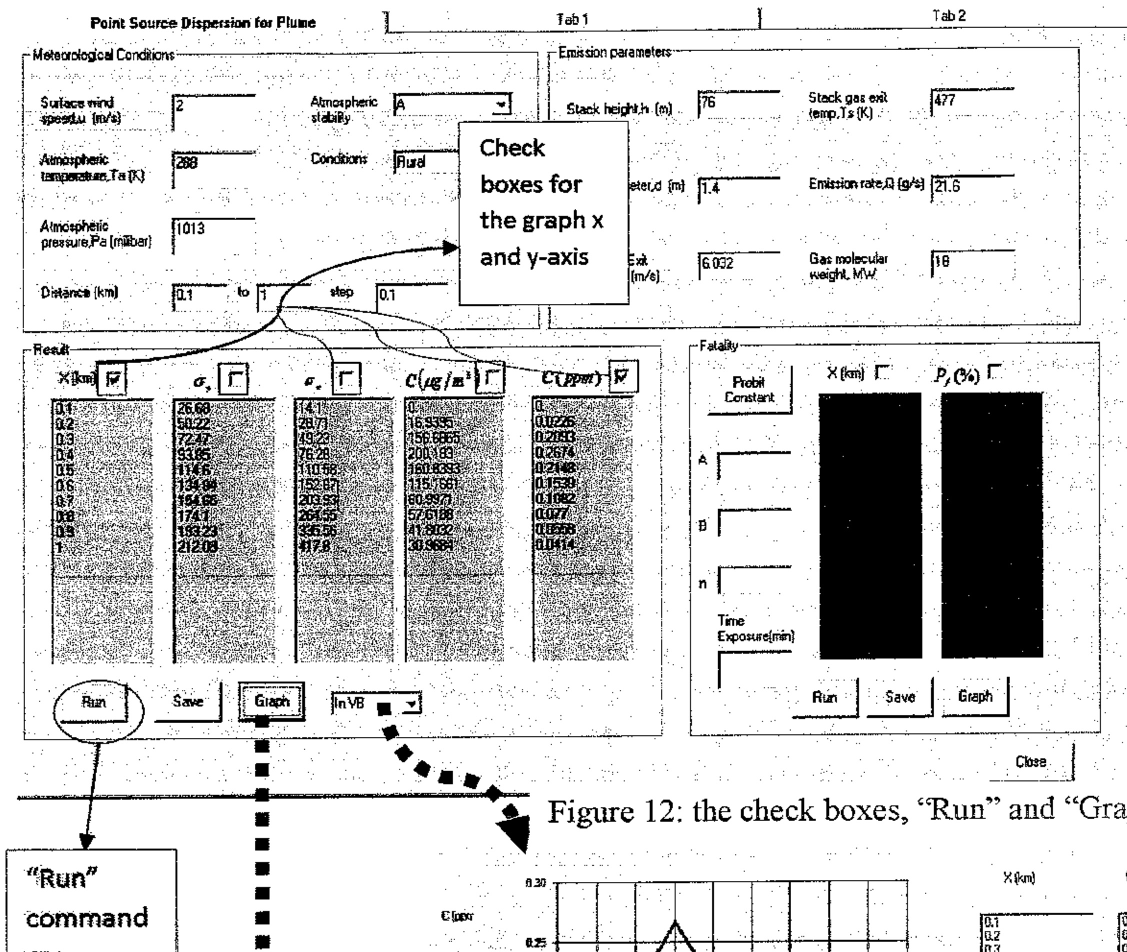


Figure 12: the check boxes, "Run" and "Graph" command

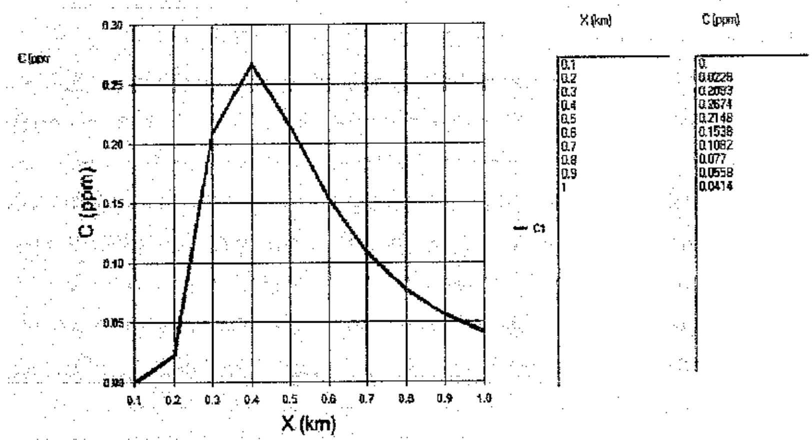


