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NUMERICAL SOLUTION OF ADVECTION-DIFFUSION OF AN AIR POLLUTANT BY THE FRACTIONAL STEP METHOD

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วิทยานิพนธ์ฉบับนี้เป็นการศึกษาคุณลักษณะของมลพิษทางอากาศในสองมิติ ที่ถูกปล่อยออกสู่ชั้นบรรยากาศจากแหล่งกำเนิดที่เป็นเส้นตรง โดยขึ้นอยู่กับเวลา ในกรณีที่มีชั้นสะท้อนกลับ เราใช้วิธีการเชิงตัวเลข ซึ่งขึ้นอยู่กับการแบ่งโดเมนของสมการการพาและการแพร่กระจายที่ขึ้นอยู่กับเวลา เพื่อหาความเข้มข้นของมลพิษทางอากาศในทิศทางใต้ลมของแหล่งกำเนิดที่มีความสูง h จากพื้นดิน ผลเฉลยของปัญหาในระบบเต็มหน่วย ได้มาจากวิธีการเชิงตัวเลขแบบแยกส่วน สมมติให้ความเข้มข้นของมลพิษ ณ เวลาเริ่มต้นมีค่าเป็นศูนย์ อัตราการไหลของความเข้มข้นที่ชั้นสะท้อนกลับ และที่พื้นดินมีค่าเป็นศูนย์ กำหนดให้ความเข้มข้นที่ถูกปล่อยออกมา จากแหล่งกำเนิดเป็นฟังก์ชันเดลต้าในอัตราคงที่ เราใช้โปรแกรมเมเปิล และโปรแกรมแมทแลบในการคำนวณหาค่าความเข้มข้นของมลพิษที่เป็นผลเฉลยของปัญหา ซึ่งได้แสดงไว้ในลักษณะของกราฟเส้นควบคุมความเข้มข้นของมลพิษ ที่สัมประสิทธิ์ของการพาและการแพร่กระจาย แตกต่างกัน

สาขาวิชาคณิตศาสตร์ ลายมือชื่อนักศึกษา.....

ปีการศึกษา 2544 ลายมือชื่ออาจารย์ที่ปรึกษา.....

SUREERAT AREERAKSAKUL: NUMERICAL SOLUTION OF ADVECTION- DIFFUSION OF AN AIR POLLUTANT BY THE FRACTIONAL STEP METHOD THESIS ADVISOR: ASSOC. PROF. SUWON TANGMANEE, Ph. D 68 PP. ISBN 974-533-039-6

The main goal of this thesis is to study the time dependent behavior in two dimensional space of an air pollutant which is released into the atmosphere from the line source in the presence of an inversion layer. We use the numerical approach, which is based on the discretization of the time dependent advection-diffusion equation governing the evolution in time of the concentration of pollutant downwind of the line source at height h above the ground. The resulting discrete problem is obtained by a fractional step method. The initial condition is taken to be zero concentration of pollutant. The flux of pollutant is assumed to be zero at the ground and at the inversion layer. The concentration of pollutant at the source is assumed to be a δ-function, which gives rise to a steady emission rate of pollutant from the source. We implement the numerical method using both Maple and Matlab in order to obtain the solution of the problems. The contour line of concentrations for different values of advection-diffusion coefficients, were presented.

สาขาวิชาคณิตศาสตร์ ลายมือชื่อนักศึกษา.....
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Sureerat Areeraksakul

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Chapter I
Introduction

Air pollution is the presence of undersirable material in air, in quantities large enough to produce harmful effects. This definition does not restrict air pollution to human causes, although we normally only talk about these. The undesirable materials may damage human health, vegetation, human property, or the global environment as well as create aesthetic insults in the form of brown or hazy air or unpleasant smells. Pollutants are known that may do all of these things. Many of these harmful materials enter the atmosphere from sources currently beyond human control. However, in the most densely inhabited parts of the globe, particularly in the industrialized countries, the principal sources of these pollutants are human activities. These activities are closely associated with our material standard of living. To eliminate these activities would cause such a drastic decrease in the standard of living that this action is seldom considered. The remedy proposed in most industrial countries is to continue the activities and control the air pollutant emissions from them.

1.1 Source of Air Pollution

From the fourteenth century until recently, the primary air pollutants have been coal smoke and gases released in industrialized areas. Unfortunately, control of pollutants rarely takes place prior to public outcry, even though the technology for controlling pollutants may be available. Early recognition of pollutants as health hazards has not resulted in pollution reduction, only when personal survival is at stake has effective action been taken against pollutants.

There are a number industrial processes which can also be source of air pollutants, with each industrial branch having its own problems with keeping the air clean. A description of the numerous processes with their specific emissions cannot be undertaken in this thesis. The interested reader is referred to special literature on this subject.

In developing countries, though, with less industrialization and motorization, the technical processes applied have not been optimized yet, so that their specific emissions are frequently higher.

A great deal of industrial pollution comes from manufacturing products from raw materials (iron from ore, lumber from trees, gasoline from crude oil, and stone from quarries) Each of these manufacturing processes produces a product, along with several waste products which we term pollutants. Occasionally, part or all of the polluting material can be recovered and converted into a unstable product.

Industrial pollution is also emitted by industries that convert products to other products (automobile bodies from steel, furniture from lumber, paint from solids and solvent, and asphaltic paving from rock and oil).

Industrial source are stationary, and each emits relatively consistent qualities and quantities of pollutants. A paper mill, for example, will be in the same place tomorrow that it is today, emitting the same quantity of the same kinds of pollutants unless a major process change in made. Control of industrial sources can usually be accomplished by applying known technology. The most effective regulatory control is that which is applied uniformly within all segments of industries in a given region, e.g., "Emission from all asphalt dryers in this region shall not exceed 230 mg of particulate matter per standard dry cubic meter of air."

1.2 Effect of Air Pollution

We control air pollution because it causes harmful effects on human health, property, aesthetics, and the global climate. Because the air pollution laws and other industrialized countries are mostly concerned with protecting human health, we will consider the effects on human health.

In Bhopal, India, in December 1984, a release of methyl isocyanate from a pesticide plant killed about 2500 people. Similar leakages of hydrogen sulfide from natural gas processing plants have killed hundreds of people. These tragic events attract wide attention. Normally, they are not considered air pollution evens, but rather industrial accidents. The damages to human health caused by air pollution are of a very different type. The materials involved are rarely as toxic as methyl isocyanate or hydrogen sulfide. They are generally not released in concentrations nearly as high as those that cause such disasters. Their effects normally do not result from a single exposure (methyl isocyanate and hydrogen sulfide can kill in minute or two), but from repeated exposure to low concentrations for long periods.

1.3 Primary Contents on Air Pollution Study

The settlements of the global environmental problem depend on the status of pollutant emissions, economic developing level, environmental investment intensity,

controlling strategy and managing level in different subregions (Asia, Africa, North America and Europe). There is abundant evidence that air pollution has adverse effects on man's health and well-being, on animal, plants and materials, and on other environmental media and climate.

East Asia is one of the regions where concentration of acid pollutant due to man-made emission and secondary pollutants are the highest in the world (Kondo 1991). Many countries in East Asia are speeding up the energy system, population and economic increase at the top speed. If the present trend is continued, Asia will become the biggest source of SO_2 and NO_2 in the world by the 21st century. A substantial portion of emission is transported by winds, hundreds to thousands of kilometers from the source. Many countries are attempting to minimize their local pollution problems by installing taller stacks. As a result, serious transnational pollution is made in broad of East Asia.

Comprehensive field experiment on environmental parameters, which include data of physical, chemical, and biological process, for different biological systems (e.g. urban, water, forest, agriculture, barren land, grass land, and sands) are very necessary to obtaining the data on air-land exchange, fluxes of mass momentum and heat, and ecological effects. The data can provide sound bases for further research on regional air pollution and biological environment (Tester 1990).

The Cross-Appalachian Tracer Experiment (Draxler 1988) consisted of seven ground-level tracer gas releases from Dayton, Ohio or Subury, Ontario during 1983. The concentration profiles measured by aircraft 600-900 km downwind of the release locations were discussed and compared with some model results. In general, concentration decreased with height in the upper PBL (planetary boundary layer) where the aircraft measurements were made. The results of a model sensitivity study suggested that the shape of the profile be primarily due to wind whose velocities increase with height and relative position of the sampling with respect to the upwind and downwind edge of the plume.

The tree-dimensional (3-D) wind, temperature and rain fields can be generated with mesoscale meteorological model (Anthes 1987, Guo 1994, Walko 1995). Different PBL models (Longhetto, Lumley 1980) can forecast turbulent vertical structures and variations of turbulence statistics with height in PBL for different terrain. The mountain and valley breeze, land and lake Breeze, land and river breeze and circulation of urban heat island are very important to correctly calculate air pollution distribution.

