Modeling, Simulation and Visualization of Air Pollution Distribution Using an Advection-Diffusion Model

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Thesis Title Modeling, Simulation and Visualization of Air Pollution Distribution Using an Advection-Diffusion Model

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I hereby certify that this work has not been accepted in substance for any other degree, and is not being currently submitted in candidature for any degree.

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ABSTRACT

Air pollution is an important problem nowadays. Mathematical modeling plays a big role to research about air pollution. Air pollution modeling is used to study the behavior of the dispersion of the pollutants in the atmosphere. The advection-diffusion equation is one of the air pollution models that can be used to describe the physical processes involved in the dispersal of pollutants in the atmosphere. The advection-diffusion equation is used in this study to understand how the pollutants disperse by observing influencing parameters, such as large-scale wind, mesoscale wind, eddy diffusivity and heat diffusion (temperature). The numerical method that was used to solve the advection-diffusion equation is the explicit finite difference method. The solution obtained is simulated and visualized by developing a program with a simple and interactive user interface using the investigated software namely “Pollution Distribution Simulation” software written by Lazarus software. The various parameters in the model are varied to see the influence of the distribution of pollutants from the simulations. The results show that the large-scale wind, the mesoscale wind, eddy diffusivity, and heat diffusion have an effect on the distribution of pollutants in all three conditions of the atmosphere, that are unstable, stable and neutral conditions.

ชื่อวิทยานิพนธ์ แบบจำลอง การจำลองแบบ และการแสดงภาพของการกระจายตัวของมลพิษในอากาศโดยใช้แบบจำลองการพา-การแพร่

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บทคัดย่อ

มลพิษทางอากาศเป็นปัญหาที่สำคัญในทุกวันนี้ แบบจำลองทางคณิตศาสตร์มีบทบาทสำคัญในการทำวิจัยเกี่ยวกับมลพิษทางอากาศ ซึ่งถูกนำมาใช้ในการศึกษาพฤติกรรมของการกระจายของสารพิษในบรรยากาศ สมการการพา-การแพร่เป็นรูปแบบหนึ่งของตัวแบบมลพิษทางอากาศที่ถูกใช้ในการอธิบายกระบวนการทางกายภาพที่เกี่ยวข้องกับการกระจายของมลพิษในบรรยากาศ สมการการพา-การแพร่ถูกนำมาใช้ในการศึกษาครั้งนี้เพื่อสร้างความเข้าใจถึงการกระจายตัวของมลพิษอย่างไรโดยการสังเกตการปรับเปลี่ยนค่าพารามิเตอร์ เช่น ลมสเกลใหญ่ (large-scale wind) ลมขนาดกลาง (mesoscale wind) การแพร่กระจายแบบเอ็ดดี้ (eddy diffusivity) และการแพร่ความร้อน (อุณหภูมิ) วิธีการคำนวณเชิงตัวเลขถูกใช้ในการแก้สมการการพา-การแพร่ด้วยวิธีการผลต่างสืบเนื่องชัดแจ้ง ผลเฉลยจากการจำลองแบบและแสดงภาพถูกพัฒนาด้วยโปรแกรมอย่างง่ายและมีการโต้ตอบกับผู้ใช้โดยการใช้โปรแกรมที่สร้างขึ้นมาชื่อว่า “Pollution Distribution Simulation” ถูกพัฒนาด้วยโปรแกรมลาซารัส พารามิเตอร์ต่างๆ ในตัวแบบจำลองถูกปรับค่าเพื่อดูอิทธิพลของการกระจายตัวของมลพิษจากการจำลองแบบ ผลจากแบบจำลองแสดงให้เห็นว่า ลมสเกลใหญ่ ลมระดับกลาง การแพร่กระจายแบบเอ็ดดี้และ การแพร่กระจายความร้อนมีผลกระทบต่อการกระจายตัวของมลพิษทั้ง 3 เงื่อนไขของบรรยากาศ ได้แก่ เงื่อนไขแบบไม่เสถียร แบบเสถียรและ แบบกลาง

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Syafika Ulfah

Table of Contents

List of Figures

List of Tables

Chapter 1

Introduction

In this research, modeling and simulation of air pollution distribution is presented. In this chapter, the problems and motivations of the research are enlightened. Moreover, the aims of the research are stated as well.

1.1 Background

Environmental issues are gaining an ever-increasing attention at local, national and international levels. Parts of the problems and challenges facing governments and institutions alike is choosing and coming up with strategies and plans to maintain a safe environment.

Pollution as an inevitable product of all industrial economies is a price for a way of life and it can generally be defined as the introduction and accumulation of contaminants into the environment. These are as a result of buildup of waste and unwanted materials which comes from the activities of living organisms and can be classified as artificial or man-made. The contaminating substances can also be from natural processes such as metal accumulation from rock dissolution but the most extreme and more severe examples of pollution, however, are usually associated with or caused by human activities. Although environmental pollution has been an alarming issue throughout the history of man and in the latter part of the century, little has been done to curb it.

Air pollution is one of the major atmospheric problems currently facing the world today. It is the introduction of undesirable substances into the air in an enormous amount to cause health issues (Noel de Nevers, 2000). Meanwhile, the World Health Organization (WHO) defines air pollution as the contamination of the indoor or outdoor environment by any chemical, physical or biological agent that modifies the natural characteristics of the atmosphere. Various studies have shown the effects of polluted air on agricultural productivity, the ecosystem, and human health.

The environment as we know is made of the atmosphere, the soil, water bodies and these play an important role in the emission of pollutants. Pollutants are always deposited in these parts of the ecosystem. The emitted pollutants undergo chemical and physical changes through interactions with the environment.

Air is a multicomponent mixture of gaseous molecules and atoms which are constantly moving about and undergoing frequent collisions. The ability of the atmosphere to reflect or absorb the concentration of pollutants depends on meteorological factors such as temperature, humidity level, pressure, wind velocity, etc. as well as the state of the atmosphere whether unstable, stable or neutral.

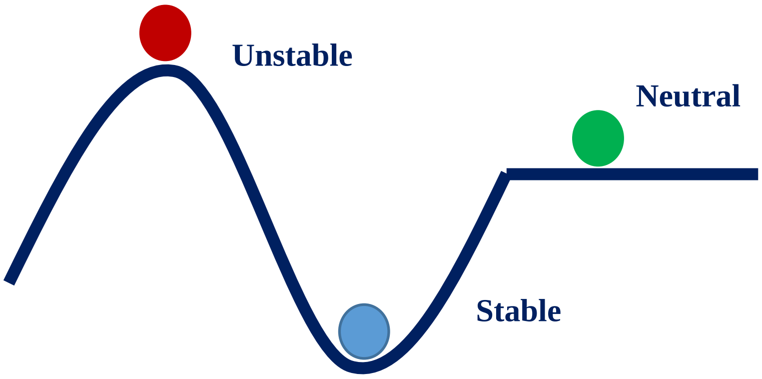
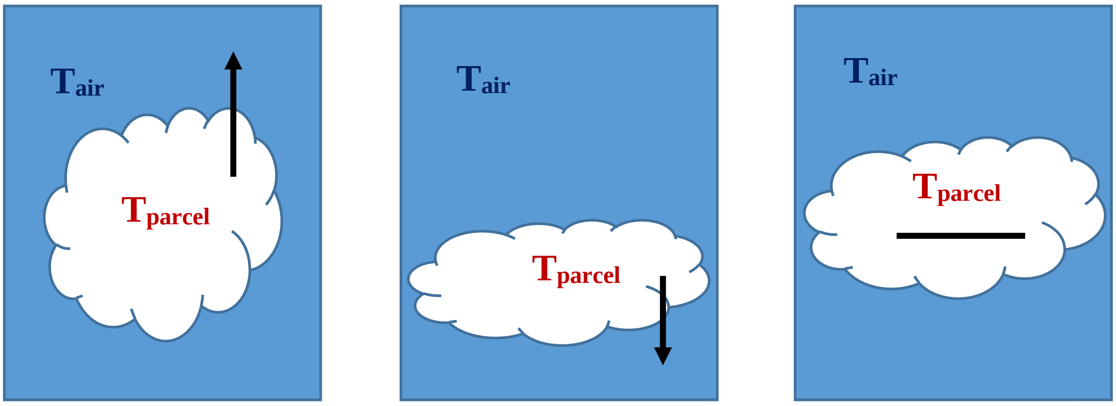


Figure 1. Stability of an object.



Unstable

$T_{parcel} > T_{air}$

Parcel is lighter and moves up.

Stable

$T_{parcel} < T_{air}$

Parcel is heavier and moves down.

Neutral

$T_{parcel} = T_{air}$

Parcel stays put.

Figure 2. Air parcel in the atmosphere.

Figure 1 shows the concept of stability of an object. The unstable, stable, and neutral state of the object can be explained with the object coming back to a state of equilibrium after any movement. Under the unstable state, the object does not come back to an equilibrium state but otherwise in the case of the stable state. In the neutral state the object remains until it is further displaced.

This concept can be used to understand atmospheric stability conditions. Figure 2 shows an air parcel in the atmosphere. The air parcel is said to be in an unstable state if the temperature of the surrounding air is greater than the temperature of the air parcel. In other words, the parcel of air becomes less dense and then moves in the upward direction. In a stable state, the air parcel moves in the downward direction when the temperature of the surrounding air becomes less than the temperature of the air parcel. This means that the parcel is heavier than the surrounding air and therefore it would sink. The air parcel is said to be in the neutral state when the temperature of the surrounding air is equal to the temperature of the air parcel. This means that the air parcel would remain at where it is until the conditions in the atmosphere change. These atmospheric conditions determine how long pollutants remain in the atmosphere whether they would be absorbed or reflected in the atmosphere in the short or long term.

The pollution pathway concept described by Holgate (1979) is a convenient way for studying and appreciating the distribution of the concentration of pollutants. Holdgate (1979) stated that there are common characteristics associated with pollutant emissions. These include the pollutants themselves ($NO_x, SO_2, etc.$), the source of the pollutants (industrial stacks, fumes from automobiles), medium of transport (either through air, water or soil) and the receptors (the living organisms, ecosystems or items or buildings affected by the pollutants).

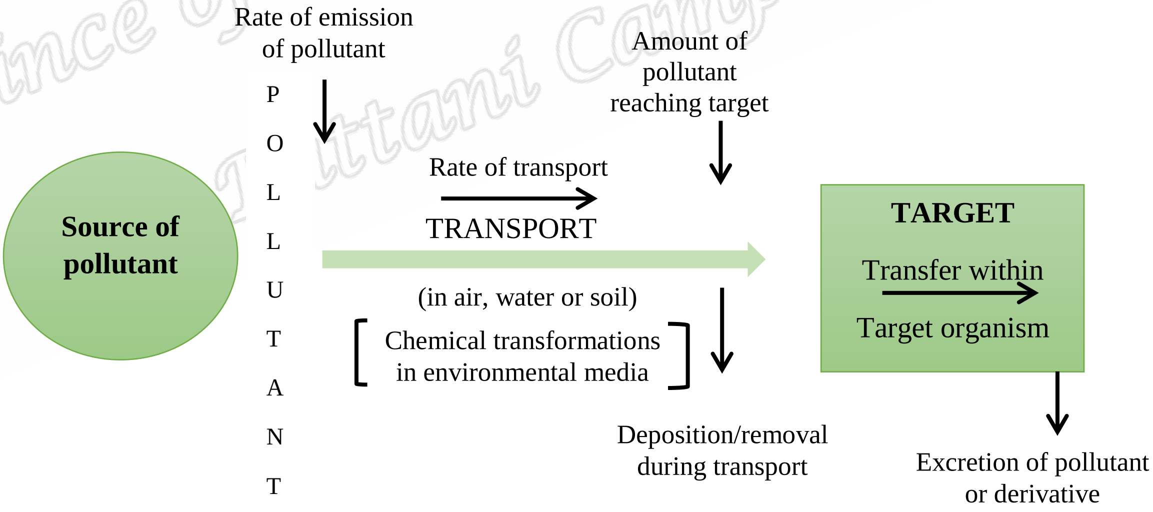


Figure 3. A simplified model of environmental pollution (Holdgate, 1979).

The distribution of pollutants can be clearly explained by other variables including the rate of emission of the pollutants from the source, the rate of the transport, physical and chemical transformations which the pollutants undergo either during transport or after deposition at the target, amounts reaching the target and its effects on the target.

Sources of pollutants can either be discrete point sources or area point sources. During pollutants emission, they are distributed through the environment either in the air (e.g. smoke, NO_x, SO_x), in water (e.g. industrial effluents) or in soil. Therefore, the transport mechanisms include movement in wind and water, gravity, and other anthropogenic transport media. Most air pollutants are released in the part of the atmosphere that is close to the earth surface (boundary layer) where normally wind blows due to turbulence. Larger particulates of pollutants of about $1 - 10\ \mu m$ are deposited in the boundary layer while smaller particles (mostly gaseous) that are normally less than $5\ \mu m$ are transported into the part which is mostly the earth's atmosphere (troposphere). These transports are as a result of the vertical movements of thermal plumes which are carried by high winds and storms that flow over mountains. Climatic changes in the atmosphere and particles size also have an effect on the transport of pollutants.

On the boundary layer, there is a continuous mixing of pollutants and the surrounding air until they attain a relatively uniform concentration. Wind velocity, solar radiations, land surface roughness and the cloud are some of the factors that determine how the concentration of pollutant dilute in the atmosphere (Masters, 1991).

The density of air is inversely proportional to its temperature and therefore warm air is less dense and rises, while cooling air becomes denser and descends. The adiabatic lapse rate (the decrease in atmospheric temperature with rising altitude) of the cooling of air masses plays a major part in determining the stability of the air into which pollutants are released. If the temperature of rising warm air decreases at a rate faster than the adiabatic lapse rate, dilution of pollutant concentration occurs as the air mass becomes unstable. However, if the temperature drops more slowly than the adiabatic lapse rate, the concentration of the pollutants would increase as the air becomes stable.

The reduction in the concentration of the pollutants depends largely on the velocity of the wind and the how far the pollutants can rise into the atmosphere. In other to explain the principal factors involved in the emission and the dispersion of pollutants, it would be convenient to use an example of the dispersion of plume of smoke from a single chimney since many atmospheric pollutants are emitted from industrial stacks (chimneys). It is also important to realize that the presence of tall buildings, other chimneys, and the urban environment can greatly complicate the pattern of dispersion of atmospheric pollutants from a single chimney.

Most models of time-averaged concentrations of pollutants downwind from a point source, such as chimney are based on a normal (Gaussian) distribution curve of the pollutants. In this research, the advection diffusion equation with time-dependent would be used to study how pollutants disperse and diffuse in the atmosphere. Some atmospheric parameters would be considered.

1.2 Problem Statement

As stated earlier, pollution has been a major problem facing governments and world leaders for decades now. The pollution problem can be viewed as affecting the quality of air, oceans and water bodies and to a large extent the ecosystem. The polluted air can affect human health and other living things. It can have a global consequence like acid rain and global warming.

WHO reported that in 2012, air pollution exposure was responsible for 7 million premature deaths, and this occurs annually. The United State Environmental Protection Agency (EPA) in 2009 reported that emissions of carbon dioxide and other long-lived greenhouse gasses that build up in the atmosphere harm the health and welfare of current and future generations by causing climate change and ocean acidification.

Ocean acidification issues occurred in Oregon as Kristin Eberhard reported. She stated that pollution has infiltrated Oregon's coasts and has caused acidification. This has created problems for the Ocean's shellfish industry. The ocean acidification reduces the pH causing high acidity which reduces the carbonate ions concentration useful to form shells of marine animals such as crab. This condition causes their shells to become fragile and makes them vulnerable.

In the economic aspects, huge sums of money are spent on air pollution issues. In China, to prevent and plan control action of the airborne pollution, it would be backed by 1,700 billion yuan ($277 billion) in total investment from the central government (China Daily, 2013).

The sources of pollution whether it is affecting the quality of air or water bodies are normally from either natural phenomenon or anthropogenic sources. In the natural phenomenon, volcanic ash, forest fires (due to excessive drought, El Nino) etc. can contribute to air pollution. As an example, on June 2015, Raung mount, one of the active volcanoes in Indonesia erupted; it is located in the province of East Java and its 2-kilometres-wide and 500-metres-deep. This mount shot out ash around 1,000 meters into the air. As a result, several airports were closed because of the decreasing visibility.

In anthropogenic sources, emissions occur from industrial stacks, vehicle combustion and sometimes forests fires. Forest fires normally occur in countries like Indonesia because of land clearing for oil palm plantations. Large acres of land are set ablaze in an attempt to clear the land and prepare it for the next planting season. Forest fires in Indonesia is a local problem has extended to a global consequence. They result in the emissions of carbon and because of that, it needs to be prevented. One of the foreign exchange earners in Indonesia is oil palm production and because of that, it becomes difficult to handle, as it is a profitable and an important commodity. Air pollution problem that has been occurring recently is from forest fires in Sumatra and this issue can be caused by either anthropogenic or natural causes. Jakarta Post reported that heavy smoke from the fires in Sumatra island has caused levels of air pollutants to spike throughout islands and some parts of Malaysia, Singapore, and even Thailand. The major concerns are that people were dying from inhaling the smoke coming out of the burning forests. Also, the blaze is destroying forests that are the lungs of the world.

El Nino in 2015 is responsible for many fire outbreaks. This phenomenon made the atmosphere warm and dry thereby increasing the number of fire outbreaks in countries like Indonesia. Many of these fires come from lands which are rich in carbon. There are a lot of peat reserves and when there is a fire outbreak, they produce huge dark smoke with carbon dioxide and other greenhouse emissions. These contribute to climatic problems. Sumatra, Indonesia might seem a world away but the haze from the fires there travel miles bringing that smoke and its accompanying degraded air quality across the globe.

Industrial stacks, a medium to release air pollutants like sulfur dioxide and nitrogen oxides rise into the atmosphere from the burning of coal in an effort to disperse pollution and decrease the impact on the local community has in the long term become a mirage. This is because wind currents are faster at higher altitudes, causing pollution to travel hundreds of miles to surrounding provinces, states, and cities. These pollutants are released into the atmosphere during the burning of fossil fuels and when it rains, the water droplets combine with these air pollutants and as a result, become acidic and then falls to the ground in the form of acid rain which can cause severe damage to humans, animals, and crops.

1.3 Motivation

Life cannot be separated from air, without it living organisms including humans would not survive. Living organisms have to breathe and accept the air as it exists in the atmosphere. We cannot choose which air to be breathe.

Every country in this world experiences the pollution problem in their cities. The distinguishing feature is the level of pollution in each country which depends on how they manage their air quality. Air pollution in high levels can affect humans, ecosystem or the climate.

Pollution, as we know, consist of contaminants which have undesired effects. Those contaminants are NO_x, SO_2, CO, PM, CO_2 and much more. Almost all respiratory diseases are caused by air pollution exposure. For instance, carbon monoxide CO can prevent oxygen from entering the various body organs of the body and tissues, $PM_{2.5}$ and PM_{10} that may be inhaled will most likely be able to be deposited within the lungs and bloodstream because of their small size. Another effect of air pollution exposure is that pollution can damage the ecosystem. The ocean acidification issue is one of the problems caused by air pollution exposure which damages the aquatic ecosystem. It is the decrease in the pH of earth's oceans. This is usually caused by the increase in carbon dioxide in the atmosphere produced by human activities (like fossil burning). Air pollution can even change the climate. CO_2, CH_4, N_2O contribute to greenhouse gasses. The particles in the haze can reflect and absorb incoming solar energy. Consequently, the atmosphere becomes warm.