Figure 12.1: Graph of C (ppm) vs distance, X (km) in Visual Basic

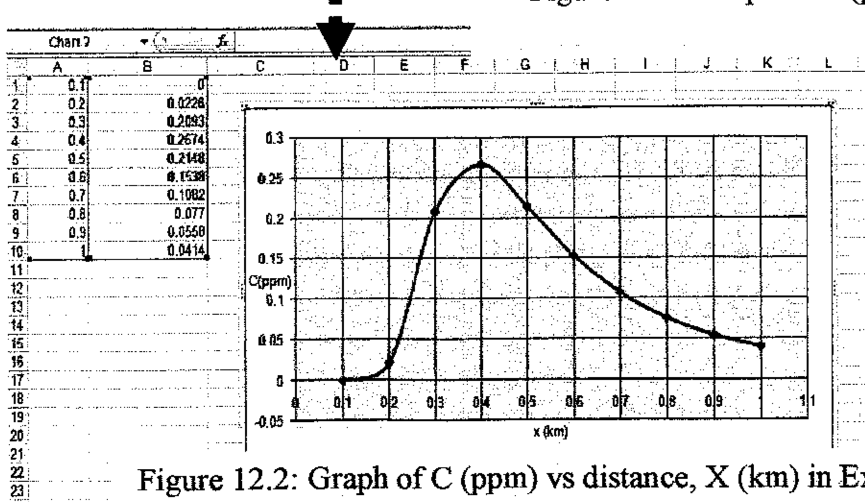
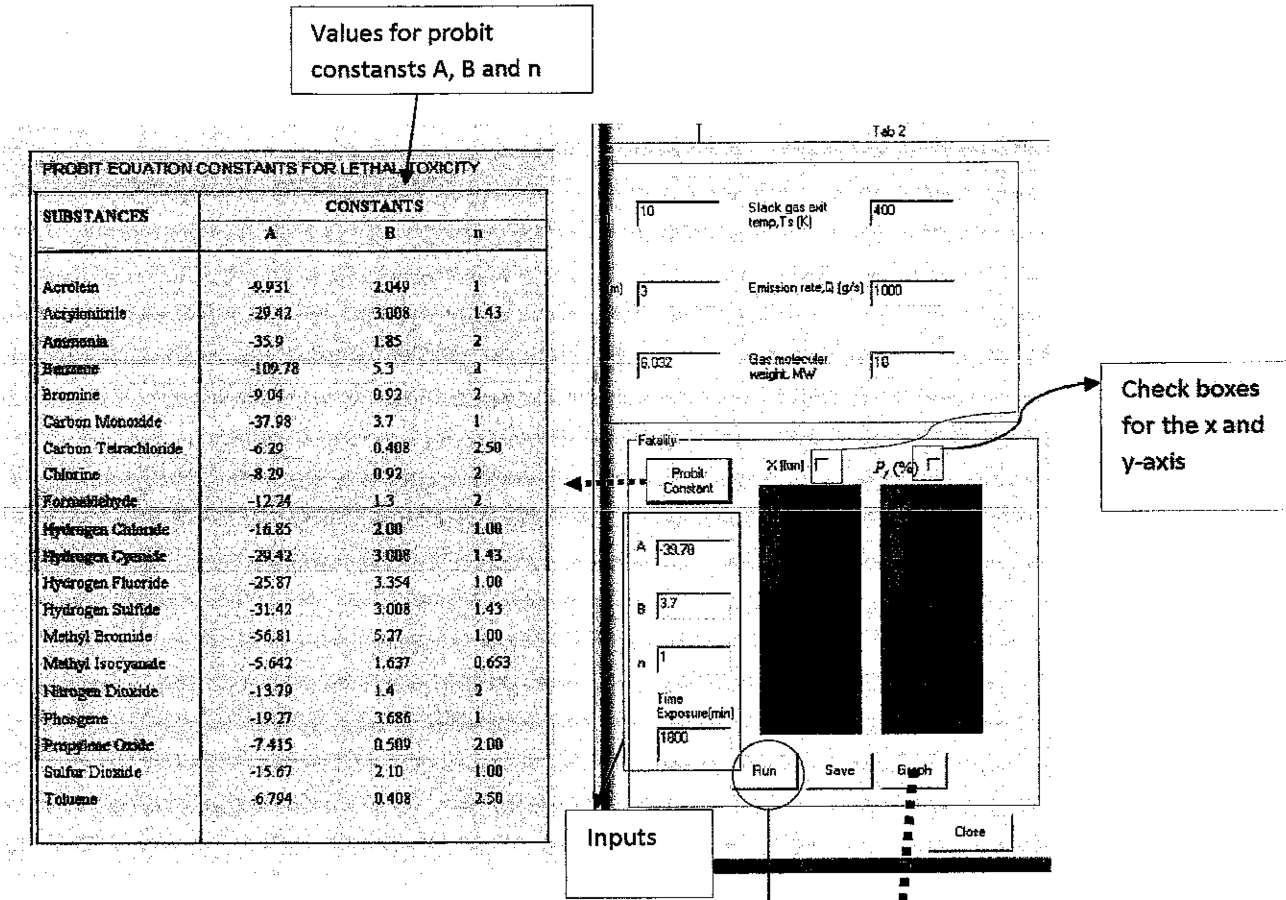