Effect of vertical inhomogeneity and non-stationary of PBL (planetary boundary layer) parameters on the mesoscale diffusion (IAP 1990) is very obvious. Vertical exchange processes of species and momentum in troposphere is very complex (Gifford

1988b). The mesoscale turbulent diffusive patterns can be derived by numerical methods (IAP 1990). Effect of the mesoscale local circulation on diurnal variation of the concentration can be studied with the meso$-\beta$ model (Walko 1995).

Air pollution law in most industrial countries is based on some kind of permitted concentration of contaminants. To plan and execute air pollution control programs designed to meet the requirements of these laws, one must predict the ambient air concentrations that will result from any planned set of emissions. Even if we did not use this type of air pollution law, we would probably use some other kind of law that made some use of predictions of ambient contaminant concentrations. These predictions are made by way of air pollutant concentration models.

The perfect air pollutant concentration model would allow us to predict the concentrations that would result from any specified set of pollutant emissions, for any specified meteorological conditions, at any location, for any time period, with total confidence in our prediction. The best currently available models are far from this ideal.

1.4 Mathematical Model Formulation in Air Pollution

Most advection-diffusion models of an air pollutant use the Gaussian plume idea, whitch also is a material balance model. In it, one considers a point source such as a factory smokestack (which is not really a point but a small area that can be satisfactorily approximated as a point) and attempts to compute the downwind concentration resulting from this point source. The schematic representation and nomenclature are show in Figure 1.1, where the origin of the coordinate system is placed at the base of the smoke stack, with the $x-$axis aligned in the downwind direction, The contaminated gas stream (normally called *plume*) is shown rising from the smokestack and then leveling off to travel in the x direction and spreading in the y and z directions as it travels.

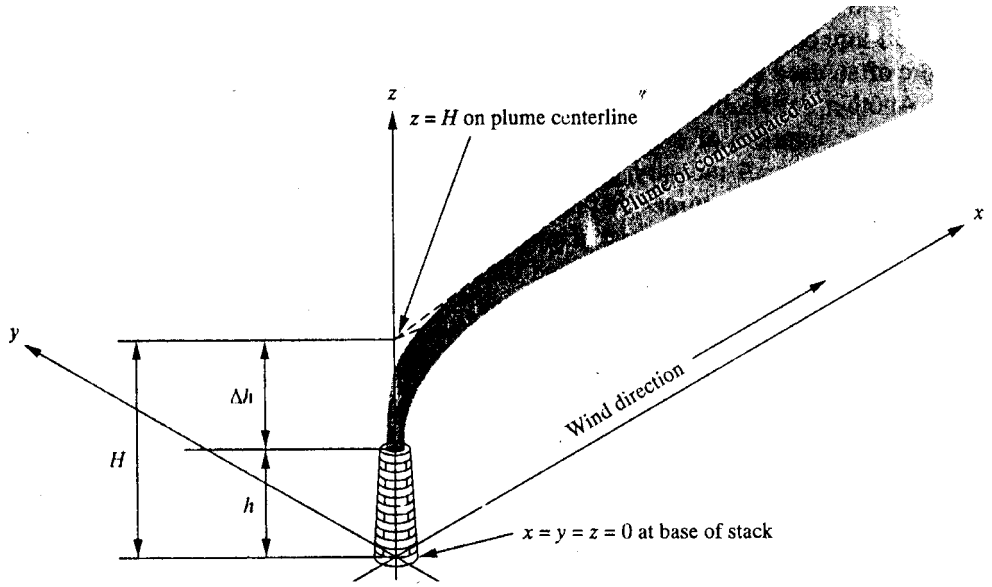


Figure:1.1 Coordinate system and nomenclature for the Gaussian plum idea.

The well known process of diffusion of pollutants downwind from a source is assumed to be governed by the differential equation

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + w\frac{\partial c}{\partial z} = \frac{\partial}{\partial x}\left(K_x\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y\frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial c}{\partial z}\right) \qquad (1.1)$$

where $c(x, y, z, t)$ is a concentration of pollutant at any point (x, y, z) and at the time t, u, w are the horizontal and vertical components of the wind velocity, and K_x, K_y, K_z are the coefficients of diffusion along the $x-, y-, z-$ directions, respectively.

We make the following assumptions:

(1) The direction of the wind is chosen along the $x-$axis.

(2) The meteorological conditions are such that horizontal advection by the wind dominates the horizontal diffusion and that vertical diffusion dominates the vertical advection by the wind.

By the assumptions, we have

$$u\frac{\partial c}{\partial x} \gg \frac{\partial}{\partial x}\left(K_x\frac{\partial c}{\partial x}\right) \quad and \quad w\frac{\partial c}{\partial z} \ll \frac{\partial}{\partial z}\left(K_z\frac{\partial c}{\partial z}\right).$$

Omitting the negligible terms of equation (1.1) , we get

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = \frac{\partial}{\partial y}\left(K_y\frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial c}{\partial z}\right). \qquad (1.2)$$

Analytic solutions of equation (1.2) for steady-state conditions have been reported by several investigators (Pasquill 1962, Rounds 1955, Sutton 1953, Smith 1957) for

different boundary conditions and different expression for u, K_y, K_z as functions of the independent variables. Time dependent analytic solutions of equation (1.2) however, are not known for arbitrary functions u, K_y, K_z. We also assume that we have a uniform line source along the $y-$axis. Thus we can eliminate the diffusion in the $y-$direction. This leads to the equation

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = \frac{\partial}{\partial z}\left(K_z \frac{\partial c}{\partial z}\right).$$

We first simplify the problem further by assuming that the wind velocity u and the diffusion coefficient K_z are independent of x, thus we can write the equation for the concentration $c = c(x, z, t)$ in the final form

$$\frac{\partial c}{\partial t} + u(z)\frac{\partial c}{\partial x} = \frac{\partial}{\partial z}\left(K_z \frac{\partial c}{\partial z}\right). \tag{1.3}$$

Suppose we have a source of pollutant at height h on the $z-$axis. We assume zero flux of concentration at ground level $z = 0$ and at height $z = H$, the bottom and the height of the inversion layers, respectively. Thus, we solve equation (1.3) for all $t > 0, x > 0$ and $0 < z < H$.

The initial condition is assumed to be zero concentration of pollutant everywhere in the domain. The flux of pollutant is assumed to be zero at the ground and at the inversion layer located at height H. The concentration of pollutant at the source is assumed to be a $\delta-$function, which gives rise to a steady emission rate Q of pollutant from the line source.

The initial condition:

$$c(x, z, 0) = 0 \qquad \text{for} \qquad x > 0, 0 < z < H \tag{1.4}$$

The boundary condition on the $z-$axis:

$$c(0, z, t) = \frac{Q}{u(h)}\delta(z - h) \qquad \text{for} \qquad t > 0, 0 < z < H \tag{1.5}$$

The boundary conditions on the inversion layers:

$$\frac{\partial c}{\partial z}(x, 0, t) = 0 \qquad \text{for} \qquad x > 0, t > 0 \tag{1.6}$$

$$\frac{\partial c}{\partial z}(x, H, t) = 0 \qquad \text{for} \qquad x > 0, t > 0 \tag{1.7}$$

1.5 Non-Dimensional Form

We now non-dimensionalize the problem by dividing the variables x, z, t, h, c, u, K respectively by the expressions $\frac{H^2 u(H)}{K(H)}, H, \frac{H^2}{K(H)}, H, \frac{QH}{u(H)}, u(H), K(H)$, so that

Remark 1.5.1

$$\frac{\partial c_{old}}{\partial t_{old}} + u_{old}\frac{\partial c_{old}}{\partial x_{old}} = \frac{\partial}{\partial z_{old}}\left(K_{z_{old}}\frac{\partial c_{old}}{\partial z_{old}}\right)$$

then

$$\frac{\partial c_{new}\cdot\frac{Q\cdot H}{u(H)}}{\partial t_{new}\cdot\frac{H^2}{K(H)}} + u_{new}\cdot u(H)\frac{\partial c_{new}\cdot\frac{Q\cdot H}{u(H)}}{\partial x_{new}\cdot\frac{H^2\cdot u(H)}{K(H)}}$$

$$= \frac{\partial\left(K_{z_{new}}\cdot K(H)\dfrac{\partial c_{new}\cdot\frac{Q\cdot H}{u(H)}}{\partial z_{new}\cdot H}\right)}{\partial z_{new}\cdot H}$$

then

$$\frac{Q\cdot H}{u(H)}\cdot\frac{K(H)}{H^2}\cdot\frac{\partial c_{new}}{\partial t_{new}} + u_{new}\cdot u(H)\cdot\frac{Q\cdot H}{u(H)}\cdot\frac{K(H)}{H^2\cdot u(H)}\cdot\frac{\partial c_{new}}{\partial x_{new}}$$

$$= K(H)\cdot\frac{Q\cdot H}{u(H)}\cdot\frac{1}{H}\cdot\frac{1}{H}\frac{\partial\left(K_{z_{new}}\dfrac{\partial c_{new}}{\partial z_{new}}\right)}{\partial z_{new}}$$

thus,

$$\frac{\partial c_{new}}{\partial t_{new}} + u_{new}\frac{\partial c_{new}}{\partial x_{new}} = \frac{\partial}{\partial z_{new}}\left(K_{z_{new}}\frac{\partial c_{new}}{\partial z_{new}}\right).$$