With the underlying effect and consequences, it is important to study the distribution of air pollution in order to know the dispersal or transport of pollutants. One of the factors affecting air pollutants distribution is air flow. Without currents of wind, the air pollutants will stick around the source of emission and as a result become increasingly concentrated, but a meteorological cycle of weather has an enormous effect on pollutants distribution and either at high or low levels it can alter the diffusion and advection processes of pollutants.

Weather refers to the state of the atmosphere with respect to the wind, temperature, pressure, humidity, etc. The pollutants can go as far as the wind carries it. Advection transports pollutants in the downwind direction and it can transfer the pollutants far away from the source of emissions. As the pollutants are being dispersed, they diffuse with time as well. Temperature, pressure, and humidity affect the diffusion process of pollutants. When the temperature is high, it increases the energy, consequently, the pollutants concentration diffuses faster than when the temperature is low. As the temperature is proportional to the atmospheric pressure, pollutants diffusion becomes faster at high pressures and slower in low-pressure conditions. When the atmosphere is very humid, it has more density, consequently, the pollutants concentration diffuses slowly.

There are some studies on the effect of NO_x, SO_2, CO, PM, CO_2 and other contaminants on human health. Zulkarnain, *et.al.*, (2010) did a study on the effect of air pollution on respiratory health and the cost of associated illness. There are lack of studies on these emission problems on modeling and simulation. Virtually, the study on this view can predict and or estimate the concentration of pollutants and how far it is distributed. There is the need to study this in order to know how the pollutants distribute in the atmosphere. Thus, this study would simulate the distribution of the pollutants by examining the meteorological parameter involved such as wind direction, wind velocity and eddy diffusivity using the simulated data.

In this research work, questions like is the pollutant being emitted from a point source and in low levels over a large area (non-point source) will be answered and thereby formulate procedures either to stop production of the pollutant or to reduce its concentration in the environment by finding other methods of manufacturing or waste handling.

As we know, not only does advection carries pollutants away in downwind direction and transport it as long as the wind blows, but diffusion also aids in the movement of the pollutants. We would, therefore, present an advection-diffusion model to describe air pollution distribution.

1.4 Objectives

The objectives of this research are:

1.1 To study air pollutants distribution using an advection-diffusion model.

1.2 To simulate the proposed mathematical model numerically by explicit finite difference method.

1.3 To create a program for simulation and visualization of air pollution distribution.

1.4 To analyze the distribution of air pollution in unstable and stable atmospheric conditions.

1.5 Expected advantages

The research work would be beneficial in the following ways.

1.1 An advection-diffusion model can help to understand the distribution of pollutants as they are dispersed through advection and diffusion processes.

1.2 The explicit finite difference method is intuitive and easy to implement to provide a quicker way of solving the proposed model which would help in the simulation of the pollutants for visualization.

1.3 A computer program would provide a way of altering the various parameters for visualization to know how the pollutants disperse.

1.4 Pollutants disperse differently in different atmospheric conditions and therefore analyzing how they disperse in these conditions would help in better policy making by governments.

Research work related to this study would be discussed in the next chapter.

Chapter 2

Literature Review

The main goal of this chapter is to relate the present study in the context of other studies and related work of air pollutants distribution modeling.

Pollution is the most serious of all environmental problems and poses a major threat to the health and well-being of millions of people and global ecosystems. For at least thirty years, people have become increasingly aware of these issues. As a result, governments and regulatory bodies have responded by taking action against grossly polluting activities in the emission of pollutants into the environment.

However, mathematicians on the other hand have approached the pollution problem through modelling of the real world situation by considering the pollutants themselves, the source of emission, the receptors (people, building, ecosystem) and how the pollutants distribute in the atmosphere and also the effects meteorological or climatic parameters or factors have on the dispersal or distribution of pollutants from a region of higher concentration to a region of lower concentration.

Quantification of the relationships between emissions and concentrations involves two steps: identifying what the most important atmospheric processes are, and representing these mathematically in a model (Bell and Treshow, 2002). Mathematical models are useful to study how pollutants behave when there are new sources of air pollution or changes in a number of pollutants emitted into the air from the presence of emission sources and help in analyzing such behaviors (Awasthi, Khare, and Gargava, 2006). Mathematical formulations of transport and dispersion are developed to identify the parameters of interest. Air quality models have become integrated tools in environmental monitoring, management and assessment of air pollution (Fenger and Tjell, 2009). The perfect air pollutant concentration model would allow us to predict the concentrations that would result from any specified set of pollutant emissions, for any specified meteorological conditions, at any location, for any time period, with total confidence in the prediction (de Nevers, 2000). A study by Arystanbekova (2004) stated that simulation of air pollution is useful in providing information about the spreading of pollutants in an area, the scale, and level of pollution and estimation.

Venkatachalappa, Khan, and Kakami (2003) studied a time-dependent two-dimensional advection-diffusion model of air pollution for an area source with an equation of the primary pollutant as follows:

$\frac{\partial C_p}{\partial t} + U(z)\frac{\partial C_p}{\partial x} = \frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_p}{\partial z}\right) - (k + k_{wp})C_p,$ where $C_p = C_p(x,z,t)$ is the ambient crosswind integrated concentration of pollutant species, U is the mean wind speed in $x-$direction, K_z is the turbulent eddy diffusivity in $z-$direction, k_{wp} is the first order rainout/washout coefficient of primary pollutant C_p, and k is the first order chemical reaction rate coefficient of primary pollutant C_p. The concentration for the secondary pollutant is $\frac{\partial C_s}{\partial t} + U(z)\frac{\partial C_s}{\partial x} = \frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_s}{\partial z}\right) - k_{ws}C_s + v_g k C_p,$ where $C_s = C_s(x,z,t)$ is the secondary pollutant, k_{ws} is the first order wet deposition coefficient of secondary pollutants, and v_g is the mass ratio of the secondary particulate species to the primary gaseous species which is being converted. The parameters they considered were variable wind velocity, eddy diffusivity, and chemical reaction. The model was solved by the implicit Crank-Nicolson finite difference technique. The model analyzed primary and secondary pollutants in stable and neutral atmospheric conditions. The result showed that the ground level concentration of primary pollutants attains peak value at the downwind end of the source region whereas, the concentration of secondary pollutants attains its peak value at the source free region in the downwind direction. The model also predicts that the ground level concentration of a secondary pollutants at a particular downwind distance is always higher in the stable atmospheric condition than that of the neutral atmospheric condition.

Sudheer, Lashminarayanachari, Prasad and Pandurangappa (2012) studied a two-dimensional mathematical model to analyze air pollutant distribution emitted from an area source. In the study, they considered chemical reaction and dry deposition for primary and secondary pollutants, with the equation of primary pollutant as follows: $\frac{\partial C_p}{\partial t}+U(z)\frac{\partial C_p}{\partial x}=\frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_p}{\partial z}\right)-kC_p,$ and for secondary pollutant,

$\frac{\partial C_s}{\partial t}+U(z)\frac{\partial C_s}{\partial x}=\frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_s}{\partial z}\right)+v_g kC_p.$ The model was solved numerically by using the implicit Crank-Nicolson finite difference technique. The results showed that the ground level concentration increases in the downwind distance within the source region and then decreases rapidly in the source free region to an asymptotic value. They noticed that the effect of deposition velocity, gravitational settling, and chemical reaction rate coefficients on primary and secondary pollutants reduces the concentration in the urban region.

Agarwal and Tandon (2009) presented a steady state two-dimensional mathematical model to study the dispersion of air pollutants. They considered mesoscale wind which is generated by urban heat island with the following equation $\frac{\partial C}{\partial x}=\frac{1}{u+u_e}\left\{\frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right)-\lambda C-w_e\frac{\partial C}{\partial z}\right\},$ where C is the air pollutant concentration at any location (x,z), u is the large-scale wind in the horizontal $x-$direction, u_e and w_e are the mesoscale wind components in the x and z direction respectively, K_z is eddy diffusivity coefficient in $z-$direction, and λ is a first order constant depletion parameter that defines the fractional loss of pollutant per unit time through various wet deposition processes existing in the atmosphere. The model is solved numerically by the implicit Crank-Nicolson finite difference scheme. The results showed that the mesoscale wind aid the pollutants to circulate and move in the upward direction, thus making the problem of air pollution more severe in urban areas.

Suresha, Lakshminarayanachari, Prasad and Pandurangappa (2013) studied a two-dimensional advection-diffusion mathematical model on pollutant distribution, with the equation of primary pollutant as follows: $\frac{\partial C_p}{\partial t}+U(z)\frac{\partial C_p}{\partial x}=\frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_p}{\partial z}\right)-kC_p,$ and for secondary pollutant $\frac{\partial C_s}{\partial t}+U(z)\frac{\partial C_s}{\partial x}=\frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_s}{\partial z}\right)+W_s\frac{\partial C_s}{\partial z}+v_gkC_p,$ where W_s is the gravitational settling velocity. They solved the model by using the implicit Crank-Nicolson finite difference technique by considering chemical reaction and gravitational settling. The results showed that the concentration of primary and secondary pollutants decreases as the removal mechanisms such as dry deposition and gravitational settling velocity increases for stable and neutral cases.

Pandurangappa, Lakshminarayanachari, and Venkatachalappa (2012) presented a two-dimensional numerical model for the dispersion of air pollutants. The study was done to find out the effect of mesoscale wind on the emission of pollutants from an area source, with the equation of the primary pollutant as follows: $\frac{\partial C_p}{\partial t}+U\left(x,z\right)\frac{\partial C_p}{\partial x}+W\left(z\right)\frac{\partial C_p}{\partial z}=\frac{\partial}{\partial z}\left(K_z\left(z\right)\frac{\partial C_p}{\partial z}\right)-\left(k+k_{wp}\right)C_p,$ where W is mean wind speed in $z-$direction, and for the secondary pollutant, $\frac{\partial C_s}{\partial t}+U\left(x,z\right)\frac{\partial C_s}{\partial x}+W\left(z\right)\frac{\partial C_s}{\partial z}=\frac{\partial}{\partial z}\left(K_z\left(z\right)\frac{\partial C_s}{\partial z}\right)+W_s\frac{\partial C_s}{\partial z}-k_{ws}C_s+v_g kC_p.$ The study was done for primary and secondary pollutants with gravitational settling velocity. The model was solved numerically using the implicit Crank-Nicolson finite difference method. The results showed that in the presence of mesoscale wind, the concentration of primary and secondary pollutants is less on the upwind side of the center of heat island and more on the downwind side of the center of heat island. It is not the case in the absence of mesoscale wind. This is because the mesoscale wind increases the velocity in the upwind direction and decreases in the downwind direction of the center of the heat island.

Lakshminarayanachari, Suresha, Siddalinga, and Pandurangappa (2013) presented a numerical model on air pollutants emitted from an area source. In the study, they considered primary and secondary pollutants with chemical reaction and gravitational settling with point source on the boundary. They analyzed the dispersion of air pollutants in an urban area in the downwind and vertical direction, with the equation of primary pollutant as follows: $\frac{\partial C_p}{\partial t}+U(z)\frac{\partial C_p}{\partial x}=\frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_p}{\partial z}\right)-kC_p,$ and for secondary pollutant, $\frac{\partial C_s}{\partial t}+U(z)\frac{\partial C_s}{\partial x}=\frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_s}{\partial z}\right)+W_s\frac{\partial C_s}{\partial z}+v_g kC_p.$ Stable and neutral atmospheric conditions were considered in the presence of large scale wind. The study showed that removal mechanisms play an important role in reducing the concentration of pollutants everywhere in the region except near the point source. Again, they showed that stable atmospheric condition is unfavorable for animals and plants in a polluted environment.

Lakshminarayanachari, Sudheer, Siddalinga, and Pandurangappa (2013) presented advection-diffusion numerical model of air pollutants emitted from an urban area source. They considered chemical reaction and dry deposition as their parameters. This was done for primary and secondary pollutants by plotting concentration contours, with the equation of primary pollutant as follows:

$\frac{\partial C_p}{\partial t}+U(z)\frac{\partial C_p}{\partial x}=\frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_p}{\partial z}\right)-kC_p,$ and for secondary pollutant,

$\frac{\partial C_s}{\partial t}+U(z)\frac{\partial C_s}{\partial x}=\frac{\partial}{\partial z}\left(K_z(z)\frac{\partial C_s}{\partial z}\right)+v_g kC_p.$ Their results showed that the removal mechanisms play an important role in reducing the concentration of the pollutants everywhere in the city region except near the point source.

Pollutants emission are governed by meteorological parameters as they undergo advection and diffusion process in the atmosphere. Meteorological parameters like temperature and wind speed have been shown to be factors that influence the dispersion of pollutants in the atmosphere. A study by Verma and Desai (2008) showed the effect of meteorological conditions on air pollution in Surat city, India. The meteorological conditions considered were wind speed, wind direction, and temperature. The result showed that as wind speed and temperature are high, the dispersion is high. Therefore, it was concluded that wind speed is the major parameter that affects the dispersion of pollutants.

Hosseinibalam and Hejazi (2012) investigated the influence of meteorological parameters on air pollution. The study was done in Isfahan, Iran, and the meteorological parameters that were observed are wind speed, temperature, air pressure and sunshine hours. The result showed that high air pollutions in December are due to low sunshine, no wind, and high atmospheric pressure.

The methodology that would be employed in solving the advection-diffusion model would be shown in Chapter 3.

Chapter 3

Methodology

This chapter presents the mathematical model that would be used to study the distribution of pollutants in the atmosphere. When the pollutants disperse in the atmosphere, some physical and removal processes like advection and diffusion take place irrespective of the atmospheric conditions.

The mathematical model for this study would be formulated by deriving the advection-diffusion model with some assumptions to clearly explain how the parameters used in the model behave. Numerical methods for solving the model would be the finite difference scheme either the explicit or implicit method. The forward, the backward and the central difference schemes are used to solve the boundary value in order to approximate the proposed model.

Figure 4 shows the work flow of this study. This starts with the emission of pollutants from sources like industrial stacks, automobiles, forest fires, etc. The pollutants are then transported and distributed through advection and diffusion processes. Advection is as a result of the wind and diffusion is when the pollutants move from a region of high concentration to a region of low concentration. This phenomenon can be modeled mathematically using an advection-diffusion equation taking into account meteorological factors like wind, temperature and eddy diffusivity. This is a boundary value problem which is coupled with initial and boundary conditions. The finite difference method is used to find the numerical solution of the advection diffusion.

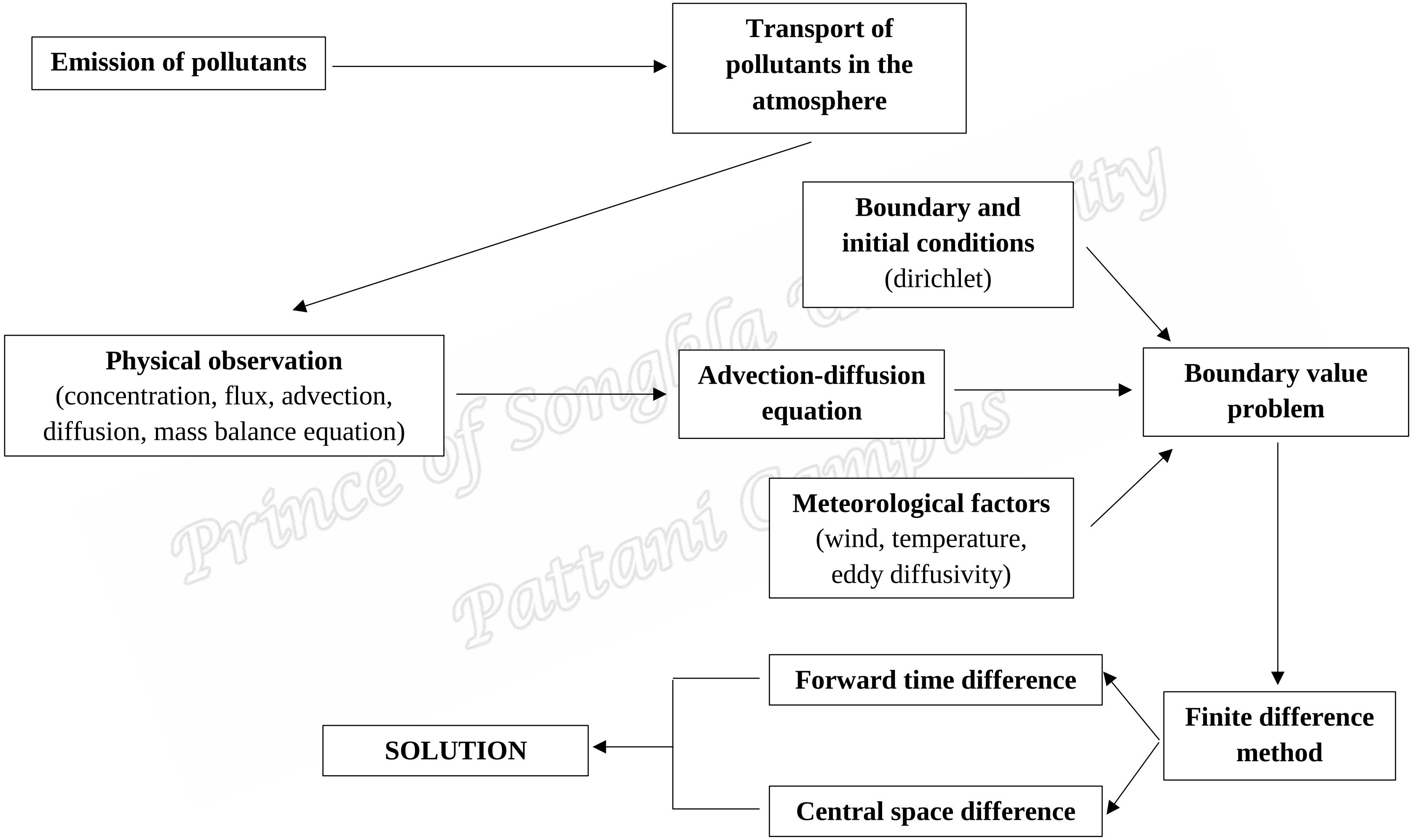


Figure 4. Work flow.

3.1 Transport of Pollutants in the Atmosphere

When pollutants are released from the source of emission, either through the soil, water or air, it disperses through advection, diffusion, and other dispersion mechanisms. Advection transports the pollutants in the downwind direction by wind. It can carry the pollutants from the source of emission through the mass movement from the area which is of high-pressure to a low-pressure area. Naturally, wind speeds increase with increasing height and thus results in the difference of dilution of pollutants concentration at a different height. Therefore, it is one of the factors that determines how fast the pollutants dilute in the atmosphere.

The diffusion process usually occurs in two ways. The first is molecular diffusion, which occurs due to the random motion of molecules within the fluid. The second is turbulent diffusion, which is the mixing due to turbulent motions in the fluid (Ramaswami, Milford, and Smal, 2005).

Most air pollutants are released into the boundary layer where they mix with the surrounding air. This surrounding air is the interaction between air flow with the surface roughness of the Earth's surface. This results in turbulence, which then results in the decrease in pollutants concentration. The degree of turbulence control how much the air pollutants dilute in the atmosphere.

The factors that determine the degree of turbulence are incoming solar radiation, wind speed, cloud cover and surface roughness. The temperature of the air also determines how much water vapor the atmosphere can hold and the form of clouds it can form. In general, surface roughness and atmospheric conditions need to be taken into account

(Jakeman, Beck, and McAlee, 1995). These conditions aggravate wind speed at ground level and at higher altitude. In the atmosphere, the atmospheric condition is categorized by three cases. The cases are an unstable, neutral and stable condition. These atmospheric conditions would result in the difference in the pattern of the puff of smoke. Consequently, it results in the varying of the diffusion capability.

