PREDICTION OF CARBON MONOXIDE CONCENTRATION DUE TO VEHICULAR EMISSION USING ROE-RIEMANN SOLVER

BY

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2004/18527EH

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SCHOOL OF ENGINEERING AND ENGINEERING TECHNOLOGY,

FEDERAL UNIVERSITY OF TECHNOLOGY,

MINNA, NIGER STATE.

NOVEMBER, 2009

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A PROJECT SUBMITTED TO THE DEPARTMENT OF CHEMICAL ENGINEERING,

SCHOOL OF ENGINEERING AND ENGINEERING TECHNOLOGY,

FEDERAL UNIVERSITY OF TECHNOLOGY, MINNA.

IN PARTIAL FULFILMENT OF THE REQUIREMENT FOR THE AWARD OF

BACHELOR OF ENGINEERING (B.ENG) DEGREE IN CHEMICAL ENGINEERING.

NOVEMBER, 2009

DECLARATION

I hereby declare that this research project '**Prediction of Carbon Monoxide Concentration due to Vehicular Emission using Roe-Riemann solver**' was carried out solely by me under the supervision of Engr. Mohammed Umar Garba of the department of Chemical Engineering, School of Engineering and Engineering Technology, Federal University of Technology Minna.

All literatures sited in this project have been duly acknowledged in the reference.

Basil

Ochigbo Basil Anebi

28-08-09

Date

CERTIFICATION

This is to certify that this research project **'PREDICTION OF CARBON MONOXIDE CONCENTRATION DUE TO VEHICULAR EMISSION USING ROE-RIEMANN SOLVER'** was carried out by **Ochigbo Basil Anebi** (2004/18527EH) and supervised, moderated and approved by the following under listed persons as a prerequisite for the award of bachelor of Engineering, (B.Eng) degree of Chemical Engineering on behalf of Chemical Engineering Department, School of Engineering and Engineering Technology, Federal University of Technology, Minna, Niger State.

Engr. M.U Garba **(Project Supervisor)**	28/08/2009 **Date**
Engr. M Alhassan **(Head of Department)**	**Date**
External Examiner	**Date**

DEDICATION

This Project is dedicated to Almighty God and my wonderful Parents, Fabian Ameh and Paulina Ochigbo, whose unflinching support, faith and encouragement saw me through the program and helped me to achieve my goals.

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I am indebted to my project supervisor, Engr. Mohammed Umar Garba for his counseling encouragement, support, and thorough review that resulted in the completion of this research work.

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I am grateful to my siblings, Kenneth, Eko, Ochanya, Okah, Ejeh Tiger, Ehi and Chief. May God bless you all. Love you all, you all are the best! And to my late sisters, may your gentle souls rest in perfect peace.

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Finally, I would like to express my sincere thanks to God, the Faithful One, who gave me the assurance that saw me through this program.

ABSTRACT

The Roe-Riemann solver, a finite volume difference method which has a great stability for prediction of fluid flow was developed for the prediction of carbon monoxide due to vehicular emission for input source strength emitted at a given value. Time, distance, air velocity and pollutant speed were the parameters considered in developing the dispersion model, which predicts the concentration profile for dispersion. The simulation of the model was carried out using the parameters (time, distance, air velocity and pollutant speed) to show the effect of air velocity and pollutant speed on concentration profile at various axial wind height/distance above ground level. From the results obtained and the graphs plotted, it shows that as the air velocity, pollutant speed and axial height/distance above ground level increases [(0.5m/s-2.5m/s), (2.50m/s-3.00m/s), (1m-11m)] respectively, the concentration of pollutant decreases (0.98mol/m^3-0.82mol/m^3) due to dispersion of pollutant. It was observed that there is a great dispersion of pollutant concentration at high air velocity, pollutant speed and axial height/distance above ground level.

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CHAPTER ONE

1.0 INTRODUCTION

The large majority of today's cars and trucks travel by using internal combustion engines that burn gasoline or other fossil fuels. The process of burning gasoline to power cars and trucks contributes to air pollution by releasing a variety of emissions such as oxides of sulphur, oxides of nitrogen, carbon monoxide, carbon dioxide, particulate matter, e.t.c, into the atmosphere. Emissions that are released directly into the atmosphere from the tailpipes of cars and trucks are the primary source of vehicular pollution. But motor vehicles also pollute the air during the processes of manufacturing, refueling, and from the emissions associated with oil refining and distribution of the fuel they burn.

Carbon monoxide being one of the major pollutants associated with motor vehicles is a very dangerous gas. Cars and trucks are the source of nearly two-thirds of this pollutant. When inhaled, it blocks the transport of oxygen to the brain, heart, and other vital organs in the human body. Newborn children and people with chronic illnesses are especially susceptible to the effects of carbon monoxide. The effect of pollution in the atmosphere to the society in general especially in the long term is very costly. Illness and premature death due wholly or in part to air pollution places a great burden upon the society by way of increased costs of medical treatment through the loss of labour. In addition, air pollution adversely affects solids, water, wildlife, weather, climate and transportation as well as reducing economic values and personal effort and well being. (Enemari, 2004).

There is a need for effective measures to mitigate the adverse impacts of motor vehicles use, the living environment in the cities of the developing world will continue to deteriorate and become increasingly unbearable if nothing is done to combat this great menace. Thus, in order to characterize the variation of these pollutants in space and time, there is need for monitoring. Air monitoring alone is expensive, time consuming and requires skilled manpower and sophisticated equipments. It is therefore necessary to develop and simulate models which must be flexible enough to determine the concentration with the changes in the source, concentration and meteorological conditions. Basically, models have a degree of control and capacity for exploring virtual realities beyond those available to us through field and laboratory experiments, particularly when dealing with atmospheric phenomenon. (Lasisi, 2007)

1.1 AIM AND OBJECTIVES

The aim of this research project is to predict the concentration of pollutants such as carbon monoxide emitted from motor vehicles for input source strength at a given distance and time. This can be achieved through actualization of the following objectives:

- Developing a mathematical model to determine the concentration of emitted carbon monoxide from motor vehicles.
- Collate data on the input source strength from motor vehicles and meteorological data on some physical parameters such as the speed of air, velocity of pollutant e.t.c.
- Collate data on the atomic diffusion volumes and molecular weight to determine the diffusivity of air-carbon monoxide system.
- Stimulate the developed model by computer program, using MATHCAD and find the interaction between these physical parameters with the concentration of carbon monoxide.

1.2 SCOPE AND LIMITATION OF STUDY

This research work focuses on the prediction of concentration of air pollutant such as carbon monoxide from vehicle emissions, taking into consideration peculiarities of the pollution pattern, their effect on human, animals and surrounding environment.

In developing the models, the equation which describes diffusion is used, this represents the change in concentration with time and space, and also to make the equation as realistic as possible.

The simulation of the developed model will be carried out to determine the concentration of carbon monoxide in atmosphere at a given distance and time, and to show the effect of some physical parameters on the concentration of carbon monoxide.

These vehicle emissions are basically hydrocarbons, carbon monoxide, oxides of nitrogen and particulates. But due to the limited scope of available data, carbon monoxide being the major exhaust gas emitted as pollutants from motor vehicles, concentration of carbon monoxide is therefore determined in this research project as a function of some physical parameters such as air velocity, pollutant's speed and source strength on the emission dispersion and concentration profile at various axial distance and height above ground level; suggestion of control measures that could eliminate or reduces pollutants from vehicle emissions to the minimum.

1.3 JUSTIFICATION OF STUDY

There is the need to preserve the land, air, and rivers especially around urban areas that has low assimilative capacity for ourselves and the younger generations. Therefore, it is morally justifiable to ensure that the health and well-being of the communities around the cities of the developing world are not threatened by these activities of vehicle emissions.

Though, advancement is being made in chemical Engineering in contributing immensely to continued global industrial growth and development, but much investigation into pollutant concentration resulting from vehicle emissions need to be undertaken because of the damaging effect of these pollutants in an environment.

Researches have being carried out on mathematical modeling for the prediction of carbon monoxide emission due to vehicular pollutant using finite difference element model (Lasisi, 2007). He recommended that other numerical methods should be used to validate the same problem.

Hence, this present research project is aimed at predicting the same concentration of carbon monoxide emitted from motor vehicle, but using another class of numerical method called **Roe-Riemann solver,** a finite volume difference method which has the ability to predict fluid flow over other finite difference formulations, and also simulating the input data with a programmed computer software called MATHCAD

Therefore, this study was carried out to develop a simulation model to validate the concentration of pollutants such as carbon monoxide from vehicle emissions with respect to some physical parameters and its effect on the environment.

CHAPTER TWO

2.0 LITERATURE REVIEW

2.1 POLLUTION

Pollution could be defined as the contamination of Earth's environment with materials that interfere with human health, the quality of life, or the natural functioning of *ecosystems* (living organisms and their physical surroundings). Although some environmental pollution is a result of natural causes, most is caused by human activities.

Pollution has received a worldwide attention; where efforts have been in existence to curb these pollution, effective international control are largely lacking. It has been difficult to achieve cooperation for pollution control in developing countries. This is even more problematic for a country like Nigeria, whose concern is to provide such basic needs as food, shelter and employment for her populace.(Enemari, 2007)

2.1.1 HISTORICAL BACKGROUND OF POLLUTION

Pollution started during the ancient times but was not a major problem because people lived in rural areas and the pollutants they produced were widely scattered.

Pollution problem started when large number of people began living together in cities. As cities grew, pollution problems grew with them. But environmental problem rarely become serious until 1700's and early 1800's during the industrial revolution period. The development of the industrial cities in 1700's and 1800's made pollution a major problem.

In the 1900's, urban areas development was on the increase and automobiles, other new inventions made pollution steadily worse. By the mid-1900's pollutants had affected the water and air quality in every major city in the world and all industrial countries.

The lives of millions of people have been endangered by pollution since the late 1960's. Measures are been taken by government to curb the situation and people are also working to reduce the extent of pollution.

2.1.2 AIR POLLUTION

Air pollution could be defined as any atmospheric condition in which certain substances are present in such a concentration that they can produce undesirable effects on man and his environment. (Susu and Gutti, 2003).

The main cause of air pollution is the combustion of fossil fuel such as petrol, coal, gasoline and gases. Most vehicles, power plants, factories, train and aircraft use fossil fuel to obtain energy, in the process, many pollutants are released into the air (Enemari, 2004). Other causes of pollution include particulate matter (i.e smoke, dust, fume, etc), radioactive materials and many others.

Most of these substances are naturally present in low concentration and are considered harmless; however, a particular substance can be considered an air pollutant only when its concentration is relatively high compared with the accepted concentration value and causes adverse effects.

The Nigerian and World Health Organization guidelines for ambient air quality standards as shown in 2.1, 2.2(i) and 2.2(ii) below;

Table 2.1 Nigerian ambient air quality standard (FEPA guidelines)

POLLUTANTS	TIME AVERAGE	LIMITS
Particulate matter	Daily average of daily Values (1 hour) Daily average of hourly	250μg/m^3 600μg/m^3 0.01ppm
Sulphur Oxide	Values 1 hour	26μg/m^3 0.1ppm (260μg/m^3)
Non-methane	Daily average of 3-hourly values	160μg/m^3
Carbon monoxide	Daily average of hourly values 8-hourly	10ppm (11.4μg/m^3) 20ppm (22.8μg/m^3)
Nitrogen Oxide (nitrogen dioxides)	Daily average of hourly value	0.04ppm-0.06ppm (11-75μg/m^3)
Photochemical oxidant	Hourly values	0.06ppm

Table 2.2(i) World Health Organization guidelines for ambient air quality standard (WHO and UNEP, 2002.)

POLLUTANTS	SAMPLING TIME	STANDARD
Particulate matter	Annual mean	40-60μg/m^3
	98 percentile	150-230μg/m^3
Thoracic particles	24 hours annual	70μg/m^3
(Pm_{10})^9	Mean	40-60μg/m^3
	10 minutes	500μg/m^3
	1 hour	350μg/m^3
CO	15 minutes	100μg/m^3
	30 minutes	60μg/m^3
NO_2	1 hour	30μg/m^3
	24 hours	10μg/m^3
Lead	1 hour	0.5-1.0μg/m^3
Photochemical	8 hours	150-200μg/m^3
Oxidants O_3	n.a	100-120μg/m^3

Table 2.2(ii) Updated WHO air quality guideline values (AQG)

POLLUTANTS	AVERAGING TIME	AQG VALUE
Particulate matter	1 year	$10\mu g/m^3$
PM_{25}	24 hours (99th percentile)	$25\mu g/m^3$
PM_{10}	1 year	$20\mu g/m^3$
	24 hours (99th percentile)	$50\mu g/m^3$
Ozone, O_3	8 hours, daily maximum	$100\mu g/m^3$
Nitrogen dioxide, NO_2	1 year	$40\mu g/m^3$
	1 hour	$200\mu g/m^3$
Sulphur dioxide, SO_2	24 hours	$20\mu g/m^3$
	10 minutes	$500\mu g/m^3$

2.1.3 SOURCES OF AIR POLLUTION

The major sources of air pollution can be classified into two;

a. **Natural sources:** these include dust from desert or land with little or no vegetation, Radon gas from radioactive decay within the earth's crust, smoke and carbon monoxide from wildfire, volcanic activities which produce sulphur, chlorine and ash particulates, electric discharge, oxidation and other reactions in the atmosphere.

b. **Human activities:** these include air pollutants (NO_x, CO, SO_x) from motor vehicles, aircrafts, diesel generators, municipal waste incinerators, power plants, etc, dust, hydrocarbons, ammonia etc from petroleum refining, etc.

2.2 VEHICULAR EMISSIONS

Vehicles derive their energies from the combustion of fossil fuel in their internal combustion chamber. If it was possible to achieve complete combustion, the fuel applied will be completely converted to energy to create the desired motion in case of automobile and to convert it to other forms of energy for various purposes like providing light etc. In the process of combustion, a number of changes occur. Some of the fuel is passed out unburned; partially burnt fuel changes form into a number of gases, impurities combine in the process principally with air to form other compounds e.g oxides of sulphur, nitrogen from the air particulate in the combustion process to form oxide of nitrogen NO, NO_2 depending on the prevailing condition in the combustion chamber. The product of combustion mainly gases/particles are then emitted into the environment as exhaust gases. (Enemari, 2004).

In urban environment that has low assimilative capacity, vehicular emission is of great concern. The emission reacts forming various species in various meteorological conditions interfering with man's activities. Vehicular emission in typical urban center constitute over 60% of total population emission compared to industries, power plants, refuse disposal, space heating, etc (W. Bach, 1965).

2.2.1 Vehicular emission is the byproducts of burning automobile fuels. There are four basic types of vehicular emissions, namely; Hydrocarbon, Carbon monoxide, Oxides of nitrogen and particulates. The three basic sources of vehicular emission are; engine crankcase blow by fumes (20%), fuel vapour (20%), and engine exhaust gases (60%). (Duffy and Smith, 1992). The major emissions from the burning of diesel are sulphur dioxide (SO_2), Lead (Pb), etc.

2.3 FACTORS INFLUENCING FUEL ECONOMY AND RATE OF GENERATION OF EXHAUST GASES LOAD.

The vehicle tare weight from manufacture has the minimum fuel. As the load increases, the engine has to do more work to pull the weight along. The energy to do this comes from burning more fuel which is accompanied by emission.

Cold and hot start; cold starting of engine has high fuel consumption. Rapid acceleration and sudden starts will result to high fuel consumption. Once the engine has been started, commence driving rather than accelerate standing which some people refer to as warming the engine.

Idling, city traffic shifting; all these result to high fuel consumption resulting in generation of exhaust gases and environmental pollution.

Speed; driving at high speed for extended period apart from wearing the engine burns more fuel and therefore vents high volume of gaseous/particulate matter with attendant environmental pollution. This is accompanied by emission. (W.Bach, 1965).

2.4 MAJOR VEHICULAR EMISSION, SOURCES AND EFFECTS

2.4.1 HYDROCARBON (HC): Hydrocarbon emissions result when fuel molecule in the engine do not burn or burn only partially. Hydrocarbon escapes into the air through fuel evaporation either from fuel system or while the vehicle is being refueled. Hydrocarbon reacts in the presence of nitrogen oxides and sunlight to form ground level ozone, the major component of smog.

2.4.1.1 HEALTH EFFECTS: Hydrocarbon emission contributes to eye, throat, and lung irritation and possibly cancer. It may lead to premature death. Ozone can lead to more frequent attack in people who have asthma and can also hurt plants and animals.

2.4.2 CARBON MONOXIDE (CO): This is a colourless, odourless gas produced by incomplete combustion of carbon containing fuel and by some biological and industrial processes. The major source of carbon emission at breathing level outdoor is the exhaust of petro-powered motor vehicle, the diesel engine (compression ignition), when properly adjusted emits little carbon monoxides.

2.4.2.1 HEALTH EFFECTS: Carbon monoxide is absorbed through the lungs and reacts with hemoglobin of the blood. This results to the formation of carboxyhemoglobin with the blood system which alters nervous system and causes changes in cardiac and pulmonary function, it causes headaches, fatigue, drowsiness, respiratory failure and even death.

2.4.3 NITROGEN DIOXIDE (NO_2): Nitrogen dioxide is a reddish-brown gas that comes from the burning of fossil fuels. It has a strong smell at high concentration. Nitrogen dioxide could be formed either by the combustion of fuel or when nitrogen in the air reacts with oxygen at high temperature. Nitrogen dioxide can react with the atmosphere to form ozone, acid rain and particles.

2.4.3.1 HEALTH EFFECTS: Atmospheric nitrogen dioxide results in acid rain which can harm plants, animals and other materials. Exposure to nitrogen dioxide results to respiratory infections.

2.4.4 PARTICULATE MATTER: This is either a solid or liquid matter that is suspended in the air. To remain in the air, particles usually must be less than 0.1mm wide and can be as small as 0.00005mm. The major sources of particulate matter are fuel burned in an automobile and power plants, road dust, sea spray etc.