Remark 1.5.2

$$\begin{aligned}
c_{new}(x_{new}, z_{new}, 0) &= 0 \qquad \forall x_{new} > 0, 0 < z_{new} < 1\\
\frac{\partial c_{new}(x_{new}, 0, t_{new})}{\partial z_{new}} &= 0 \qquad \forall x_{new} > 0, t_{new} > 0\\
\frac{\partial c_{new}(x_{new}, 1, t_{new})}{\partial z_{new}} &= 0 \qquad \forall x_{new} > 0, t_{new} > 0
\end{aligned}$$

and

$$\begin{aligned}
c_{old}(0, z_{old}, t_{old}) &= \frac{Q}{u_{old}(h)}\delta(z_{old} - h_{old}) \qquad \forall x_{old} > 0, 0 < z_{old} < H\\
c_{new}(0, z_{new}, t_{new}) &= \frac{Q}{u_{new}(h)\cdot u(H)}\delta(z_{new}\cdot H - h_{new}\cdot H)\cdot\frac{u(H)}{Q\cdot H}\\
&= \frac{Q\cdot H}{u_{new}(h)\cdot u(H)}\delta(z_{new} - h_{new})\cdot\frac{u(H)}{Q\cdot H}\\
&= \frac{\delta(z_{new} - h_{new})}{u_{new}(h)} \qquad \forall x_{new} > 0, 0 < z_{new} < 1.
\end{aligned}$$

We use the same notation for the non-dimensionalized variables. In these new variables the resulting system is

$$\frac{\partial c}{\partial t} + u(z)\frac{\partial c}{\partial x} = \frac{\partial}{\partial z}\left(K_z \frac{\partial c}{\partial z}\right) \qquad \forall x > 0, 0 < z < 1, t > 0 \tag{1.8}$$

with the initial condition:

$$c(x, z, 0) = 0 \qquad \text{for} \qquad x > 0, 0 < z < 1 \tag{1.9}$$

and the boundary condition on the $z-$axis:

$$c(0, z, t) = \frac{\delta(z - h)}{u(h)} \qquad \text{for} \qquad t > 0, 0 < z < 1 \tag{1.10}$$

and the boundary conditions on the inversion layers:

$$\frac{\partial c}{\partial z}(x, 0, t) = 0 \qquad \text{for} \qquad x > 0, t > 0 \tag{1.11}$$

$$\frac{\partial c}{\partial z}(x, 1, t) = 0 \qquad \text{for} \qquad x > 0, t > 0. \tag{1.12}$$

(Note that in this representation both the emission rate and the height of the inversion layer base are normalized to unity.)

1.6 The Objective of This Thesis

The main goals of this thesis as follows:

(1) To find the numerical approximation to the solution of the mathematical model of an air pollutant released into the atmosphere from the line source in the presence of an inversion layer. The mathematical model consists of the time dependent advection-diffusion equation. The inversion layer acts as an impermeable barrier to the flux of the pollutant to higher levels of the atmosphere.

(2) To develop a computer program for predicting the scattering of an air pollutant by mathematical model.

(3) To use this computer codes to calculated behaviour of an air pollutant for difference from of wind profiles.

1.7 The Scope and Limitations of This Thesis

We will restrict to the problem given by equations (1.8), (1.9), (1.10), (1.11) and (1.12). The wind profile and the diffusion coefficient are constants or are functions of z only.

Chapter II
Preliminaries

2.1 Fractional Step Method

In Yanenko, 1961 the method of splitting (fractional steps) was formulated as a method for the construction of economical implicit schemes for a system of partial differential equations. In Yanenko, 1961 only the two-layer systems in fractional steps were studied. In the paper of G.I. Marchuk and N.N. Yanenko (Marchuk, Yanenko 1966), this method was formulated for systems of differential equations and many-layer schemes in fractional step for a linear system of integro-differential equations with respect to an unknown vector function of the form

$$\frac{\partial u}{\partial t} = \Omega u + f, \tag{2.1}$$

for which the Cauchy problem is correctly posed in some Banach space

$$u(x,0) = u_0(x), \tag{2.2}$$

where

$$\Omega = \Omega_1 + \Omega_2 + ... + \Omega_p, \tag{2.3}$$

is the representation of integro-differential operator Ω as the sum of p operators $\Omega_1, \Omega_2, ..., \Omega_p$; the operators $\Omega_1, \Omega_2, ..., \Omega_p$ are approximated by operators Λ_{ij} in such a way that the following approximate representations are valid

$$\left.\begin{array}{c} \Lambda_{10} + \Lambda_{11} \sim \Omega_1; \\ \Lambda_{20} + \Lambda_{21} + \Lambda_{22} \sim \Omega_2; \\ ..... \\ \Lambda_{p0} + \Lambda_{p1} + ... + \Lambda_{pp} \sim \Omega_p. \end{array}\right\} \tag{2.4}$$

(Operators Λ_{ij} can be of arbitrary structure both difference and integro-differential.)

The method of splitting is

$$\left.\begin{array}{c} \dfrac{u^{n+1/p}-u^{n}}{\tau}=\Lambda_{10}u^{n}+\Lambda_{11}u^{n+1/p}+F_1; \\ \dfrac{u^{n+2/p}-u^{n+2/p}}{\tau}=\Lambda_{20}u^{n}+\Lambda_{21}u^{n+1/p}+\Lambda_{22}u^{n+2/p}+F_2; \\ \cdots\cdots\cdots\cdots \\ \dfrac{u^{n+1}-u^{n+(p-1)/p}}{\tau}=\Lambda_{p0}u^{n}+\Lambda_{p1}u^{n+1/p}+....+\Lambda_{pp}u^{n}+F_p; \end{array}\right\} \tag{2.5}$$

where

$$F_s=\Lambda_s f \quad ; \quad \sum_{s=1}^{p}\Lambda_s \sim E. \tag{2.6}$$

2.2 Partial Differential Equations

The subject of PDEs was practically a branch of physics until the twentieth century.

2.2.1 General Form of Partial Differential Equation

The key defining property of a partial differential equation (PDE) is that there is more than one independent variable $x, y, \ldots$. There is a dependent variable u, that is unknown function of these independent variables $u(x, y, ...)$. We will often denote its derivatives by subscripts; thus $\dfrac{\partial u}{\partial x}=u_x$, and so on. A PDE is an identity that relates the independent variables, the dependent variable u, and the partial derivatives of u. It can be written as

$$F(x, y, u(x, y), u_x(x, y), u_y(x, y))=F(x, y, u, u_x, u_y)=0. \tag{2.7}$$

This is the most general PDE in two independent variables of first order. The *order* of an equation is the highest derivative that appears. Second-order PDE in general case can be written as

$$F(x, y, u, u_x, u_y, u_{xx}, u_{xy}, u_{yy})=0. \tag{2.8}$$

A *solution* of a PDE is a function $u(x, y, ...)$ that satisfies the equation identically, at least in some region of the $x, y, \ldots$ variables.

2.2.2 First Order Linear Equation

Let us solve

$$a\,u_t+b u_x=0, \tag{2.9}$$

where a and b are constants not both zero.

Geometric method The quantity $au_t + bu_x$ is the directional derivative of u in the direction of the vector $V = (a, b) = a\hat{\imath} + b\hat{\jmath}$ where $\imath$ and $\jmath$ are unit vector of t and x axes. The directional derivative must be zero. This means that $u(t, x)$ must be constant in the direction of V. The vector $(b, -a)$ is orthogonal to V. The lines parallel to V have the equations $bt - ax =$ constant. They are called *the characteristic lines*. The solution is constant on each such line. Therefore, $u(t, x)$ depends on $bt - ax$ only. Thus the solution is

$$u(t, x) = f(bt - ax) \tag{2.10}$$

where f is any function of one variable. Let's explain this conclusion more explicitly. On the line $bt - ax = c$, the solution u has a constant value. Call this value $f(c)$. Then $u(t, x) = f(c) = f(bt - ax)$. Since c is arbitrary, we have formula (2.10) for all values of t and x.