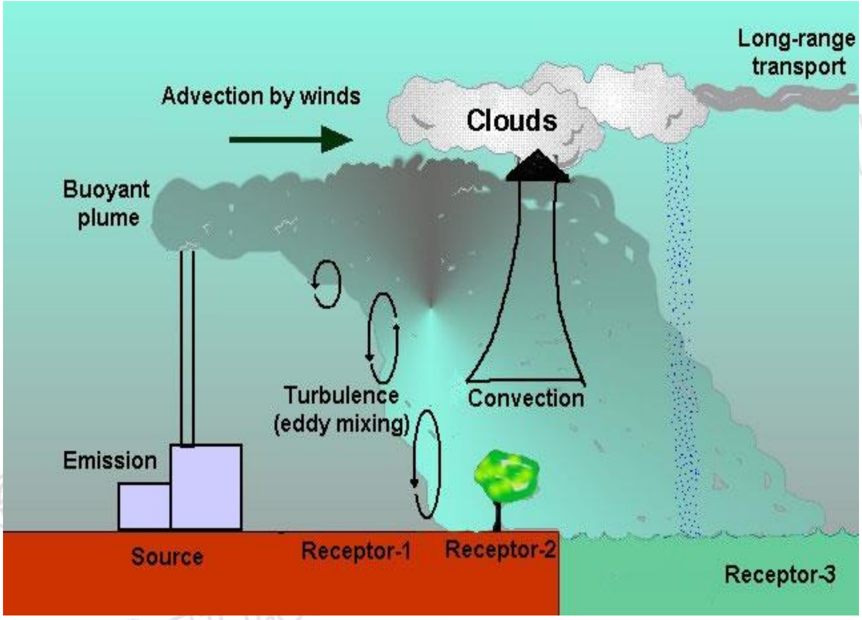


Figure 5. Transport of pollutants in the atmosphere.

Figure 5 describes the transport of pollutants in the atmosphere right from the source of emission through to the transport by advection coupled with turbulence and finally the effect on receptors, that is the living organisms, ecosystem, building, etc.

3.2 Derivation of the Advection-Diffusion Equation

3.2.1 Physical observation of pollutant transport

The application of the conservation of mass equation to the analysis of physical systems is essential for studying materials leaving and entering a system. What this means is that if the level of pollutants in the atmosphere increases, then that increase can only be attributed to the fact that the pollutant came from a source and had been carried into the atmosphere or maybe produced through chemical reaction from other compounds that were already in the atmosphere. This phenomenon is widely used in engineering analysis. For example, the conservation of mass can be used to model pollution dispersion and other physical processes.

Pollutants are measured by their levels of concentration which is defined as the amount of substance per unit volume of a fluid. This is given by:

$$C = \frac{m}{V},$$

where C is the concentration of pollutants $\left(\mu g / m^3\right)$, m is the amount of substance $\left(\mu g\right)$ and V is the volume $\left(m^3\right)$. In the "air" which is compressible, the concentration of pollutants changes due to the volume of air present which changes due to pressure change but not because of the mass variation of the contaminants.

The movement of pollutants is essential to know as this defines the flux which is the quantity of that substance passing through a section perpendicular to that direction per unit area and per unit time.

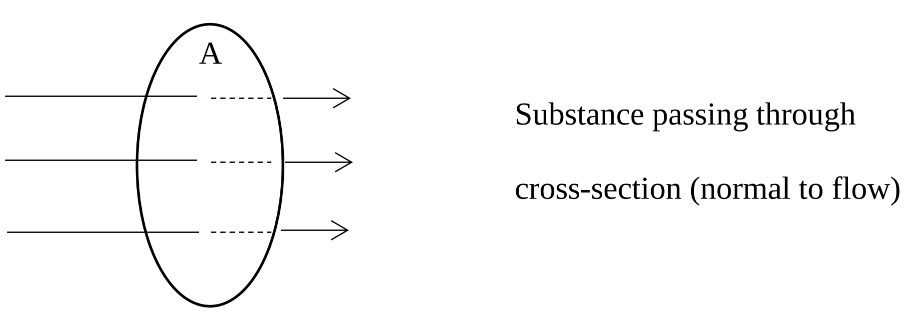


Figure 6. An air mass through an ellipse.

As shown in Figure 6 above, the ellipse corresponds to an area A, and air mass is denoted by m which passes through the ellipse in time t so that we have the following equation:

$$Q_a = \frac{m}{A\Delta t},$$

where Q_a is the flux $(\mu g/m^2 s)$ or a rate of mass per area per time, m is a mass (μg), A is a cross sectional area (m^2) and t is time (s). Flux can be related to concentration (C) and the fluid velocity (U) through the following equation:

$$Q_a = \frac{m}{V}\frac{V}{A\Delta t} = CU ,$$

This process is called an advection.

The flux of the pollutant carries the pollutant from place to place and also causes the decrease of concentration over the random fluctuation. It can be illustrated as shown in Figure 7.

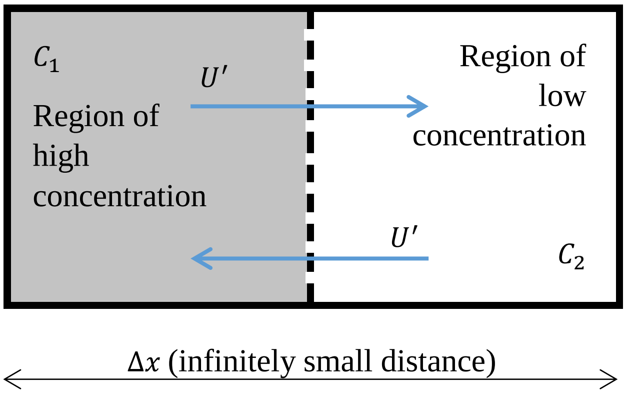


Figure 7. Diffusion process in a flux

If C_1 is a region of high concentration of pollutant and C_2 is a region of low concentration of pollutant, then C_1 diffuses to surrounding area of C_2 with the fluctuating flow $U^{'}$ till it reaches the equilibrium. Therefore, the flux of diffusive $\left(Q_d\right)$ component is as follows

$$\begin{aligned} Q_d &= C_1U^{'} - C_2U^{'}, \\ &= -U^{'}\left(C_2 - C_1\right), \\ &= -U^{'}\Delta C. \end{aligned}$$

Multiplying and dividing by Δx on the right hand side in the above equation, and taking the limit toward an infinitely small distance $\left(\Delta x\right)$ results in

$$\begin{aligned} Q_d &= -U^{'}\Delta x\frac{\Delta C}{\Delta x}, \\ &= -D\frac{dC}{dx}, \end{aligned}$$

where $D = U^{'}\Delta x$ is the diffusivity $\left(m^2 / s\right)$. The flux of a substance $\left(Q\right)$ consists of “advective” component $\left(Q_a\right)$ and diffusive component $\left(Q_d\right)$. So, the flux can be expressed as,

$$\begin{aligned} Q &= Q_a + Q_d, \\ &= CU - D\frac{dC}{dx}. \end{aligned}$$

3.2.2 Mass balance equation

The mass balance equation also known as the conservation of mass states that mass can neither be created nor destroyed, where the mass before reaction is equal to the mass after reaction.

Total mass in a system = total mass out of a system

+ total mass accumulated in the system

Total mass accumulated in the system = total mass in a system – total mass out of a system

$$V\frac{dC}{dt} = AQ(x,t) - AQ(x+\Delta x,t),$$

since $V = A\Delta x$, then it is obtained

$$A\Delta x\frac{dC}{dt} = AQ(x,t) - AQ(x+\Delta x,t),$$

$$\Delta x\frac{dC}{dt} = Q(x,t) - Q(x+\Delta x,t),$$

$$\frac{dC}{dt} = \frac{Q(x,t) - Q(x+\Delta x,t)}{\Delta x},$$

$$= -\left(\frac{Q(x+\Delta x,t) - Q(x,t)}{\Delta x}\right),$$

$$= -\frac{\Delta Q}{\Delta x}.$$

As shown in Figure 7, the diffusion occurs over a distance Δx and in order to know the area it covers, the flux (Q) needs to be differentiated with respect to the distance Δx,

$$\frac{dC}{dt} = -\frac{dQ}{dx}.$$

The independent variables are time (t) and distance (x) and so it would partially be differentiated and also taking the limit of $\Delta x \to 0$ gives

$$\frac{\partial C}{\partial t} = -\frac{\partial Q}{\partial x} = -\frac{\partial\left(CU - D\frac{dC}{dx}\right)}{\partial x},$$

Since U the fluctuating flow and D the diffusivity are constant, the above equation can be written as,

$$\frac{\partial C}{\partial t} = -U\frac{\partial C}{\partial x} + D\frac{\partial^2 C}{\partial x^2},$$

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2}.$$

Agarwal and Tandon (2009) showed the case of air pollution distribution for a three dimensional conservation of mass equation in a steady state condition, assuming the wind velocity U, V, W as well as the eddy diffusivity K_x, K_y, K_z depend on x, y, z directions respectively. This is expressed as follows,

$$U\frac{\partial C}{\partial x} + V\frac{\partial C}{\partial y} + W\frac{\partial C}{\partial z} = \frac{\partial}{\partial x}\left(K_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right) + R,$$

where R is the removal/reaction term.

Moreover, Lakshminarayanachari, Sudheer, Siddalinga, and Pandurangappa (2013) has showed that the dispersion of pollutant with time dependent can be expressed by the following equation:

$$\frac{\partial C}{\partial t}+U\frac{\partial C}{\partial x}+V\frac{\partial C}{\partial y}+W\frac{\partial C}{\partial z}=\frac{\partial}{\partial x}\left(K_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right)+S,$$

where S is the source or sink of the air pollution.

The advection term $U\frac{\partial C}{\partial x}+V\frac{\partial C}{\partial y}+W\frac{\partial C}{\partial z}$ depicts the movement of the pollutants which is transported by bulk motion, in this case the wind velocity and the diffusion term $\frac{\partial}{\partial x}\left(K_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right)$ depicts the spreading of the random motion of the molecules.

In this study, a two-dimensional advection diffusion equation would be considered with some assumptions as follows:

1. The chemical properties of the pollutants are not considered.
2. The mean of pollutants concentration is considered to be constant in the crosswind (y) direction because of the homogeneity of urban terrain. Therefore, it is ignored.
3. The emission of pollutants is continuous.

The equation only considers the downwind direction ($x-$axis) and the upwind direction ($z-$axis) with removal mechanism. In the downwind direction, the wind velocity is denoted by U and in the vertical direction, it is denoted by W with the removal term denoted by λC. The two dimensional advection-diffusion equation would have the following form:

$$\frac{\partial C}{\partial t}+U\frac{\partial C}{\partial x}+W\frac{\partial C}{\partial z}=K_x\frac{\partial^2 C}{\partial x^2}+K_z\frac{\partial^2 C}{\partial z^2}-\lambda C, \qquad (1)$$

where C is the concentration of pollutants dependent of distance in the x and z direction as well as time t. In other words $C(x,z,t)$ is the concentration function and its independent variables. This equation is complicated to be solved analytically and because of this, it would be solved using numerical method to approximate the solution.

3.2.3 Meteorological factors

As discussed earlier, meteorological factors play an important role in determining the air quality in a particular area. Meteorological factors such as wind profile (speed and direction), temperature, air pressure, humidity, mesoscale wind, etc. determine pollutant concentration in a particular area. The present study would only consider wind speed, wind direction, mesoscale wind and temperature as most of these parameters are related. For instance, high temperature results in low humidity. Also eddy diffusivity would be considered although it is not a meteorological factor. Temperature affects the diffusion rate which makes it ideal for it to be considered.

The wind speed and direction determines how high or low the concentration of pollutants would be in a particular area. Wind speed is considered to be the parameter majorly affecting the dispersion of pollutants (Vermal and Desai, 2008).

When the air pollutants are emitted, they are transported horizontally by a large-scale wind which is taken to be a function of altitude (vertical distance). Again, the pollutants are transported both horizontally and vertically by mesoscale wind. The large-scale wind (U) and the vertical diffusivity (K_z) are parameterized as a function of vertical height z in the same way as shown by Lin and Hildemann (1996).

$$u = u(z) = u_r \left(\frac{z}{z_r} \right)^{\alpha},$$

$$K_z = K_z(z) = K_r \left(\frac{z}{z_r} \right)^{\beta},$$

where $u = u(z_r)$ and $K_z = K_z(z_r)$ are the measured wind speed and vertical diffusivity at a reference height z_r and α, β are the constants that depend on the atmospheric stability and surface roughness.

According to Dilley and Yen (1971), the mathematical representation of mesoscale wind in the horizontal (u_e) and vertical directions (w_e) are,

$$u_e = -ax\left(\frac{z}{z_r} \right)^{\alpha},$$

$$w_e = \frac{az}{(\alpha+1)}\left(\frac{z}{z_r} \right)^{\alpha},$$

respectively, where a is a proportionality constant.

Temperature affects the rate of dispersal of pollutants as at high temperatures, pollutants tend to diffuse faster. In this section, a temperature formula is proposed as it affects turbulence thereby affecting the mesoscale wind. The proposed temperature formula is

$$\frac{\partial T}{\partial t} = Q_r\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial z^2}\right), \tag{2}$$

where T is the temperature, Q_r is heat diffusion.

3.2.4 Boundary and initial conditions of the advection-diffusion equation

To obtain a unique solution of the time-dependent advection-diffusion equation, the initial and boundary conditions are needed which are appropriate to the domain. Boundary value problems of any physical relevance have these characteristics: (1) the conditions are imposed at two different points, (2) the solution is of interest only between those two points, and (3) the independent variable is a space variable (Powers, 2010). For the equation of the type:

$$\frac{\partial^2 C}{\partial x^2} = \frac{1}{k}\frac{\partial C}{\partial t}; \qquad 0 < x < a, 0 < t \tag{3}$$

$$C(x,0) = f(x); \qquad 0 < x < a \tag{4}$$

$$C(x_0,t) = \alpha(t); \tag{5}$$

$$\frac{\partial C}{\partial x}(x_0,t) = \beta(t); \tag{6}$$

$$const_1 C(x_0,t) + const_2 \frac{\partial C}{\partial x}(x_0,t) = \gamma(t). \tag{7}$$

The condition in equation (4) is the initial value which is given at every point in the domain of interest where $f(x)$ is a given function of x alone. If x_0 is denoted as an endpoint then the concentration at the boundary may be controlled in the same way.

Let $\alpha(t)$ be a function of time, then the condition in equation (5) is called a Dirichlet condition. When the flow rate is controlled by a function of time β, the condition in equation (6) is called a Neumann condition. Another possibility of the boundary condition is the condition in equation (7) which is called Robin condition. In this study the zero Dirichlet boundary condition is used.

3.3 Finite Difference Method

The equation (1) is complicated to be solved analytically. One of the numerical method for solving boundary value problems is to use finite difference methods. The principle of finite difference methods is almost like numerical schemes used in solving ordinary differential equations. It consists of approximating the differential operator by replacing the derivatives in the equation using differential quotients. The domain is partitioned in space and in time. The approximations of the solution are computed at the space or time points.

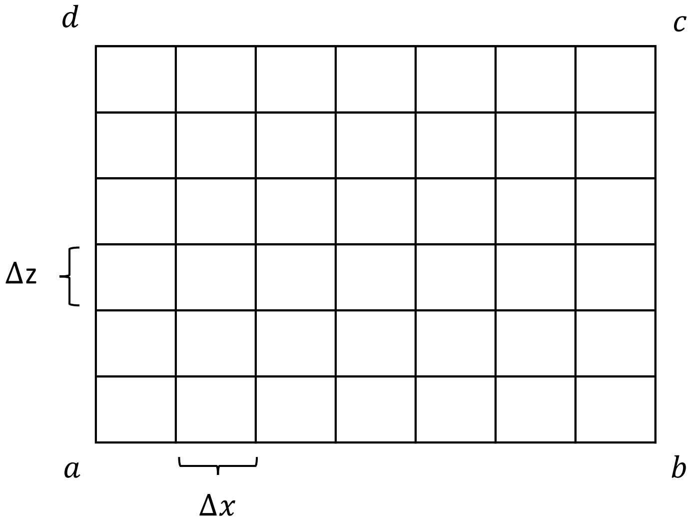


Figure 8. Domain.

The domain of interest will be determined in a rectangular manner, the corner points are a,b,c and d as shown in Figure 8 and it is divided into subinterval with spacing $\frac{b-a}{N}=\Delta x$ and $\frac{d-a}{N}=\Delta z$ for the spatial dimension, Δt for the time dimension where N is the number of grid points and a uniform grid would be obtained. Finite difference approximations are used to replace the derivatives using Taylor series with the reference point at x:

$$f\left(x+\Delta x\right)=f\left(x\right)+\frac{\left(\Delta x\right)^1}{1!}\frac{\partial f}{\partial x}+\frac{\left(\Delta x\right)^2}{2!}\frac{\partial^2 f}{\partial x^2}+\frac{\left(\Delta x\right)^3}{3!}\frac{\partial^3 f}{\partial x^3}+...+\frac{\left(\Delta x\right)^n}{n!}\frac{\partial^n f}{\partial x^n}+....$$

There are three finite difference methods that can be used to find the value of $f\left(x+\Delta x\right)$, they are forward difference, backward difference and central difference.