2.4.4.1 HEALTH EFFECTS: Particulate matter could result to respiratory problems and eye irritation.

2.4.5 SULPHUR DIOXIDE (SO_2): Sulphur dioxide is a colourless and corrosive gas that cannot be seen or smelled at low levels but can have a 'rotten egg' smell at high levels. Sulphur dioxide is sourced from the combustion of coal or oil plant. It could also be gotten from factories that make chemicals, paper or fuel. It can react in the atmosphere to form acid rain.

2.4.5.1 HEALTH EFFECTS: Sulphur dioxide irritates eyes and respiratory system, reduces pulmonary functions and aggravates respiratory diseases. Sulphur dioxides can harm trees and crops as well as damaging buildings.

2.4.6 LEAD (Pb): This is a blue-gray metal that is very toxic and is found in a number of forms and locations. Lead paint is an important source of lead, especially in houses where lead paint is peeling. Lead in old pipes can be a source of lead in drinking water. Lead can also be found in cars where leaded gasoline or fuels are used.

2.4.6.1 HEALTH EFFECTS: Heart attacks or stroke could result from exposure to lead in adults. Lead could lead to low intelligent quotients (IQs) in children. Ingestion of lead has been linked to several physiological disorders in man such as gastro-intestinal disorder, nausea, circulatory collapse, blindness, anemia, etc.

2.4.7 GREENHOUSE GASES: These are gases that stay in the air for a longtime and warm up the planet by trapping sunlight. This is called the 'greenhouse effect' because the gases act like the gases in a greenhouse. Some of the important greenhouse gases are carbon dioxide (CO_2), methane (CH_4) and nitrous oxide.

Carbon dioxide is the most important greenhouse gas. It is produced from the burning of fossil fuels in cars, power plants, houses and industries. Plants convert carbon dioxide back to oxygen, but its release from human activities is higher than the world's plant can process. Thus, the amount of carbon dioxide in air continues to increase. This build up acts like a blanket and traps heat close to the surface of the earth.

2.4.7.1 HEALTH EFFECTS: It leads to changes in climate, high temperature, high sea levels, changes in forest composition and damage to land.

2.4.8 STRATOSPHERIC OZONE depletes: These are chemicals that can destroy the ozone in the stratosphere. The chemicals include chlorofluorocarbons (CFCs), halons, etc. CFCs are used in air conditioners and refrigerators since they work well as coolants. They could be found in aerosol cans and fire extinguishers. Other stratospheric ozone depletes are used as solvents in industries.

2.4.8.1 HEALTH EFFECTS: If the ozone layer is destroyed, people are exposed to more ultraviolet radiation from the sun. This can lead to skin cancer and eye problems. High ultraviolet radiation can also harm plants and animals.

2.5 CONTROL OF AIR POLLUTION

Some air pollution controlling measures include;

1. Sensitization and educating the people about the causes and dangers of pollution.
2. Machineries and vehicles should be improved so that more efficient fuel combustion occurs.

3. Strict laws should be passed and enforced to make factories and users of motor vehicles keep air pollution down by using anti-pollution devices and taking anti-pollution measures.

2.6 VEHICULAR EMISSION CONTROL

This falls into two basic categories; Tailpipe emission control and Evaporative emission control.

2.6.1 Tailpipe emission: this is the product of burning fuel in the vehicle's engine, emitted from the vehicles exhaust system such as hydrocarbon (HC), NO_x, CO, CO_2, and particulates. Tailpipe emission control can be categorized into four parts; Increasing engine efficiency, increasing vehicle efficiency, increasing driving efficiency, and cleaning up the emission.

2.6.1.1 Catalytic converters: this is a device placed in the exhaust pipe which converts various emissions into less harmful ones using generally, a combination of platinum, palladium and rhodium as catalyst. Catalytic converters have been steadily improved over the years. They make for a significant and easily applied method for reducing tailpipe emissions.

2.6.2 Evaporative emissions: these emissions are produces from the evaporation of fuel in the following ways: gas tank venting, ruining losses and refueling losses. Efforts at the reduction of evaporative emission include the following:

2.6.2.1 CAPTURING VENTED VAPOURS

Within the vehicle, vapours from the tank are channeled through canister containing activated carbon instead of being vented to the atmosphere. The vapours are absorbed within the canister, which feeds into the inlet manifold of the engine. When the vehicle is running, the vapour absorbed from the carbon are drawn into the engine and burned.

2.6.2.2 REDUCING REFUELING LOSSES

All modern vehicles have tank filler necks that instead of just being a tube into the tank, as in easier vehicles, now have a small-diameter hinged and spring loaded door only large enough for the tip of the filler nozzle. This prevents vapour leakage when the filler cap is removed, and also prevent as catalytic converter-fitted vehicle being refueled with leaded fuel. This modification also applies to the filling station pumps. They are now equipped to suck the vapour back into the pumps as they are displaced by fuel.

2.7 THE NEED TO CONTROL POLLUTION

The control of air pollution is needed due to its;

1. Potential danger to human, animal and plant lives.
2. Economic losses due to irreversible loss of large quantity of useful products-organic solvents, metals and their oxides, acidic oxides such as SO_2, CO, Cl_2, P_2O_5 etc.
3. Loss due to corrosion mainly from acidic oxide in air.

2.8 MATHEMATICAL MODELS AND MODELING

This is the use of simplified mathematical representation of real world system, process or theory. Mathematical models are developed in order to enhance our ability to understand, predict and possibly control the behavior of the system being modeled. Mathematical models are symbolic and help to express ideals and problems clearly.

Mathematical modeling can be defined as a phenomenon by mathematical equations (called models) and extracting from the useful information which can be used for prediction or process analysis. Mathematical models may be dynamic (changing with time) or static, and they may involve random process.

Consider the problem of human inhalation of pollutant gas (i.e exhaust gas from vehicular emission) and its consequent impact on health. If mathematical and statistical techniques are used to determine the magnitude of the concentration, the duration of inhalation (time) and the frequent of exposure, then, this description is the simultaneous occurrence of two events, the presence of people and pollutant concentration (x, t) at point x and time t, (Ryan) Exposure = f [P(x, t), C(x, t)] where P(x, t) is the number of people at point x and time t of inhaling the exhaust gas, e.g carbon monoxide at the concentration, C(x, t). The magnitude C(x, t) of the concentration as function of the path of the subject characterized by his or her position "x" at all time "t" for the duration of time interval in which exposure takes place. There are many other situations like this where the use of mathematics provide valuable information concerning the behavior of a system at much lower cost than the alternative trial and error approach.

Generally, in air pollution modeling, many experimental data have been generated and analyzed theoretically before now but the use of mathematical and statistical techniques to evaluate and correct these data gives rise to mathematical modeling of air quality. Therefore, the use of light model of air pollution not only predict the pollutant concentration at the initial stage and the dispersion, but the minimum permissible limit with which the pollutant will be considered harmless to human health and as well as short term and long term effect for long exposure. From examination and interpretation of the result using these mathematical models, for a particular pollutant e.g carbon monoxide vehicle exhaust gas, we say that the research has built a model of carbon monoxide from vehicular emission not a physical model but a mathematical model.

Mathematical models represent pollutants behavior in the atmosphere. These are techniques to estimate concentration of pollutants in ambient air with respect to time and space for a given set of meteorological and emission conditions. Mathematical model used in air quality may be either source models (dispersion model) or receptor model type.

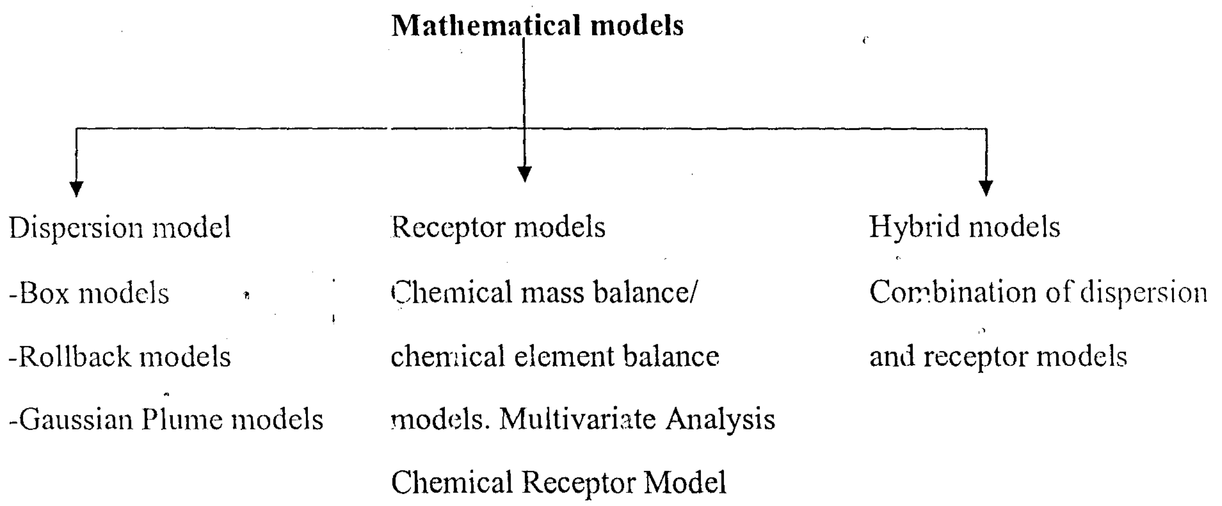

Fig 2.1 Mathematical models used in a quality modeling.

2.8.1 DISPERSION MODELS

The dispersion model states that the contribution of source to a receptor is the product of emission rate and a dispersion factor. (Henry, 1984). Dispersion can be classified into geometric form of the emission, given rise to expression for point, line and area source. Based upon emission conditions, these are subdivided into instantaneous (Puff) model and continuous (Plumel model). Some of the dispersion models are describe as follows:

2.8.1.1 Box Models: These are the simplest form of dispersion and are useful for preliminary and rough order calculation for area sources. In these models, dispersion is neglected and area source is assumed to be enclosed in a box and pollutants are considered to be instantaneously and homogenously mixed within the box.

2.8.1.2 Rollback Models: The basic assumption of these models is that air quality is proportional to emission from all sources. They are based upon proportional scaling method, that is, all emission sources are curtailed method by same level. They are useful for global scale problem.

2.8.1.3 Gaussian Plume Models: In theses models, the dispersion is considered inversely proportional to the wind velocity. i.e concentration of pollutant, $\mathbf{C} \alpha\, {}^{1}/\mathrm{v}$ where v is the wind velocity. The basic assumption followed is that diffusion can represented by Gaussian function.

The conventional dispersion model have been well studied and widely used. However, one of the major draw back of these models is that they need accurate emission inventories for various sources as input which are difficult to measure and involve significant errors. They are not useful for aerosols.

2.8.1.4 Receptor Model: Receptor model is in contrast to dispersion model, starts with observed ambient air-borne particle concentration at a receptor and seek to apportion the observed concentration among several sources type based on the knowledge of the composition of the receptor material. Receptor modeling methods have become feasible due to advancement in sampling and analytical techniques (Gordon, 1980).

2.9 STEPS IN USING MATHEMATICAL MODELS

The major steps in modeling and using mathematical models are:

- Observing real world phenomena.
- Recognizing the problem.
- Familiarization with system to be modeled.
- Construction of the model.
- Assumption and constraints.
- Solution technique (simulation).
- Interpretation analysis.
- Validation of the model.
- Implementation.
- Monitoring of the system model.

2.10 SIMULATION

This is the representation of a process by mathematical model, generally in the form of a computer program. This is an acceptable tool for understanding chemical process. Simulation in general is to pretend that one deals with real thing while really working with an initiator. In operation research, the imitation is computer knowledge of the simulated reality.

Simulation, however, may be performed manually, most often, the system model is written either as computer program or a kind of input simulator software.

2.11 ROE-RIEMANN SOLVER

The Roe-Riemann solver provides a very nice scheme for calculating solution of time dependent problems in one dimension. But once a dimensional Riemann solver is constructed for a particular system of equation, it is easy to extend it to multiple dimensions. The simplest multidimensional Riemann solver treats each other of the directions dimensionally as if it were a set of one dimensional problem.

CHAPTER THREE

3.0 DEVELOPMENT OF MODEL

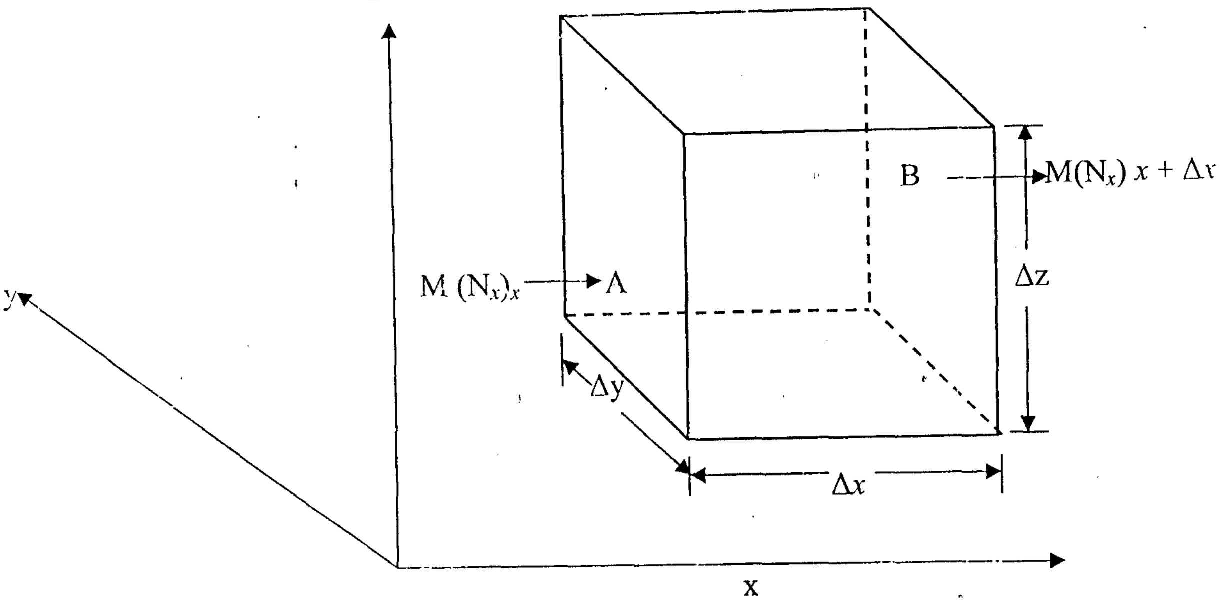

Fig 3.1 Region of volume Δx, Δy, Δz fixed in space through which a fluid is flowing.

For a small volume element Δx, Δy, Δz, fixed in space as shown in figure 3.1, a material balance based on continuity equation can be developed. The mathematical model for the prediction of carbon monoxide due to vehicular emission is based on this continuity equation.

3.1 THE MATERIAL BALANCE

From fig 3.1, the material balance can be written as:

(Rate of mass input) – (Rate of mass output) + (Net rate of amount of mass introduced by the source strength) = (Rate of accumulation) --3.1

The mass flow rate of pollutants into the three (3) phases with a common corner at A is

$M(N_x)\Delta y\Delta z + M(N_y)\Delta x\Delta z + M(N_z)\Delta x\Delta y$ --3.2

The equation 3.2 above can be written as

$M[(N_x)\Delta y\Delta z + (N_y)\Delta x\Delta z + (N_z)\Delta x\Delta y$ --3.3

Where:

N_x is the flux in x-direction (mol/m^{2}s)

$(N_x)X$ is the value at location x and,

M is the molecular weight of the pollutant CO (g/mol)

In a similar manner, the mass rate of flow out of the three (3) phases with a common corner B is:

$M[(N_x)_{x+\Delta x}\Delta Y\Delta Z + (N_y)_{y+\Delta y}\Delta X\Delta Z + (N_z)_{z+\Delta z}\Delta X\Delta Y]$ --3.4

The total pollutant in the element is Δx, Δy, $\Delta z\ \rho$; its rate of accumulation is therefore

$\Delta x\Delta y\Delta z\,\frac{\delta \rho}{\delta t}$ --3.5

Where;

ρ is the density of carbon monoxide in (g/m^3)

Now, the net rate of amount of mass introduced by source strength is $\Delta x\ \Delta y\ \Delta zq$ --------------3.6

Where;

q is the source strength in (g/m^{3}s)

Substituting equation 3.3 through equation 3.6 into equation 3.1, we have,

$M(N_x)\Delta y\Delta z + M(N_y)\Delta x\Delta z + M(N_z)\Delta x\Delta y - M[(N_x)_{x+\Delta x}\Delta Y\Delta Z + (N_y)_{y+\Delta y}\Delta x\Delta z + (N_z)_{z+\Delta z}\Delta x\Delta y] + \Delta x\Delta y\Delta zq = \Delta x\Delta y\Delta z\,\frac{\delta \rho}{\delta t}$ --3.7

By multiplying through equation 3.7 by (-1) gives:

$-M(N_x)\Delta y\Delta z - M(N_y)\Delta x\Delta z - M(N_z)\Delta x\Delta y + M(N_x)_{x+\Delta x}\Delta y\Delta z + M(N_y)_{y+\Delta y}\Delta x\Delta z + M(N_z)_{z+\Delta z}\Delta x\Delta y - \Delta x\Delta y\Delta zq = -\Delta x\Delta y\Delta z\,\frac{\delta \rho}{\delta t}$ --3.8

$M[(N_x)_{x+\Delta x} - (N_x)_x]\,\Delta y\Delta z + M[(N_y)_{y+\Delta y} - (N_y)_y]\,\Delta x\Delta z + M[(N_z)_{z+\Delta z} - (N_z)_z]\,\Delta x\Delta y - \Delta x\Delta y\Delta xq = -\,\Delta x\Delta y\Delta zq\,\frac{\delta \rho}{\delta t}$ --3.9

$M\{[(N_x)_{x+\Delta x} - (N_x)_x]\Delta y\Delta z + [(N_y)_{y+\Delta y} - (N_y)y]\Delta x\Delta z + [(N_z)_{z+\Delta z} - (N_z)_z]\Delta x\Delta y\} + \Delta x\Delta y\Delta z\,\frac{\delta \rho}{\delta t} = \Delta x\Delta y\Delta zq$ --3.10

Dividing equation 3.10 through by Δx, Δy, Δz and taking limit as the three distances become zero gives;

$$M\left[\frac{\delta Nx}{\delta x}+\frac{\delta Ny}{\delta y}+\frac{\delta Nz}{\delta z}\right]+\frac{\delta \rho}{\delta t}=q \quad \text{------------}3.11$$

In another form, equation 3.11 can be written as;

$$\frac{\delta(MNx)}{\delta x}+\frac{\delta(MNy)}{\delta y}+\frac{\delta(MNz)}{\delta z}+\frac{\delta \rho}{\delta t}=q \quad \text{------------}3.12$$

Note that the flux (N_x) for the pollutant, CO is made of two parts namely; the one resulting from the bulk of the fluid pollutant, CO motion and the one resulting from diffusion of CO. This implies that flux N = bulk motion of CO + diffusion motion of CO.