Coordinate Method Change variables(or "make a change of coordinates") to

$$t' = at + bx \qquad x' = bt - ax. \tag{2.11}$$

Replace all t and x derivatives by t' and x' derivatives. By the chain rule,

$$u_t = \frac{\partial u}{\partial t} = \frac{\partial u}{\partial t'}\frac{\partial t'}{\partial t} + \frac{\partial u}{\partial x'}\frac{\partial x'}{\partial t} = au_{t'} + bu_{x'}$$

and

$$u_x = \frac{\partial u}{\partial x} = \frac{\partial u}{\partial x'}\frac{\partial x'}{\partial x} + \frac{\partial u}{\partial t'}\frac{\partial t'}{\partial x} = bu_{t'} - au_{x'}.$$

Hence $au_t + bu_x = a(au_{t'} + bu_{x'}) + b(bu_{t'} - au_{x'}) = (a^2 + b^2)u_{t'}$. So, since $a^2 + b^2 \neq 0$, the equation takes the form $u_{t'} = 0$ in the new (primed) variables. Thus the solution is $u = f(x') = f(bt - ax)$, with f an arbitrary function of one variable. This is exactly the same answer as before.

Now for the sake of simplicity assume that $\dfrac{a}{b} > 0$. Let us study the following initial-boundary value problem for the equation (2.9), the unknown function $u(t, x)$ is given on the sets $X = \{t = t_0, x > x_0\}$ and $T_0 = \{t > t_0, x = x_0\}$. Because the solution of equation (2.9) is a constant along characteristic, then the solution of the initial-boundary problem can be constructed as follows.

In the domain

$$\left\{(t, x) | x > x_0 + \frac{b}{a}(t - t_0)\right\}$$

the solution is found from the boundary conditions on X.

In the domain

$$\left\{(t,x)|x_0 \leq x < x_0 + \frac{b}{a}(t-t_0)\right\}$$

the solution is found from the initial conditions on T_0.

2.2.3 Example of Simple Partial Differential Equation

In this section we present a series of examples of PDEs as they occur in physics. They provided the basic motivation for all the PDE problems. We shall see that most often in physical problems the independent variables are those of space x, y, z and time t.

Example 2.2.1 Transport equation

Consider an air pollution, say, flowing at a constant rate u along a horizontal pipe of fixed cross section in the positive x direction. A substance, say a pollutant, is suspended in the air. Let $c(x,t)$ be its concentration at time t. The amount of pollutant in the interval $[0,b]$ at the time t is $M = \int_0^b c(x,t)dx$. At the later time $t+h$, the same molecules of pollutant have moved to the right by $u \cdot h$. Hence

$$M = \int_0^b c(x,t)dx = \int_{uh}^{b+uh} c(x,t+h)dx.$$

Differentiating with respect to b, we get

$$c(b,t) = c(b+uh, t+h).$$

Differentiating with respect to h and putting $h = 0$, we get

$$0 = uc_x(b,t) + c_t(b,t),$$

which is equation

$$c_t + uc_x = 0. \tag{2.12}$$

That is, the rate of change c_t of concentration is proportional to the gradient c_x. Diffusion is assumed to be negligible. Solving this equation as in Section 2.2.2, we find that the concentration is a function of $(x-ut)$ only. This means that the substance is transported to the right at a fixed speed u. Each individual particle moves to the right at speed u, that is, in the xt plane, it moves precisely along a characteristic line (see Figure 2.1).

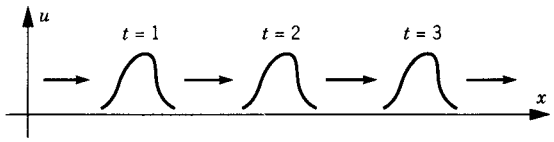


Figure:2.1 $c(x,t)$.

Example 2.2.2 Parabolic Partial Differential Equation

Parabolic PDEs occur when propagation problems include dissipative mechanisms, such as viscous shear or heat conduction. The classical example of a parabolic PDE is the diffusion or heat conduction equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \tag{2.13}$$

Interpretation on a Physical Basis Parabolic problems are typified by solutions which march forward in time but diffuse is space. Thus a disturbance to the solution introduced at P (in Figure 2.2) can influence any part of the computational domain for $t \geq t_i$. However, the magnitude of the disturbance quickly attenuates in moving away from P.

The incorporation of a dissipative mechanism also implies that even if the initial conditions include a discontinuity, the solution in the interior will always be continuous.

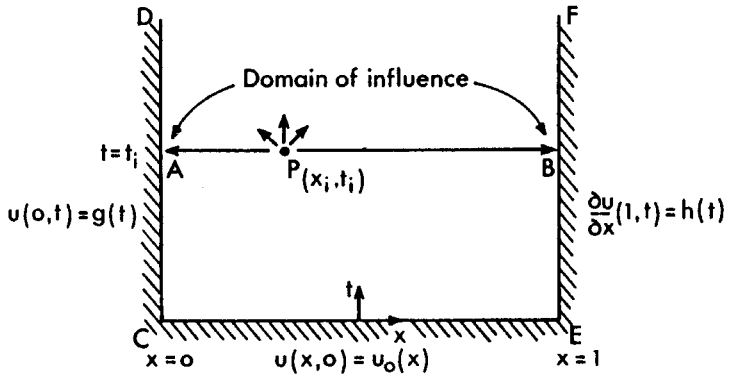


Figure:2.2 Computational domain for a parabolic PDE.

Appropriate Boundary (and Initial) Conditions For (2.13) it is necessary to specify Dirichlet initial conditions, e.g.

$$u(x,0) = u_0(x) \qquad \text{for} \qquad 0 \leq x \leq 1. \tag{2.14}$$

Appropriate boundary conditions would be

$$u(0,t) = g(t) \qquad \text{and} \qquad \frac{\partial u}{\partial x}(1,t) = h(t). \tag{2.15}$$

For the boundaries CD and EF (Figure 2.2) any combination of Dirichlet, Neumann or mixed boundary conditions is acceptable. However, it is desirable, in specifying Dirichlet boundary conditions, to ensure continuity with the initial conditions at C and E. Failure to do so will produce a solution with severe gradients adjacent to C and E, which may create difficulties for the computational algorithm. For systems of parabolic PDEs, initial conditions on CE and boundary conditions on CD and EF are necessary for all dependent variables.

2.3 Finite Difference Approximations

There are several choices that must be made when developing a finite difference solution to a partial difference equation. Foremost among these are the choice of the discrete finite difference grid used to represent the continuous solution domain and the choice of the finite difference approximations used to represent the exact partial derivatives in the partial differential equation.

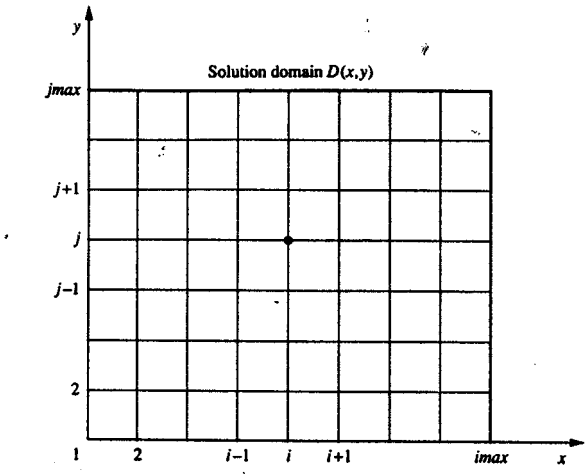


Figure:2.3 Solution domain $D(x, y)$ and finite difference grid.

The solution domain $D(x, y)$ in xy space for a two dimensional equilibrium problem is illustrated in Figure 2.3. The solution domain must be covered by a two-dimensional grid of lines, called the *finite difference grid.* The intersection of these grid lines are the grid points at which the finite difference solution to the partial differential equation is to be obtained. For the present, let these grid lines be equally spaced lines, perpendicular to the x and y axes and having uniform spacings $\triangle x$ and $\triangle y$, respectively. The resulting finite difference grid is illustrated in Figure 2.3. Nonuniform grids, in which $\triangle x$ and $\triangle y$ are variable, and generalized grids, in which the grid lines are not parallel to the coordinate axes. The subscript i is used to denote

the physical grid lines corresponding to constant values of x [i.e., $x_i = (i-1)\triangle x$], and the subscript j is used to denote the physical grid lines corresponding to constant values of y [i.e., $y_i = (j-1)\triangle y$]. Thus, grid point (i,j) corresponds to location (x_i, y_j) in the solution domain $D(x,y)$. The dependent variable at a grid point is denoted by the same subscript notation that is used to denote the grid points themselves. Thus, the function $f(x,y)$ at grid point (i,j) is denoted by

$$f(x_i, y_j) = f_{i,j}. \tag{2.16}$$

In a similar manner, derivatives are denoted by

$$\frac{\partial f(x_i,y_j)}{\partial x} = \left.\frac{\partial f}{\partial x}\right|_{i,j} = f_x|_{i,j} \quad \text{and} \quad \frac{\partial^2 f(x_i,y_j)}{\partial x^2} = \left.\frac{\partial^2 f}{\partial x^2}\right|_{i,j} = f_{xx}|_{i,j}\,. \tag{2.17}$$

In the development of finite difference methods, a distinction must be made between the exact solution of the partial differential equation and the approximate solution of the partial differential equation. For the remainder of this section exact solutions will be denoted by an overbar on the symbol for the dependent variable [e.g., $\overline{f}(x,y)$], and the approximate solution will be denoted by the symbol for the dependent variable without an overbar [e.g., $f(x,y)$]. This very precise distinction between the exact solution and the approximate solution of a partial differential equation is required for studies of consistency, order, and convergence.