3.3.1 Forward difference method

To find the value of a function, the independent variable is shifted forward by Δx, therefore the Taylor series expansion can be written as

$$f\left(x+\Delta x\right)=f\left(x\right)+\frac{\left(\Delta x\right)^1}{1!}\frac{\partial f}{\partial x}+\frac{\left(\Delta x\right)^2}{2!}\frac{\partial^2 f}{\partial x^2}+\frac{\left(\Delta x\right)^3}{3!}\frac{\partial^3 f}{\partial x^3}+...+\frac{\left(\Delta x\right)^n}{n!}\frac{\partial^n f}{\partial x^n}+....$$

Lets' find the first derivative $\frac{\partial f}{\partial x}$

$$\frac{\left(\Delta x\right)^1}{1!}\frac{\partial f}{\partial x}=f\left(x+\Delta x\right)-f\left(x\right)-\frac{\left(\Delta x\right)^2}{2!}\frac{\partial^2 f}{\partial x^2}-\frac{\left(\Delta x\right)^3}{3!}\frac{\partial^3 f}{\partial x^3}-...-\frac{\left(\Delta x\right)^n}{n!}\frac{\partial^n f}{\partial x^n}-....$$

$$\frac{\partial f}{\partial x}=\frac{f\left(x+\Delta x\right)-f\left(x\right)}{\Delta x}-\frac{\Delta x}{2}\frac{\partial^2 f}{\partial x^2}-\frac{\left(\Delta x\right)^2}{6}\frac{\partial^3 f}{\partial x^3}-...-\frac{\left(\Delta x\right)^{n-1}}{n!}\frac{\partial^n f}{\partial x^n}-....$$

To find the first derivative of the function, the second and higher derivative will be truncated as $\Delta x \to 0$, it can then be written as,

$$\frac{\partial f}{\partial x} \approx \frac{f\left(x+\Delta x\right)-f\left(x\right)}{\Delta x}-\frac{\Delta x}{2}\frac{\partial^2 f}{\partial x^2}$$

$$\frac{\partial f}{\partial x} \approx \frac{f\left(x+\Delta x\right)-f\left(x\right)}{\Delta x}+O\left(\Delta x\right).$$

3.3.2 Backward difference method

The backward difference is used when we want to find the value of the function if the independent variable is shifted backward by Δx. Applying the Taylor series, gives,

$$f\left(x-\Delta x\right)=f\left(x\right)+\frac{\left(-\Delta x\right)^1}{1!}\frac{\partial f}{\partial x}+\frac{\left(-\Delta x\right)^2}{2!}\frac{\partial^2 f}{\partial x^2}+\frac{\left(-\Delta x\right)^3}{3!}\frac{\partial^3 f}{\partial x^3}+\ldots+\frac{\left(-\Delta x\right)^n}{n!}\frac{\partial^n f}{\partial x^n}+\ldots,$$

$$\frac{\left(\Delta x\right)^1}{1!}\frac{\partial f}{\partial x}=f\left(x\right)-f\left(x-\Delta x\right)+\frac{\left(\Delta x\right)^2}{2!}\frac{\partial^2 f}{\partial x^2}-\frac{\left(\Delta x\right)^3}{3!}\frac{\partial^3 f}{\partial x^3}+\ldots-\frac{\left(\Delta x\right)^n}{n!}\frac{\partial^n f}{\partial x^n}+\ldots,$$

$$\frac{\partial f}{\partial x}=\frac{f\left(x\right)-f\left(x-\Delta x\right)}{\Delta x}+\frac{\Delta x}{2}\frac{\partial^2 f}{\partial x^2}-\frac{\left(\Delta x\right)^2}{6}\frac{\partial^3 f}{\partial x^3}+\ldots-\frac{\left(\Delta x\right)^{n-1}}{n!}\frac{\partial^n f}{\partial x^n}+\ldots,$$

As in the case of the forward difference method, to find the first derivative of the function, the second and higher derivative will be truncated as $\Delta x \to 0$, it can be written as,

$$\frac{\partial f}{\partial x} \approx \frac{f\left(x\right)-f\left(x-\Delta x\right)}{\Delta x}+\frac{\Delta x}{2}\frac{\partial^2 f}{\partial x^2},$$

$$\frac{\partial f}{\partial x} \approx \frac{f\left(x\right)-f\left(x-\Delta x\right)}{\Delta x}+O\left(\Delta x\right).$$

3.3.3 Central difference method

Mathematically, the central difference method is the summation of the forward

$$\frac{\partial f}{\partial x}=\frac{f\left(x+\Delta x\right)-f\left(x\right)}{\Delta x}-\frac{\Delta x}{2}\frac{\partial^2 f}{\partial x^2}-\frac{\left(\Delta x\right)^2}{6}\frac{\partial^3 f}{\partial x^3}-\ldots-\frac{\left(\Delta x\right)^{n-1}}{n!}\frac{\partial^n f}{\partial x^n}-\ldots.$$

and the backward difference

$$\frac{\partial f}{\partial x}=\frac{f\left(x\right)-f\left(x-\Delta x\right)}{\Delta x}+\frac{\Delta x}{2}\frac{\partial^2 f}{\partial x^2}-\frac{\left(\Delta x\right)^2}{6}\frac{\partial^3 f}{\partial x^3}+\ldots-\frac{\left(\Delta x\right)^{n-1}}{n!}\frac{\partial^n f}{\partial x^n}+\ldots,$$

Lets' find the first derivative $\frac{\partial f}{\partial x}$

$$2\frac{\partial f}{\partial x}\approx\frac{f\left(x+\Delta x\right)-f\left(x\right)}{\Delta x}+\frac{f\left(x\right)-f\left(x-\Delta x\right)}{\Delta x}-\frac{2\left(\Delta x\right)^2}{6}\frac{\partial^3 f}{\partial x^3},$$

$$\frac{\partial f}{\partial x}\approx\frac{f\left(x+\Delta x\right)-f\left(x-\Delta x\right)}{2\Delta x}-\frac{\left(\Delta x\right)^2}{6}\frac{\partial^3 f}{\partial x^3},$$

$$\frac{\partial f}{\partial x}\approx\frac{f\left(x+\Delta x\right)-f\left(x-\Delta x\right)}{2\Delta x}-O\left(\Delta x^2\right).$$

This means that the central difference method has a smaller error than the other methods.

3.3.4 The explicit finite difference scheme

The explicit method, which is also known as the *Forward Time Center Space* evaluates the variable of interest at time $n+1$ depending on the variable in the previous time n.

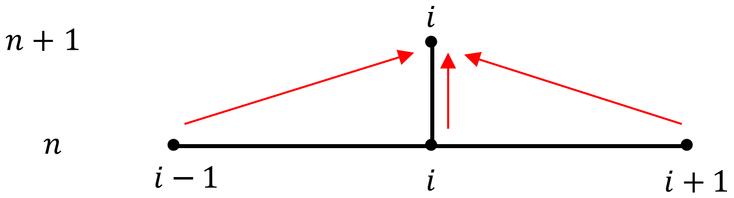


Figure 9. Explicit finite difference scheme.

Consider the equation,

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}; \qquad 0<x<1; \qquad 0<t<\infty; \tag{8}$$

with boundary condition: $u(0,t)=0;$ $\quad 0<t<\infty;$

and initial condition: $u(x,0)=\sin\pi x+x;$ $\quad 0\le x\le 1.$

Discretizing the domain by $\left(x_i,t_j\right)$ and the value of the function u is denoted by $u_{i,j}$.

Using the forward difference approximation for $\dfrac{\partial u}{\partial t}$ gives,

$$\frac{\partial u}{\partial t}\approx\frac{u_{i,j+1}-u_{i,j}}{\Delta t},$$

and the central difference approximation for $\dfrac{\partial^2 u}{\partial x^2}$,

$$\frac{\partial^2 u}{\partial x^2}\approx\frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{\Delta x^2},$$

then substituting to equation (8) gives,

$$\frac{u_{i,j+1}-u_{i,j}}{\Delta t}=\frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{\Delta x^2},$$

$$u_{i,j+1} = \frac{\Delta t}{\Delta x^2}\left(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}\right) + u_{i,j},$$

$$u_{i,j+1} = \left(1 - 2\frac{\Delta t}{\Delta x^2}\right)u_{i,j} + \frac{\Delta t}{\Delta x^2}\left(u_{i+1,j} + u_{i-1,j}\right).$$

The method gives the new values $u_{i,j+1}$ explicitly in terms of previous values $u_{i,j}, u_{i+1,j}$ and $u_{i-1,j}$.

3.4 Numerical Solution of the Proposed Mathematical Model

This section focuses on the discretization of equation (1). The explicit method is used in the discretization. We consider the domain for a two dimensional advection-diffusion $[0, X] \times [0, Z]$ for spatial domain and the interval $[0, T]$ for the time domain. The x and z intervals are divided into M and N subintervals which are $0 = x_0 < x_1 < x_2 < \ldots < x_M = X$ and $0 = z_0 < z_1 < z_2 < \ldots < z_N = Z$ and the interval of time t is partitioned into L subinterval $0 = t_0 < t_1 < t_2 < \ldots < t_N = T.$ Then the coordinate for the grid is defined by $x_i = i\Delta x,\ z_j = j\Delta z$ for the spatial grid.

3.4.1 The advection-diffusion equation

The equation (1) would be solved explicitly by using the forward difference approximation for time variable t.

$$\frac{\partial C}{\partial t} \approx \frac{C_{i,j}^{n+1} - C_{i,j}^{n}}{\Delta t}, \tag{9}$$

and central difference approximation for advection and diffusion term,

$$\frac{\partial C}{\partial x} \approx \frac{C_{i+1,j}^{n} - C_{i-1,j}^{n}}{2\Delta x}, \tag{10}$$

$$\frac{\partial C}{\partial z} \approx \frac{C_{i,j+1}^{n} - C_{i,j-1}^{n}}{2\Delta z}, \tag{11}$$

$$\frac{\partial^2 C}{\partial x^2} \approx \frac{C_{i+1,j}^{n} - 2C_{i,j}^{n} + C_{i-1,j}^{n}}{\Delta x^2}, \tag{12}$$

$$\frac{\partial^2 C}{\partial z^2} \approx \frac{C_{i,j+1}^{n} - 2C_{i,j}^{n} + C_{i,j-1}^{n}}{\Delta z^2}. \tag{13}$$

Substitute equation (9), (10), (11), (12) and (13) into equation (1)

$$\frac{C_{i,j}^{n+1} - C_{i,j}^{n}}{\Delta t} + U\frac{C_{i+1,j}^{n} - C_{i-1,j}^{n}}{2\Delta x} + W\frac{C_{i,j+1}^{n} - C_{i,j-1}^{n}}{2\Delta z} = K_x\frac{C_{i+1,j}^{n} - 2C_{i,j}^{n} + C_{i-1,j}^{n}}{\Delta x^2}$$

$$+K_z\frac{C_{i,j+1}^{n} - 2C_{i,j}^{n} + C_{i,j-1}^{n}}{\Delta z^2} - \lambda C_{i,j}^{n}.$$

Separating the time and spatial term gives,

$$\frac{C_{i,j}^{n+1} - C_{i,j}^{n}}{\Delta t} = -U\frac{C_{i+1,j}^{n} - C_{i-1,j}^{n}}{2\Delta x} - W\frac{C_{i,j+1}^{n} - C_{i,j-1}^{n}}{2\Delta z} + K_x\frac{C_{i+1,j}^{n} - 2C_{i,j}^{n} + C_{i-1,j}^{n}}{\Delta x^2}$$

$$+K_z\frac{C_{i,j+1}^{n} - 2C_{i,j}^{n} + C_{i,j-1}^{n}}{\Delta z^2} - \lambda C_{i,j}^{n}.$$

Multiplying all terms by Δt gives,

$$C_{i,j}^{n+1} - C_{i,j}^{n} = -\frac{U\Delta t}{2\Delta x}\left(C_{i+1,j}^{n} - C_{i-1,j}^{n}\right) - \frac{W\Delta t}{2\Delta z}\left(C_{i,j+1}^{n} - C_{i,j-1}^{n}\right) + \frac{K_x\Delta t}{\Delta x^2}\left(C_{i+1,j}^{n} - 2C_{i,j}^{n} + C_{i-1,j}^{n}\right)$$

$$+\frac{K_z\Delta t}{\Delta z^2}\left(C_{i,j+1}^{n} - 2C_{i,j}^{n} + C_{i,j-1}^{n}\right) - \lambda\Delta t C_{i,j}^{n}.$$

Classifying each term results in,

$$C_{i,j}^{n+1} = -\frac{U\Delta t}{2\Delta x}C_{i+1,j}^{n} + \frac{U\Delta t}{2\Delta x}C_{i-1,j}^{n} - \frac{W\Delta t}{2\Delta z}C_{i,j+1}^{n} + \frac{W\Delta t}{2\Delta z}C_{i,j-1}^{n} + \frac{K_x\Delta t}{\Delta x^2}C_{i+1,j}^{n} - 2\frac{K_x\Delta t}{\Delta x^2}C_{i,j}^{n} + \frac{K_x\Delta t}{\Delta x^2}C_{i-1,j}^{n}$$

$$+\frac{K_z\Delta t}{\Delta z^2}C^n_{i,j+1}-2\frac{K_z\Delta t}{\Delta z^2}C^n_{i,j}+\frac{K_z\Delta t}{\Delta z^2}C^n_{i,j-1}-\lambda\Delta t C^n_{i,j}+C^n_{i,j}.$$

Grouping each term by the same position gives,

$$C^{n+1}_{i,j}=\left(-\frac{U\Delta t}{2\Delta x}+\frac{K_x\Delta t}{\Delta x^2}\right)C^n_{i+1,j}+\left(\frac{U\Delta t}{2\Delta x}+\frac{K_x\Delta t}{\Delta x^2}\right)C^n_{i-1,j}+\left(-\frac{W\Delta t}{2\Delta z}+\frac{K_z\Delta t}{\Delta z^2}\right)C^n_{i,j+1}$$

$$+\left(\frac{W\Delta t}{2\Delta z}+\frac{K_z\Delta t}{\Delta z^2}\right)C^n_{i,j-1}+\left(-2\frac{K_x\Delta t}{\Delta x^2}-2\frac{K_z\Delta t}{\Delta z^2}-\lambda\Delta t+1\right)C^n_{i,j}.$$

The equation above can be written as follows:

$$C^{n+1}_{i,j}=A_1C^n_{i+1,j}+A_2C^n_{i-1,j}+A_3C^n_{i,j+1}+A_4C^n_{i,j-1}+A_5C^n_{i,j}, \qquad (14)$$

for $i=1,2,3,\dots,M$ and $j=1,2,3,\dots,N,$ where,

$$A_1=-\frac{U\Delta t}{2\Delta x}+\frac{K_x\Delta t}{\Delta x^2},$$

$$A_2=\frac{U\Delta t}{2\Delta x}+\frac{K_x\Delta t}{\Delta x^2},$$

$$A_3=-\frac{W\Delta t}{2\Delta z}+\frac{K_z\Delta t}{\Delta z^2},$$

$$A_4=\frac{W\Delta t}{2\Delta z}+\frac{K_z\Delta t}{\Delta z^2},$$

$$A_5=-2\frac{K_x\Delta t}{\Delta x^2}-2\frac{K_z\Delta t}{\Delta z^2}-\lambda\Delta t+1.$$

The explicit scheme will converge and be stable when $0\le\frac{\Delta t}{\Delta x^2}\le\frac{1}{4}.$

The source of emission is supposed to be 9 point grids in the middle of the domain whereby the values come from the input from the user.

Initial concentration value $C^n_{i,j}$ is an input data from user, for $i=\left(\dfrac{M}{2}-1\right),\ldots,\left(\dfrac{M}{2}+1\right)$ and $j=\left(\dfrac{N}{2}-1\right),\ldots,\left(\dfrac{N}{2}+1\right)$ whereby M and N must be even number.

Boundary conditions for the concentration of pollutants are as follows:

$$C^n_{i,0}=C^n_{i,N}=0,\ \text{for } i=0,1,2,\ldots,M \ \text{ and } \ j=0,1,2,\ldots,N,$$

$$C^n_{0,j}=C^n_{M,j}=0,\ \text{for } i=0,1,2,\ldots,M \ \text{ and } \ j=0,1,2,\ldots,N.$$

3.4.2 Temperature

The equation (2) is solved in the same way as the advection-diffusion equation in Equation (1).

$$\frac{T^n_{i,,j}-T^{n+1}_{i,j}}{\Delta t}=Q_r\left(\frac{T^{n-1}_{i+1,j}-2T^{n-1}_{i,j}+T^{n-1}_{i-1,j}}{\Delta x^2}+\frac{T^{n-1}_{i,j+1}-2T^{n-1}_{i,j}+T^{n-1}_{i,j-1}}{\Delta z^2}\right).$$

Multiplying all terms by Δt gives,

$$T^n_{i,j}-T^{n-1}_{i,j}=\frac{Q_r\Delta t}{\Delta x^2}\left(T^{n-1}_{i+1,j}-2T^{n-1}_{i,j}+T^{n-1}_{i-1,j}\right)+\frac{Q_r\Delta t}{\Delta z^2}\left(T^{n-1}_{i,j+1}-2T^{n-1}_{i,j}+T^{n-1}_{i,j-1}\right).$$

Classifying each term gives,

$$T^n_{i,j}=\frac{Q_r\Delta t}{\Delta x^2}T^{n-1}_{i+1,j}-2\frac{Q_r\Delta t}{\Delta x^2}T^{n-1}_{i,j}+\frac{Q_r\Delta t}{\Delta x^2}T^{n-1}_{i-1,j}+\frac{Q_r\Delta t}{\Delta z^2}T^{n-1}_{i,j+1}-2\frac{Q_r\Delta t}{\Delta z^2}T^{n-1}_{i,j}+\frac{Q_r\Delta t}{\Delta z^2}T^{n-1}_{i,j-1}+T^{n-1}_{i,j}.$$

Grouping each term by the same position,

$$T^n_{i,j}=\frac{Q_r\Delta t}{\Delta x^2}T^{n-1}_{i+1,j}+\frac{Q_r\Delta t}{\Delta x^2}T^{n-1}_{i-1,j}+\frac{Q_r\Delta t}{\Delta z^2}T^{n-1}_{i,j+1}+\frac{Q_r\Delta t}{\Delta z^2}T^{n-1}_{i,j-1}+\left(-2\frac{Q_r\Delta t}{\Delta x^2}-2\frac{Q_r\Delta t}{\Delta z^2}+1\right)T^{n-1}_{i,j}.\quad(15)$$

In this work, temperature at the ground level (lower part) is different from the temperature in the atmosphere (upper part). Hence, the temperature between them is calculated by using linear interpolation. The following is the initial conditions of the temperature:

1) Lower temperature (LowT): $T_{i,j}^{n}$ are given by input data from user for $i = 0,1,2,...,M$ and $j = 0,1,2,3.$
2) Upper temperature (UpperT): $T_{i,j}^{n}$ are given by input data from user for $i = 0,1,2,...,M$ and $j = N-2, N-1, N,$
3) Temperature between ground level and atmosphere

   $$\Delta Temperature = \frac{LowT - UpperT}{N-7},$$

   $T_{i,j}^{n} = \left(LowT - \Delta Temperature\right) * \left(j-3\right),$ for $i = 0,1,2,...,M$ and $j = 4,...,N-3.$

While for the boundary conditions are:

1) $T_{i,j}^{n} =$ LowT, for $i = 0,1,2,...,M$ and $j = 0,1,2,3,$
2) $T_{i,j}^{n} =$ UpperT, for $i = 0,1,2,...,M$ and $j = N-2, N-1, N,$
3) $T_{i,j}^{n} = \left(LowT - \Delta Temperature\right) * \left(j-3\right),$ for $i = 0$ and $j = 4,...,N-3,$
4) $T_{i,j}^{n} = \left(LowT - \Delta Temperature\right) * \left(j-3\right),$ for $i = M$ and $j = 4,...,N-3.$

3.4.3 Parameters involved in the advection-diffusion equation

The large-scale wind, mesoscale wind and eddy diffusivity have effect on air pollution distribution directly and temperature determines how much turbulence occur which would influence the mesoscale wind, in other words temperature has an indirect effect on air pollution distribution. Heat diffusion and air flow which is generated by temperature would be considered as parameters in the model in equation (15).

The large-scale wind U is a combination of the function of altitude and distance, it is taken into account as

$$U_{i,j} = u_r\left(\frac{j}{z_r}\right)^{\alpha} + qi\left(\frac{j}{z_r}\right)^{\alpha}, \tag{16}$$

where u_r is the mean wind speed and q is a proportionality constant, and eddy diffusivity

$$K_{z_j} = K_r\left(\frac{j}{z_r}\right)^{\beta}, \tag{17}$$

$$K_{x_i} = K_r\left(\frac{i}{z_r}\right)^{\beta}, \tag{18}$$

where K_r is the diffusivity at a reference height z_r, for the mesoscale wind W, it would be,

$$W_{i,j} = \frac{aj}{(\alpha+1)}\left(\frac{j}{z_r}\right)^{\alpha} + b\left(\frac{T_{i,j}^{n} - \min T}{\max T - \min T}\right), \tag{19}$$

where a is the proportionality constant and b is the air flow constant which is caused by temperature, and all these parameters are applied for each $i = 1, 2, 3..., M$ and $j = 1, 2, 3..., N.$

3.5 The Proposed Modeling of Air Pollution Distribution

This section is talk about modeling of the work we have mentioned so far. It is enlightened from the mathematical model to the solution.