Therefore, N = K + J --3.13

where K = bulk motion of CO

J = diffusion motion of CO

If the pollutant is in the same direction and that of the wind, equation 3.13 in terms of masses and in the x-direction is;

$MN_x = U_x\rho m + V_x\rho + MJ_x$ --3.14a

while if the pollutant is in the opposite direction to the wind, i.e taking the direction of the wind as positive x-direction and the pollutant negative x-direction, in terms of masses and in the x-direction, equation 3.13 gives,

$MN_x = U_x\rho m - V_x\rho + MJ_x$ --3.14b

where,

ρm is the density of the mixture of air and the pollutant as the pollutant mixed with the air thus changing the density of air (g/m^3)

ρ is the density of the pollutant which is constant (g/m^3)

U_x is the velocity of wind in x-direction (m/s)

V_x is the velocity of pollutant in x-direction (m/s)

Now, since ρm is the density of the mixture of air and the pollutant mixed with the air, thus changing the density of air. It can be represented through the following general relationship;

$$PV = nRT$$

$$PV = \frac{m}{M} RT$$

$$PM = \frac{m}{V} RT$$

$$PM = \rho RT$$

$$P = \frac{PM}{RT} \quad \text{--} 3.15$$

By

$$\rho m = \frac{M_{air} P_{air}}{RT} + \frac{MP_{CO}}{RT} \quad \text{--} 3.16$$

or

$$\frac{1}{RT} [M_{air} P_{air} + MP_{CO}]$$

Where;

$\frac{M_{air} P_{air}}{RT} = \frac{M_{air}(P_T - P_{CO})}{RT}$ is the density of air (g/m^3)

$\frac{MP_{CO}}{RT}$ is the density of carbon monoxide (g/m^3)

$P_{air} = P_T - P_{CO}$, Partial pressure of air (atm)

P_T = Total pressure of mixture of air and CO (atm)

P_{CO} = Pressure of carbon monoxide (atm)

M = molecular weight of CO (g/mol)

M_{air} = molecular weight of air (g/mol)

R = gas constant (atm.cm^3/mol.k)

T = Temperature of which a sample of dry air would have density as the mixture (k)

J_x = diffusion flux (i.e by using partial differential method).

$$J_x = -\Delta \frac{\delta c}{\delta x} \text{ ---------- } 3.17$$

Differentiating equation 3.14a gives;

$$\frac{\delta MNx}{\delta x} = \rho m \frac{\delta Ux}{\delta x} + U_x \frac{\delta \rho m}{\delta x} + \rho \frac{\delta Vx}{\delta x} + V_x \frac{\delta \rho}{\delta x} + M \frac{\delta Jx}{\delta x} \text{ ---------- } 3.18$$

Since $\frac{\delta MNx}{\delta x}$ has been obtained in the equation 3.18, then equation 3.12 can be written in three (3) dimensional forms as:

$$\rho m \left[\frac{\delta Ux}{\delta x} + \frac{\delta Uy}{\delta y} + \frac{\delta Uz}{\delta z}\right] + \left[Ux \frac{\delta \rho m}{\delta x} + Uy \frac{\delta \rho m}{\delta y} + Uz \frac{\delta \rho m}{\delta z}\right] + \left[Vx \frac{\delta \rho}{\delta x} + Vy \frac{\delta \rho}{\delta y} + Vz \frac{\delta \rho}{\delta z}\right] +$$

$$M \left[\frac{\delta Jx}{\delta x} + \frac{\delta Jy}{\delta y} + \frac{\delta Jz}{\delta z}\right] + \frac{\delta \rho m}{\delta t} = q \text{ ---------- } 3.19$$

Also from equation 3.14a differentiation becomes;

$$M \frac{\delta Nx}{\delta x} = \rho m \frac{\delta Ux}{\delta x} + Ux \frac{\delta \rho m}{\delta x} + \rho \frac{\delta Vx}{\delta x} + Vx \frac{\delta \rho}{\delta x} + M \frac{\delta Jx}{\delta x}$$

Since

$J_x = -\Delta \frac{\delta c}{\delta x}$ from equ. 3.17, substituting in the above equation, we have,

$$M \frac{\delta Nx}{\delta x} = \rho m \frac{\delta Ux}{\delta x} + Ux \frac{\delta \rho m}{\delta x} + \rho \frac{\delta Vx}{\delta x} + Vx \frac{\delta \rho}{\delta x} - MD \frac{\delta 2c}{\delta x2} \text{ ---------- } 3.20$$

Substituting equation 3.17 into 3.19, we have,

$$\rho m \left[\frac{\delta Ux}{\delta x} + \frac{\delta Uy}{\delta y} + \frac{\delta Uz}{\delta z}\right] + \left[Ux \frac{\delta \rho m}{\delta x} + Uy \frac{\delta \rho m}{\delta y} + Uz \frac{\delta \rho m}{\delta z}\right] + \rho \left[\frac{\delta Vx}{\delta x} + \frac{\delta Vy}{\delta y} + \frac{\delta Vz}{\delta z}\right] + \left[Vx \frac{\delta \rho}{\delta x} +\right.$$

$$\left. Vy \frac{\delta \rho}{\delta y} + Vz \frac{\delta \rho}{\delta z}\right] - MD \left[\frac{\delta^2 c}{\delta x^2} + \frac{\delta^2 c}{\delta y^2} + \frac{\delta^2 c}{\delta z^2}\right] + \frac{\delta \rho m}{\delta t} = q \text{ ---------- } 3.21$$

Applying the equation of continuity,

$\frac{\delta Ux}{\delta x} + \frac{\delta Uy}{\delta y} + \frac{\delta Uz}{\delta z}$ and $\frac{\delta Vx}{\delta x} + \frac{\delta Vy}{\delta y} + \frac{\delta Vz}{\delta z}$ tends to zero, then equation 3.21 becomes

$$Ux\frac{\delta\rho m}{\delta x} + Uy\frac{\delta\rho m}{\delta y} + Uz\frac{\delta\rho m}{\delta z} + Vx\frac{\delta\rho}{\delta x} + Vy\frac{\delta\rho}{\delta y} + Vz\frac{\delta\rho}{\delta z} - MD\left[\frac{\delta^2 c}{\delta x^2} + \frac{\delta^2 c}{\delta y^2} + \frac{\delta^2 c}{\delta z^2}\right] +$$

$$\frac{\delta\rho m}{\delta t} = q \text{ ------------------------------------3.22}$$

Dividing density by molecular weight i.e ρ/M (mol/dm^3) results to concentration, the equation 3.22 becomes:

$$Ux\frac{\delta c}{\delta x} + Uy\frac{\delta c}{\delta y} + Uz\frac{\delta c}{\delta z} + Vx\frac{\delta c}{\delta x} + Vy\frac{\delta c}{\delta y} + Vz\frac{\delta c}{\delta z} - \Delta\left[\frac{\delta^2 c}{\delta x^2} + \frac{\delta^2 c}{\delta y^2} + \frac{\delta^2 c}{\delta z^2}\right] + \frac{\delta c}{\delta t} = q \text{ -----------3.23}$$

i.e $Ux\frac{\delta\rho m}{\delta x} + \frac{1}{M} \Rightarrow \frac{Ux}{\delta x} \text{X} \frac{\delta\rho m}{M} \Rightarrow Ux\frac{\delta c}{\delta x}$

Rearranging equation 3.23 gives;

$$Ux\frac{\delta c}{\delta x} + Uy\frac{\delta c}{\delta y} + Uz\frac{\delta c}{\delta z} + Vx\frac{\delta c}{\delta x} + Vy\frac{\delta c}{\delta y} + Vz\frac{\delta c}{\delta z} + \frac{\delta c}{\delta t} = \Delta\left[\frac{\delta^2 c}{\delta x^2} + \frac{\delta^2 c}{\delta y^2} + \frac{\delta^2 c}{\delta z^2}\right] + q \text{ ----------3.24}$$

Thus,

$$\frac{\delta c}{\delta t} = -\left[Ux\frac{\delta c}{\delta x} + Uy\frac{\delta c}{\delta y} + Uz\frac{\delta c}{\delta z}\right] - \left[Vx\frac{\delta c}{\delta x} + Vy\frac{\delta c}{\delta y} + Vz\frac{\delta c}{\delta z}\right] + \Delta\left[\frac{\delta^2 c}{\delta x^2} + \frac{\delta^2 c}{\delta y^2} + \frac{\delta^2 c}{\delta z^2}\right] + q \text{ ----3.25}$$

The variables *Ux, Uy, Uz, Vx, Vy, Vz,* and *c* can each be described as the sum of the mean and a turbulent composition as follows;

$$\left.\begin{aligned} U_x &= \bar{U}_x + U_x' \\ U_y &= \bar{U}_y + U_y' \\ U_z &= \bar{U}_z + U_z' \\ V_x &= \bar{V}_x + V_x' \\ V_y &= \bar{V}_y + V_y' \\ V_z &= \bar{V}_z + V_z' \\ C &= \bar{C} + C' \end{aligned}\right] \text{ ------------------------------------3.26}$$

Where:

U_x and V_x are the instantaneous measurement of the east and west component velocities, $\bar{U}_x$ and V_x' are the deviation of U and V from the mean.

Substituting 3.26 into 3.25 and assuming an incompressible, non divergent atmosphere (reasonable assumption for the most scales of motion affecting vehicles emission produced).

$$\frac{\delta c}{\delta t} = - \left[\frac{\delta \bar{U}x\bar{C}}{\delta x} + \frac{\delta \bar{U}y\bar{C}}{\delta y} + \frac{\delta \bar{U}z\bar{C}}{\delta z}\right] - \left[\frac{\delta \bar{V}x\bar{C}}{\delta x} + \frac{\delta \bar{V}y\bar{C}}{\delta y} + \frac{\delta \bar{V}z\bar{C}}{\delta z}\right] - \left[\frac{\delta U_x'C'}{\delta x} + \frac{\delta U_y'C'}{\delta y} + \frac{\delta U_z'C'}{\delta z}\right] + \left[\frac{\delta V_x'C'}{\delta x} + \frac{\delta V_y'C'}{\delta y} + \frac{\delta V_z'C'}{\delta z}\right] + \Delta x \frac{\delta^2 c}{\delta x^2} + \Delta y \frac{\delta^2 c}{\delta y^2} + \Delta z \frac{\delta^2 c}{\delta z^2} + q \text{ -------------------- } 3.27$$

The term on the left hand side describe the change of concentration with time. The first two terms in the bracket on the right hand side describes the change due to mean motion (transport), the second two terms in the brackets describe the changes due to turbulent (dispersion) and the third term wit the derivative of concentration square describes the molecular diffusion.

The Reynold's number of molecular diffusion is small compared to that of turbulent diffusion thus, we can ignore the molecular diffusion term in equation 3.27 above to zero. i.e

$$\Delta x \frac{\delta^2 c}{\delta x^2} + \Delta y \frac{\delta^2 c}{\delta y^2} + \Delta z \frac{\delta^2 c}{\delta z^2} = 0 \text{ -------------------- } 3.28$$

The turbulence fluxes ($V_x'C', V_y'C', V_z'C'$) defined as the mass of pollutant deposition per unit area per unit time due to turbulence are difficult to measure directly, then

$$\frac{\delta V_x'C'}{\delta x} + \frac{\delta V_y'C'}{\delta y} + \frac{\delta V_z'C'}{\delta z} = 0 \text{ -------------------- } 3.29$$

It is common therefore to assume that turbulence is proportional to the gradient of the mean concentration.

$$\left.\begin{aligned} U_x'C' &= -\,Kx\left(\frac{\delta c}{\delta x}\right) \\ U_y'C' &= -\,Ky\left(\frac{\delta c}{\delta x}\right) \\ U_z'C' &= -\,Kz\left(\frac{\delta c}{\delta x}\right) \end{aligned}\right\} \text{-----------------------------------3.30}$$

Where Kz is proportionality constant called the **eddy diffusion.**

Equation 3.27 becomes;

$$\frac{\delta c}{\delta t} = -\left[\frac{\bar{U}x\delta\bar{C}}{\delta x} + \frac{\bar{U}y\delta\bar{C}}{\delta y} + \frac{\bar{U}z\delta\bar{C}}{\delta z}\right] - \left[\frac{\bar{V}x\delta\bar{C}}{\delta x} + \frac{\bar{V}y\delta\bar{C}}{\delta y} + \frac{\bar{V}z\delta\bar{C}}{\delta z}\right] + \frac{\delta}{\delta x}\left[Kx\frac{\delta\bar{c}}{\delta x}\right] + \frac{\delta}{\delta y}\left[Ky\frac{\delta\bar{c}}{\delta y}\right]$$

$$+\frac{\delta}{\delta z}\left[Kz\frac{\delta\bar{c}}{\delta z}\right] + q \text{ -----------------------------------3.31}$$

Further assuming that the eddy diffusivity values Kx, Ky, and Kz are invariant along their respective axis, an assumption often made to simplify the calculation, but not necessarily physically realistic, this expression can be simplified to the parabola form as:

$$\frac{\delta c}{\delta t} = Kx\frac{\delta^2\bar{c}}{\delta x^2} + Ky\frac{\delta^2\bar{c}}{\delta y^2} + Kz\frac{\delta^2\bar{c}}{\delta z^2} - \left[\frac{\bar{U}x\delta\bar{C}}{\delta x} + \frac{\bar{U}y\delta\bar{C}}{\delta y} + \frac{\bar{U}z\delta\bar{C}}{\delta z}\right] - \left[\frac{\bar{V}x\delta\bar{C}}{\delta x} + \frac{\bar{V}y\delta\bar{C}}{\delta y} + \frac{\bar{V}z\delta\bar{C}}{\delta z}\right] + q \text{ -----3.32}$$

3.2 CONSIDERING A CONTINUOUS SOURCE STRENGTH

For a continuous source strength of pollutant, the emission of the pollutant source strength (q) remains constant. This means that the source strength (q) of pollutant e.g carbon monoxide from car exhaust gas to the atmosphere is considered not increasing with time. The source strength versus time graph is shown in figure 3.2 below;

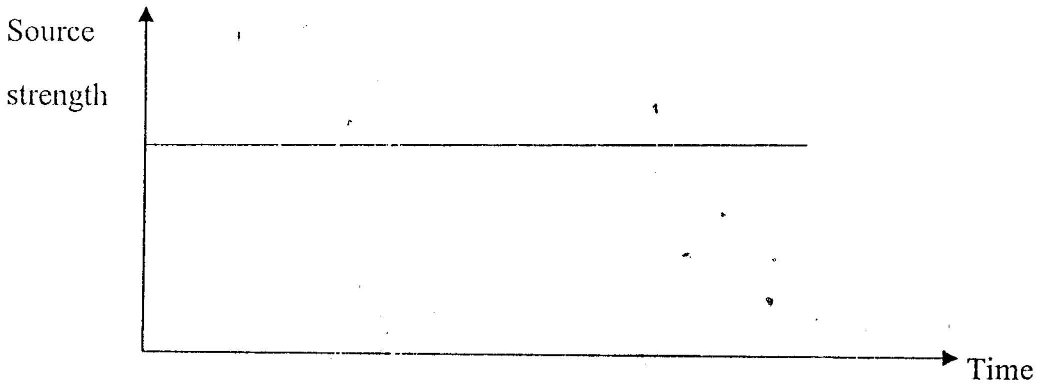

Figure 3.2 illustration of continuous source strength. Therefore, equation 3.32 remain unchanged, that is;

$$\frac{\delta c}{\delta t} = Kx\frac{\delta^2 \bar{c}}{\delta x^2} + Ky\frac{\delta^2 \bar{c}}{\delta y^2} + Kz\frac{\delta^2 \bar{c}}{\delta z^2} - \left[\frac{\bar{U}x\delta\bar{C}}{\delta x} + \frac{\bar{U}y\delta\bar{C}}{\delta y} + \frac{\bar{U}z\delta\bar{C}}{\delta z}\right] - \left[\frac{\bar{V}x\delta\bar{C}}{\delta x} + \frac{\bar{V}y\delta\bar{C}}{\delta y} + \frac{\bar{V}z\delta\bar{C}}{\delta z}\right] + q \text{-----}3.3.2$$

3.3 PULSE INPUT (POLLUTANT RELEASED INTERMITTENTLY)

This is a situation where the pollutant is released in disorderly manner at different intervals of time and still the source strength (q) of the pollutant is maintained constant.

$$\frac{\delta c}{\delta t} = Kx\frac{\delta^2 \bar{c}}{\delta x^2} + Ky\frac{\delta^2 \bar{c}}{\delta y^2} + Kz\frac{\delta^2 \bar{c}}{\delta z^2} - \left[\frac{\bar{U}x\delta\bar{C}}{\delta x} + \frac{\bar{U}y\delta\bar{C}}{\delta y} + \frac{\bar{U}z\delta\bar{C}}{\delta z}\right] - \left[\frac{\bar{V}x\delta\bar{C}}{\delta x} + \frac{\bar{V}y\delta\bar{C}}{\delta y} + \frac{\bar{V}z\delta\bar{C}}{\delta z}\right] + q \text{-------}3.3.3$$

Where q is equal to equation 3.3.2

3.4 PULSE INPUT POLLUTANT RELEASED ONCE

This is a solution whereby the velocity of the pollutant is zero (i.e V_n=0) thus our model equation becomes;

$$\frac{\delta c}{\delta t} = Kx\frac{\delta^2 \bar{c}}{\delta x^2} - Ky\frac{\delta^2 \bar{c}}{\delta y^2} - Kz\frac{\delta^2 \bar{c}}{\delta z^2} - \left[\frac{\bar{U}x\delta\bar{C}}{\delta x} + \frac{\bar{U}y\delta\bar{C}}{\delta y} + \frac{\bar{U}z\delta\bar{C}}{\delta z}\right] + q \text{------------------------------------}3.3.4$$

3.5 NUMERICAL SOLUTION

There are various approximate methods of numerical solution available for solving model equation. The major ones among the numerical solution methods are Crank Nicholson method, explicit finite difference scheme, implicit finite difference scheme, finite volume scheme, e.t.c.