Figure 12.2: Graph of C (ppm) vs distance, X (km) in Excel

The software is also able to estimate the human fatality, or the percentage of the people affected by the concentration of gas over distance predicted in the "Result" section. The user has to key in the variables needed in the "Fatality" section in order for the software to predict the fatality. The variables involved are the constants A, B and n and the time exposure in minutes. The values for the mentioned constants may be obtained from the constant table by clicking the "Probit constants" command as shown on figure (13). The user may also plot a graph of fatality (Pf) versus the distance via Visual Basic or Microsoft Excel as shown in figure (13.1).



PROBIT EQUATION CONSTANTS FOR LETHAL TOXICITY

SUBSTANCES	CONSTANTS		
	A	B	n
Acrolein	-9.931	2.049	1
Acrylonitrile	-29.42	3.008	1.43
Ammonia	-35.9	1.85	2
Benzene	-109.78	5.3	2
Bromine	-9.04	0.92	2
Carbon Monoxide	-37.98	3.7	1
Carbon Tetrachloride	-6.29	0.408	2.50
Chlorine	-8.29	0.92	2
Formaldehyde	-12.24	1.3	2
Hydrogen Chloride	-16.85	2.00	1.00
Hydrogen Cyanide	-29.42	3.008	1.43
Hydrogen Fluoride	-25.87	3.354	1.00
Hydrogen Sulfide	-31.42	3.008	1.43
Methyl Bromide	-56.81	5.27	1.00
Methyl Isocyanate	-5.642	1.637	0.653
Nitrogen Dioxide	-13.79	1.4	2
Phosgene	-19.27	3.686	1
Propylene Oxide	-7.415	0.509	2.00
Sulfur Dioxide	-15.67	2.10	1.00
Toluene	-6.794	0.408	2.50