Exact derivatives such as $\overline{f}_{xx}$ may be approximated at grid point (i,j) in term of the values of f at grid point (i,j) itself and adjacent grid points in a number of ways. For example, consider the partial derivative $\overline{f}_{xx}$. Writing the Taylor series (see the Appendix) for $\overline{f}_{i+1,j}$ and $\overline{f}_{i-1,j}$ using grid point (i,j) as the base point gives

$$\left.\begin{aligned}\overline{f}_{i+1,j} = \overline{f}_{i,j} + \overline{f}_x|_{i,j}\,\triangle x + \frac{1}{2}\,\overline{f}_{xx}|_{i,j}\,\triangle x^2 \\ + \frac{1}{6}\,\overline{f}_{xxx}|_{i,j}\,\triangle x^3 + \frac{1}{24}\,\overline{f}_{xxxx}|_{i,j}\,\triangle x^4 + \ldots.\end{aligned}\right\} \tag{2.18}$$

$$\left.\begin{aligned}\overline{f}_{i-1,j} = \overline{f}_{i,j} - \overline{f}_x|_{i,j}\,\triangle x + \frac{1}{2}\,\overline{f}_{xx}|_{i,j}\,\triangle x^2 \\ - \frac{1}{6}\,\overline{f}_{xxx}|_{i,j}\,\triangle x^3 + \frac{1}{24}\,\overline{f}_{xxxx}|_{i,j}\,\triangle x^4 + \ldots.\end{aligned}\right\} \tag{2.19}$$

where the convention $(\triangle x)^n \longrightarrow \triangle x^n$ has been used for compactness. Equations (2.18) and (2.19) can be expressed as Taylor formulas with remainders (see the Appendix A). Thus,

$$\left.\begin{aligned}\overline{f}_{i+1,j} = \overline{f}_{i,j} + \overline{f}_x|_{i,j}\,\triangle x + \frac{1}{2}\,\overline{f}_{xx}|_{i,j}\,\triangle x^2 \\ + \frac{1}{6}\,\overline{f}_{xxx}|_{i,j}\,\triangle x^3 + \frac{1}{24}\,\overline{f}_{xxxx}|_{i,j}\,\triangle x^4 + \ldots + R_{n+1}(\xi_+)\end{aligned}\right\} \tag{2.20}$$

$$\left.\begin{aligned} \overline{f}_{i-1,j} = \overline{f}_{i,j} - \overline{f}_x\big|_{i,j}\,\triangle x + \frac{1}{2}\,\overline{f}_{xx}\big|_{i,j}\,\triangle x^2 \\ -\frac{1}{6}\,\overline{f}_{xxx}\big|_{i,j}\,\triangle x^3 + \frac{1}{24}\,\overline{f}_{xxxx}\big|_{i,j}\,\triangle x^4 + ... + R_{n+1}(\xi_-) \end{aligned}\right\} \tag{2.21}$$

where the remainder term R_{n+1} is given by

$$R_{n+1} = \frac{1}{(n+1)!}\frac{\partial^{n+1}\overline{f}(\xi)}{\partial x^{n+1}}\triangle x^{n+1} \tag{2.22}$$

where $x_i \quad \xi_+ \quad x_{i+1}$ and $x_{i-1} \quad \xi_- \quad x_i$. If the infinite Taylor series are truncated after the nth derivative to obtain approximations of $\overline{f}_{i+1,j}$ and $\overline{f}_{i-1,j}$, then the remainder term R_{n+1} is the error associated with the truncated Taylor series. In many cases, our main concern will be the *order* of the error, which is the rate at which the error goes to zero as $\triangle x \longrightarrow 0$. The remainder term depends on $\triangle x^{n+1}$. Consequently, as $\triangle x \longrightarrow 0$, the error goes to zero as $\triangle x^{n+1}$. Thus, the order of the truncated Taylor series approximation of $\overline{f}_{xx}\big|_{i,j}$ is $n+1$, which is denoted by the symbol $O(\triangle x^{n+1})$.

Adding equations (2.18) and (2.19) and solving for $\overline{f}_{xx}\big|_{i,j}$ yields

$$\overline{f}_{xx}\big|_{i,j} = \frac{\overline{f}_{i+1,j} - 2\overline{f}_{i,j} + \overline{f}_{i-1,j}}{\triangle x^2} - \frac{1}{12}\,\overline{f}_{xxxx}\big|_{i,j}\,\triangle x^2 + ... \tag{2.23}$$

Equivalently, from equations (2.20) and (2.21),

$$\overline{f}_{xx}\big|_{i,j} = \frac{\overline{f}_{i+1,j} - 2\overline{f}_{i,j} + \overline{f}_{i-1,j}}{\triangle x^2} + ... + \frac{R_{n+2}}{\triangle x^2} \tag{2.24}$$

which can be written as

$$\overline{f}_{xx}\big|_{i,j} = \frac{\overline{f}_{i+1,j} - 2\overline{f}_{i,j} + \overline{f}_{i-1,j}}{\triangle x^2} + ... + O(\triangle x^n) \tag{2.25}$$

where

$$\frac{R_{n+2}}{\triangle x^2} = \frac{1}{(n+2)!}\frac{\partial^{n+2}\overline{f}(\overline{\xi})}{\partial x^{n+2}}\frac{\triangle x^{n+2}}{\triangle x^2} = O(\triangle x^n) \tag{2.26}$$

where $x_{i-1} \quad \overline{\xi} \quad x_{i+1}$. If the Taylor series is truncated after the second derivative term (i.e., $n = 2$), then equations (2.24) and (2.25) give

$$\overline{f}_{xx}\big|_{i,j} = \frac{\overline{f}_{i+1,j} - 2\overline{f}_{i,j} + \overline{f}_{i-1,j}}{\triangle x^2} - \frac{1}{12}\overline{f}_{xxxx}(\overline{\xi})\triangle x^2 \tag{2.27}$$

which can be written as

$$\left.\begin{aligned} \overline{f}_{xx}\big|_{i,j} &= \frac{\overline{f}_{i+1,j} - 2\overline{f}_{i,j} + \overline{f}_{i-1,j}}{\triangle x^2} + E(\overline{f}_{xx}\big|_{i,j}) \\ &= \frac{\overline{f}_{i+1,j} - 2\overline{f}_{i,j} + \overline{f}_{i-1,j}}{\triangle x^2} + O(\triangle x^2) \end{aligned}\right\} \tag{2.28}$$

where the remainder term $E(\overline{f}_{xx}\big|_{i,j})$ is given by

$$E(\overline{f}_{xx}\big|_{i,j}) = -\frac{1}{12}\overline{f}_{xxxx}(\overline{\xi})\triangle x^2 = O(\triangle x^2). \tag{2.29}$$

A finite difference approximation of $\overline{f}_{xx}|_{i,j}$, which will be denoted by $f_{xx}|_{i,j}$, can be obtained from equation (2.28) by neglecting the remainder term. Thus,

$$f_{xx}|_{i,j} = \frac{\overline{f}_{i+1,j} - 2\overline{f}_{i,j} + \overline{f}_{i-1,j}}{\triangle x^2}. \tag{2.30}$$

The remainder term which has been neglected in equation (2.30) is a the *truncation error* of the finite difference approximation of $\overline{f}_{xx}|_{i,j}$. Equation (2.30) is called *second-order centered-difference* approximation of $\overline{f}_{xx}$ at grid point (i,j).