In this project, Roe-Riemann solver is used. This method takes its basis from finite volume scheme.

3.5.1 NUMERICAL SIMULATION

Recall equation 3.3.3

$$\frac{\delta c}{\delta t} = - \left[\frac{\bar{U}x\delta\bar{C}}{\delta x} + \frac{\bar{U}y\delta\bar{C}}{\delta y} + \frac{\bar{U}z\delta\bar{C}}{\delta z}\right] - \left[\frac{\bar{V}x\delta\bar{C}}{\delta x} + \frac{\bar{V}y\delta\bar{C}}{\delta y} + \frac{\bar{V}z\delta\bar{C}}{\delta z}\right] + Kx\frac{\delta^2\bar{c}}{\delta x^2} + Ky\frac{\delta^2\bar{c}}{\delta y^2} + Kz\frac{\delta^2\bar{c}}{\delta z^2} + \mathrm{q} \text{ -------3.3.3}$$

The discertisation of our system of equation can be written in vector form which will be shown in section 3.5.2. Assuming fluxing in x-direction, equation 3.3.3 becomes

$$\frac{\delta c}{\delta t} + \frac{\bar{U}x\delta\bar{C}}{\delta x} + \frac{\bar{V}x\delta\bar{C}}{\delta x} - \frac{kx\,\delta^2\bar{c}}{\delta x^2} = \mathrm{q} \text{ ----------------------------------3.5.1}$$

3.5.2 ROE-RIEMANN APPLICATION TO EQUATION

The numerical approximation to equation 3.3.3 begins by dividing space into cell with edges at $X_i + {}^1/_2$ and uniform width Δx, although this restriction can be relaxed. Integration C(*x*,t) over a spatial cell and dividing by Δx, we get space average data in cell (1) and time (t).

The general Roe-Riemann equation in one dimension (i.e along x-direction) is shown below;

$$\frac{\delta U}{\delta t} + \frac{\delta \Lambda U}{\delta x} = S(u) \text{ ----------------------------------3.5.2}$$

Where $U_i\ (t) = \frac{1}{\Delta x}\int_{x-{}^1/_2}^{x+{}^1/_2} U\ (x,t)\delta x$ ------------------------------3.5.3

Integrating over cell (1) gives;

$$\frac{\delta Ui}{\delta t} + \frac{\Lambda U_{i-1/2} - \Lambda U_{i-1/2}}{\Delta x} = Si \text{ ----------------------------------3.5.4}$$

Where

U*i*(t) is a vector of the spatial averages at time (t)

S (u) is source vector

$AU_{i-1/2}$ is the flux of each of the moment in the x-direction

AU is flux (rate of flow of state (u) across an interface).

U_i is cell state

$U_{i+1/2}$ is intercell state.

U (x,t) is vector state of variable.

Given AU is flux of U

$$\text{i.e } AU = F \text{ ------------------------------------ } 3.5.6$$

$$\frac{\delta AU}{\delta U} + \frac{\delta F}{\delta U} \text{ ------------------------------------ } 3.5.7$$

$$A = \frac{\delta F}{\delta U} \text{ ------------------------------------ } 3.5.8$$

$$A_x = \frac{\delta Fx}{\delta U(t)} \text{ ------------------------------------ } 3.5.9$$

Similarly equation 3.5.7 becomes:

$$\frac{\delta (AU)x}{\delta U} = \frac{\delta Fx}{\delta U} \text{ ------------------------------------ } 3.5.10$$

Now, recall the model equation, equation 3.3.3

$$\frac{\delta c}{\delta t} = -\left[\frac{\bar{U}x\delta\bar{C}}{\delta x} + \frac{\bar{U}y\delta\bar{C}}{\delta y} + \frac{\bar{U}z\delta\bar{C}}{\delta z}\right] - \left[\frac{\bar{V}x\delta\bar{C}}{\delta x} + \frac{\bar{V}y\delta\bar{C}}{\delta y} + \frac{\bar{V}z\delta\bar{C}}{\delta z}\right] + Kx\frac{\delta^2\bar{c}}{\delta x^2} + Ky\frac{\delta^2\bar{c}}{\delta y^2} + Kz\frac{\delta^2\bar{c}}{\delta z^2} + q \text{ -------} 3.3.3$$

Note, the equation 3.3.3 above is in 3-dimensional form. By rearranging we have;

$$\frac{\delta c}{\delta t} + \frac{\delta}{\delta x}\left[UxC + VxC - \frac{\delta}{\delta t}(KxC)\right] + \frac{\delta}{\delta y}\left[UyC + VyC - \frac{\delta}{\delta y}(KyC)\right] +$$

$$\frac{\delta}{\delta z}\left[UzC + VzC - \frac{\delta}{\delta z}(KzC)\right] = q \text{ ------------------------------------ } 3.5.11$$

Relating equation 3.5.10 to 3.5.11, then equation 3.5.11 in another form can be written as

$$U_t + F_x + F_y + F_z = S \text{ ------------------------------------ } 3.5.12$$

Where

$$U = \begin{pmatrix} C \\ 0 \end{pmatrix} \text{ ------------------------------------ } 3.5.13$$

$$F_x = \left(U_xC + \begin{matrix}V_xC\\0\end{matrix} - {}^{\delta}/_{\delta x}\ K_xC\right) \text{------------------------------}3.5.14$$

$$F_y = \left(U_yC + \begin{matrix}V_yC\\0\end{matrix} - {}^{\delta}/_{\delta y}\ K_yC\right) \text{------------------------------}3.5.15$$

$$F_z = \left(U_zC + \begin{matrix}V_zC\\0\end{matrix} - {}^{\delta}/_{\delta z}\ K_zC\right) \text{------------------------------}3.5.16$$

$$S = \begin{pmatrix}q\\0\end{pmatrix}$$

The Jacobian matrix A in equation 3.5.9 in 3-dimensional form can be computed as;

$$A_x = \frac{\delta F_x}{\delta t} = \begin{pmatrix}U_x + V_x\\0\end{pmatrix} \text{------------------------------}3.5.17$$

$$A_y = \frac{\delta F_y}{\delta t} = \begin{pmatrix}U_y + V_y\\0\end{pmatrix} \text{------------------------------}3.5.18$$

$$A_z = \frac{\delta F_z}{\delta t} = \begin{pmatrix}U_z + V_z\\0\end{pmatrix} \text{------------------------------}3.5.19$$

From equation 3.5.17, 3.5.18 and 3.5.19, the eigen values in 3-dimension as well are:

$$\left.\begin{aligned}\lambda_x &= U_x + V_x\\ \lambda_y &= U_y + V_y\\ \lambda_z &= U_z + V_z\end{aligned}\right\} \text{------------------------------}3.5.20$$

We have determined an approximate value which must satisfy the flux (F).

$$F = AU = \sum \bar{\alpha}_x \bar{e}_x \bar{\lambda}_x \text{------------------------------}3.5.21$$

Where $\bar{e}_n$ is the eigen vector

Note,

$$\Delta C = \bar{\alpha} \text{ (i.e change in concentration)} \text{------------------------------}3.5.22$$

$$\Delta C.V = \bar{\alpha}\,\lambda \text{------------------------------}3.5.23$$

Then, $F = \sum \Delta C \lambda_x \bar{e}_x$ ------------------------------3.5.24

Since in equation 3.18, the only axis considered in the solution is the x-axis, therefore, the use of summation will not affect any changes in flux.

$$\Delta F = \Delta C\lambda_x \bar{e}_x \text{ --3.5.25}$$

$$\Delta F = \Delta C\lambda_x \text{ i.e } \bar{e}_x = 1 \text{ for unit vector ------------------------3.5.26}$$

For a unidirectional system, the flux at the cell interface is given by,

$$A_xU_{i+1/2} = \tfrac{1}{2}\,[A_xU_i + A_xU_{i+1}] - \tfrac{1}{2}\sum \bar{\alpha}_x\bar{\lambda}_x\bar{e}_x \text{ ---------------------3.5.27}$$

The flux $F_{i\pm 1/2}$ in one dimension can be computed as:

$$F_{i\pm 1/2} = \tfrac{1}{2}\,[F_{i+1} + F_i] - \tfrac{1}{2}\sum \bar{\alpha}_n\bar{\lambda}\bar{e}_n \text{ ---------------------------3.5.28}$$

Using *i, j, k* for the direction of *x, y, z* respectively, the flux at the cell interface in three dimensional forms can be written respectively as:

$$\left.\begin{aligned} F_{i\pm 1/2} &= \tfrac{1}{2}[F_{i+1} + F_i] - \tfrac{1}{2}\sum \bar{\alpha}_{xn}\bar{\lambda}_{xn}\bar{e}_{xn} \\ F_{j\pm 1/2} &= \tfrac{1}{2}[F_{j+1} + F_j] - \tfrac{1}{2}\sum \bar{\alpha}_{yn}\bar{\lambda}_{yn}\bar{e}_{yn} \\ F_{k\pm 1/2} &= \tfrac{1}{2}[F_{k+1} + F_k] - \tfrac{1}{2}\sum \bar{\alpha}_{zn}\bar{\lambda}_{zn}\bar{e}_{zn} \end{aligned}\right\} \text{ ---------------------3.5.29}$$

Substituting equation 3.5.25 into the first equation of 3.5.29 gives

$$F_{i+1/2} = \tfrac{1}{2}[F_{i+1} + F_i] - \tfrac{1}{2}\,\Delta F_{i+1/2} \text{ ---------------------------3.5.30}$$

Where $\Delta F_{i\pm 1/2}$, change in flux between the grid point *i* and *i* + ½ is computed by

$$\Delta F_{i+1/2} = \frac{\Delta F}{2} \text{ --3.5.31}$$

Rewriting equation 3.5.4 in the form of

$$\frac{\delta U}{\delta t} = -\frac{[F_{i+1/2} + F_{i-1/2}]}{\Delta x} + S_i \text{ -----------------------------3.5.32}$$

i.e $AU_{i\pm 1/2} = F_{i\pm 1/2}$

Within the finite volume scheme, the simplest way to incorporate source term (i.e source strength) into numerical method is to add on a point wise approximate of each cell. The resulting Riemann scheme is corporate with the source term can be written in three dimensions in the form of equation 3.5.33 below;

$$U^n_{i+1,j,k} = U^n_{ijk} - \frac{\Delta t}{\Delta x}(F_{i+1/2,j,k} - F_{i-1/2,j,k}) - \frac{\Delta t}{\Delta y}(F_{i,j+1/2,k} - F_{i,j+1/2,k})$$

$$- \frac{\Delta t}{\Delta z}(F_{i,j,k+1/2} - F_{i,j,k-1/2}) + \Delta t q^n_{i+1} \text{ --3.5.33}$$

For a unidirectional system, (i.e one dimension axis), the above discretised model solving equation reduces to the form of

$$\boxed{U^n_{i+1} = U^n_i - \frac{\Delta t}{\Delta x}(F_{i+1/2} + F_{i-1/2}) + \Delta t q^n_{i+1}} \text{ --3.5.34}$$

Equation 3.5.34 is the general model solving equation known as Roe-Riemann solver equation.

Rewriting equation 3.5.24 in terms of concentration, we have;

$$\boxed{C^n_{i+1} = C^n_i - \frac{\Delta t}{\Delta x}(F_{i+1/2} + F_{i-1/2}) + \Delta t q^n_{i+1}} \text{ --3.5.35}$$

Equation 3.5.35 is the general developed model Roe-Riemann solver equation for determining the concentration of carbon monoxide, CO emitted from motor vehicles.

3.5.3 BOUNDARY CONDITIONS

1. C (Xo, Yo, Zo, t) > 0

   For t ≥ 0, Xo = 0, Yo = 0, Zo = 0

   or C (i, j, k) for t ≥ 0, I = 0, j = 0, k = 0

2. q (i, j, k) > 0

for all $i \geq 0, j \geq 0, k \geq 0, t \geq 0$

3.5.4 SIMULATION OF THE MODEL

The above developed model was simulated manually and by visual basic program. The manual simulation and the code for the program were presented as appendix A and B respectively.

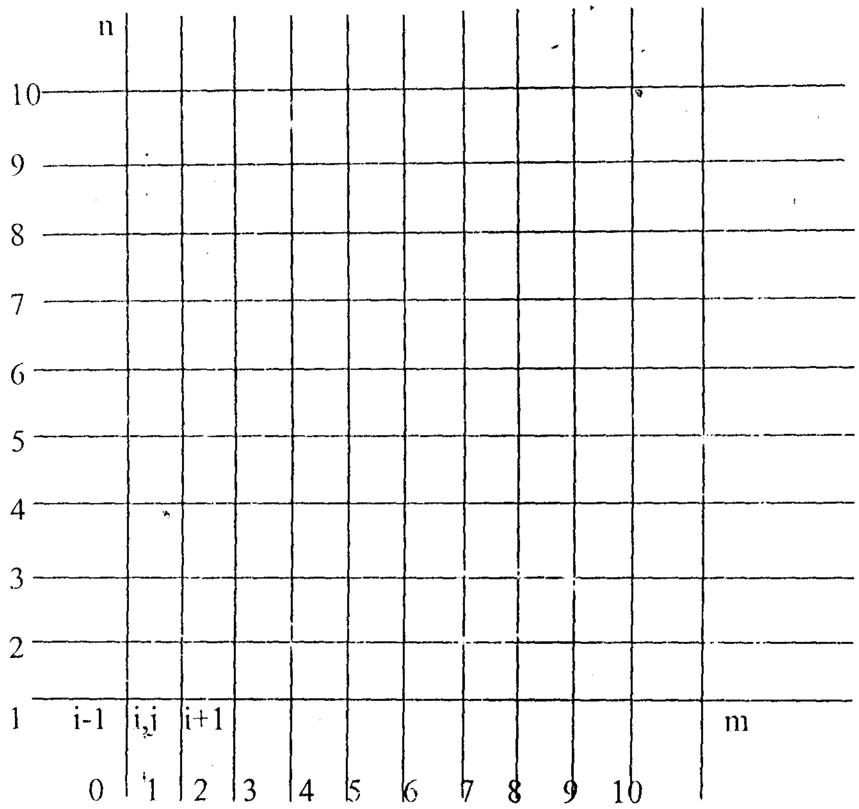

Fig 3.5.1 Rectangular net mesh x, y for finite difference derivative.

i, j = equal cell location in grid

n = time level

i+1 = nest grid point

$C_{i,j}^{n}$ = concentration at the node i, j.

$C_{i+1,j}^{n}$ = concentration at the node i+1, j.

$F_{i,j}$ = flux in the cell grid node i, j.

$F_{i+1,j}$ = flux in the cell grid node i+1, j.

$F_{i-1,j}$ = flux in the cell grid node i-1, j.

$F_{i,j+1}$ = flux in the cell grid node i, j+1.

$F_{i,j-1}$ = flux in the cell grid node i, j-1.

3.5.5 ASSUMPTION MADE AND SOURCE OF DATA USED IN CALCULATION

Assumptions

1. A constant car speed is assumed
2. Density of air is constant at 30°C
3. Emission of carbon monoxide is constant at constant car speed.
4. Diffusion coefficient of carbon monoxide/air system is constant at atmospheric pressure and temperature.
5. A unit-directional transport of carbon monoxide in air is assumed.
6. Velocity of air is constant at a given height in the atmosphere.
7. Assuming the variation in concentration is determined over 10 equal spatial of both time and distance (i.e height) at i, j.

3.5.6 DATA USED IN CALCULATION

a) Velocity of air (U); range of value of velocity (0.5m/s – 2.5m/s) was considered so as to show the effect of change in wind velocity to concentration distribution. This is based on the assumption that we have calm and light velocity in the environment considered.

b) Density of air; a value of 1.16kg/m^3 applies for condition of atmospheric temperature and pressure (1atm 30°C).

c) Velocity of carbon monoxide existing depends on the vehicle operating condition. Values range from 2.3m/s to 3.0m/s is considered in the conditions. The basis of the consideration of two stroke engine cars operating at a speed of 25km/hr, (6.94m/s) and temperature and pressure of 2300k and 1000kpa to 2250kpa, the correlation was given by Metghalachi and Keck 1982.

d) Source strength (q); it could also be called the generation term. It is obtained under the condition of constant car speed of 25km/hr and emission factor of 56.89km. A range of 0.00458g/m^{3}s to 0.0103g/m^{3}s applies for 2300k temperature for a pressure range of 1000 – 2250KPa. The basis is the consideration of stroke engine operating at the condition stated earlier.

e) Diffusion coefficient (K); for purpose up to about 10 atmosphere or even higher, the diffusion coefficient for a binary mixture of gases, A and B may be estimated from Fuller, Schettler and Girding relation.

$$K_{AB} = \frac{1.0 \text{ X } 10^{-7} \text{ X } T^{1.75} \text{ X } [\frac{1}{M_A} \text{ X } \frac{1}{M_B}]^{\frac{1}{2}}}{P[(\Sigma V_A)^{0.33} + (\Sigma V_B)^{0.33}]^2}$$

A value of $K_{AB} = 2.05 \times 10^{-5}$m^2/s applies for the carbon monoxide/air system. This is based on the diffusion coefficient of carbon monoxide/air system is constant at atmospheric temperature and pressure.