Figure 13: Probit constants table and fatality section of PluDMS

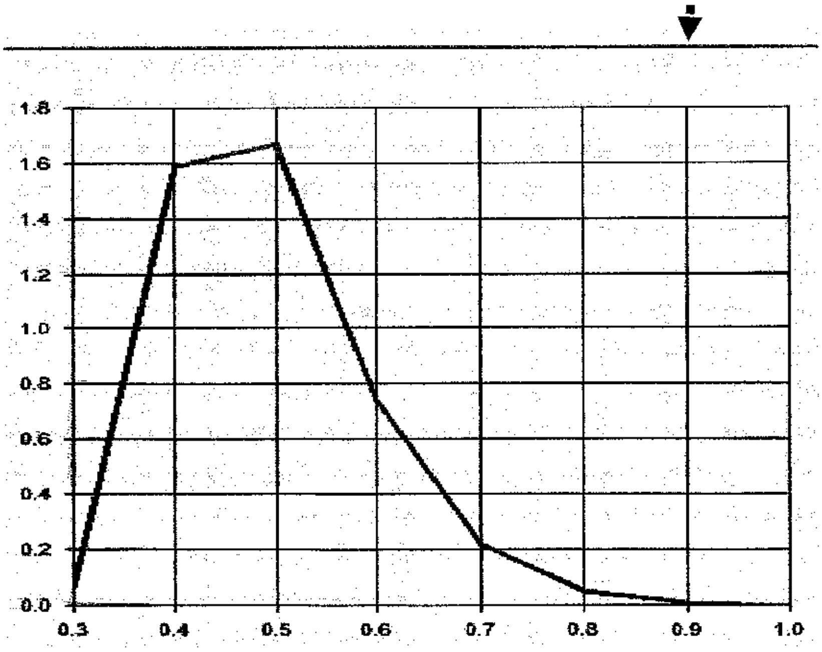


Figure 13.1: Graph of P_f(%) vs Distance,X (km)

4.3 Case Study

The software has to be validated with established dispersion model software which is SCREEN3 by using the data from a selected case study. The case study is from Milton R Beychok's *Fundamentals of Stack Gas Dispersion (2005).*

Calculate the ground level, centerline concentration downwind from a source stack. The given conditions are:

Type of terrain: Rural

Surface wind velocity: 2m/sec

Ambient temperature: 288 K

Ambient Pressure: 1013 milibar

Pasquill stability class: A

Source stack:

Emission rate: 21.6 g/s

Exit diameter: 1.4m

Exit height: 76 m

Exit temperature: 477 K

Distance: 0.1 to 2 km

4.4 Result and Discussion

The results obtained from the software and SCREEN3 for the case study are shown and compared in this section.

The results obtained from the PluDMS and SCREEN3 are tabulated (Table 8) and plotted (Figure 14):

Table 8: Results from PluDMS and SCREEN3

	PluDMS			SCREEN3		
X (km)	σ_y (m)	σ_z (m)	C (ppm)	σ_y (m)	σ_z (m)	C (ppm)
0.1	26.68	14.1	0	28.53	16.95	0
0.2	50.22	28.71	0.0145	52.26	33.06	0.0004
0.3	72.47	49.23	0.1345	73.56	50.25	0.0198
0.4	93.85	76.28	0.1719	94.18	73.07	0.0693
0.5	114.6	110.58	0.1381	114.25	105.95	0.0951
0.6	138.84	152.87	0.0989	133.90	154.83	0.0849
0.7	154.65	203.93	0.0695	153.21	213.97	0.0642
0.8	174.1	264.55	0.0495	172.19	283.49	0.0469
0.9	193.23	335.56	0.0359	190.90	363.51	0.0348
1	212.09	417.8	0.0266	209.36	454.15	0.0271
1.1	230.69	512.13	0.0201	227.60	555.54	0.0229
1.2	249.06	619.46	0.0155	245.64	667.79	0.0206
1.3	267.22	740.68	0.0121	263.46	791.01	0.0191
1.4	285.2	876.74	0.0096	281.12	925.29	0.0178
1.5	302.99	1028.56	0.0077	298.61	1070.73	0.0168
1.6	320.61	1197.21	0.0063	315.95	1227.42	0.0159
1.7	338.08	1383.63	0.0051	333.15	1395.44	0.0151
1.8	355.41	1588.83	0.0043	350.22	1574.88	0.0143
1.9	372.6	1813.89	0.0036	367.16	1765.80	0.0137