The proposed mathematical model is shown in Equation (1) as follows:

$$\frac{\partial C}{\partial t} + U_{i,j}\frac{\partial C}{\partial x} + W_{i,j}\frac{\partial C}{\partial z} = K_{x_i}\frac{\partial^2 C}{\partial x^2} + K_{z_j}\frac{\partial^2 C}{\partial z^2} - \lambda C,$$

This model is solved explicitly by using forward time difference and central space difference and we then obtain the discrete equation as in Equation (14); such that

$$C_{i,j}^{n+1} = A_1 C_{i+1,j}^{n} + A_2 C_{i-1,j}^{n} + A_3 C_{i,j+1}^{n} + A_4 C_{i,j-1}^{n} + A_5 C_{i,j}^{n},$$

The initial condition $C_{i,j}^{n}$ are given by input data from user for $i = \left(\frac{M}{2}-1\right),\ldots,\left(\frac{M}{2}+1\right)$ and $j = \left(\frac{N}{2}-1\right),\ldots,\left(\frac{N}{2}+1\right)$, and the boundary conditions are following:

$C_{i,0}^{n} = C_{i,N}^{n} = 0,$ for $i = 0,1,2,\ldots,M$ and $j = 0,1,2,\ldots,N,$

$C_{0,j}^{n} = C_{M,j}^{n} = 0,$ for $i = 0,1,2,\ldots,M$ and $j = 0,1,2,\ldots,N.$

Simulations for the numerical solution of the advection-diffusion model would be carried out in the next chapter. Discussion on the various figures would be shown as well.

Chapter 4

Result and Discussion

This study is to analyze the distribution of pollutants under the influence of large-scale wind, heat diffusion, air flow which is caused by temperature, mesoscale wind and eddy diffusivity. The equations (15), (16), (17), (18), and (19) have some unknown parameters which are $Q_r, U_r, z_r, q, K_r, a, b, \alpha$ and β, therefore for the computation of air pollutants concentration, these input parameters are required. Some of the values used in this study come from the previous study by Agarwal and Tandon (2009), like the reference height $z_r = 10m$ and proportionality constant $q = 0.002s^{-1}$. The rest of the parameters have range of values as follows: $Q_r = 0$ to $5\,m^2/s$, $U_r = -50$ to $50\,m/s$, $K_r = 0$ to $5\,m^2/s$, a from -1 to $1s^{-1}$ and b from -1 to 1, these give an opportunity to test for a wider parameter value. The values of other unknown parameters α and β are taken according to the stability conditions of the atmosphere and surface roughness as shown by Irwin (1979) in table 1, with these values of α (table 1) corresponding to different stability classes, the value of β can be obtained by $\beta = 1 - \alpha$, based on Schmidt's conjugate power law.

Table 1. Stability and surface roughness constants.

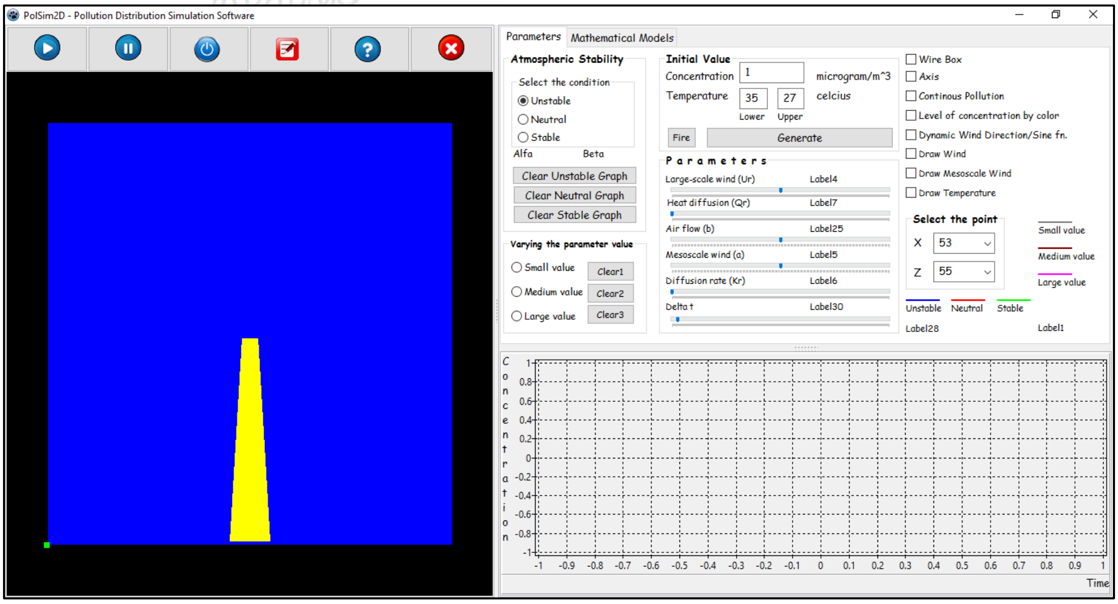
Atmospheric Stability	α	β
Unstable	0.17	0.83
Neutral	0.27	0.73
Stable	0.61	0.39

It is assumed that pollutants are emitted at a constant rate in a uniformly distributed domain. The area extends up to 500 m downwind and 500 m in the vertical direction. The removal of pollutants is assumed to be taking place by either dry deposition or wet deposition processes. The value for the removal parameter $\lambda = 10^{-6} s^{-1}$ is assumed to be constant in all atmospheric conditions.

An explicit finite difference scheme requires solutions to be within their range of validity. Therefore, this analysis is done for $M = 100$ and $N = 100$ independent grid points with each grid equal to 5 meters.

4.1 User Interface of the "Pollution Distribution Simulation" Software

In this section, the program user interface developed is shown as well as the simulations that were carried out to study the distribution of pollutants in the atmosphere. The various buttons are described to show how the program works and the simulations carried out, are done by varying the atmospheric conditions and the parameter values.



Atmospheric Stability – Select the condition: ● Unstable ○ Neutral ○ Stable

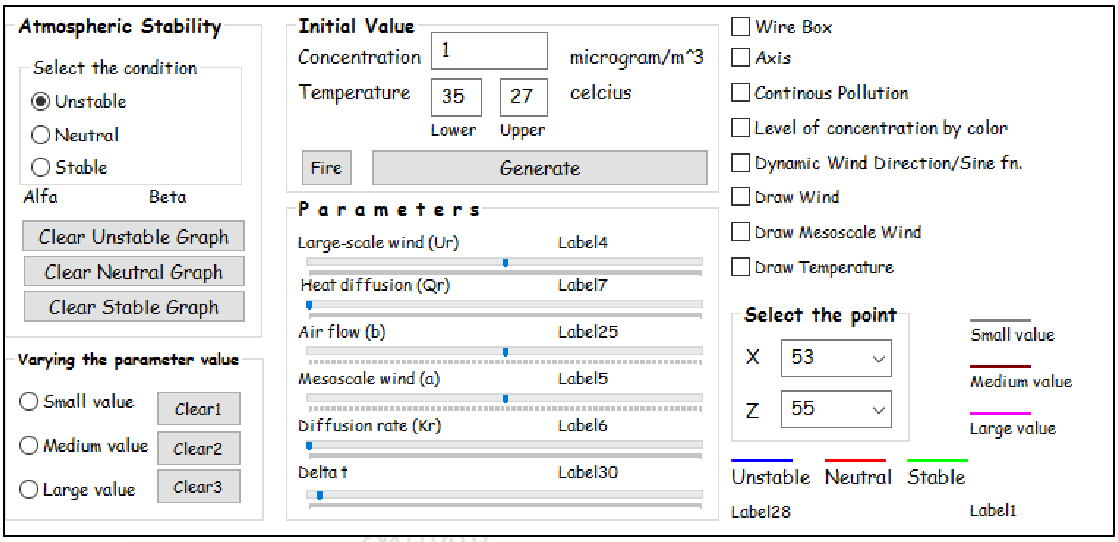
Initial Value: Concentration 1 microgram/m^3

Temperature 35 (Lower) 27 (Upper) celcius

Select the point: X 53, Z 55

Figure 10. User interface of the program.

Figure 10 shows the user interface of the program used in carrying out the various simulation of this study. The program was developed using the Lazarus programming software. The program presents a simple user interface that is very interactive.



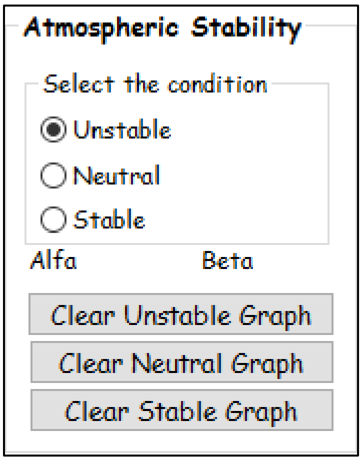
Select the condition
● Unstable
○ Neutral
○ Stable

Initial Value
Concentration 1 microgram/m^3
Temperature 35 Lower 27 Upper celcius

Select the point
X 53
Z 55

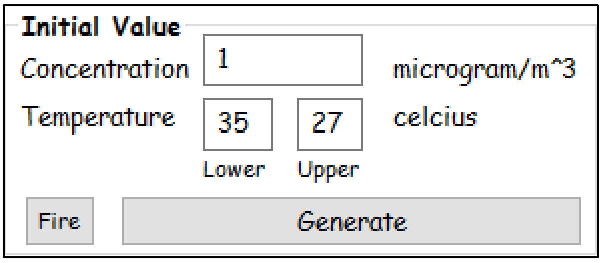
Figure 11. Parameter adjusting panel.

The various buttons and check boxes of the program are shown in Figure 11. This is the part where all the parameters are adjusted in order to have a clear understanding of how the pollutants distribute.



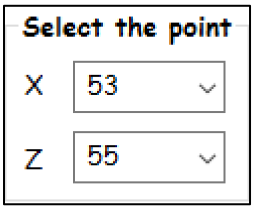
Select the condition
● Unstable
○ Neutral
○ Stable

Figure 12. Atmospheric condition panel.



Concentration 1 microgram/m^3
Temperature 35 27 celcius
Lower Upper

Figure 13. Initial value panel



X 53
Z 55

Figure 14. Arbitrary point panel

Figure 12, 13 and 14 show the detailed description of the user interface. Figure 12 represents the section where the atmospheric conditions can be changed by choosing unstable, neutral or stable conditions. The atmospheric conditions depend on the atmospheric stability (α) and surface roughness (β), the values will appear at label *Alfa* and *Beta* respectively when the program is run. The Clear Unstable Graph, Clear Neutral Graph and Clear Stable Graph buttons are used to remove the graph for each condition in accordance with their label. This conditions would be described later in the chapter. Figure 13 describes the section where the initial concentration of pollutants as well the temperature can be inputted. The initial temperature is needed as it affects the degree or intensity of turbulence in the atmosphere. In natural cases, the temperature at each altitude is different. Therefore, in this study the temperature is differentiated to lower and upper temperature whereby for temperature in the ground level and in the atmosphere respectively. Figure 14 shows the section where arbitrary points are chosen in order to measure the level of concentration in at particular point.

This is done in the x (horizontal) and z (vertical) directions, this arbitrary points will be shown in the visualization panel as a green dot after choosing.

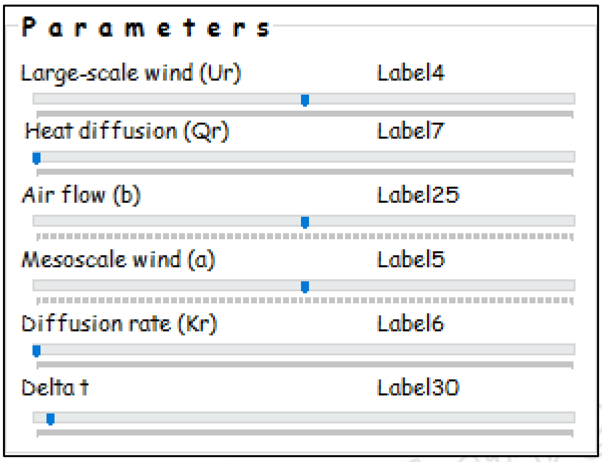


Figure 15. Model parameters panel.

Figure 15 shows the part where the parameters for the mathematical model can be varied. The parameters for the large-scale wind, heat diffusion, flow of air which is generated by temperature, mesoscale wind and diffusion rate can be varied using the slider to any considerable value of choice. Delta t slider is used to increase or decrease Δt. The greater the value of Δt, the faster the distribution of pollutants in the atmosphere. But note that, the explicit method is satisfied for the small number of Δt, if the Δt is very large, there is a possibility that the program would crash.

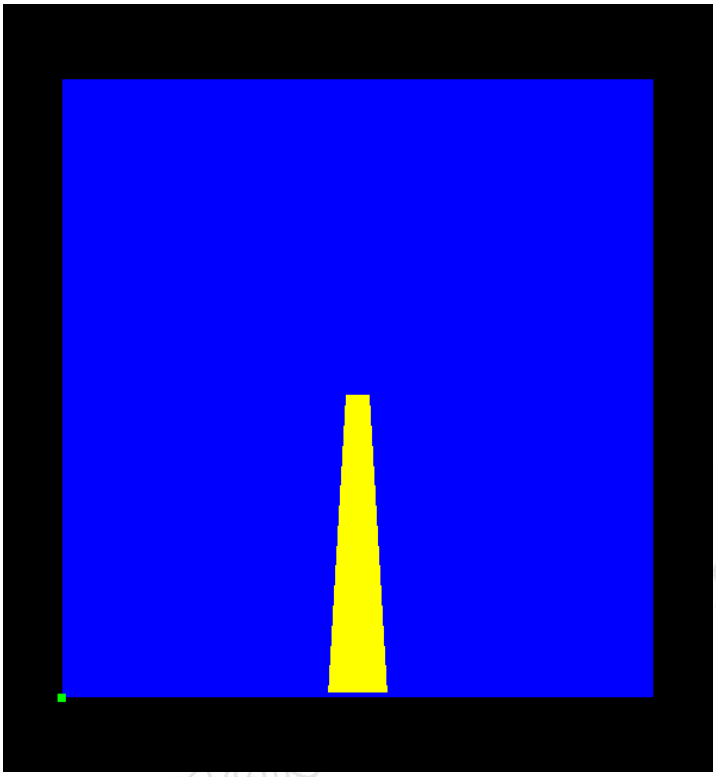


Figure 16. Visualization panel.

Figure 16 shows the visualization part of the program. The yellow stack represents the source of pollutant emission. When the program is initialized and run, pollutants are emitted from the stack and as the model parameters are adjusted, they then distributed in the plane. With this, the concentration can be measured when an arbitrary point is chosen.

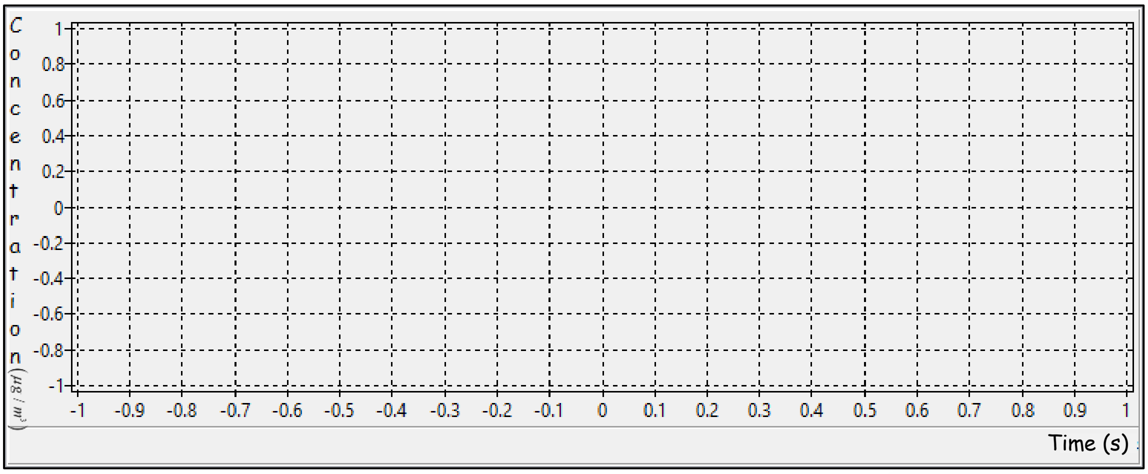


Figure 17. Graph panel.

Figure 18. Execution buttons.

Figure 17 shows the plotting area where the concentration is plotted against time. Figure 18 shows the various execution buttons like play, pause, stop, notes, help and close. Each of these buttons can be used to alter the simulation process either in running, pausing or stopping the program. The concentration values are kept in a text file and can be viewed by pressing the note button. The change in the level of concentration of pollutants can be viewed as a plot in Figure 17 for each of the atmospheric conditions.

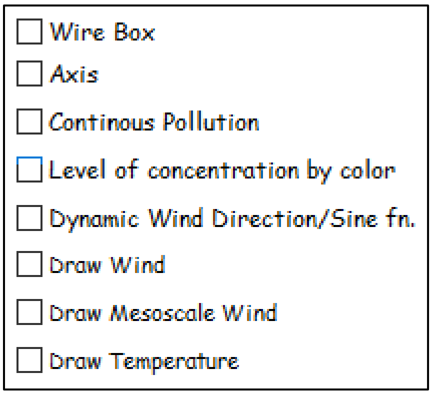


Figure 19. Check boxes panel.

Figure 19 shows some features of the program. Wire box check box shows the domain in a wire form in order for the user to be able to see the grids. Axis check box is to show the X – axis and Z – axis. Continuous pollution check box is to keep the pollutant in a continuous emission. Level of concentration by color check box is to show the level of concentration by different colors. Dynamic wind direction check box is created in order for the mean wind speed to move dynamically by a sine function. Draw wind, draw mesoscale wind and draw temperature check box are to show that the magnitude of the large-scale wind, mesoscale wind and temperature respectively are different with height.

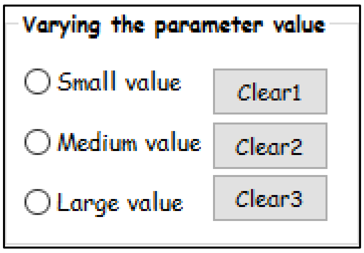


Figure 20. Graphic value panel.

Figure 20 shows the panel to plot the graph in the different value for the same parameter from the small value to the large value.

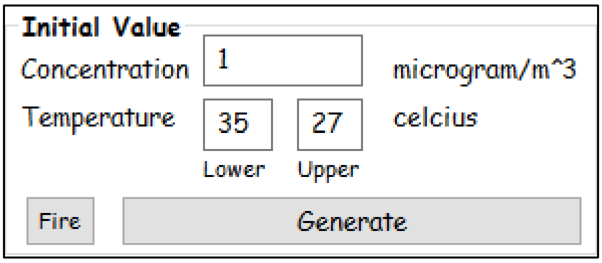
The next section shows the simulation that were carried out by the program.

4.2 Simulation

The advection-diffusion model described in chapter 3 depends on some parameters as well as the atmospheric condition at a particular point in time. The atmospheric condition considered are the unstable, neutral and stable which intern depend on some constants. The constants are the atmospheric stability represented in the model as α and the surface roughness of the earth as β in the model (see Table 1).

To be able to gain insight clearly on air pollutants distribution under the effect of the various model parameters like the large-scale wind, heat diffusion, air flow from the temperature, mesoscale wind and diffusion rate simulations are carried out and then visualized using the program developed. The program is run by choosing an atmospheric parameter, inputting the initial concentration, temperature and the various model parameters. Arbitrary points are then chosen and the system is activated by clicking on the generate button (see Figure 10). The concentration of pollutants is simulated using equation (14) and (15).

This section presents the various graphs that were plotted under the atmospheric conditions considered in this study. Different concentration-time plots would be shown to explain how the level of concentration of pollutants are affected by the model parameters.