3.5.7 NUMERICAL SIMULATION INPUT DATA

From the assumptions stated in 3.5.5 and source of data used in the calculation (i.e the numerical simulation input data) are generated at equal intervals and tabulated as shown in table 3.1 below.

Velocity of air (U); Range of values of velocity (0.5m/s – 2.5m/s).

Velocity of carbon monoxide ; Range of value of velocity (2.5m/s – 3.0m/s)

Source strength (q): Range of values from 0.00458g/m^{3}s to 0.0103g/m^{3}s, which is 0.000164mol/m^{3}s to 0.000368mol/m^{3}s after dividing by the molecular weight of carbon monoxide, CO (28g/mol).

Diffusion coefficient (K) is 2.95 x 10^{-5}m/s from the Fuller, Schettler and Girding relation.

Height (m)	Velocity of Air U (m/s)	Velocity of CO V (m/s)	Source Strength q (mol/m^{3}s)
1	0.50	2.50	0.000164
2	0.70	2.55	0.000186
3	0.90	2.60	0.000208
4	1.10	2.65	0.000231
5	1.30	2.70	0.000253
6	1.50	2.70	0.000275
7	1.70	2.75	0.000297
8	1.90	2.80	0.000320
9	2.10	2 85	0.000342
10	2.30	2.90	0.000364
11	2.50	3.00	0.000368

TABLE 3.1 Numerical simulation input data

Source: From Literature based on the correlation given by Metghalachi and Keck, 1982.

The numerical simulations were carried out at ground level. The concentrations were determined as function of axial distance 10m for a simulation time of 10seconds. The simulation results were presented in table 4.1a and 4.1b.

CHAPTER FOUR

4.0 RESULTS AND DISCUSSION

4.1 RESULTS

Table 4.1 (a) and (b) shows the results of the numerical solution of the model.

The manually generated numerical simulation results are presented in table 4.1 (a) while table 4.1 (b) shows the numerical simulation results generated by computer programming.

From the results obtained, various plot of concentration with velocities of air, pollutant speeds at different heights above the ground level/axial distance for input source strength were made.

Table 4.1 (a): manually simulated result

Height above the ground/ axial distance (m)	Velocity of Air U (m/s)	Velocity of CO V (m/s)	Source Strength q (mol/m^{3}s)	Concentration of CO mol/m^3
1	0.50	2.50	0.000164	0.98
2	0.70	2.55	0.000186	0.95
3	0.90	2.60	0.000208	0.94
4	1.10	2.65	0.000231	0.92
5	1.30	2.70	0.000253	0.90
6	1.50	2.70	0.000275	0.89
7	1.70	2.75	0.000297	0.87
8	1.90	2.80	0.000320	0.86
9	2.10	2.85	0.000342	0.85
10	2.30	2.90	0.000364	0.84
11	2.50	3.00	0.000368	0.82

Table 4.1 (b): programmed simulated result

Height above the ground/ axial distance (m)	Velocity of Air U (m/s)	Velocity of CO V (m/s)	Source Strength q (mol/m^{3}s)	Concentration of CO mol/m^3
1	0.50	2.50	0.000164	0.98
2	0.70	2.55	0.000186	0.95
3	0.90	2.60	0.000208	0.94
4	1.10	2.65	0.000231	0.92
5	1.30	2.70	0.000253	0.90
6	1.50	2.70	0.000275	0.89
7	1.70	2.75	0.000297	0.87
8	1.90	2.80	0.000320	0.86
9	2.10	2.85	0.000342	0.85
10	2.30	2.90	0.000364	0.84
11	2.50	3.00	0.000368	0.82

4.2 DISCUSSION

4.2.1 Effects of Air Velocity

The plots of concentration against velocity of air and axial distance/height above the ground level are shown in figure 4.1 and 4.3 of appendix D. The concentration profiles for all the components exhibit exponential distribution. The exponential nature of the profile shows there is a considerable decrease (0.98mol/m^3 – 0.82mol/m^3) in the concentration of pollutant as it is being dispersed above the ground level, if only we consider the horizontal axis of figure 4.3 as the height above the ground level. As the height above the ground level increases (1m – 11m), the air velocity also increases (0.5m/s – 2.5m/s), thus leading to decrease (0.98mol/m^3 – 0.82mol/m^3) in pollutant concentration (Boubbel, Fox, Turner and Stern, 1994).

This shows that there is better pollution dispersion as air velocity increases (0.5m/s – 2.5m/s), thus diluting the pollutant. Also, from the figures, it was observed that at the same height above the ground level, but at different air velocities, the pollutant concentration shows an inverse relation with velocity.

Considering figure 4.1 and 4.3, and taking the horizontal axis of figure 4.3 as the axial wind distance, as the air velocity increases (0.50m/s – 2.50m/s), the pollutant concentration decreases (0.98mol/m^3 – 0.82mol/m^3)along the axial wind distance as a result of better dispersion of the pollutant which leads to its dilution. Also, at the same axial wind distance, higher concentration of pollutant occurred at a low air velocity than at a higher velocity. It thus shows that the higher the air velocity, the more the pollutant is being dispersed and the lower the pollutants concentration.

4.2.2 Effects of pollutant speed

Figure 4.2 illustrates the effect of pollutant speed. The concentration profile for figure 4.2 is similar to figure 4.1 (i.e they both exhibit exponential distribution profile), this implies that as the pollutant speed increases (2.50m/s – 3.00m/s), there is a considerable decrease (0.98mol/m^3 – 0.82mol/m^3) in pollutant concentration as the height above the ground level increases (1m – 11m) as a result of dilution of pollutant as it rises up (Boubbel, Fox, Turner and Stern, 1994).

At the same height above the ground level but at different pollutant speed, the concentration is inversely proportional to the pollutant speed. Also, at the same speed but at different height above the ground level, the pollutant concentration decreased with height.

CHAPTER FIVE

5.0 CONCLUSIONS AND RECOMMENDATIONS

5.1 CONCLUSIONS

The prediction of carbon monoxide concentration due to vehicular emissions as a function of some physical parameters such as velocity of air, velocity of pollutant, height above the ground level/axial distance and source strength was satisfactory due to the mathematical model generated from Roe-Riemann based on the continuity equation.

Thus;

- ❖ Increase in air velocity (0.50m/s – 2.50m/s) decreases the concentration of pollutant ($0.98 mol/m^3$ – $0.82 mol/m^3$) as the axial wind distance and height above the ground level increases (1m – 11m).
- ❖ Increase in pollutant speed (2.50m/s – 3.00m/s) decreases the concentration of pollutant ($0.98 mol/m^3$ – $0.82 mol/m^3$) as the axial wind distance and height above the ground level increases.

Lastly, the model equation for the determination of carbon monoxide from vehicular emission is;

$$C^n_{i+1} = C^n_i - \frac{\Delta t}{\Delta x}\left(F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}\right) + \Delta t\, q^n_{i+1}$$

Where

$$F_{i+\frac{1}{2}} = \tfrac{1}{2}\left[F_{i+1} + F_i\right] - \tfrac{1}{2}\,\Delta F_i + \tfrac{1}{2}$$

$F_{i-\frac{1}{2}}$ = Previously calculated $F_{i+\frac{1}{2}}$

RECOMMENDATIONS

1. To reduce pollution problems caused by vehicular emission of carbon monoxide, high operating engine temperature and pressure should be avoided to prevent the generation of carbon monoxide caused by incomplete combustion of unburned fuels which are emitted at great speed.

2. The most advanced air quality model should be compared against one another and against field experimental observation results using a detailed and accurate set of input and verification data.
3. Further research is needed into the use of model that relates indoor exposure to outdoor air quality. One that will show relationship between emission source and human exposure.
4. Simulation should be carried out using other computer programs like ChemCad to check their accuracies.
5. Reliable mass transport system will greatly reduce the number of vehicles on our roads at any given time and therefore emissions.
6. In Nigeria, the refineries should be fully evaluated with the aim of redesigning them to produce entirely unleaded petrol in the very near future.
7. Importation to supplement local production of petrol in Nigeria if necessary should be unleaded as far as possible.
8. Communication systems particularly wire and wireless will greatly reduce travelling within and outside our places of abode and will reduce emission.
9. Individuals can also make a difference in the effort to reduce pollution from cars by;
    - Simple vehicle maintenance.
    - Parking vehicles in shade during warm periods with strong sunlight can keep a car cooler and can minimize the evaporation of fuel.
    - Choosing a place to live that reduces the need to drive.

NOMENCLATURE

Ax	Jacobian matrix in x-direction
C	Concentration of pollutant, mol/m^3
D	Diffusivity of the pollutant, m^2/s
Jx	Flux of diffusion relative to motor average velocity, mol/m^{2}s
K	Eddy diffusion m^2/s
M	Molecular weight of pollutant, g/mol
M_{air}	Molecular weight of air, g/mol
Nx	x-direction flux, mol/m^{2}s
q	Source strength, g/m^{3}s
t	Time of dispersion, s
T	Temperature of the surrounding, k
Ux	Velocity of air in x-direction, m/s
$\bar{U}$	Mean component of the wind velocity, m/s
U'	Deviation of pollutant speed from mean component, m/s
Vx	Pollutant speed in x-direction, m/s
$\bar{V}$	Mean of pollutant speed from component, m/s
V'	Deviation of pollutant speed from component, m/s
ρ	Density of pollutant kg/m^3
λ_x	Eigen value in x-direction
$\bar{\rho}_n$	Eigenvector

α_n	Change in concentration
Σv	Diffusion volumes for simple molecule
K_{AB}	Diffusion coefficient of air-co system.

Subscript

A	Air component
B	Pollutant component
n	Time level
i, j	Cell location in grid
i + 1	Next point in the grid
x	in the x-direction
y	in the y-direction
z	in the z-direction

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APPENDIX A

NUMERICAL SIMULATION CALCULATION

A.1 Using the boundary conditions stated in section 3.5.3 and figure 3.5.1, **n** is the time level (0 to 10seconds) where $\Delta t = 0.1$sec, M is the division in axial distance of 10 equal parts and simulation time of 10seconds. The length of each axis is 10m and the change in distance between two points is 1m (i.e $\Delta x = 1$m). Taking the change in concentration between two points in grid is equal to change in time level. Then;

$$\Delta t = \Delta C = 0.1$$

Where

$$\Delta t = 0.1\text{sec}$$

And $\Delta C = 0.1\text{mol/m}^3$

A.1.1 From table 3.1, using the first set of input data

$U = 0.5$m/s, $V = 2.5$m/s, $q = 0.000164\text{mol/m}^3\text{s}$, $K = 2.05 \times 10^{-5}\text{m}^2/\text{s}$ (this value is constant throughout).

Note; $\Delta t = \Delta C = 0.1$, $\Delta x = 1$m and let $C_0^0 = 0.1\text{mol/m}^3$ (initial concentration at time level zero).

From equation 3.5.22, $\Delta C = 01\text{mol/m}^3$

From equation 3.5.20, the eigenvalues is calculated as

$$\lambda x = U_x + V_x = 0.5 + 2.5 = 3.0\text{m/s}$$

From equation 3.5.14, flux of grid point $i + 1$ is calculated

$$F_{i+1} = U_x C_0^0 + C_0^0 V_x - K \frac{\Delta C}{\Delta x}$$

$$F_{i+1} = C_0^0 (U_x + V_x) - K \frac{\Delta C}{\Delta x}$$

Where

$U_x = 0.5\text{m/s}$, $V_x = 2.5\text{m/s}$, $C = 0.1\text{mol/m}^3$, $K = 2.05 \times 10^{-5}\text{m}^2/\text{s}$, $\Delta C = 0.1\text{mol/m}^3$

$$\left.\begin{array}{l}\Delta t = 0.1\text{sec} \\ \Delta x = 1\text{m}\end{array}\right] \text{these values are constant all through the calculation.}$$

By substituting into the above equation 3.5.14,

$$F_{i+1} = 1(0.5 + 2.5) - \frac{2.05 \times 10^{-5} \times 0.1}{1}$$

$$= 3.000\text{mol/m}^2\text{s}$$

Change in grid flux between the grid point i and $i + 1$ is calculated from equation 3.5.24

$$\Delta F = \sum \Delta C \lambda_x \bar{e}_n$$

Equation 3.5.25 considers only one axis, therefore, the use of summation will not affect any change.

Hence, $\Delta F = \Delta_x \lambda_x \bar{e}_n$ for a unit eigenvector i.e $\bar{e}_1 = 1$, the change in flux equation reduced to the form;

$$\Delta F = \lambda_x \Delta C$$

$$= 3 \times 0.1$$

$$= 0.3\text{mol/m}^2\text{s}$$

Now, flux at grid point i can be calculated as;

$$F_i = F_{i+1} - \Delta F$$

$$= 3.000 - 0.3$$

$$= 2.700\text{mol/m}^2\text{s}$$

Change in flux between the grid point i and $i + ½$ is

$\Delta F_{i+1/2} = \frac{\Delta F}{2} = \frac{0.3}{2} = 0.15\text{mol/m}^2\text{s}$

The flux at grid point i +1/2 can be calculated from 3.5.19

$F_{i+½} = ½\,[F_{i+1} + F_i] - ½ \times \Delta F_{i+½}$

$= ½\,[3.000 + 2.700] - ½ \times 0.15$

$= 2.775\text{mol/m}^2\text{s}$

Now, we assume the change in flux between the grid points i and i + ½ is equal to the opposite side flux (i.e $\Delta F_{i+1/2} = \Delta F_{i-1/2}$).

Hence, $\Delta F_{i-½} = F_i - \Delta F_{i+½}$

$= 2.700 - 0.15$

$= 2.550\text{mol/m}^2\text{s}$

Using Roe-Riemann solver (equation 3.5.35), concentration at the grid point can be calculated as:

$$C^n_{i+1,j,k} = C^n_{i,j,k} - \frac{\Delta t}{\Delta x}(F_{i+1/2,j,k} - F_{i-1/2,j,k}) + \Delta t q^o_1$$

Where

$C^o_1 = 1\text{mol/m}^3$, $\Delta t = 0.1\text{sec}$, $\Delta x = 1\text{m}$, $F_{i+½} = 2.775\text{mol/m}^2\text{s}$, $F_{i-½} = 2.550\text{mol/m}^2\text{s}$,

$q^o = 0.000164\text{mol/m}^3\text{s}$

Substituting,

$C^o_1 = 1 - \frac{0.1}{1}(2.775 - 2.550) + 0.1 \times 0.000164$

$= 0.98\text{mol/m}^3$

A.1.2 Using the same procedure for the second set of input data (from table 3.1)

$U_x = 0.7\text{m/s}$, $V_x = 2.55\text{m/s}$, $q_2 = 0.000186\text{mol/m}^3\text{s}$, $K = 2.05 \times 10^{-5}\text{m}^2\text{/s}$

The new change in concentration is;

$$\Delta C = C_0^o - C_1^o$$

$$= 1 - 0.978 = 0.022\text{mol/m}^3$$

$$\lambda_x = U_x + V_x$$

$$= 0.7 + 2.55 = 3.25\text{m/s}$$

New flux at next grid point $i + 1$ is;

$$F_{i+1} = C_1^o\,(U_x + V_x) - K\frac{\Delta C}{\Delta x}$$

$$F_{i+1} = 0.978 \text{ x } 3.25 - \frac{2.05 \text{ x } 10^{-5} \text{ x } 0.022}{1} \qquad = 3.1785\text{mol/m}^2\text{s}$$

Flux at grid point i will be flux previously calculated as $i + 1$ (i.e new F_i = old F_{i+1} calculated before).

Therefore, $F_i = 3.000\text{mol/m}^2\text{s}$ (calculated previously as F_{i+1})

New flux at grid point $i + ½$ is

$$F_{i+½} = ½\,[F_{i+1} + F_i] - ½\,\Delta F$$

ΔF is change in flux between the grid points i and $i + 1$ is computed as:

$$\Delta F = \lambda_x\,\Delta C = 3.25 \text{ x } 0.022$$

$$= 0.0715\text{mol/m}^2\text{s}$$

$$F_{i+½} = ½\,[3.176 + 3.000] - ½ \text{ x } 0.0715$$

$$= 3.0535\text{mol/m}^2\text{s}$$

$F_{i-½} = 2.775\text{mol/m}^2\text{s}$ (previously calculated $F_{i+½}$).