First-order one-sided approximations of $\overline{f}_{xx}$ at grid point (i,j) can be obtained by writing Taylor series for $\overline{f}_{i+1,j}$, $\overline{f}_{i+2,j}$, $\overline{f}_{i-1,j}$ and $\overline{f}_{i-2,j}$ using grid point (i,j) as the base point and proceeding in a similar manner. The results are

$$\overline{f}_{xx}|_{i,j} = \frac{\overline{f}_{i+2,j} - 2\overline{f}_{i+1,j} + \overline{f}_{i,j}}{\triangle x^2} + O(\triangle x) \tag{2.31}$$

$$\overline{f}_{xx}|_{i,j} = \frac{\overline{f}_{i,j} - 2\overline{f}_{i-1,j} + \overline{f}_{i-2,j}}{\triangle x^2} + O(\triangle x). \tag{2.32}$$

The terms $O(\triangle x)$ and $O(\triangle x^2)$ are truncation error terms. The notation $O(\triangle x)$, read as order $\triangle x$, denotes that truncation error is proportional to $\triangle x$ (i.e., first-order). Similarly, the notation $O(\triangle x^2)$, reads as order $\triangle x^2$, denotes a second-order truncation error. In some cases, our only concern will be with the order of the truncation error. In other cases, we will need to know the exact form of the truncation error. Equation (2.31) is a first-order forward-difference approximation and equation (2.32) is a first-order backward-difference approximation. They are rarely used, except at boundaries. Equation (2.28) is a second-order centered-difference approximation. It is the most commonly used finite difference approximation of a second derivative.

Performing the analogous procedures in the y direction yields the following result:

$$\overline{f}_{yy}|_{i,j} = \frac{\overline{f}_{i,j+1} - 2\overline{f}_{i,j} + \overline{f}_{i,j-1}}{\triangle y^2} - \frac{1}{12}\overline{f}_{yyyy}(\overline{\eta})\triangle y^2 \tag{2.33}$$

$$\overline{f}_{yy}|_{i,j} = \frac{\overline{f}_{i,j+2} - 2\overline{f}_{i,j+1} + \overline{f}_{i,j}}{\triangle y^2} + O(\triangle y) \tag{2.34}$$

$$\overline{f}_{yy}|_{i,j} = \frac{\overline{f}_{i,j} - 2\overline{f}_{i,j-1} + \overline{f}_{i,j-2}}{\triangle y^2} + O(\triangle y). \tag{2.35}$$

Finite difference solutions of a partial differential equation are obtained by replacing the exact partial derivatives in the partial differential equation by finite difference approximations, such as equation (2.28) and (2.33), to obtain a finite difference equation that approximates the partial differential equation.

2.3.1 The Crank-Nicolson Method

The backward-time centered-space (BTCS) approximation of the diffusion equation $\overline{f}_t = \alpha \overline{f}_{xx}$ has a major advantage over explicit methods. It is unconditionally stable. It is an implicit, two-level, single-step method. The finite difference approximation of $\overline{f}_{xx}$ derivative is second order. However, the finite difference approximation of the time derivative is only first-order. Using a second-order finite difference approximation of the time derivative would be an obvious improvement.

Crank and Nicolson (Crank, Nicolson 1974) proposed approximating the partial derivative $\overline{f}_t$ at grid point $(i, n+\frac{1}{2})$ by the second-order centered difference approximation and the partial derivative $\overline{f}_{xx}$ by the average value

$$\overline{f}_{xx}\Big|_t^{n+1/2} = \frac{1}{2}\left(\overline{f}_{xx}\Big|_t^{n+1} + \overline{f}_{xx}\Big|_t^{n}\right). \tag{2.36}$$

The order of this approximation is expected to be $O(\triangle t^2)$. The partial derivatives $\overline{f}_{xx}$ at time level n and $n+1$ are approximated by the second-order centered-difference approximations. The resulting finite difference approximation of the one-dimensional diffusion equation is

$$\frac{f_i^{n+1} - f_i^n}{\triangle t} = \alpha \frac{1}{2}\left(\frac{f_{i+1}^{n+1} - 2f_i^{n+1} + f_{i-1}^{n+1}}{\triangle x^2} + \frac{f_{i+1}^{n} - 2f_i^{n} + f_{i-1}^{n}}{\triangle x^2}\right). \tag{2.37}$$

Rearranging equation (2.37) yields the finite difference equation

$$-df_{i-1}^{n+1} + 2(1+d)f_i^{n+1} - df_{i+1}^{n+1} = df_{i-1}^{n} + 2(1-d)f_i^{n} + df_{i+1}^{n} \tag{2.38}$$

where $d = \alpha(\triangle t/\triangle x^2)$ is the diffusion number.

Chapter III
Numerical Scheme

Air pollution law in most industrial countries is based on some kind of permitted concentration of contaminants (NAAQS in the United States). To plan the execute air pollution control programs designed to meet the requirements of these laws, one must predict the ambient air concentrations that will result from any planned set of emission. Even if we did not use this type of air pollution law, we would probably use some other kind of law that made some use of predictions of ambient contaminant concentrations. These predictions are made by way of air pollutant concentration models.

The perfect air pollutant concentration model would allow us to predict the concentration that would result from any specified set of pollutant emission, for any specified meteorological conditions, at any location, for any specified meteorological conditions, at any location, for any time period, with total confidence in our prediction. The best currently available models are far from thus ideal. In this chapter we consider the mathematical model (1.8), (1.9), (1.10), (1.11) and (1.12).

We use the numerical approach descriebed in (Runca, Sardei 1975), which is based on the discretization of the time dependent advection-diffusion equation governing the evolution in time of the concentration of pollutant downwind of the line source at height h above the ground. Problem (1.8), (1.9), (1.10), (1.11) and (1.12) is solved with the method of fractional step (Yanenko 1971). According to this technique, the concentration field at the time $t + \triangle t$ is obtained from that at the time t by separating the contributions due to advection and diffusion terms as follows:

In the first step the advection equation

$$\frac{\partial c}{\partial t} + u(z)\frac{\partial c}{\partial x} \quad = 0 \tag{3.1}$$

is solved in the whole $x - z$ integration region over the time interval $\triangle t$ with the concentration field at the time t as initial conditions (1.9) and (1.10) as boundary condition. The diffusion equation

$$\frac{\partial c}{\partial t} - \frac{\partial}{\partial z}\left(K_z \frac{\partial c}{\partial z}\right) \quad = \quad 0 \tag{3.2}$$

is then solved in the second step over the same time interval. Here the initial condition is provided by the concentration field obtained from the first step and the boundary conditions by the relation (1.11) and (1.12). Let us show that the solution of (3.1) and (3.2) is an approximation of the concentration field at the time $t + \triangle t$.
If we denote

$$\begin{aligned} \Lambda_1 c &= -u(z)\frac{\partial c}{\partial x} \\ \Lambda_2 c &= \frac{\partial}{\partial z}\left(K_z \frac{\partial c}{\partial z}\right) \end{aligned}$$

the Cauchy problem for equation (1.8) is

$$\begin{cases} \dfrac{\partial c}{\partial t} = (\Lambda_1 + \Lambda_2)\, c \\ c(x, z, 0) = c_0(x, z). \end{cases}$$

We can split the previous problem into two problems

$$\begin{cases} \dfrac{\partial c^*}{\partial t} = \Lambda_1 c^* \\ c^*(x, z, t_n) = c(x, z, t_n) \end{cases}$$

and

$$\begin{cases} \dfrac{\partial \widetilde{c}}{\partial t} = \Lambda_2 \widetilde{c} \\ \widetilde{c}(x, z, t_n) = c^*(x, z, t_n + \tau). \end{cases}$$

By Tarlor series, we have

$$\begin{aligned} c(x, z, t_n + \tau) &= c(x, z, t_n) + \frac{\partial c}{\partial \tau} + O(\tau^2) \\ &= c(x, z, t_n) + \tau\,(\Lambda_1 + \Lambda_2)\, c + O(\tau^2) \\ &= [E + \tau\,(\Lambda_1 + \Lambda_2)]\, c + O(\tau^2) \end{aligned}$$

where E is identity operator. In the same way, we get

$$\begin{aligned} c^*(x, z, t_n + \tau) &= (E + \tau\Lambda_1) c^*(x, z, t_n) + O(\tau^2) \\ &= (E + \tau\Lambda_1) c(x, z, t_n) + O(\tau^2) \\ \widetilde{c}(x, z, t_n + \tau) &= (E + \tau\Lambda_2) \widetilde{c}(x, z, t_n) + O(\tau^2) \\ &= (E + \tau\Lambda_2) c^*(x, z, t_n + \tau) + O(\tau^2) \\ &= (E + \tau\Lambda_2)(E + \tau\Lambda_1) c(x, z, t_n) + O(\tau^2) \\ &= [E + \tau(\Lambda_1 + \Lambda_2)] c(x, z, t_n) + O(\tau^2) \\ &= c(x, z, t_n + \tau) + O(\tau^2). \end{aligned}$$

If we take $\tau \to 0$ then $O(\tau^2) \to 0$ and

$$\widetilde{c}(x, z, t_n + \tau) \to c(x, z, t_n + \tau)$$

For equation (3.1) a Lagrangian technique is used in order to avoid artificial diffusion errors associated with the advection step. The diffusion equation (3.2) is solved with a conventional Eulerian finite-difference scheme.