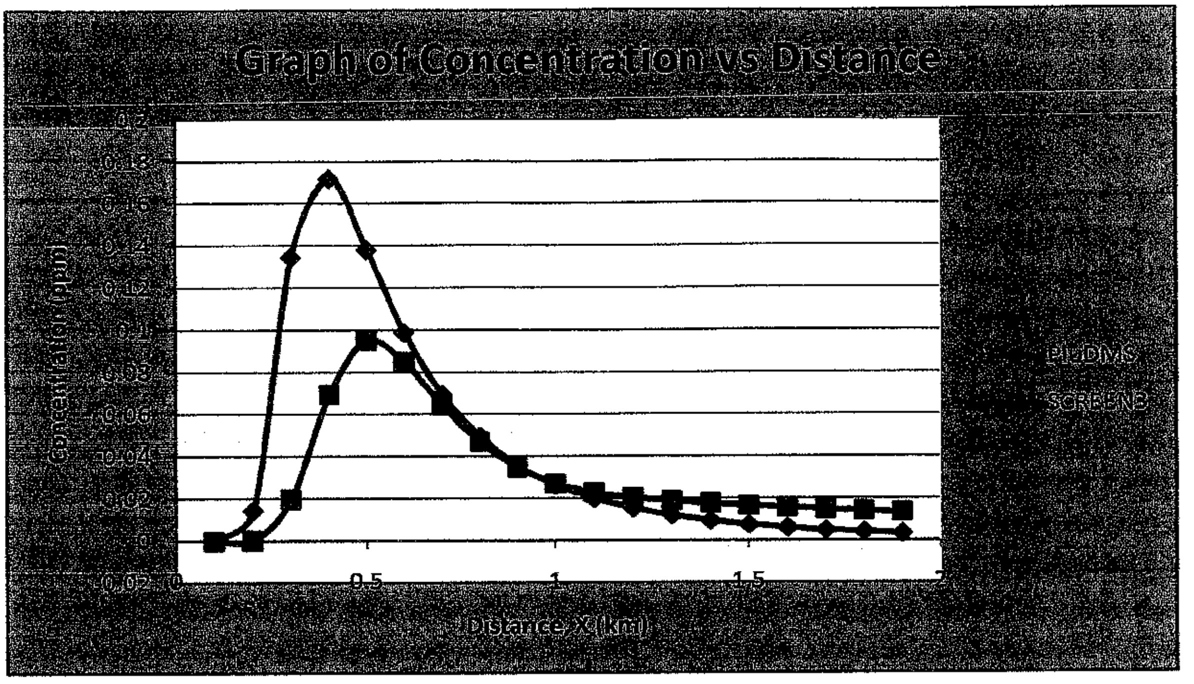


Figure 14: Graph of Concentration vs Distance for PluDMS and SCREEN3

As can be seen from Figure (14) above, the result obtained using the PluDMS and SCREEN3 are slightly different. The concentration predicted by PluDMS is higher than SCREEN3. Referring to table (8), the maximum concentration predicted by PluDMS is 0.1719 ppm while SCREEN3 predicted 0.0951.

The difference in results from PluDMS and SCREEN3 could be due to the different equations used in the softwares. Both PluDMS and SCREEN3 use the Pasquill-Gifford dispersion model. However, the parameters involved in the model have several variations. For example, the dispersion coefficients, σ_y and σ_z , can be calculated using the equations provided in table 6, the power law function (Eqn 7), or the Turner version of the rural Pasquill dispersion coefficients (Eqn 5) which is used in PluDMS. The values of σz and σy from PluDMS and SCREEN3 are compared in table 8 and the graph is plotted in figure (15) and (16).