The concentration at the next point in the grid $C_i^{\hat{o}}$ can be calculated using equation 3.5.35 (discretized reduced form of Roe-Riemann solver equation).

$$C_2^1 = C_1^o - \frac{\Delta t}{\Delta x}\,(F_{i+½} - F_{i-½}) + \Delta t\, q_2^1$$

$C_2^1 = 0.978 - \frac{0.1}{1}(3.054 - 2.775) + 0.1 \text{ x } 0.000186$

$C_2^1 = 0.95\text{mol/m}^3$

A.1.3 Using the same procedure for the third set of input data

$U_x = 0.9\text{m/s}$, $V_x = 2.6\text{m/s}$, $q_3^2 = 0.0002082\text{mol/m}^3\text{s}$, $K = 2.05\text{x}10^{-5}\text{m}^2/\text{s}$

$\Delta C = 0.978 - 0.950 = 0.028\text{mol/m}^3$

$\lambda_x = 0.9 + 2.6 = 3.5\text{m/s}$

$F_{i-1} = 0.950 \text{ x } 3.5 - \frac{2.05 \text{ x } 10^{-5} \text{ x } 0.028}{1} = 3.3250\text{mol/m}^2\text{s}$

$F_i = 3.1785\text{mol/m}^2\text{s}$ (calculated previously as F_{i+1})

$\Delta F = \lambda_x \Delta C = 3.50 \text{ x } 0.28 = 0.098\text{mol/m}^2\text{s}$

$F_{i+½} = ½\,[3.3250 + 3.1785] - ½ \text{ x } 0.098 = 3.20275\text{mol/m}^2\text{s}$

$F_{i-½} = 3.0535\text{mol/m}^2\text{s}$ (calculated previously as $F_{i+½}$)

Hence, C_3^2 can be calculated as

$C_3^2 = C_2^1 - \frac{\Delta t}{\Delta x}(F_{i+½} - F_{i-½}) + \Delta t\, q_3^2$

$C_3^2 = 0.950 - \frac{0.1}{1}(3.20275 - 3.0535) + 0.1 \text{ x } 0.0002305$

$C_3^2 = 0.94\text{mol/m}^3$

A.1.4 Fourth set of input data

$U_x = 1.1\text{m/s}$, $V_x = 2.65\text{m/s}$, $q_4^2 = 0.0002305\text{mol/m}^3\text{s}$, $K = 2.05 \text{ x } 10^{-5}\text{m}^2/\text{s}$

Now, $\Delta C = 0.950 - 0.935 = 0.015\text{mol/m}^3$

$\lambda_x = 1.1 + 2.65 = 3.75\text{m/s}$

$F_{i+½} = 0.935 \text{ x } 3.75 - 2.05 \text{ x } 10^{-5} \text{ x } 0.015 = 3.5062\text{mol/m}^2\text{s}$

$F_i = 3.3250 \text{mol/m}^2\text{s}$ (calculated previously as $F_{i+½}$ in A.1.3)

$\Delta F = 3.75 \times 0.015 = 0.05625 \text{mol/m}^2\text{s}$

$F_{i+½} = ½ [3.5062 + 3.3250] - ½ \times 0.05625 = 3.387475 \text{mol/m}^2\text{s}$

Hence, $C_4^3 = C_3^2 - \frac{\Delta t}{\Delta x} (F_{i+½} - F_{i-½}) + \Delta t\, q_4^3$

$C_4^3 = 0.935 - \frac{0.1}{1} (3.387475 - 3.20275) + 0.1 \times 0.0002305$

$C_4^3 = 0.92 \text{mol/m}^3$

A.1.5 For the fifth set of input data.

$U_x = 1.3 \text{m/s}$, $V_y = 2.7 \text{m/s}$, $q_5^4 = 0.0002528 \text{mol/m}^3\text{s}$, $K = 2.05 \times 10^{-5} \text{m}^2\text{/s}$

$\Delta C = 0.935 - 0.917 = 0.018 \text{mol/m}^3$

$\lambda_x = 1.3 + 2.7 = 4.0 \text{m/s}$

$F_{i+1} = 0.917 \times 4.0 - 2.05 \times 10^{-5} \times 0.018 = 3.6680 \text{mol/m}^2\text{s}$

$F_i = 3.5062 \text{mol/m}^2\text{s}$ (F_{i+1} in A.1.4)

$\Delta F = 4.0 \times 0.018 = 0.072 \text{mol/m}^2\text{s}$

$F_{i+½} = ½ [3.6680 + 3.5062] - ½ \times 0.072 = 3.5511 \text{mol/m}^2\text{s}$

$F_{i-½} = 3.387475 \text{mol/m}^2\text{s}$ ($F_{i+½}$ in A.1.4)

Hence,

$C_5^4 = C_4^3 - \frac{\Delta t}{\Delta x} (F_{i+½} - F_{i-½}) + \Delta t\, q_5^4$

$C_5^4 = 0.917 - 0.1 (3.5511 - 3.387475) + 0.1 \times 0.000258$

$C_5^4 = 0.90 \text{mol/m}^3$

A.1.6 For the sixth set of input data

$U_x = 1.5\text{m/s}$, $V_x = 2.75\text{m/s}$, $q_6^5 = 0.0002751\text{mol/m}^3\text{s}$, $K = 2.05 \times 10^{-5}\text{m}^2\text{/s}$

$\Delta C = 0.917 - 0.901 = 0.016\text{mol/m}^3$

$\lambda_x = 1.50 + 2.75 = 4.25\text{m/s}$

$F_{i+1} = 0.901 \times 4.25 - 2.05 \times 10^{-5} \times 0.016 = 3.8292\text{mol/m}^2\text{s}$

$F_i = 3.6680\text{mol/m}^2\text{s}$ (from previous calculation)

$\Delta F = 4.25 \times 0.016 = 0.068\text{mol/m}^2\text{s}$

$F_{i+½} = ½ [3.8292 + 3.6680] - ½ \times 0.068 = 3.7146\text{mol/m}^2\text{s}$

$F_{i-½} = 3.5511\text{mol/m}^2\text{s}$ (previous calculation of $F_{i+½}$).

Hence,

$$C_6^5 = C_5^4 - \frac{\Delta t}{\Delta x}(F_{i+½} - F_{i-½}) + \Delta t\, q_6^5$$

$$C_6^5 = 0.901 - 0.1\,(3.7146 - 3.5511) + 0.1 \times 0.0002751$$

$$C_6^5 = 0.89\text{mol/m}^3$$

A.1.7 Using the seventh set of input data from the table 3.1

$U_x = 1.7\text{m/s}$, $V_x = 2.80\text{m/s}$, $q_7^6 = 0.0002974\text{mol/m}^3\text{s}$, $K = 2.05 \times 10^{-5}\text{m}^2\text{/s}$

$\Delta C = 0.901 - 0.885 = 0.016\text{mol/m}^3$

$\lambda_x = 1.7 + 2.80 = 4.5\text{m/s}$

$F_{i+1} = 0.885 \times 4.5 - 2.05 \times 10^{-5} \times 0.016 = 3.9825\text{mol/m}^2\text{s}$

$F_i = 3.8292\text{mol/m}^2\text{s}$ (from previous calculation of F_{i+1})

$\Delta F = 4.5 \times 0.016 = 0.072\text{mol/m}^2\text{s}$

$F_{i+½} = ½ [3.9825 + 3.8292] - ½ \times 0.072 = 3.8699\text{mol/m}^2\text{s}$

$F_{i-½}$ = 3.7146mol/m^{2}s (previous calculation of $F_{i+½}$).

Hence,

$C_7^6 = C_6^5 - \frac{\Delta t}{\Delta x}(F_{i+½} - F_{i-½}) + \Delta t\, q_7^6$

$C_7^6 = 0.885 - 0.1\,(3.8699 - 3.7146) + 0.1 \times 0.0002974$

$C_7^6 = 0.87$mol/m^3

A.1.8 From table 3.1, the 8th sets of input data are:

$U_x = 1.9$m/s, $V_x = 2.85$m/s, $q_8^7 = 0.0003197$mol/m^{3}s, $K = 2.05 \times 10^{-5}$m^2/s

$\Delta C = 0.885 - 0.869 = 0.016$mol/m^3

$\lambda_x = 1.9 + 2.85 = 4.75$m/s

$F_{i+1} = 0.869 \times 4.75 - 2.05 \times 10^{-5} \times 0.016 = 4.1277$mol/m^{2}s

F_i = 3.9825mol/m^{2}s (taken from F_{i+1} in A.1.7)

$\Delta F = 4.75 \times 0.016 = 0.076$mol/m^{2}s

$F_{i+½} = ½\,[4.1277 + 3.9825] - ½ \times 0.076 = 4.0171$mol/m^{2}s

$F_{i-½}$ = 3.6899mol/m^{2}s (from $F_{i+½}$ in A.1.7)

Hence,

$C_8^7 = C_7^6 - \frac{\Delta t}{\Delta x}(F_{i+½} - F_{i-½}) + \Delta t\, q_8^7$

$C_8^7 = 0.869 - 0.1\,(4.0171 - 3.6899) + 0.1 \times 0.0003197$

$C_8^7 = 0.86$mol/m^3

A.1.9 Using the 9th sets of data from table 3.1

$U_x = 2.1$m/s, $V_x = 2.90$m/s, $q_9^8 = 0.0003420$mol/m^{3}s, $K = 2.05 \times 10^{-5}$m^2/s

$\Delta C = 0.869 - 0.854 = 0.015$mol/m^3

$\lambda_x = 2.1 + 2.90 = 5.0\text{m/s}$

$F_{i+1} = 0.854 \text{ x } 5.0 - 2.05 \text{ x } 10^{-5} \text{ x } 0.015 = 4.2700\text{mol/m}^2\text{s}$

$F_i = 4.1277\text{mol/m}^2\text{s}$ (previous F_{i+1})

$\Delta F = 5.0 \text{ x } 0.015 = 0.075\text{mol/m}^2\text{s}$

$F_{i+½} = ½\,[4.2700 + 4.1277] - ½ \text{ x } 0.075 = 4.16135\text{mol/m}^2\text{s}$

$F_{i-½} = 4.0171\text{mol/m}^2\text{s}$ (previous $F_{i+½}$).

Hence,

$C_9^8 = C_8^7 - \frac{\Delta t}{\Delta x}(F_{i+½} - F_{i-½}) + \Delta t\, q_9^8$

$C_9^8 = 0.854 - 0.1\,(4.16135 - 4.0171) + 0.1 \text{ x } 0.0003420$

$C_9^8 = 0.85\text{mol/m}^3$

A.1.10 The tenth set of data from the table 3.1

$U_x = 2.3\text{m/s}$, $V_x = 2.95\text{m/s}$, $q_{10}^9 = 0.0003643\text{mol/m}^3\text{s}$, $K = 2.05 \text{ x } 10^{-5}\text{m}^2\text{/s}$

$\Delta C = 0.854 - 0.840 = 0.014\text{mol/m}^3$

$\lambda_x = 2.3 + 2.95 = 5.25\text{m/s}$

$F_{i+1} = 0.840 \text{ x } 5.25 - 2.05 \text{ x } 10^{-5} \text{ x } 0.014 = 4.4100\text{mol/m}^2\text{s}$

$F_i = 4.2700\text{mol/m}^2\text{s}$ (previous F_{i+1})

$\Delta F = 5.25 \text{ x } 0.014 = 0.0735\text{mol/m}^2\text{s}$

$F_{i+½} = ½\,[4.4100 + 4.2700] - ½ \text{ x } 0.0735 = 4.30325\text{mol/m}^2\text{s}$

$F_{i-½} = 4.16135\text{mol/m}^2\text{s}$ (previous $F_{i+½}$).

Thus,

$C_{10}^9 = C_9^8 - \frac{\Delta t}{\Delta x}(F_{i+½} - F_{i-½}) + \Delta t\, q_{10}^9$

$C_{10}^{9} = 0.840 - 0.1\ (4.30325 - 4.16135) + 0.1 \times 0.0003643$

$C_{10}^{9} = 0.84\text{mol/m}^3$

A.1.11 The eleventh set of data from the table 3.1

$U_x = 2.5\text{m/s}$, $V_x = 3.0\text{m/s}$, $q_{11}^{10} = 0.0003679\text{mol/m}^3\text{s}$, $K = 2.05 \times 10^{-5}\text{m}^2\text{/s}$

$\Delta C = 0.840 - 0.826 = 0.014\text{mol/m}^3$

$\lambda_x = 2.5 + 3.0 = 5.5\text{m/s}$

$F_{i+1} = 0.826 \times 5.5 - 2.05 \times 10^{-5} \times 0.014 = 4.5430\text{mol/m}^2\text{s}$

$F_i = 4.4100\text{mol/m}^2\text{s}$ (previous F_{i+1})

$\Delta F = 5.5 \times 0.014 = 0.077\text{mol/m}^2\text{s}$

$F_{i+½} = ½\ [4.5430 + 4.4100] - ½ \times 0.077 = 4.4380\text{mol/m}^2\text{s}$

$F_{i-½} = 4.30325\text{mol/m}^2\text{s}$ (previous $F_{i+½}$).

Thus,

$C_{11}^{10} = C_{10}^{9} - \frac{\Delta t}{\Delta x}\ (F_{i+½} - F_{i-½}) + \Delta t\ q_{11}^{10}$,

$C_{11}^{10} = 0.826 - 0.1\ (4.4380 - 4.30325) + 0.1 \times 0.0003679$

$C_{11}^{10} = 0.82\text{mol/m}^3$

APPENDIX B

$x := 1..11$

$u_x :=$ "velocity of air in m/s"

$v_x :=$ "velocity of CO in m/s"

$q_x :=$ "Source strenght in mol/m^3*s"

$u_x :=$	$v_x :=$	$q_x :=$
0.50	2.50	0.000164
0.70	2.55	0.000186
0.90	2.60	0.000208
1.10	2.65	0.000231
1.30	2.70	0.000253
1.50	2.75	0.000275
1.70	2.80	0.000297
1.90	2.85	0.000320
2.10	2.90	0.000342
2.30	2.95	0.000364
2.50	3.00	0.000368

$$(C_{i+1})^n = (C_i)^n - \frac{\Delta t}{\Delta x} \cdot \left(F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}\right) + \Delta t \cdot (q_{i+1})^n$$ Roe-Riemann Solver

$\Delta t := 0.1 \cdot s$

$\Delta x := 1 \cdot m$

$k := 2.05 \cdot 10^{-5} \cdot \frac{m^2}{s}$

first_value

$\Delta c := 0.1 \cdot \frac{mol}{m^3}$

$C_0 := 1.0 \frac{mol}{m^3}$ this is initial concentration at time level zero

$\lambda_x := u_x + v_x$

$\lambda_x =$

3
3.25
3.5
3.75
4
4.25
4.5
4.75
5
5.25
5.5

Flux at grid point i+1 is $i := 0$

$u_{x_1} := 0.50 \cdot \frac{m}{s}$ $v_{x_1} := 2.50 \cdot \frac{m}{s}$

$$F_{i+1} := C_0 \cdot \left(u_{x_1} + v_{x_1}\right) - k \cdot \frac{\Delta c}{\Delta x}$$

$$F_{i+1} = 3 \frac{mol}{m^2 \cdot s}$$

Change in grid flux between the grid point i and i+1 is

Let $en := 1$

$\lambda_{x_1} := 3.0 \cdot \frac{m}{s}$

$$\Delta F = \sum \lambda_{x_1} \cdot \Delta c \cdot en$$

since we are considering one axis, unit eigen vector, en = 1

$$\Delta F := \lambda_{x_1} \cdot \Delta c$$

$$\Delta F = 0.3 \frac{mol}{m^2 \cdot s}$$

Flux at grid point i is

$$F_i := F_{i+1} - \Delta F$$

$$F_i = 2.7\,\frac{mol}{m^2 \cdot s}$$

change in flux between the grid point i and i+ 1/2 is

$$\Delta F_{i+\frac{1}{2}} = \frac{\Delta F}{2} \qquad \frac{\Delta F}{2} = 0.15\,\frac{mol}{m^2 \cdot s} \qquad \Delta F_{i+\frac{1}{2}} = \Delta F_{\frac{i}{2}}$$

$$\Delta F_{\frac{i}{2}} := 0.15 \cdot \frac{mol}{m^2 \cdot s}$$

The flux at grid point i+ 1/2 is

$$F_{i+\frac{1}{2}} = \frac{1}{2} \cdot \left(F_{i+1} + F_i\right) - \frac{1}{2} \cdot \Delta F_{i+\frac{1}{2}}$$

Let $F_{i+\frac{1}{2}} = F_{\frac{i}{2}}$

$$F_{\frac{i}{2}} := \frac{1}{2} \cdot \left(F_{i+1} + F_i\right) - \frac{1}{2} \cdot \Delta F_{\frac{i}{2}}$$

$$F_{\frac{i}{2}} = 2.77\,\frac{mol}{m^2 \cdot s}$$

Let $\Delta F_{i-\frac{1}{2}} = \Delta F_{-\frac{i}{2}}$

$$\Delta F_{\frac{i}{2}} := 0.15 \cdot \frac{mol}{m^2 \cdot s} \qquad F_i := 2.7 \cdot \frac{mol}{m^2 \cdot s}$$

$$F_{-\frac{i}{2}} := F_i - \Delta F_{\frac{i}{2}}$$

$$F_{-\frac{i}{2}} = 2.55\,\frac{mol}{m^2 \cdot s}$$

Using Roe- Riemann Solver:

Concentration at the grid point can be calculated as

$$\left(C^n\right)_{i+1,jk} = \left(C^n\right)_{i,jk} - \left[\frac{\Delta t}{\Delta x} \cdot \left(F_{i+\frac{1}{2},jk} - F_{i-\frac{1}{2},jk}\right)\right] + \Delta t \cdot \left(q^n\right)_1$$

$$q_{x_1} := 0.000164 \cdot \frac{mol}{m^3 \cdot s} \qquad F_{\frac{i}{2}} := 2.775 \cdot \frac{mol}{m^2 \cdot s} \qquad F_{-\frac{i}{2}} := 2.550 \cdot \frac{mol}{m^2 \cdot s}$$

$C_0 := 1 \cdot \frac{mol}{m^3}$ $\Delta t := 0.1 \cdot s$ $\Delta x := 1 \cdot m$

$$C_1 := C_0 - \frac{\Delta t}{\Delta x} \cdot \left(F_{\frac{i}{2}} - F_{\frac{-i}{2}} \right) + \Delta t \cdot q_{x_1}$$

$$C_1 := 1 \cdot \frac{mol}{m^3} - \left[\frac{0.1 \cdot s}{1 \cdot m} \cdot (2.775 - 2.550) \cdot \frac{mol}{m^2 \cdot s} \right] + 0.1 \cdot s \cdot 0.000164 \cdot \frac{mol}{m^3 \cdot s}$$

$$C_1 = 0.98 \frac{mol}{m^3}$$

Second_value

$u_{x_2} := 0.7 \cdot \frac{m}{s}$ $v_{x_2} := 2.55 \cdot \frac{m}{s}$ $q_{x_2} := 0.000186 \cdot \frac{mol}{m^3 \cdot s}$