3.1 The advection step

The solution of equation (3.1) in the Lagrangian formulation

$$\frac{\partial c(\zeta, z, t)}{\partial t} = 0 \qquad \text{with} \qquad \zeta = x - ut. \tag{3.3}$$

is obvious. Equation (3.3) simply means that in a reference frame moving with the velocity u the concentration does not change in time. Thus equation (3.1) is exactly satisfied by translating the concentration field at any time step $\triangle t$ to the distance $u\triangle t$. This procedure is evidently mass conserving.

If the wind velocity is constant in space and time, equation (3.3) can directly be represented in the Eulerian frame used for equation (3.2) simply by choosing $\triangle x = u\triangle t$. A further simplification is provided by the fact that for u =constant equation (3.1) and (3.2) can be integrated separately not only over a single time interval, but over the whole integration time. In fact, the advection-diffusion equation (1.8) can be transformed by introducing Lagrangian coordinates to a pure diffusion equation valid in frame moving with the velocity u.

If the wind velocity is not constant, the described Lagrangian treatment of equation (3.1) becomes problematic in connection with the Eulerian difference scheme used for equation (3.2). In fact, for constants $\triangle t$ and a variable u, the condition $\dfrac{u \cdot \triangle t}{\triangle x} = 1$ means a variable $\triangle x$. Thus, positions not coincident with grid points will be reached by all particles whose velocity is different from the chosen ratio $\dfrac{\triangle x}{\triangle t}$. In other words, equation (3.1) cannot be satisfied by translating the whole concentration field to the next grid points of an Eulerian frame.

To overcome this difficulty, the given velocity profile $u(z)$ is approximated by a step function whose discrete values u_k are defined at any vertical grid point k, as fractions of the maximum wind velocity $u_{\max}$:

$$u_k = \frac{p_k}{q} u_{\max}, \quad p_k \leq q, \quad k = 1, 2, ..., n \tag{3.4}$$

where p_k and q are positive integers and n is the number of vertical grid points. For a given distribution of the vertical intervals $\triangle z_k$ and a given q, the integers p_k are determined from the condition that the step function becomes as close as possible to the original velocity profile $u(z)$. More precisely, the single u_k values are chosen from

equation (3.4) as the best approximations to the mean values of $u(z)$ over any vertical step. Figure 3.1 shows as an example, how the velocity profile $u = z^{0.2}$ is approximated for a constant interval $\triangle z = 0.05$ and $q = 5$. For sufficiently small $\triangle z$ and sufficiently large $q = 5$, the approximation error of the step function is arbitrarily small.

The horizontal interval $\triangle x$ is defined as

$$\triangle x = \frac{u_{\max}}{q} \triangle t. \tag{3.5}$$

Consequently, the pollutant moving with the velocity u_k is translated at any time step to the distance $p_k \triangle x$, that is, to positions coincident with grid points. In particular, the pollutant with the maximum velocity $u_{\max}$ is translated to a distance $q \triangle x$. The front of the advancing material, separating the polluted from the "clean" region, moves with the maximum velocity $u_{\max}$ and is located at $x = u_{\max}\ t$. The described procedure can be immediately extended to include downwind variations of the wind velocity. (Note that downwind variations of the diffusion coefficient K are already included.) In this case the given velocity function $u(x, z)$ has to be approximated by a two dimensional step function u_{kj}. The u_{kj} matrix is related to a corresponding integer matrix p_{kj} according to equation (3.4). The parameters $u_{\max}$ and q can still be taken as constant. Equation (3.5) shows that the horizontal interval $\triangle x$ is then constant as well. For $u_{\max}$ we can choose, for example. the absolute maximum value of $u(x, z)$. The discretization parameter q has to be chosen large enough to ensure a sufficient approximation of the given velocity in the whole field.

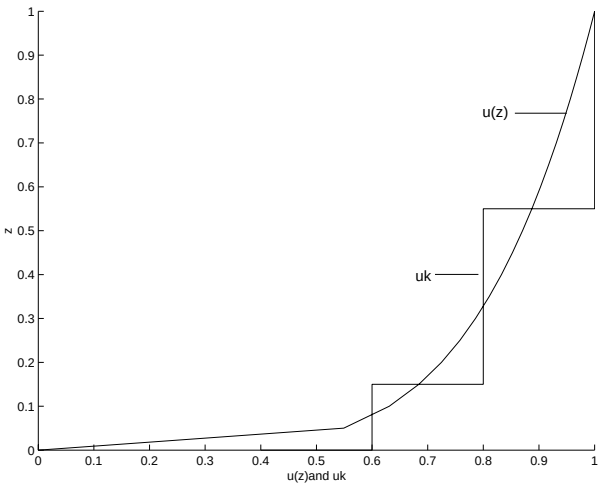


Figure:3.1 Wind profile $u = z^{0.2}$ and approximating step function u_k for $q = 5$ and uniform vertical grid spacing $\triangle z = 0.05$.

3.2 The Diffusion Step

The diffusion equation (3.2) is solved with an implicit centered-space difference scheme allowing for a variable grid spacing. Let we define $\triangle z_k$ is the first interval above the k grid point

$$\triangle z_k = z_{k+1} - z_k$$

and for any mesh function v_k, δ is defined by

$$\delta v_k = \frac{v_{k+1/2} - v_{k-1/2}}{z_{k+1/2} - z_{k-1/2}}$$

then the second partial derivative of (3.2) as follow,

$$\begin{aligned}
& \delta(K_k \delta(c_k)) \\
= & \frac{K_{k+1/2} \cdot \delta(c_{k+1/2}) - K_{k-1/2} \cdot \delta(c_{k-1/2})}{z_{k+1/2} - z_{k-1/2}} \\
= & \frac{K_{k+1/2} \cdot \dfrac{c_{k+1} - c_k}{z_{k+1} - z_k} - K_{k-1/2} \cdot \dfrac{c_k - c_{k-1}}{z_k - z_{k-1}}}{z_{k+1/2} - z_{k-1/2}} \\
= & \frac{K_{k+1/2} \cdot \dfrac{c_{k+1} - c_k}{\triangle z_k} - K_{k-1/2} \cdot \dfrac{c_k - c_{k-1}}{\triangle z_{k-1}}}{\dfrac{\triangle z_{k-1} + \triangle z_k}{2}} \\
= & \frac{2}{\triangle z_{k-1} + \triangle z_k} \left[K_{k+1/2} \cdot \frac{c_{k+1} - c_k}{\triangle z_k} - K_{k-1/2} \cdot \frac{c_k - c_{k-1}}{\triangle z_{k-1}} \right] \\
= & \frac{2}{\triangle z_k \left(\triangle z_{k-1} + \triangle z_k \right)} \left[K_{k+1/2} \left(c_{k+1} - c_k \right) - \frac{\triangle z_k}{\triangle z_{k-1}} \cdot K_{k-1/2} \left(c_k - c_{k-1} \right) \right] \\
= & \frac{2}{\triangle z_k \left(\triangle z_{k-1} + \triangle z_k \right)} \cdot \\
& \cdot \left[K_{k+1/2} \cdot c_{k+1} - K_{k+1/2} \cdot c_k - \frac{\triangle z_k}{\triangle z_{k-1}} \cdot K_{k-1/2} \cdot c_k + \frac{\triangle z_k}{\triangle z_{k-1}} \cdot K_{k-1/2} \cdot c_{k-1} \right] \\
= & \frac{2}{\triangle z_k \left(\triangle z_{k-1} + \triangle z_k \right)} \cdot \\
& \cdot \left[\frac{\triangle z_k}{\triangle z_{k-1}} \cdot K_{k-1/2} \cdot c_{k-1} - \left(\frac{\triangle z_k}{\triangle z_{k-1}} \cdot K_{k-1/2} + K_{k+1/2} \right) c_k + K_{k+1/2} \cdot c_{k+1} \right]
\end{aligned}$$

Thus the approximation equation of diffusion equation (3.2) is

$$\frac{c_k^{t+\triangle t} - c_k^t}{\triangle t} = \theta \delta(K_k \delta(c_k^{t+\triangle t})) + (1-\theta) \delta(K_k \delta(c_k^t)) \tag{3.7}$$

with appropriate discrete initial and boundary conditions. Here, for any mesh function v_k, δ is defined by

$$\delta v_k = \frac{v_{k+1/2} - v_{k-1/2}}{z_{k+1/2} - z_{k-1/2}}$$

This method is always stable for $\frac{1}{2} \leq \theta \leq 1$ in our computations we used $\theta = \frac{1}{2}$, thus the Crank-Nicholson finite difference method for diffusion equation (3.6) is

$$\frac{c_k^{t+\triangle t} - c_k^t}{\triangle t} = \frac{1}{2}\delta(K_k\delta(c_k^{t+\triangle t})) + \frac{1}{2}\delta(K_k\delta(c_k^t)). \tag{3.8}$$