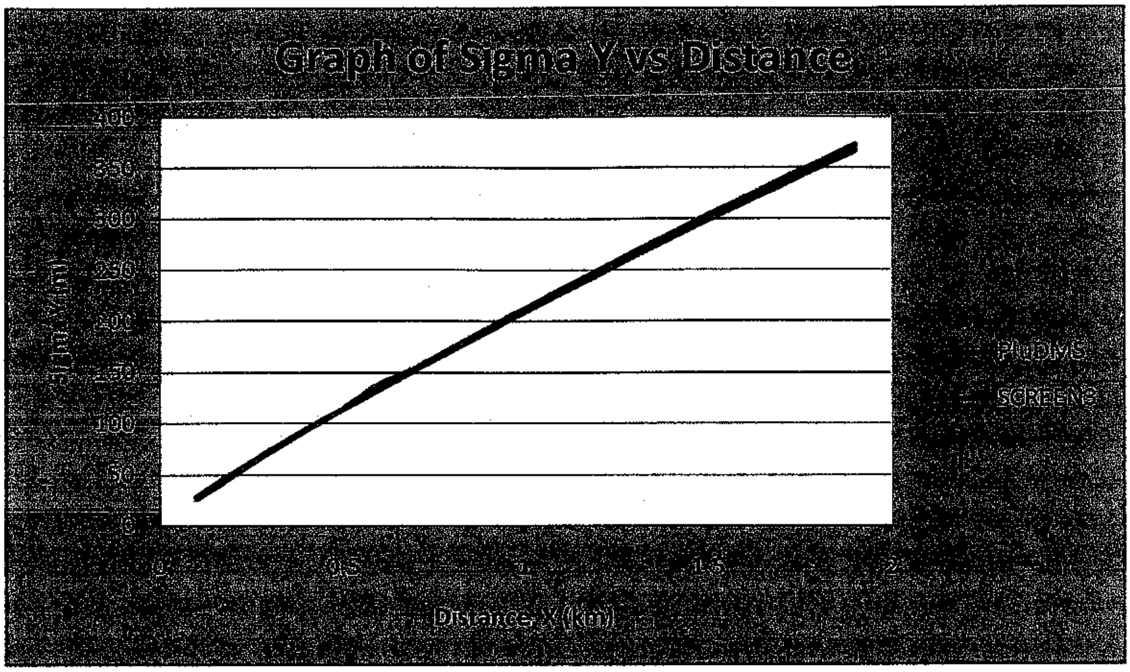


Figure 15: Graph of Sigma Y (m) vs Distance, X (km) PluDMS And SCREEN3

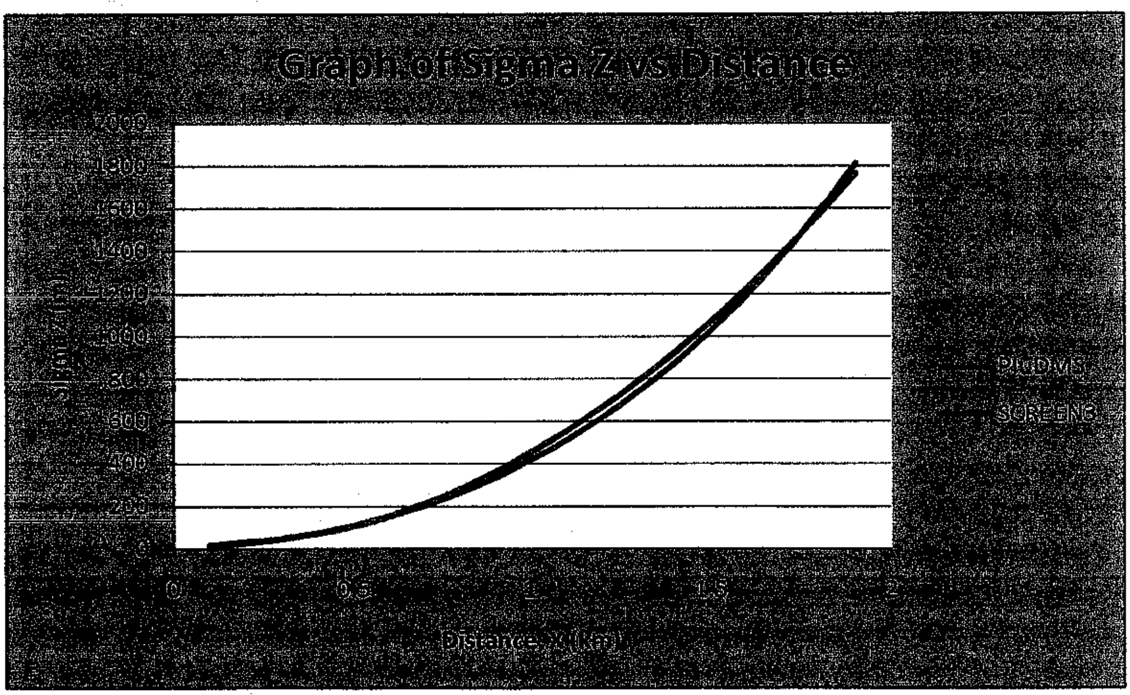


Figure 16: Graph Of Sigma Z(m) Vs Distance, X (km) For PluDMS And SCREEN3

Based on figures (15) and (16), the dispersion coefficient values calculated by PluDMS and SCREEN3 are similar. The other parameter that affects the difference between the two softwares is the plume rise calculation. The most commonly known equations for the plume rise are the Brigg's and Holland's equation. SCREEN3 software is known to use the Briggs' equation while the PluDMS uses Holland's equation. According to Schnelle and Dey (1999), the concentration predicted using the Hollands equation is higher compared to using the Briggs' equation. The Briggs' equation is more complicated than Holland's equation. Due to this, the difference of the concentration values between PluDMS and SCREEN3 exists.

4.4.1 Fatality

The fatality is also calculated and it is found that no fatality occurs for the same data inputs.

CHAPTER 5

CONCLUSION AND RECOMMENDATIONS

5.1 Conclusion

Pollutant gases from industrial activities are released into the atmosphere every day. The concentration released by a point source can be predicted using mathematical model. The mathematical model is hard to implement manually, thus it is easier to use air pollution computer software such as PluDMS. By knowing the concentration of the gas released, the assessment of the gas potential hazard to human can be done.

PluDMS has been developed using the Visual Basic language. It has been simulated and the concentration of CO dispersion over a specified distance has been predicted. It is also able to estimate the fatality the pollutant gas might cause to humans.