The new change in concentration is

$$\Delta C_2 := C_0 - C_1$$

$$\Delta C_2 = 0.02 \frac{mol}{m^3}$$

$$\lambda_{x_2} := 3.25 \cdot \frac{m}{s}$$

New flux at next grid point i + 2 is

$$F_{i+2} := C_1 \cdot \left(u_{x_2} + v_{x_2} \right) - k \cdot \frac{\Delta C_2}{\Delta x}$$

$$F_{i+2} = 3.18 \frac{mol}{m^2 \cdot s}$$

Flux at grid point i will be flux previous calculated as i + 1, that is

$$F_{i_2} := F_{i+1}$$

$$F_{i_2} = 3 \frac{mol}{m^2 \cdot s}$$

New flux at grid point i + 1/2 is

$$\Delta F_2 := \lambda_{x_2} \cdot \Delta C_2$$

$$\Delta F_2 = 0.07\,\frac{mol}{m^2 \cdot s}$$

$$F_{(i)2_2} := \frac{1}{2} \cdot \left(F_{i+2} + F_{i_2}\right) - \frac{1}{2} \cdot \Delta F_2$$

$$F_{(i)2_2} = 3.05\,\frac{mol}{m^2 \cdot s}$$ $$F_{i_2} := 2.775 \cdot \frac{mol}{m^2 \cdot s}$$

$$F_{-(i)2_2} := F_{i_2}$$

$$F_{-(i)2_2} = 2.77\,\frac{mol}{m^2 \cdot s}$$

Using Roe-Riemann Solver

$$\Delta t := 0.1 \cdot s \qquad \Delta x := 1 \cdot m$$

$$C_1 := 0.978 \cdot \frac{mol}{m^3}$$

$$q_{x_2} := 0.000186 \cdot \frac{mol}{m^3 \cdot s} \qquad F_{(i)2_2} := 3.052 \cdot \frac{mol}{m^2 \cdot s} \qquad F_{-(i)2_2} := 2.775 \cdot \frac{mol}{m^2 \cdot s}$$

$$C_2 := C_1 - \frac{\Delta t}{\Delta x} \cdot \left[F_{(i)2_2} - F_{-(i)2_2}\right] + \Delta t \cdot q_{x_2}$$

$$C_2 := 0.978 \cdot \frac{mol}{m^3} - \frac{0.1 \cdot s}{1 \cdot m} \cdot \left(3.052 \cdot \frac{mol}{m^2 \cdot s} - 2.775 \cdot \frac{mol}{m^2 \cdot s}\right) + 0.1 \cdot s \cdot \left(0.000186 \cdot \frac{mol}{m^3 \cdot s}\right)$$

$$C_2 = 0.95\,\frac{mol}{m^3}$$

Third_value

$$u_{x_3} := 0.90 \cdot \frac{m}{s} \qquad v_{x_3} := 2.60 \cdot \frac{m}{s} \qquad q_{x_3} := 0.000208 \cdot \frac{mol}{m^3 \cdot s}$$

The new change in concentration is

$$\Delta C_3 := C_1 - C_2$$

$$\Delta C_3 = 0.03\,\frac{mol}{m^3}$$

$$\lambda_{x_3} := 3.5 \cdot \frac{m}{s}$$

New flux at next grid point i + 3 is

$$F_{i+3} := C_2 \cdot \left(u_{x_3} + v_{x_3}\right) - k \cdot \frac{\Delta C_3}{\Delta x}$$

$$F_{i+3} = 3.33 \, \frac{mol}{m^2 \cdot s}$$

Flux at grid point i will be flux previous calculated as i + 2, that is

$$F_{i_3} := F_{i+2} \qquad F_{i_3} = 3.18 \, \frac{mol}{m^2 \cdot s}$$

New flux at grid point i + 1/2 is

$$\Delta F_3 := \lambda_{x_3} \cdot \Delta C_3$$

$$\Delta F_3 = 0.1 \, \frac{mol}{m^2 \cdot s}$$

$$F_{(i)\frac{3}{2}} := \frac{1}{2} \cdot \left(F_{i+3} + F_{i_3}\right) - \frac{1}{2} \cdot \Delta F_3$$

$$F_{(i)\frac{3}{2}} = 3.2 \, \frac{mol}{m^2 \cdot s}$$

$$F_{-(i)\frac{3}{2}} := F_{(i)\frac{2}{2}} \qquad F_{(i)\frac{2}{2}} := 3.052 \cdot \frac{mol}{m^2 \cdot s}$$

$$F_{-(i)\frac{3}{2}} = 3.05 \, \frac{mol}{m^2 \cdot s}$$

Using Roe-Riemann Solver

$$\Delta t := 0.1 \cdot s \qquad \Delta x := 1 \cdot m \qquad C_2 := 0.95 \cdot \frac{mol}{m^3}$$

$$q_{x_3} := 0.000208 \cdot \frac{mol}{m^3 \cdot s}$$

$$C_3 := C_2 - \frac{\Delta t}{\Delta x} \cdot \left[F_{(i)\frac{3}{2}} - F_{-(i)\frac{3}{2}}\right] + \Delta t \cdot q_{x_3}$$

$$C_3 := 0.95 \cdot \frac{mol}{m^3} - \frac{0.1 \cdot s}{1 \cdot m} \cdot (3.203 - 3.053) \cdot \frac{mol}{m^2 \cdot s} + 0.1 \cdot s \cdot \left(0.000208 \cdot \frac{mol}{m^3 \cdot s}\right)$$

$$C_3 = 0.91\,\frac{mol}{m^3}$$

Fourth_value

$$u_{x_4} := 1.10 \cdot \frac{m}{s} \qquad v_{x_4} := 2.65 \cdot \frac{m}{s} \qquad q_{x_4} := 0.000231 \cdot \frac{mol}{m^3 \cdot s}$$

The new change in concentration is

$$\Delta C_4 := C_2 - C_3 \qquad \Delta C_4 = 0.01\,\frac{mol}{m^3}$$

$$\lambda_{x_4} := 3.75 \cdot \frac{m}{s}$$

New flux at next grid point i + 4 is

$$F_{i+4} := C_3 \cdot \left(u_{x_4} + v_{x_4}\right) - k \cdot \frac{\Delta C_4}{\Delta x} \qquad F_{i+4} = 3.51\,\frac{mol}{m^2 \cdot s}$$

Flux at grid point i will be flux previous calculated as i + 3, that is

$$F_{i_4} := F_{i+3} \qquad F_{i_4} = 3.33\,\frac{mol}{m^2 \cdot s}$$

New flux at grid point i + 1/2 is

$$\Delta F_4 := \lambda_{x_4} \cdot \Delta C_4$$

$$\Delta F_4 = 0.06\,\frac{mol}{m^2 \cdot s}$$

$$F_{\frac{(i)4}{2}} := \frac{1}{2} \cdot \left(F_{i+4} + F_{i_4}\right) - \frac{1}{2} \cdot \Delta F_4 \qquad F_{\frac{(i)4}{2}} = 3.39\,\frac{mol}{m^2 \cdot s}$$

$$F_{-\frac{(i)4}{2}} := F_{\frac{(i)3}{2}} \qquad F_{\frac{(i)3}{2}} := 3.2 \cdot \frac{mol}{m^2 \cdot s}$$

$$F_{-\frac{(i)4}{2}} = 3.2\,\frac{mol}{m^2 \cdot s}$$

Using Roe-Riemann Solver

$\Delta t := 0.1 \cdot s$ $\Delta x := 1 \cdot m$ $C_3 := 0.94 \cdot \frac{mol}{m^3}$

$$C_4 := C_3 - \frac{\Delta t}{\Delta x} \cdot \left[F_{\frac{(i)4}{2}} - F_{\frac{(i)4}{2}} \right] + \Delta t \cdot q_{x_4}$$

$$C_4 := 0.94 \cdot \frac{mol}{m^3} - \frac{0.1 \cdot s}{1 \cdot m} \cdot (3.39 - 3.2) \cdot \frac{mol}{m^2 \cdot s} + 0.1 \cdot s \cdot \left(0.000231 \cdot \frac{mol}{m^3 \cdot s} \right)$$

$$C_4 = 0.92 \frac{mol}{m^3}$$

Fifth_value

$u_{x_5} := 1.30 \cdot \frac{m}{s}$ $v_{x_5} := 2.70 \cdot \frac{m}{s}$ $q_{x_5} := 0.000253 \cdot \frac{mol}{m^3 \cdot s}$

The new change in concentration is

$\Delta C_5 := C_3 - C_4$ $\Delta C_5 = 0.02 \frac{mol}{m^3}$

$\lambda_{x_5} := 4 \cdot \frac{m}{s}$

New flux at next grid point i + 5 is

$$F_{i+5} := C_4 \cdot \left(u_{x_5} + v_{x_5} \right) - k \cdot \frac{\Delta C_5}{\Delta x}$$

$$F_{i+5} = 3.68 \frac{mol}{m^2 \cdot s}$$

Flux at grid point i will be flux previous calculated as i + 4, that is

$F_{i_5} := F_{i+4}$ $F_{i_5} = 3.51 \frac{mol}{m^2 \cdot s}$

New flux at grid point i + 1/2 is

$\Delta F_5 := \lambda_{x_5} \cdot \Delta C_5$ $\Delta F_5 = 0.08 \frac{mol}{m^2 \cdot s}$

$F_{\frac{(i)5}{2}} := \frac{1}{2} \cdot \left(F_{i+5} + F_{i_5} \right) - \frac{1}{2} \cdot \Delta F_5$ $F_{\frac{(i)5}{2}} = 3.56 \frac{mol}{m^2 \cdot s}$

$$F_{\substack{-(i)5\\2}} := F_{\substack{(i)4\\2}}$$

$$F_{\substack{(i)4\\2}} := 3.39 \cdot \frac{mol}{m^2 \cdot s}$$

$$F_{\substack{-(i)5\\2}} = 3.39 \frac{mol}{m^2 \cdot s}$$

Using Roe-Riemann Solver

$$\Delta t := 0.1 \cdot s \qquad \Delta x := 1 \cdot m \qquad C_4 := 0.92 \cdot \frac{mol}{m^3}$$

$$C_5 := C_4 - \frac{\Delta t}{\Delta x} \cdot \left[F_{\substack{(i)5\\2}} - F_{\substack{-(i)5\\2}} \right] + \Delta t \cdot q_{x_5}$$

$$C_5 := 0.92 \cdot \frac{mol}{m^3} - \frac{0.1 \cdot s}{1 \cdot m} \cdot (3.56 - 3.39) \cdot \frac{mol}{m^2 \cdot s} + 0.1 \cdot s \cdot \left(0.000253 \cdot \frac{mol}{m^3 \cdot s} \right)$$

$$C_5 = 0.9 \frac{mol}{m^3}$$

Sixth_value

$$u_{x_6} := 1.50 \cdot \frac{m}{s} \qquad v_{x_6} := 2.75 \cdot \frac{m}{s} \qquad q_{x_6} := 0.000275 \cdot \frac{mol}{m^3 \cdot s}$$

The new change in concentration is

$$\Delta C_6 := C_4 - C_5$$

$$\Delta C_6 = 0.02 \frac{mol}{m^3}$$

$$\lambda_{x_6} := 4.25 \cdot \frac{m}{s}$$

New flux at next grid point i + 6 is

$$F_{i+6} := C_5 \cdot \left(u_{x_6} + v_{x_6} \right) - k \cdot \frac{\Delta C_6}{\Delta x}$$

$$F_{i+6} = 3.84 \frac{mol}{m^2 \cdot s}$$

Flux at grid point i will be flux previous calculated as i + 5, that is

$$F_{i_6} := F_{i+5}$$

$$F_{i_6} = 3.68 \frac{mol}{m^2 \cdot s}$$

New flux at grid point i + 1/2 is

$$\Delta F_6 := \lambda_{x_6} \cdot \Delta C_6$$

$$\Delta F_6 = 0.07 \frac{mol}{m^2 \cdot s}$$

$$F_{(i)6_{2}} := \frac{1}{2} \cdot \left(F_{i+6} + F_{i_6}\right) - \frac{1}{2} \cdot \Delta F_6$$

$$F_{(i)6_{2}} = 3.72 \frac{mol}{m^2 \cdot s}$$

$$F_{-(i)6_{2}} := F_{(i)5_{2}}$$

$$F_{(i)5_{2}} := 3.56 \cdot \frac{mol}{m^2 \cdot s}$$

$$F_{-(i)6_{2}} = 3.56 \frac{mol}{m^2 \cdot s}$$

Using Roe-Riemann Solver

$\Delta t := 0.1 \cdot s$ $\Delta x := 1 \cdot m$ $C_5 := 0.90 \cdot \frac{mol}{m^3}$

$$C_6 := C_5 - \frac{\Delta t}{\Delta x} \cdot \left[F_{(i)6_{2}} - F_{-(i)6_{2}}\right] + \Delta t \cdot q_{x_6}$$

$$C_6 := 0.90 \cdot \frac{mol}{m^3} - \frac{0.1 \cdot s}{1 \cdot m} \cdot (3.64 - 3.56) \cdot \frac{mol}{m^2 \cdot s} + 0.1 \cdot s \cdot \left(0.000275 \cdot \frac{mol}{m^3 \cdot s}\right)$$

$$C_6 = 0.89 \frac{mol}{m^3}$$

Seventh_value

$u_{x_7} := 1.70 \cdot \frac{m}{s}$ $v_{x_7} := 2.80 \cdot \frac{m}{s}$ $q_{x_7} := 0.000297 \cdot \frac{mol}{m^3 \cdot s}$

The new change in concentration is

$$\Delta C_7 := C_5 - C_6$$

$$\Delta C_7 = 7.97 \times 10^{-3} \frac{mol}{m^3}$$

$$\lambda_{x_7} := 4.50 \cdot \frac{m}{s}$$

New flux at next grid point i + 7 is

$$F_{i+7} := C_6 \cdot \left(u_{x_7} + v_{x_7}\right) - k \cdot \frac{\Delta C_7}{\Delta x}$$

$$F_{i+7} = 4.01 \frac{mol}{m^2 \cdot s}$$

Flux at grid point i will be flux previous calculated as i + 6, that is

$$F_{i_7} := F_{i+6}$$

$$F_{i_7} = 3.84 \frac{mol}{m^2 \cdot s}$$

New flux at grid point i + 1/2 is

$\Delta F_7 := \lambda_{x_7} \cdot \Delta C_7$ $\qquad \Delta F_7 = 0.04 \frac{mol}{m^2 \cdot s}$

$F_{\frac{(i)7}{2}} := \frac{1}{2} \cdot \left(F_{i+7} + F_{i_7}\right) - \frac{1}{2} \cdot \Delta F_7$

$F_{\frac{(i)7}{2}} = 3.91 \frac{mol}{m^2 \cdot s}$

$F_{\frac{(i)6}{2}} := 3.72 \cdot \frac{mol}{m^2 \cdot s}$

$F_{-\frac{(i)7}{2}} := F_{\frac{(i)6}{2}}$

$F_{-\frac{(i)7}{2}} = 3.72 \frac{mol}{m^2 \cdot s}$

Using Roe-Riemann Solver

$\Delta t := 0.1 \cdot s$ $\qquad \Delta x := 1 \cdot m$ $\qquad C_6 := 0.89 \cdot \frac{mol}{m^3}$

$$C_7 := C_6 - \frac{\Delta t}{\Delta x} \cdot \left[F_{\frac{(i)7}{2}} - F_{-\frac{(i)7}{2}}\right] + \Delta t \cdot q_{x_7}$$

$$C_7 := 0.89 \cdot \frac{mol}{m^3} - \frac{0.1 \cdot s}{1 \cdot m} \cdot (3.91 - 3.72) \cdot \frac{mol}{m^2 \cdot s} + 0.1 \cdot s \cdot \left(0.000297 \cdot \frac{mol}{m^3 \cdot s}\right)$$

$C_7 = 0.87 \frac{mol}{m^3}$

Eighth_value

$u_{x_8} := 1.90 \cdot \frac{m}{s}$ $\qquad v_{x_8} := 2.85 \cdot \frac{m}{s}$ $\qquad q_{x_8} := 0.000320 \cdot \frac{mol}{m^3 \cdot s}$

The new change in concentration is

$\Delta C_8 := C_6 - C_7$ $\qquad \Delta C_8 = 0.02 \frac{mol}{m^3}$

$\lambda_{x_8} := 4.75 \cdot \frac{m}{s}$

New flux at next grid point i + 8 is

$F_{i+8} := C_7 \cdot \left(u_{x_8} + v_{x_8}\right) - k \cdot \frac{\Delta C_8}{\Delta x}$ $\qquad F_{i+8} = 4.14 \frac{mol}{m^2 \cdot s}$