Initial Value

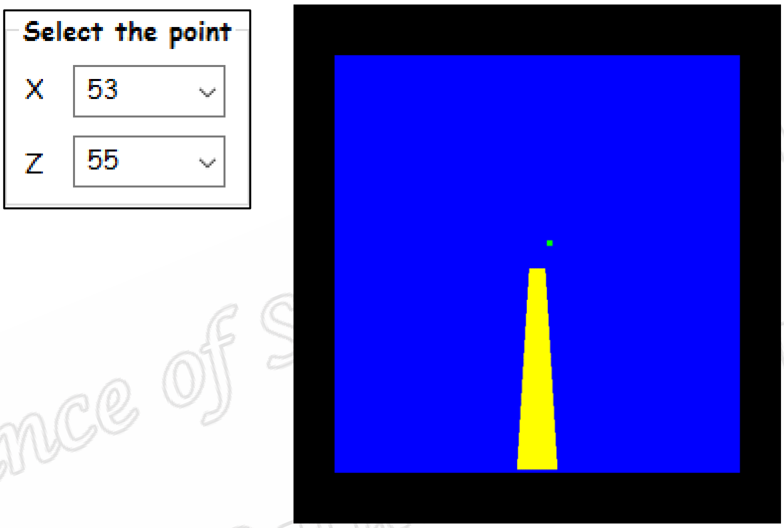
Concentration 1 microgram/m^3

Temperature 35 27 celcius

Lower Upper

Figure 21. Initial value panel.

In this simulation, Figure 21 shows the initial values inputted to the program.



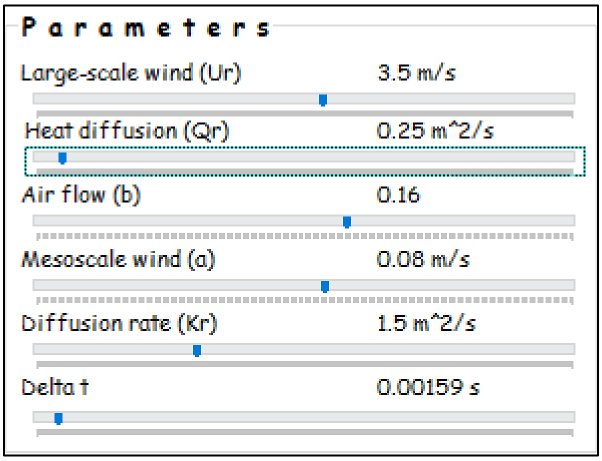
Select the point

X 53

Z 55

Figure 22. Position of the arbitrary point.

An arbitrary point is chosen by using X and Z labels in the program and the corresponding position is shown with a green dot in the visualization panel as shown in Figure 22.



Parameters

Large-scale wind (Ur) 3.5 m/s

Heat diffusion (Qr) 0.25 m^2/s

Air flow (b) 0.16

Mesoscale wind (a) 0.08 m/s

Diffusion rate (Kr) 1.5 m^2/s

Delta t 0.00159 s

Figure 23. Parameters values for simulation.

The parameters values used in Figure 24 are shown in Figure 23. This is done by adjusting the slider for each of the parameters.

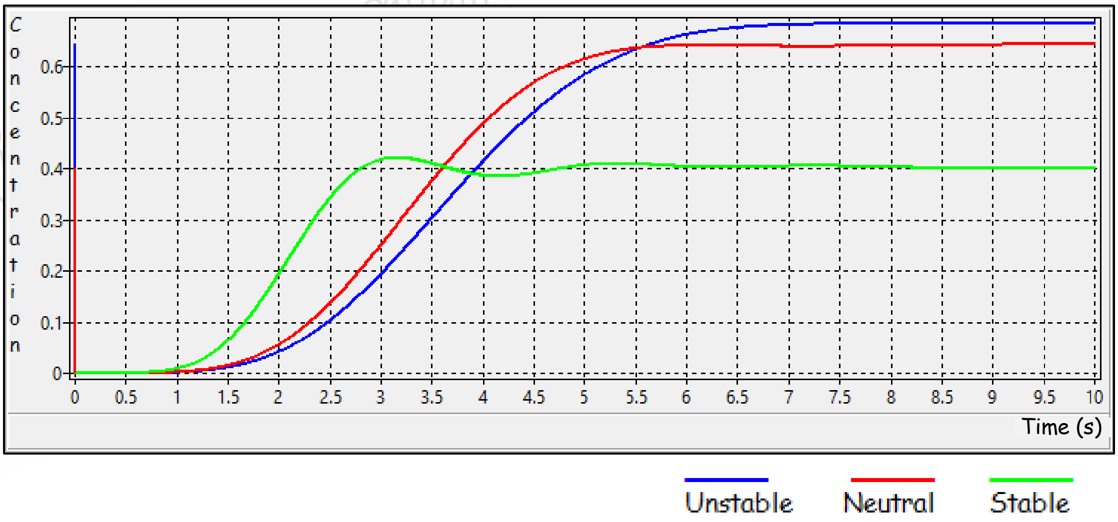
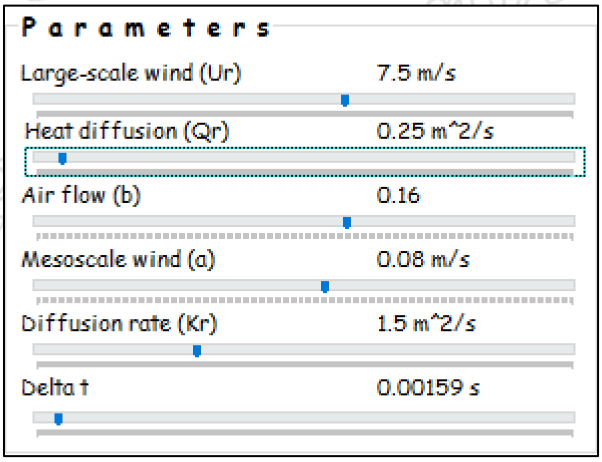


Figure 24. Pollutants distribution in all atmospheric conditions.

Figure 24 presents the distribution of pollutants in unstable, neutral and stable atmospheric conditions. When the emission starts, the level of concentration of pollutants is measured and a graph is plotted in the plotting panel. The simulation is done with the time interval of $0 \le t \le 10$. The level of concentration decreases as the emission continuous and this can be seen in figure 22 at a $0.7\,\mu g/m^3$ level under the unstable condition, $0.64\,\mu g/m^3$ under the neutral condition and $0.44\,\mu g/m^3$ under the stable condition. This is due to the difference in the atmospheric conditions as they all have different atmospheric stability and surface roughness values. From the graph it can be seen that at time 4.5, 5.5 and 6 unit of time for stable, neutral and unstable conditions respectively, the concentration of pollutants maintains some level of constancy. This is due to the fact that, the emission is continuous and at the point the change in concentration of the pollutants and the atmosphere is the same so there is not any significance change. Also, the pollutants undergo an advection and diffusion process and therefore there would always be a drop or increase in the concentration levels in the presence of the model parameters.



Large-scale wind (Ur) 7.5 m/s
Heat diffusion (Qr) 0.25 m^2/s
Air flow (b) 0.16
Mesoscale wind (a) 0.08 m/s
Diffusion rate (Kr) 1.5 m^2/s
Delta t 0.00159 s

Figure 25. The parameters value for simulation when the large-scale wind is increased.

Subsequently the simulation is carried out by increasing large-scale wind to $7.5\,m/s$ but the rest of the model parameters are maintained from the simulation was carried out in Figure 24. The values of the parameters are shown in Figure 25.

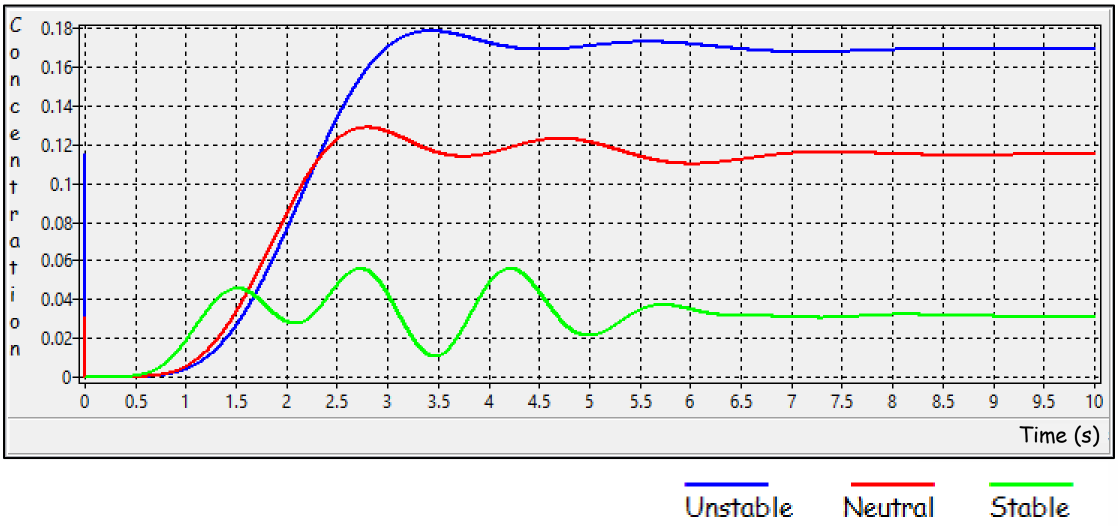


Figure 26. Varying mean wind speed in all atmospheric condition.

Figure 26 shows that in each of the atmospheric conditions, the peak level of the level of concentration of pollutants has decreased. This is evident from the previous figures with a $0.7\mu g/m^3$ to $0.18\mu g/m^3$ under the unstable condition, $0.64\mu g/m^3$ to $0.13\mu g/m^3$ under the neutral condition and finally $0.44\mu g/m^3$ to $0.044\mu g/m^3$ under the stable condition. The level of concentration of pollutants has decreased due to an increase in the large-scale wind. This fact would be explored more later in the chapter, as each of the parameters would be varied in one atmospheric condition. The level of constancy in the concentration of pollutants at 6.5, 7 and 6.8 unit of time for the stable, neutral and unstable conditions is a result of the reasons given under the Figure 24.

4.3 Visualizing the Effects of the Model Parameters on the Concentration of Pollutants

The model parameters are varied and used for the unstable atmospheric condition. This is done to see the effect they have on the distribution of pollutants in the atmosphere. In the simulations, one particular parameter is varied whiles the others are kept constant.

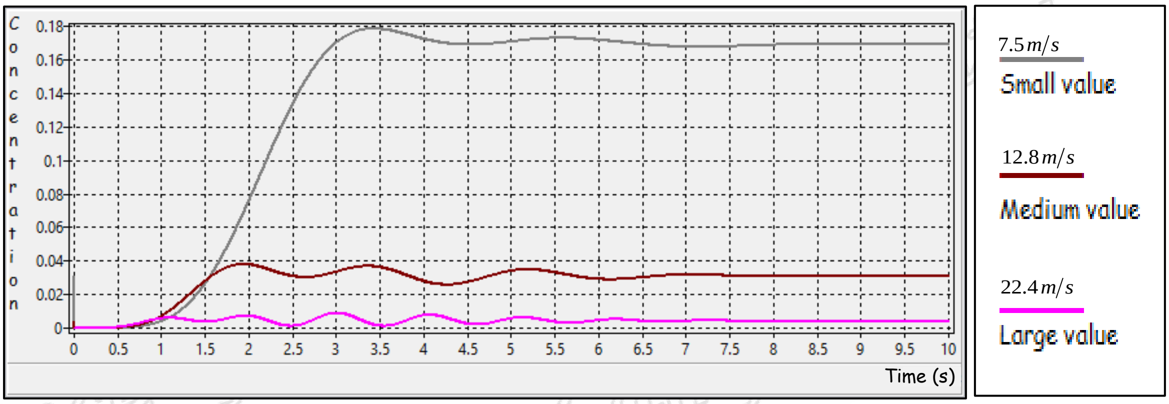


Figure 27. Pollutant distribution by varying the large-scale wind.

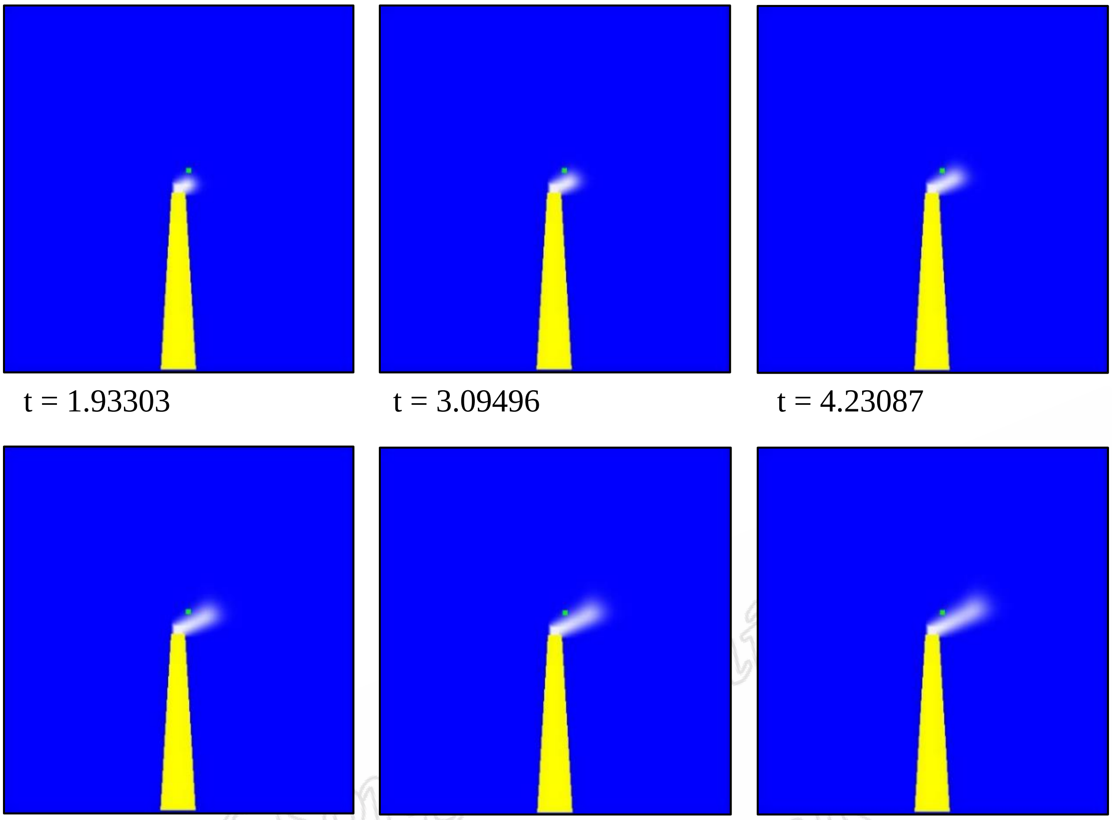
The simulations carried out in Figure 27 start with a large-scale wind of $7.5\ m/s$ and this value is varied to $12.8 m/s$ and $22.4 m/s$ whiles the other parameters are kept constant. Also the level of constancy in the concentration of pollutants at 8, 7.5 and 6.5 unit of time for the small value, medium value and large value respectively in unstable condition is as a result of the reason given under the Figure 24. Table 2 shows the model parameters and their values.

Table 2. Varying large-scale wind

Large-scale wind (U_r)	7.5	12.8	22.4
Heat diffusion (Q_r)	0.2		
Air flow (b)	0.16		
Mesoscale wind (a)	0.08		
Diffusion rate (K_r)	1.5		
Delta t	0.00159		

From the figures, it can be seen that as the large-scale wind increases the level of concentration decreases. This is because the bulk transfer of pollutants is as a result of the intensity of the wind in a particular area. As the speed of wind increases, pollutants are carried farther away from the source of emission.

In the program, the sign of the mean wind speed determines the direction of the pollutants. Figure 28 show the direction of the concentration of pollutants when the mean wind speed is positive 7.5 m/s. As a result, the movement of the pollutants from the stack can be seen from the left to right. The figures were captured at different time intervals as indicated under each of them. The movement of the pollutants would continue this way until the direction of the mean wind speed is changed.

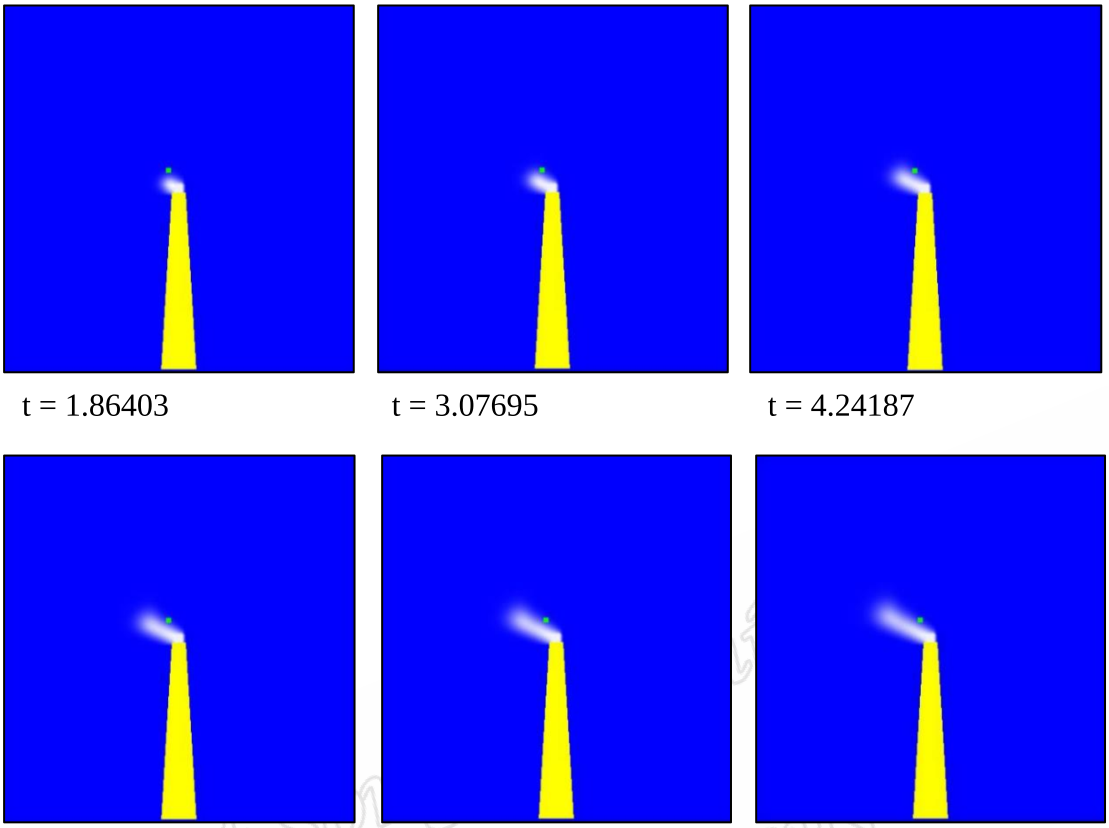


t = 1.93303 t = 3.09496 t = 4.23087

t = 5.30379 t = 6.34072 t = 7.38364

Figure 28. Visualization of pollutants distribution with positive large-scale wind.

As opposed to Figure 28, Figure 29 shows visualization of the emission of pollutants from stack with a negative mean wind speed $-7.5\,m/s$. The negative sign represents the direction of the pollutants. It can therefore be seen at different time intervals the direction of the pollutants from the right to the left and this can be changed when the mean wind speed becomes positive.


t = 1.86403

t = 3.07695

t = 4.24187

t = 5.34879

t = 6.41371

t = 7.50263

Figure 29. Visualization of pollutants distribution with negative large-scale wind.