PluDMS has successfully been simulated and the results have been obtained. The validation of the software is done using another air dispersion software, SCREEN3. PluDMS produces slightly different values than SCREEN3 but the trends produced by both softwares are similar.

The objectives of the project are accomplished.

5.2 Recommendations

The recommendations for future work are:

- Use a more complicated equation for the dispersion model to increase the accuracy of the software

- Evaluate PluDMS using actual data to evaluate the accuracy of the software
- Evaluate PluDMS with other established air pollution dispersion softwares.

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APPENDICES

Table (A.1)

Material	a	b	n
Acrolein	-9.93	2.05	1.0
Acrylonitrile	-7.81	1.00	1.3
Allyl Alcohol	-4.22	1.00	1.0
Ammonia	-16.14	1.00	2.0
Benzene	-109.78	5.30	2.0
Bromine	-10.50	1.00	2.0
Carbon Disulfide	-46.56	4.20	1.0
Carbon Monoxide	-7.25	1.00	1.0
Carbon Tetrachloride	-6.29	0.41	2.5
Chlorine	-13.22	1.00	2.3
Ethylene Oxide	-6.19	1.00	1.0
Hydrogen Chloride	-6.20	1.00	1.0
Hydrogen Cyanide	-9.68	1.00	2.4
Hydrogen Sulfide	-11.15	1.00	1.9
Methyl Bromide	-5.92	1.00	1.0
Methyl Isocyanate	-0.34	1.00	0.7
Nitrogen Dioxide	-17.95	1.00	3.7
Parathion	-2.84	1.00	1.0
Phosgene	-27.20	5.10	1.0
Phosphamidon	-3.14	1.00	0.7
Phosphine	-2.25	1.00	1.0
Propylene Oxide	-7.42	0.51	2.0
Sulfur Dioxide	-1.22	1.00	2.40
Tetraethyl Lead	-1.50	1.00	1.0
Toluene	-6.79	0.41	2.50

Source: Louvar, J.F. and Louvar, B.D., 1998.*Health and Environmental Risk Analysis: Fundamentals with Applications.*

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	MID SEMESTER BREAK	8	9	10	11	12	13	14
1	Project Work Continue	■	■	■												
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