Flux at grid point i will be flux previous calculated as i + 7, that is

$F_{i_8} := F_{i+7}$

$$F_{i_8} = 4.01 \frac{mol}{m^2 \cdot s}$$

New flux at grid point i + 1/2 is

$\Delta F_8 := \lambda_{x_8} \cdot \Delta C_8$

$$\Delta F_8 = 0.09 \frac{mol}{m^2 \cdot s}$$

$$F_{\frac{(i)8}{2}} := \frac{1}{2} \cdot \left(F_{i+8} + F_{i_8}\right) - \frac{1}{2} \cdot \Delta F_8$$

$$F_{\frac{(i)8}{2}} = 4.03 \frac{mol}{m^2 \cdot s}$$

$F_{-\frac{(i)8}{2}} := F_{\frac{(i)7}{2}}$ $\qquad F_{\frac{(i)7}{2}} := 3.91 \cdot \frac{mol}{m^2 \cdot s}$

$$F_{-\frac{(i)8}{2}} = 3.91 \frac{mol}{m^2 \cdot s}$$

Using Roe-Riemann Solver

$$C_8 := C_7 - \frac{\Delta t}{\Delta x} \cdot \left[F_{\frac{(i)8}{2}} - F_{-\frac{(i)8}{2}}\right] + \Delta t \cdot q_{x_8}$$

$$C_8 := 0.87 \cdot \frac{mol}{m^3} - \frac{0.1 \cdot s}{1 \cdot m} \cdot (4.03 - 3.91) \cdot \frac{mol}{m^2 \cdot s} + 0.1 \cdot s \cdot \left(0.000320 \cdot \frac{mol}{m^3 \cdot s}\right)$$

$$C_8 = 0.86 \frac{mol}{m^3}$$

Ninth_value

$u_{x_9} := 2.10 \cdot \frac{m}{s}$ $\qquad v_{x_9} := 2.90 \cdot \frac{m}{s}$ $\qquad q_{x_9} := 0.000342 \cdot \frac{mol}{m^3 \cdot s}$

The new change in concentration is

$\Delta C_9 := C_7 - C_8$

$$\Delta C_9 = 0.01 \frac{mol}{m^3}$$

$\lambda_{x_9} := 5.0 \cdot \frac{m}{s}$

New flux at next grid point i + 9 is

$$F_{i+9} := C_8 \cdot \left(u_{x_9} + v_{x_9}\right) - k \cdot \frac{\Delta C_9}{\Delta x}$$

$$F_{i+9} = 4.29 \frac{\mathrm{mol}}{\mathrm{m}^2 \cdot \mathrm{s}}$$

Flux at grid point i will be flux previous calculated as i + 8, that is

$$F_{i_9} := F_{i+8}$$

$$F_{i_9} = 4.14 \frac{\mathrm{mol}}{\mathrm{m}^2 \cdot \mathrm{s}}$$

New flux at grid point i + 1/2 is

$$\Delta F_9 := \lambda_{x_9} \cdot \Delta C_9$$

$$\Delta F_9 = 0.06 \frac{\mathrm{mol}}{\mathrm{m}^2 \cdot \mathrm{s}}$$

$$F_{\frac{(i)9}{2}} := \frac{1}{2} \cdot \left(F_{i+9} + F_{i_9}\right) - \frac{1}{2} \cdot \Delta F_9$$

$$F_{\frac{(i)9}{2}} = 4.18 \frac{\mathrm{mol}}{\mathrm{m}^2 \cdot \mathrm{s}}$$

$$F_{-\frac{(i)9}{2}} := F_{\frac{(i)8}{2}}$$

$$F_{\frac{(i)8}{2}} := 4.03 \cdot \frac{\mathrm{mol}}{\mathrm{m}^2 \cdot \mathrm{s}}$$

$$F_{-\frac{(i)9}{2}} = 4.03 \frac{\mathrm{mol}}{\mathrm{m}^2 \cdot \mathrm{s}}$$

Using Roe-Riemann Solver

$$C_9 := C_8 - \frac{\Delta t}{\Delta x} \cdot \left[F_{\frac{(i)9}{2}} - F_{-\frac{(i)9}{2}}\right] + \Delta t \cdot q_{x_9}$$

$$C_9 := 0.86 \cdot \frac{\mathrm{mol}}{\mathrm{m}^3} - \frac{0.1 \cdot \mathrm{s}}{1 \cdot \mathrm{m}} \cdot (4.18 - 4.03) \cdot \frac{\mathrm{mol}}{\mathrm{m}^2 \cdot \mathrm{s}} + 0.1 \cdot \mathrm{s} \cdot \left(0.000342 \cdot \frac{\mathrm{mol}}{\mathrm{m}^3 \cdot \mathrm{s}}\right)$$

$$C_9 = 0.85 \, \mathrm{mol\,m}^{-3}$$

Tenth_value

$$u_{x_{10}} := 2.30 \cdot \frac{\mathrm{m}}{\mathrm{s}} \qquad v_{x_{10}} := 2.95 \cdot \frac{\mathrm{m}}{\mathrm{s}} \qquad q_{x_{10}} := 0.000364 \cdot \frac{\mathrm{mol}}{\mathrm{m}^3 \cdot \mathrm{s}}$$

The new change in concentration is

$$\Delta C_{10} := C_8 - C_9$$

$$\Delta C_{10} = 0.01 \frac{\mathrm{mol}}{\mathrm{m}^3}$$

$$\lambda_{x_{10}} := 5.25 \cdot \frac{\mathrm{m}}{\mathrm{s}}$$

New flux at next grid point i + 10 is

$$F_{i+10} := C_9 \cdot \left(u_{x_{10}} + v_{x_{10}}\right) - k \cdot \frac{\Delta C_{10}}{\Delta x} \qquad F_{i+10} = 4.44 \frac{mol}{m^2 \cdot s}$$

Flux at grid point i will be flux previous calculated as i + 9, that is

$$F_{i_{10}} := F_{i+9} \qquad F_{i_{10}} = 4.29 \frac{mol}{m^2 \cdot s}$$

New flux at grid point i + 1/2 is

$$\Delta F_{10} := \lambda_{x_{10}} \cdot \Delta C_{10} \qquad \Delta F_{10} = 0.07 \frac{mol}{m^2 \cdot s}$$

$$F_{\substack{(i)10\\2}} := \frac{1}{2} \cdot \left(F_{i+10} + F_{i_{10}}\right) - \frac{1}{2} \cdot \Delta F_{10} \qquad F_{\substack{(i)10\\2}} = 4.33 \frac{mol}{m^2 \cdot s}$$

$$F_{-\substack{(i)10\\2}} := F_{\substack{(i)9\\2}} \qquad F_{\substack{(i)9\\2}} := 4.18 \cdot \frac{mol}{m^2 \cdot s}$$

$$F_{-\substack{(i)10\\2}} = 4.18 \frac{mol}{m^2 \cdot s}$$

Using Roe-Riemann Solver

$$C_{10} := C_9 - \frac{\Delta t}{\Delta x} \cdot \left[F_{\substack{(i)10\\2}} - F_{-\substack{(i)10\\2}}\right] + \Delta t \cdot q_{x_{10}}$$

$$C_{10} := 0.85 \cdot \frac{mol}{m^3} - \frac{0.1 \cdot s}{1 \cdot m} \cdot (4\ 33 - 4.18) \cdot \frac{mol}{m^2 \cdot s} + 0.1 \cdot s \cdot \left(0.000364 \cdot \frac{mol}{m^3 \cdot s}\right)$$

$$C_{10} = 0.84 \frac{mol}{m^3}$$

Eleventh_value

$u_{x_{11}} := 2.50 \cdot \frac{m}{s}$ $\quad v_{x_{11}} := 3.00 \cdot \frac{m}{s}$ $\quad q_{x_{11}} := 0.000368 \cdot \frac{mol}{m^3 \cdot s}$

The new change in concentration is

$\Delta C_{11} := C_9 - C_{10}$ $\quad \Delta C_{11} = 10 \times 10^{-3} \frac{mol}{m^3}$

$\lambda_{x_{11}} := 5.5 \cdot \frac{m}{s}$

New flux at next grid point i + 11 is

$F_{i+11} := C_{10} \cdot \left(u_{x_{11}} + v_{x_{11}}\right) - k \cdot \frac{\Delta C_{11}}{\Delta x}$ $\quad F_{i+11} = 4.59 \frac{mol}{m^2 \cdot s}$

Flux at grid point i will be flux previous calculated as i + 10, that is

$F_{i_{11}} := F_{i+10}$ $\quad F_{i_{11}} = 4.44 \frac{mol}{m^2 \cdot s}$

New flux at grid point i + 1/2 is

$\Delta F_{11} := \lambda_{x_{11}} \cdot \Delta C_{11}$ $\quad \Delta F_{11} = 0.05 \frac{mol}{m^2 \cdot s}$

$F_{(i)\frac{11}{2}} := \frac{1}{2} \cdot \left(F_{i+11} + F_{i_{11}}\right) - \frac{1}{2} \cdot \Delta F_{11}$ $\quad F_{(i)\frac{11}{2}} = 4.49 \frac{mol}{m^2 \cdot s}$

$F_{-(i)\frac{11}{2}} := F_{(i)\frac{10}{2}}$ $\quad F_{(i)\frac{10}{2}} := 4.33 \cdot \frac{mol}{m^2 \cdot s}$

$F_{-(i)\frac{11}{2}} = 4.33 \frac{mol}{m^2 \cdot s}$

Using Roe-Riemann Solver

$$C_{11} := C_{10} - \frac{\Delta t}{\Delta x} \cdot \left[F_{(i)\frac{11}{2}} - F_{-(i)\frac{11}{2}} \right] + \Delta t \cdot q_{x_{11}}$$

$$C_{11} := 0.84 \cdot \frac{mol}{m^3} - \frac{0.1 \cdot s}{1 \cdot m} \cdot (4.49 - 4.33) \cdot \frac{mol}{m^2 \cdot s} + 0.1 \cdot s \cdot \left(0.000368 \cdot \frac{mol}{m^3 \cdot s} \right) \qquad C_{11} = 0.82 \frac{mol}{m^3}$$

APPENDIX C

a. Density of Air (ρ)

From the general gas equation,

$PV = nRT$

$PV = \frac{m}{M}RT$

$P = \frac{m}{V} \times \frac{RT}{M}$

$P = \rho\frac{RT}{M}$

$\rho = \frac{PM}{RT}$

where

P = atmospheric pressure (atm)

M = molecular mass of air (g/mol)

m = mass of air (g)

R = gas constant ($atm.cm^3/mol.k$)

T = temperature = 30°C = 303K

Therefore, $\rho = \frac{1 \text{ X } 2.9}{82.1 \text{ X } 303} = 1.1658 \text{ x } 10^{-3} g/cm^3 = 1.1658 kg/m^3$

b. Diffusion coefficient (K_{AB}) of carbon monoxide/air system from the Fuller, Schettler and

$$K_{CO/air} = \frac{1.0 \text{ X } 10^{-7} \text{ X } T^{1.75} \text{ X } [\frac{1}{M_A} \text{ X } \frac{1}{M_B}]^{\frac{1}{2}}}{P[(\Sigma V_A)^{0.33} + (\Sigma V_B)^{0.33}]^2}$$

Where

T = atmospheric temperature of 30°C

P = atmospheric pressure of 1atm

ΣV_A = atomic diffusion volume of air = 18.9

ΣV_B = atomic diffusion of CO = 20.1

M_A = molecular weight of air = 29g/mol

M_B = molecular weight of CO = 28g/mol

$$K_{CO/air} = \frac{1.0 \times 10^{-7} \times 303^{1.75} \times (1/2 + 1/2)^{1/2}}{28.40481004} = 2.05 \times 10^{-5}\ m^2/s$$

PPENDIX D

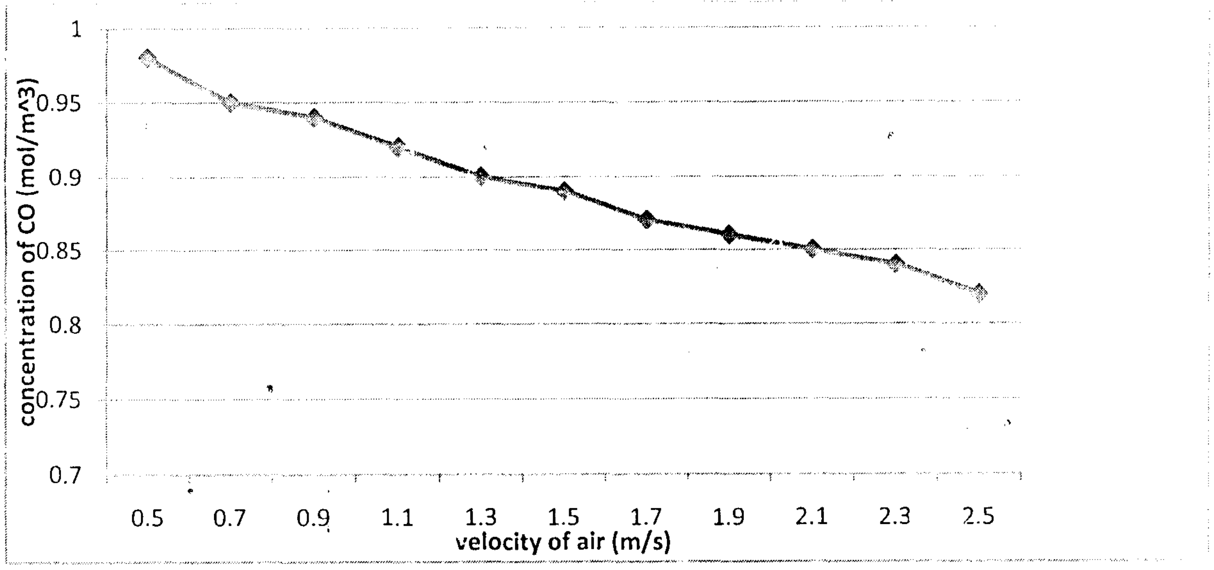

Figure 4.1 Concentration of CO (mol/m^3) against velocity of air, V (m/s).

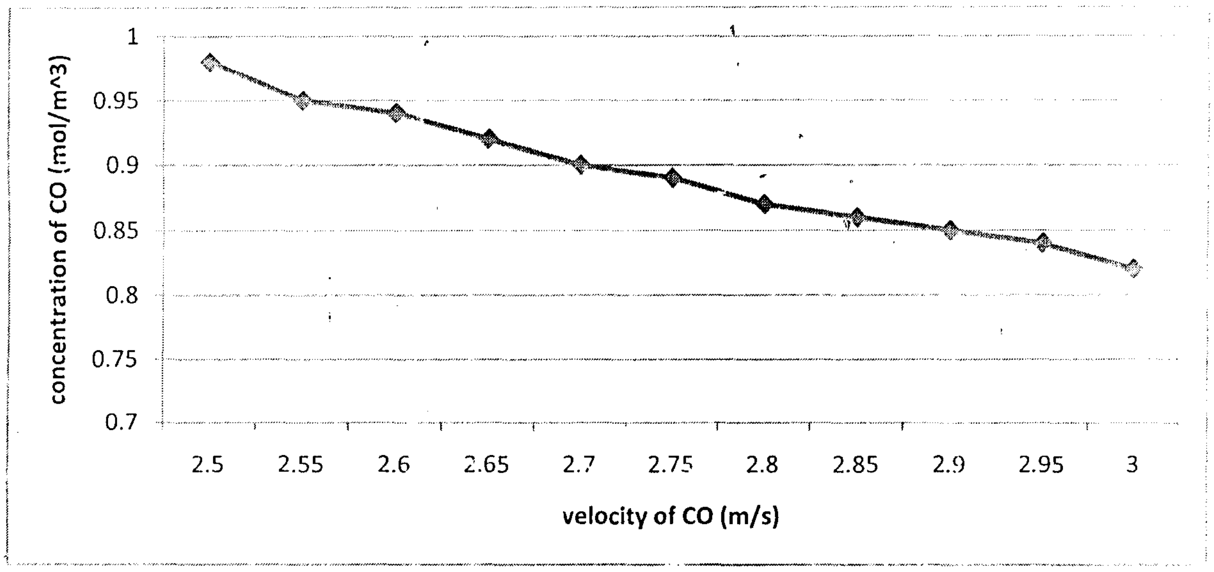

Figure 4.2 Concentration of CO (mol/m^3) against velocity of CO, U (m/s).

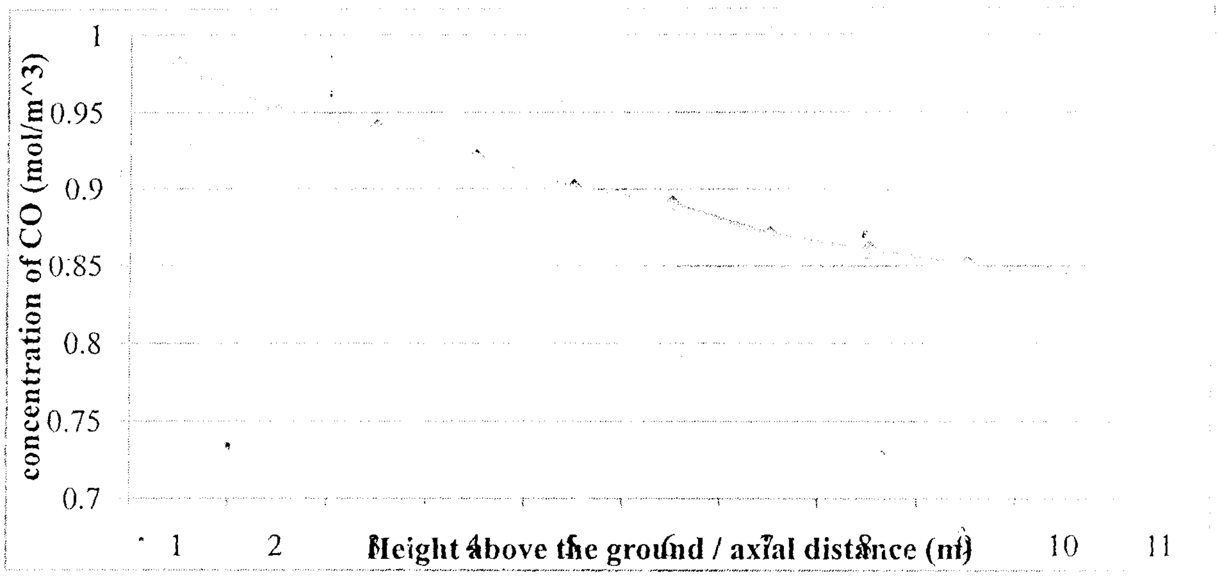

Figure 4.3 Concentration of CO (mol/m^3) against Height/axial distance above ground level (m)