The effect of heat diffusion in the distribution of pollutants is observed with the following simulations.

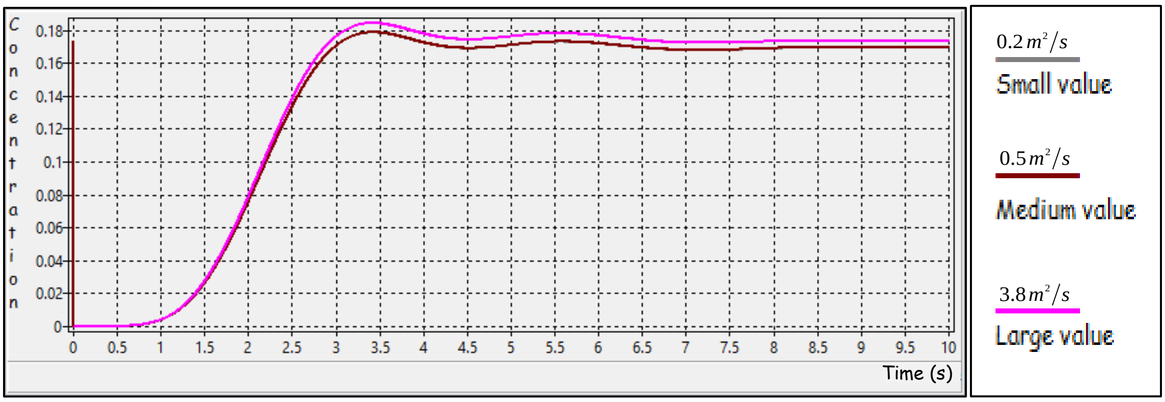


Figure 30. Pollutant distribution by varying the heat diffusion.

In the transport of pollutants, advection is dominant over diffusion and therefore from Figure 30 even though the heat diffusion is increased from 0.2 m^2/s to 0.5 m^2/s and then finally to 3.8 m^2/s, there is no significant difference in the level of concentration of pollutants. The level of constancy in the concentration of pollutants for all values from small to large value at 8 unit of time has been explained earlier (see Figure 24). Table 3 shows the parameter values for each of the figures.

Table 3. Varying heat diffusion rate

Large-scale wind (U_r)	7.5		
Heat diffusion (Q_r)	0.2	0.5	3.8
Air flow (b)	0.16		
Mesoscale wind (a)	0.08		
Diffusivity (K_r)	1.5		
Delta t	0.00159		

The air flow generated by the temperature in the atmosphere is considered as part of the model parameters. This is a constant that is varied to see the effect it has on the distribution of pollution.

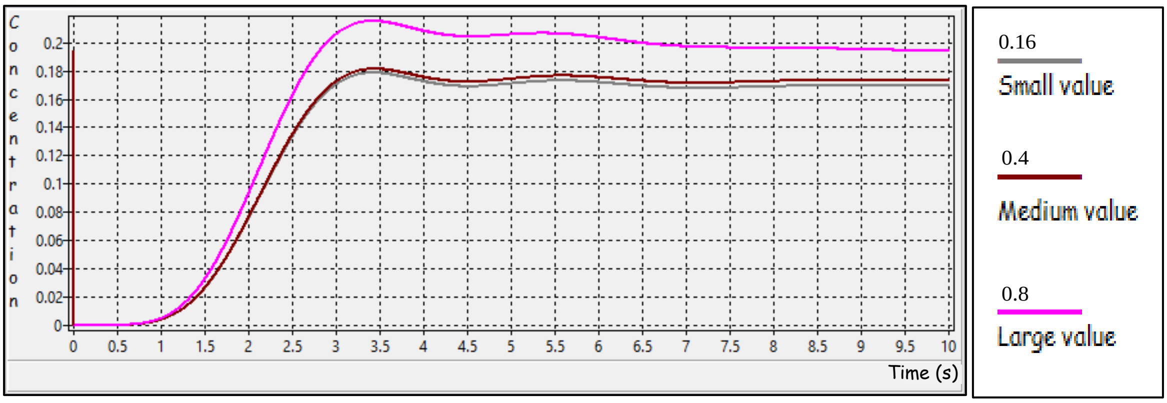


Figure 31. Pollutant distribution by varying air flow.

From Figure 31, the level of concentration increases in the unstable atmospheric condition as the value of air flow is increased from 0.16 to 0.4 and then 0.8. Therefore, an increase or decrease in this value results in a corresponding increase or decrease in the level of concentration of pollutants. In Figure 30, the level of constancy in the concentration of pollutants for all values are the same which is at 7 unit of time. The reason is the same as explained in Figure 24. Table 4 shows the various values for the simulation.

Table 4. Varying air flow

Large-scale wind (U_r)	7.5		
Heat diffusion (Q_r)	0.2		
Air flow (b)	0.16	0.4	0.8
Mesoscale wind (a)	0.08		
Diffusivity (K_r)	1.5		
Delta t	0.00159		

The temperature of the atmosphere has an effect on the turbulence and this turbulence creates a mesoscale wind which is responsible for carrying the pollutants into the atmosphere. The figures show that the concentration of pollutants increase when air flow is increased.

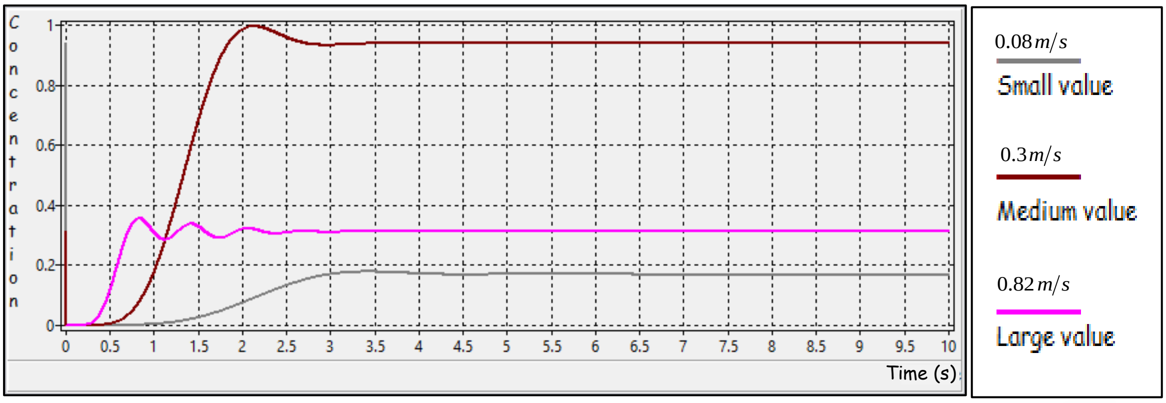


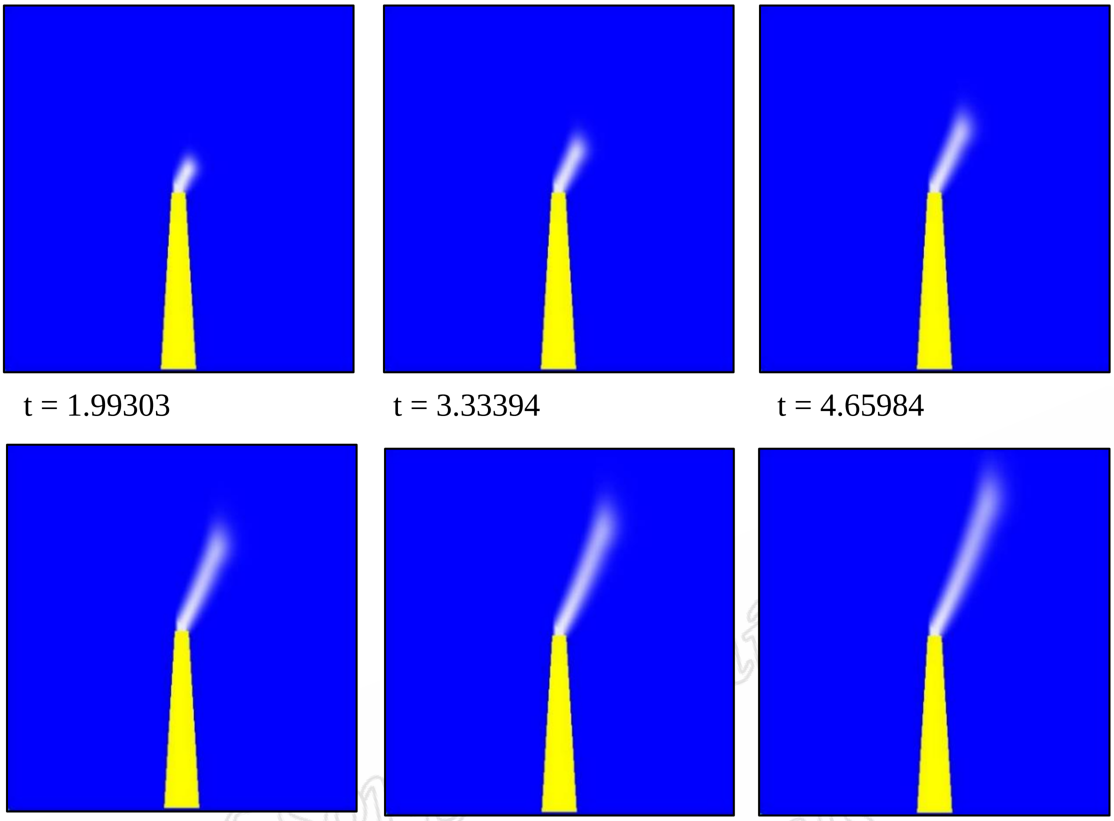
Figure 32. Pollutant distribution by varying mesoscale wind.

As studied by M. Agarwal and Tandon (2009), the mesoscale wind prevents the dispersal of pollutants which results in the increase of pollution concentration in the atmosphere. From Figure 32, the level of concentration of pollutants increase as the mesoscale wind is increased from 0.08 m/s to 0.3 m/s but decreased when it was increased to 0.82 m/s. This is because of the position of the arbitrary point that was chosen. The concentration of the pollutants was far from the arbitrary point and hence a decrease in the concentration level. The other model parameters are kept constant as the value of the mesoscale wind is varied. The level of constancy in the concentration of pollutants at 5, 3.5 and 3 for the small value, medium value and large value respectively is as a result of the same reason given under Figure 24. Table 5 shows the values used in each of the simulations carried out.

Table 5. Varying mesoscale wind.

Large-scale wind (U_r)	7.5		
Heat diffusion (Q_r)	0.2		
Air flow (b)	0.16		
Mesoscale wind (a)	0.08	0.3	0.82
Diffusivity (K_r)	1.5		
Delta t	0.00159		

The mesoscale wind is responsible for carrying the pollutants in the upwind and downwind directions. The mesoscale wind is positive 0.3 m/s and so the pollutants would move up but the mean wind speed is positive so from Figure 33, the pollutants move in the northeast direction at different time intervals.

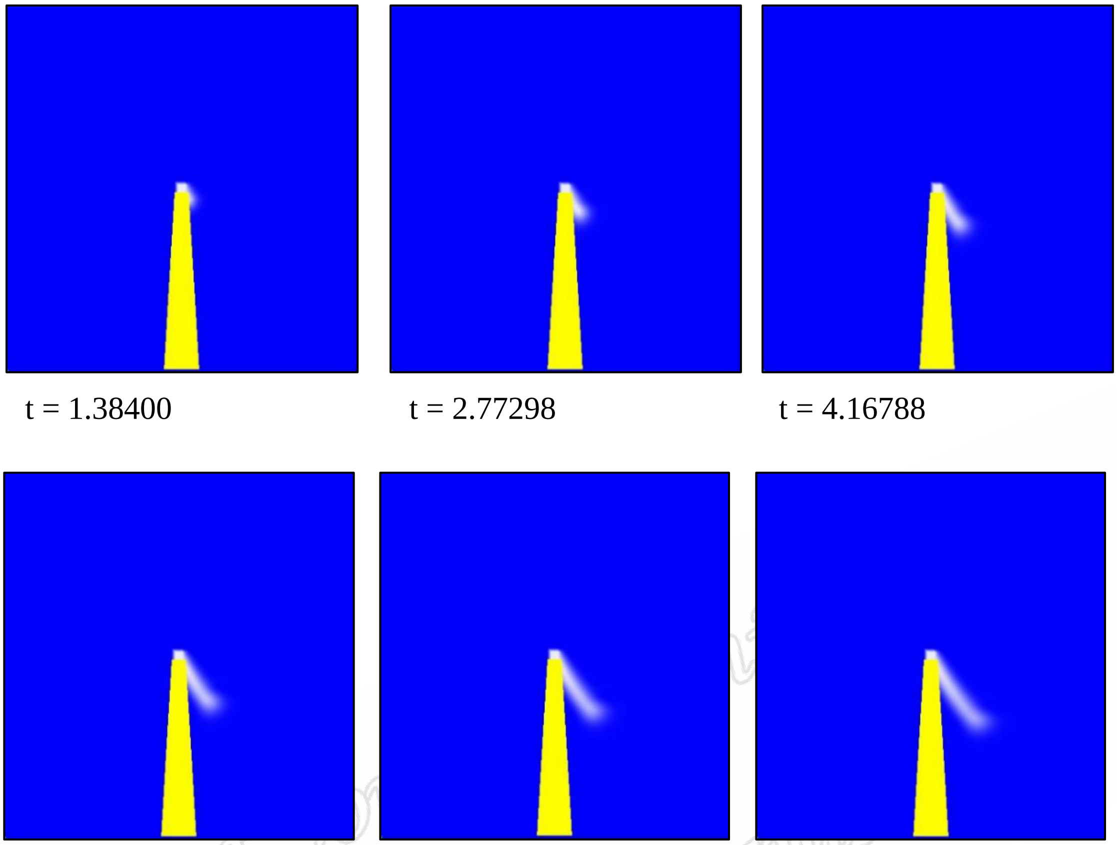


t = 1.99303 t = 3.33394 t = 4.65984

t = 5.91975 t = 7.16066 t = 8.42977

Figure 33. Visualization of pollutants distribution with positive mesoscale wind $0.3 m/s$.

With a negative value of the mesoscale wind $-0.3\ m/s$, the pollutants move in the downwind direction at different times intervals as shown in Figure 34.



t = 1.38400 t = 2.77298 t = 4.16788

t = 5.49778 t = 6.77169 t = 8.10464

Figure 34. Visualization of pollutants distribution with positive mesoscale wind $-0.3 m/s$.

Diffusion is the movement of molecules from a higher concentration to a lower concentration. In this study, the higher concentration point is the source of emission of pollutants and the lower concentration is the arbitrary point that was chosen. As the diffusivity is increased from 0.6 m^2/s to 1.5 m^2/s and the finally to 3.7 m^2/s, the level of concentration of pollutants increase as shown in Figure 35. In this case, the level of constancy in the concentration of pollutants at 9.5, 6.5 and 4.5 unit of time for the small value, medium value and large value respectively can be explained in the same way as that of Figure 24.

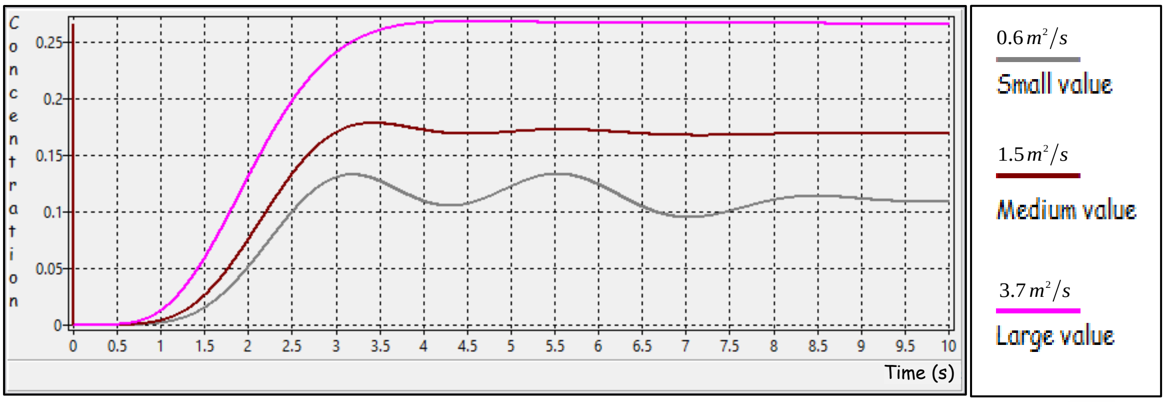


Figure 35. Pollutant distribution by varying diffusion rate.

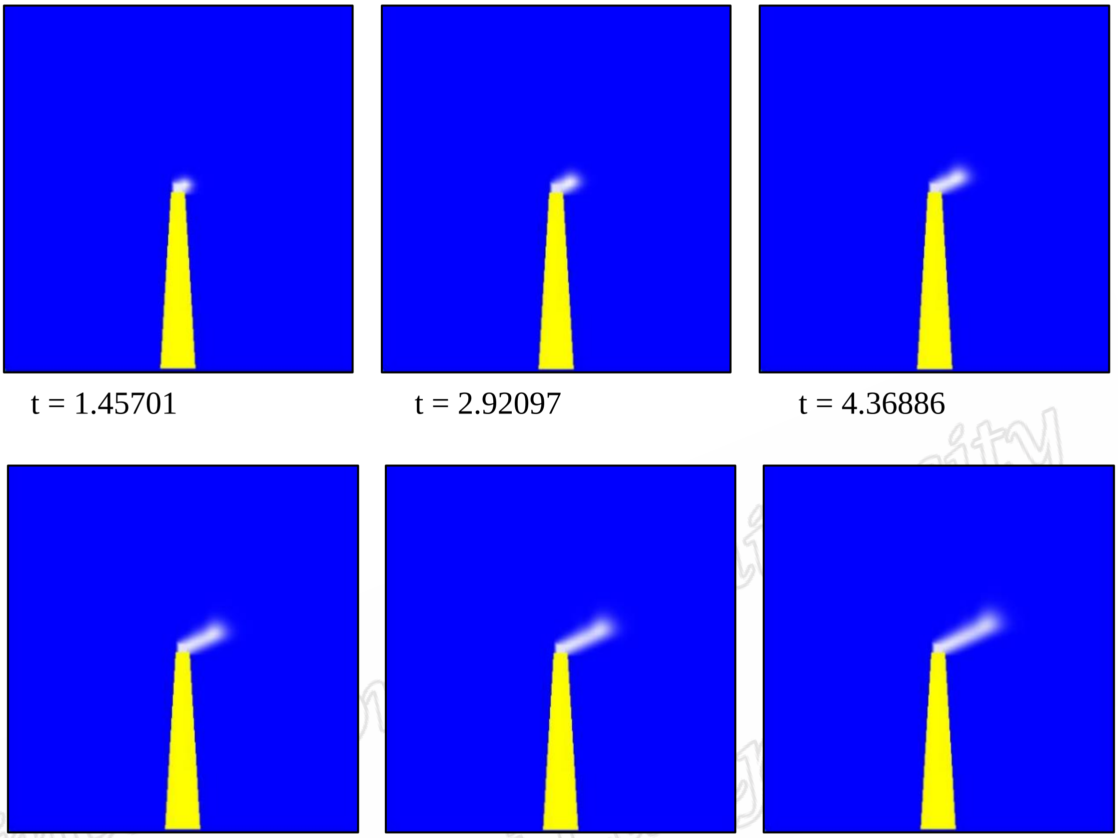
This due to the fact that the pollutants are diffusing at a faster rate to the arbitrary point which tend to increase the concentration at that point. Table 6 shows the model values that were used to carry out the simulations.

Table 6. Varying diffusivity.

Large-scale wind (Ur)	7.5		
Heat diffusion (Qr)	0.2		
Air flow (b)	0.16		
Mesoscale wind (a)	0.08		
Diffusivity (Kr)	0.6	1.5	3.7
Delta t	0.00159		

Simulations for the model parameters have been carried out for each of the atmospheric conditions and then visualized in the various figures shown. Inferences and conclusions would be discussed in the next chapter.

The diffusivity is varied and visualized at different time intervals. This cannot be seen clearly in movement of the pollutants from Figure 36 with diffusivity 0.6 m^2/s.

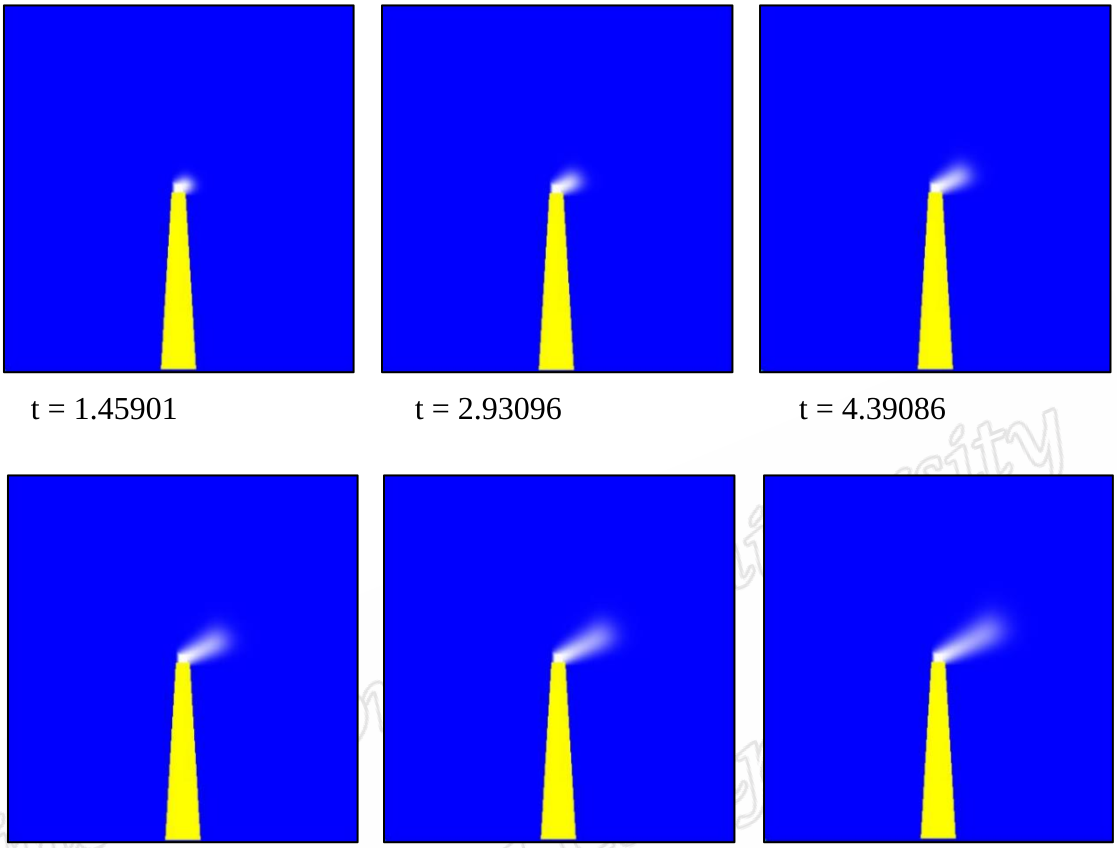


t = 1.45701 t = 2.92097 t = 4.36886

t = 5.74976 t = 7.09066 t = 8.47479

Figure 36. Visualization of pollutants distribution with diffusion rate of $0.6\,m^2/s$.

Figure 37 shown the movement of pollutants as the diffusivity is varied to be 3 m^2/s. This cannot be seen clearly as advection is dominant over diffusion in the transport of pollutants in the atmosphere.



t = 1.45901

t = 2.93096

t = 4.39086

t = 5.78976

t = 7.15466

t = 8.54282

Figure 37. Visualization of pollutants distribution with diffusion rate of $0.6\, m^2/s$.

The next chapter presents the conclusion as well as further research of the study.

Chapter 5

Conclusion and Further Research

5.1 Conclusion

Air pollution is one of the major atmospheric problems the world faces nowadays. The WHO estimates millions of people dying each year as a result of pollution problems. Dispersion models are essential in managing the ambient air quality. The dispersion models are used to estimate the impact of the concentration of air pollutants which have on the living organisms as well the entire ecosystem.

By using a mathematical model, it becomes easier to learn the basic concept of the physical phenomena that takes place during the distribution of pollutants as they undergo advection and diffusion processes under the influence of meteorological factors. In this study, these parameters represent large-scale wind, mesoscale wind, eddy diffusivity and temperature. These parameters have been incorporated into the model to understand how pollutants distribute in different atmospheric stability conditions.

The finite difference method is used to solve the model numerically. The results are simulated and visualized using the program developed. Various simulations were carried out in order to access how the distribution of pollutants are affected when any of the model parameters are varied. The large-scale wind shows a significant change in the level of concentration of pollutants. The increase or decrease in the large-scale wind resulted in a corresponding increase or decrease in the level of concentration of pollutants. The mesoscale wind however showed different results. An increase in the mesoscale wind resulted in an increase in the concentration levels. Therefore, the transport of pollutants from the source of emission depends largely on the large-scale wind as advection is dominant over diffusion in this process.

Through the various simulations, the effect of the parameters on the distribution of pollutants can be appreciated as it makes it easier to understand the pollution distribution concept. Although the concentration of pollutants cannot be reduced after it has been released into the atmosphere, but through this study, the government and other stake holders can be advised in order to make policies that would cut down the production of NO_2, SO_s and other harmful pollutants through coal power plants by going green. That is encouraging the use of renewable energy. The visualization of the pollutants can be used to explain the pollution problems to communities on how meteorological parameters affect the distribution of pollutants.

5.2 Further research

The entire study of pollutants distribution is largely based on simulations but in further research, real meteorological data can be used to confirm the validity of the model. Again, some removal mechanisms can be added to the simulation in order to know the actual concentration of pollutants after these physical processes.

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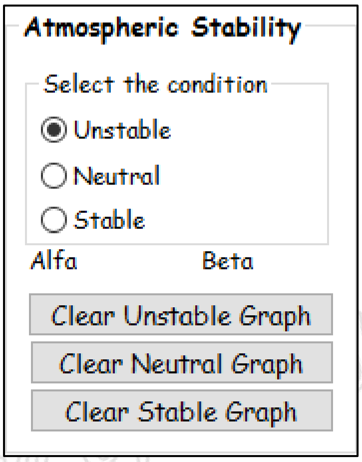
APPENDIX

How to use the program?

The pollution distribution simulation software can be used by going through the following steps. Getting familiarized with the program takes a few seconds. The steps are outlined below.

1. Select one of the atmospheric conditions.



Atmospheric Stability

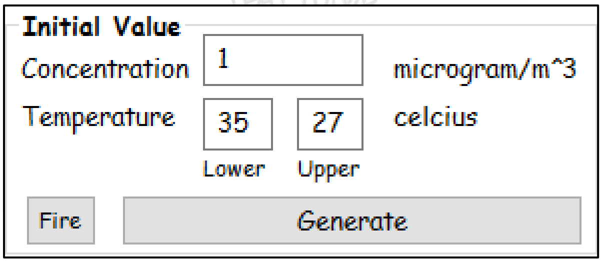
Select the condition

● Unstable

○ Neutral

○ Stable

2. Input the initial value of concentration and temperature.



Initial Value

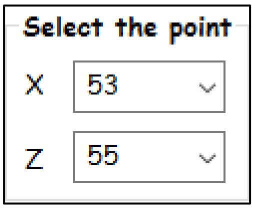
Concentration 1 microgram/m^3

Temperature 35 27 celcius

Lower Upper

Then, to activate it click the generate button.

3. The concentration of the pollutants can be known at a particular point by choosing the X and Z labels.

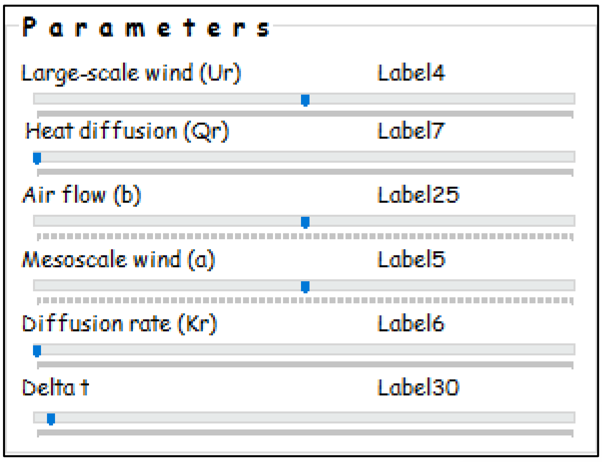


Select the point

X 53

Z 55

4. The mean wind speed, heat diffusion, flow from the temperature, turbulence, diffusion rate can be varied by using the slider.



Parameters

Large-scale wind (Ur) Label4

Heat diffusion (Qr) Label7

Air flow (b) Label25

Mesoscale wind (a) Label5

Diffusion rate (Kr) Label6

Delta t Label30

5. Click the play button ▶ to run the program, button ⏸ to pause the program, button ⏻ to stop the program, button ✎ to save the concentration value of pollutants in a file, button ? to as a guide in using the program and button ✖ to close the program.

Algorithm of the program

```
Var                                               {variables for the model}

{the variables for the model are defined in order to be used in the various procedure}

Const WD   = 100                                  {the number of grid horizontally}
Const HD   = 100                                  {the number of grid vertically}
Const $z_r$   = 10                                   {reference height}
Const IVC  = 1                                    {initial value of concentration}
Const IVT  = 27                                   {initial value of temperature}

{defining the data types for the variables}

Time          : single
dt            : single
dh            : single
Lamda         : single
$U_r$            : real
a             : real
$K_r$            : real
$Q_r$            : real
alfa, beta    : real
b             : real

{creating an array}

wind          : array [1..WD, 1..HD] of single
$w_e$            : array [1..WD, 1..HD] of real
$K_x$, $K_z$        : array [1..HD] of real
Tnew, Tnow    : array [0..WD, 0..HD] of single
Cnew, Cnow    : array [0..WD, 0..HD] of single
```

Algorithm

{simulation}

Procedure 1.

```
{in this procedure, the initial values are set for subsequent calculation in the program}

begin
    $U_r$    ←—  0.01
    a     ←—  0.01
    $K_r$    ←—  0.01
    $Q_r$    ←—  0.0007
```

```
    b       ← 0.01
    Time    ← 0                        {initial computational time}
    dt      ← 0.001                    {time increment}
    dh      ← 5                        {spatial increment dx = dz = dh}
    Lamda   ← 0.000001

        for j ←  0 to HD do
            for i ←  0 to WD do
                begin
                    Tnow [i,j] ← IVT
                end
end procedure.
```

Procedure 2.

{in order to run the program, the various atmospheric parameters are enabled. This is done by using a check box}

```
    read (radiogroup)
        if unstable.checked then
            alfa ←  0.17
            beta ←  0.83
        end if
        if neutral.checked then
            alfa ←  0.27
            beta ←  0.73
        end if
        if stable.checked then
            alfa ←  0.61
            beta ←  0.39
        end if
```

{this section calculates the various parameters for the model using the formula from the model}

```
    for j ←  1 to HD-1 do
        begin
            $K_z[j]$ ← $K_r\left(\frac{j}{z_r}\right)^{\beta}$

            for i ← 1 to WD-1 do
                begin
                    $K_x[i]$ ← $K_r\left(\frac{i}{z_r}\right)^{\beta}$
```

```
            Wind [i,j]  ←  $u_r\left(\frac{j}{z_r}\right)^{\alpha} + a\,i\left(\frac{j}{z_r}\right)^{\alpha}$
            Tnew [i,j]  ←  $\frac{Q_r\,\Delta t}{\Delta x^2}T^{n-1}_{i+1,j} + \frac{Q_r\,\Delta t}{\Delta x^2}T^{n-1}_{i-1,j} + \frac{Q_r\,\Delta t}{\Delta z^2}T^{n-1}_{i,j+1} + \frac{Q_r\,\Delta t}{\Delta z^2}T^{n-1}_{i,j-1} + \left(-2\frac{Q_r\,\Delta t}{\Delta x^2} - 2\frac{Q_r\,\Delta t}{\Delta z^2}T^{n-1}_{i,j} + 1\right)T^{n-1}_{i,j}$
            w_e [i,j]   ←  $\frac{a\,j}{(\alpha+1)}\left(\frac{j}{z_r}\right)^{\alpha} + b\left(\frac{T^{n}_{i,j}-minT^{n}_{i,j}}{maxT^{n}_{i,j}-minT^{n}_{i,j}}\right)$
        end
    end
end procedure.
```

Procedure 3.

{the initial concentration is inputted in this procedure and procedure 2 is called to use the atmospheric condition. Procedure 5 is then used in order to draw the corresponding graphs}

```
Call procedure 2
Call procedure 5

{input the initial concentration}

Cnow [50,50] ← IVP
Cnow [49,50] ← IVP
Cnow [49,51] ← IVP
Cnow [51,50] ← IVP
Cnow [51,51] ← IVP
Cnow [50,49] ← IVP
Cnow [49,49] ← IVP
Cnow [50,51] ← IVP
Cnow [51,49] ← IVP

{calculating concentration with the concentration formula}

  for j ← 1 to HD-1 do
    begin
      for i ← 1 to WD-1 do
        begin
          Cnew [i,j] ← $A_1C^{n}_{i+1,j} + A_2C^{n}_{i-1,j} + A_3C^{n}_{i,j+1} + A_4C^{n}_{i,j-1} + A_5C^{n}_{i,j}.$
        end
    end
end procedure.
```

Procedure 4.

{activate the initial value}

```
Call procedure 1.
Call procedure 2.
```

{setting the selected point to measure the concentration of pollutant using the combo box}

```
for i ←  0 to WD do                              {for setting point X}
    begin
        Combobox1 [i]  ←  0 … 100
    end

for j ←  0 to HD do                              {for setting point Z}
    begin
        Combobox2 [j]  ←  0 … 100
    end
```

{visualization}

Procedure 5.

{in this procedure, the graph for the three atmospheric condition can be drawn for visualization}

```
begin
    if Unstable.Checked then
        begin
            UnstableSeries1.
        end;
    if Neutral.Checked then
        begin
            NeutralSeries1.
        end;
    if Stable.Checked then
        begin
            StableSeries1.
        end;
end;
```

Procedure 6.

{this procedure use openGL utility to draw the image for visualization}

```
Var                                   {local variable for procedure 6 only}

Speed       : double
```

```
DataRange  : double
begin
    glClearColor(0.0, 0.0, 0.0, 1.0);
    glClear(GL_COLOR_BUFFER_BIT or GL_DEPTH_BUFFER_BIT);
    glEnable(GL_DEPTH_TEST);
    glMatrixMode(GL_PROJECTION);
    glLoadIdentity();
    gluPerspective(45.0, double(Width) / height, 0.2, 100.0);
    glMatrixMode(GL_MODELVIEW);
    glLoadIdentity();
    glTranslatef(-1.0, 0.0,-3.0);
    glTranslatef(Tran_X,Tran_Y,Tran_Z);
    glRotatef(alpha+dx,0.0,1.0,0.0);
    glRotatef(betha+dy,1.0,0.0,0.0);

    if Axis.Checked then
        begin
            glBegin(GL_LINES);
                glColor3f(1.0,0.0,0.0);
                glVertex3f(-1.0,0.0,0.0);
                glVertex3f( 1.0,0.0,0.0);

                glColor3f(0.0,1.0,0.0);
                glVertex3f(0.0,-1.0,0.0);
                glVertex3f(0.0, 1.0,0.0);

                glColor3f(0.0,0.0,1.0);
                glVertex3f(0.0,0.0,-1.0);
                glVertex3f(0.0,0.0, 1.0);
            glEnd();
        end;

    if (MaxC-MinC) = 0 then
        begin
            MaxC ←— 1;
            MinC ←— 0;
        end;

    if WireBox.Checked then
        begin
            glPolygonMode(GL_FRONT_AND_BACK,GL_LINE)    {to show grid}
        end else
        begin
```

```
        glPolygonMode(GL_FRONT_AND_BACK,GL_FILL);   {to show plane}
    end;

DataRange ← MaxC-MinC;

{drawing source of emission}

glPointSize(7);   { size of the point }
glBegin(GL_POINTS);
    glcolor3f(0,1,0);
    glPointSize(10);
    glvertex3f(-1+(PointX)*(4/WD), -1+PointZ*(2/HD), 0.01);
    glpointsize(1);
glEnd();

{drawing the stack}

glBegin(GL_POLYGON);
    glColor3f(1.0,1.0,0);
    glvertex3f(-1+((WD div 2)-5)*(4/WD), -1+(1)*(2/HD), 0.01);
    glvertex3f(-1+((WD div 2)-2)*(4/WD), -1+((HD div 2)-1)*(2/HD), 0.01);
    glvertex3f(-1+((WD div 2)+2)*(4/WD), -1+((HD div 2)-1)*(2/HD), 0.01);
    glvertex3f(-1+((WD div 2)+5)*(4/WD), -1+(1)*(2/HD), 0.01);
glEnd();

{configurating the 4 boundary condition}

{North}

for j ← 0 to 0 do
    for i ← 0 to WD do
        begin
            Cnow[i,j] ← Cnow[i,j+1];
        end;

{South}

for j ← HD to HD do
    for i ← 0 to WD do
        begin
            Cnow[i,j] ← Cnow[i,j-1];
        end;

{West}

for j ← 0 to HD do
    for i ← 0 to 0 do
```

```
        begin
            Cnow[i,j]  ←  Cnow[i+1,j];
        end;

{East}

for j  ←  0 to HD do
    for i  ←  WD to WD do
        begin
            Cnow[i,j]  ←  Cnow[i-1,j];

    end;

{tranfer the Cnew to Cnow and Tnew to Tnow}

for j  ←  1 to HD-1 do
    for i  ←  1 to WD-1 do
        begin
            Cnow[i,j]  ←  Cnew[i,j];
            Tnow[i,j]  ←  Tnew[i,j];
        end;

Speed := double(OpenGLControl1.FrameDiffTimeInMSecs)/10;

cube_rotationx += 5.15 * Speed;
cube_rotationy += 5.15 * Speed;
cube_rotationz += 20.0 * Speed;
Time  ←  Time + dt;

{finalize with swap buffer / refresh openGL}

OpenGLControl1.SwapBuffers;

end;
```

Procedure 7.

{to call procedure 3 and procedure 6}

Call procedure 3.
Call procedure 6.

Procedure 8.

{to run the program}

```
begin
    MaxC    := 0;
    MinC    := 0;
```

```
    Ur      := TrackBar1.Position/100;   {The Mean Wind Speed (Ur)}
    a       := TrackBar2.Position/100;   {Turbulence (a = proportionality constant)}
    Kr      := TrackBar3.Position/100;   {Diffusion Rate (Kx / Kz)}
    Qr      := TrackBar4.Position/100;   {Heat Diffusion (Qx / Qz)}
    b       := TrackBar5.Position/100;   {b = the flow caused by the temperature}

    call procedure 2.

    Timer1.Enabled  := True;
end;
```

Vitae

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International Conference

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