We can write (3.8) in the form

$$M \begin{pmatrix} c_1^{t+\triangle t} \\ c_2^{t+\triangle t} \\ \cdot \\ \cdot \\ \cdot \\ c_{21}^{t+\triangle t} \end{pmatrix} = A \begin{pmatrix} c_1^t \\ c_2^t \\ \cdot \\ \cdot \\ \cdot \\ c_{21}^t \end{pmatrix}$$

where M is tridiagonal dominant matrix, which garantee the exist of M^{-1}, then

$$\begin{pmatrix} c_1^{t+\triangle t} \\ c_2^{t+\triangle t} \\ \cdot \\ \cdot \\ \cdot \\ c_{21}^{t+\triangle t} \end{pmatrix} = M^{-1}A \begin{pmatrix} c_1^t \\ c_2^t \\ \cdot \\ \cdot \\ \cdot \\ c_{21}^t \end{pmatrix}$$

we can find M and A by take a system of 21 equations for 21 unknowns, as

$$\begin{aligned}
\frac{c_k^{t+\triangle t} - c_k^t}{\triangle t} &= \frac{\delta(K_k\delta(c_k^{t+\triangle t})) + \delta(K_k\delta(c_k^t))}{2} \\
c_k^{t+\triangle t} - c_k^t &= \frac{\triangle t}{2} \cdot \frac{2}{\triangle z_k\left(\triangle z_{k-1} + \triangle z_k\right)} \cdot \\
&\quad \cdot \left[\begin{array}{c} \left(\frac{\triangle z_k}{\triangle z_{k-1}} \cdot K_{k-1/2}\right) c_{k-1}^{t+\triangle t} - \left(\frac{\triangle z_k}{\triangle z_{k-1}} \cdot K_{k-1/2} + K_{k+1/2}\right) c_k^{t+\triangle t} \\ + \left(K_{k+1/2}\right) c_{k+1}^{t+\triangle t} + \left(\frac{\triangle z_k}{\triangle z_{k-1}} \cdot K_{k-1/2}\right) c_{k-1}^t \\ - \left(\frac{\triangle z_k}{\triangle z_{k-1}} \cdot K_{k-1/2} + K_{k+1/2}\right) c_k^t + \left(K_{k+1/2}\right) c_{k+1}^t] \end{array} \right] \\
&= Q_k \cdot c_{k-1}^{t+\triangle t} - R_k \cdot c_k^{t+\triangle t} + S_k \cdot c_{k+1}^{t+\triangle t} + Q_k \cdot c_{k-1}^t - R_k \cdot c_k^t + S_k \cdot c_{k+1}^t
\end{aligned}$$

where

$$\begin{aligned}
\mu_k &= \frac{\triangle z_{k-1} + \triangle z_k}{\triangle t} \\
Q_k &= \frac{K_{k-1/2}}{\triangle z_{k-1}} \cdot \frac{1}{\mu_k} \\
R_k &= \left(\frac{K_{k-1/2}}{\triangle z_{k-1}} + \frac{K_{k+1/2}}{\triangle z}\right) \cdot \frac{1}{\mu_k} \\
S_k &= \frac{K_{k+1/2}}{\triangle z} \cdot \frac{1}{\mu_k}
\end{aligned}$$

so equation (3.18) for $k = 2...20$, as follow

$$-Q_k \cdot c_{k-1}^{t+\Delta t} + (1 + R_k)\, c_k^{t+\Delta t} - S_k \cdot c_{k+1}^{t+\Delta t} = Q_k \cdot c_{k-1}^{t} + (1 - R_k)\, c_k^{t} + S_k \cdot c_{k+1}^{t}$$

from the boundary conditions (1.11) and (1.12) we take the second order of boundary conditions,
equation (3.8) for $k = 1$,

$$\left(\frac{-(2\Delta z_1 + \Delta z_2)}{\Delta z_1(\Delta z_1 + \Delta z_2)}\right) c_1 + \left(\frac{\Delta z_1 + \Delta z_2}{\Delta z_1 \Delta z_2}\right) c_2 - \left(\frac{\Delta z_1}{\Delta z_2(\Delta z_1 + \Delta z_2)}\right) c_3 = 0$$

equation (3.8) for $k = 21$,

$$\left(\frac{2\Delta z_{20} + \Delta z_{19}}{\Delta z_{20}(\Delta z_{20} + \Delta z_{19})}\right) c_{21} + \left(\frac{\Delta z_{20} + \Delta z_{19}}{\Delta z_{19} \Delta z_{20}}\right) c_{20} - \left(\frac{\Delta z_{20}}{\Delta z_{19}(\Delta z_{20} + \Delta z_{19})}\right) c_{19} = 0.$$

Let

$$M_{1,1} = \left(\frac{-(2\Delta z_1 + \Delta z_2)}{\Delta z_1(\Delta z_1 + \Delta z_2)}\right)$$
$$M_{1,2} = \left(\frac{\Delta z_1 + \Delta z_2}{\Delta z_1 \Delta z_2}\right)$$
$$M_{1,3} = -\left(\frac{\Delta z_1}{\Delta z_2(\Delta z_1 + \Delta z_2)}\right)$$
$$M_{21,19} = \left(\frac{\Delta z_{20}}{\Delta z_{19}(\Delta z_{20} + \Delta z_{19})}\right)$$
$$M_{21,20} = -\left(\frac{\Delta z_{20} + \Delta z_{19}}{\Delta z_{19} \Delta z_{20}}\right)$$
$$M_{21,21} = \left(\frac{2\Delta z_{20} + \Delta z_{19}}{\Delta z_{20}(\Delta z_{20} + \Delta z_{19})}\right)$$

finally, we have

$$\begin{pmatrix} M_{1,1} & M_{1,2} & M_{1,3} & . & . & . & 0 \\ -Q_2 & 1+R_2 & -S_2 & 0 & . & . & 0 \\ 0 & -Q_3 & 1+R_3 & -S_3 & 0 & . & . \\ . & 0 & . & . & . & 0 & . \\ . & & 0 & . & . & . & 0 \\ . & & & 0 & -Q_{20} & 1+R_{20} & -S_{20} \\ 0 & . & . & . & M_{21,19} & M_{21,20} & M_{21,21} \end{pmatrix} \begin{pmatrix} c_1^{t+\triangle t} \\ c_2^{t+\triangle t} \\ . \\ . \\ . \\ c_{20}^{t+\triangle t} \\ c_{21}^{t+\triangle t} \end{pmatrix}$$

$$= \begin{pmatrix} 0 & 0 & 0 & . & . & . & 0 \\ Q_2 & 1-R_2 & S_2 & 0 & . & . & 0 \\ 0 & Q_3 & 1-R_3 & S_3 & 0 & . & . \\ . & 0 & . & . & . & 0 & . \\ . & & 0 & . & . & . & 0 \\ . & & & 0 & Q_{20} & 1-R_{20} & S_{20} \\ 0 & . & . & . & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} c_1^t \\ c_2^t \\ . \\ . \\ . \\ c_{20}^t \\ c_{21}^t \end{pmatrix}$$

3.3 Vertical Grid Geometry

In order to provide good resolution of the concentration profile near the source, where the strongest diffusion occurs, we used a Gaussian distribution of the vertical grid point "spacing", centered at the source location, as expressed by

$$\frac{1}{\triangle z_\upsilon} = \frac{1}{\triangle z_s} e^{-A_i (z_k - h)^2} \begin{cases} {}_\upsilon = k, i = 1 \quad for \quad z_k \geqslant h \\ {}_\upsilon = k-1, i = 2 \quad for \quad z_k \leqslant h \\ k = 2, 3, ..., n-1 \end{cases} \tag{3.9}$$

with

$$\left.\begin{array}{l} z_1 = 0 \\ z_k = \sum_{j=1}^{k-1} \triangle z_j, \quad k = 2, 3, ..., n-1 \\ z_n = 1 \end{array}\right\} \tag{3.10}$$

$\triangle z_s$ is the size of the first interval above and below the source. A_1 and A_2 are parameters of the distribution, n is the number of vertical grid points. $\triangle z_s$ and n are taken as independent parameters.

Example 3.3.3

$$n = 21, h = 0.2$$

choose $\triangle z_s$ *in the range*

$$\begin{aligned} \frac{1}{2(21-1)} &< \triangle z_s < \frac{1}{21-1} \\ \frac{1}{40} &< \triangle z_s < \frac{1}{20} \\ 0.025 &< \triangle z_s < 0.05 \end{aligned}$$

if we choose $\triangle z_s = 0.033$ *and choose the point at source* $z_6 = h = 0.2$ *then* $\triangle z_5 = \triangle z_6 = 0.033$.

For grid below the source

$$z_k \leqslant h \quad i.e. \quad v = k-1, i = 2, k = 6,5,4,3,2$$

from (3.9) and (3.10),

$$\frac{1}{\triangle z_{k-1}} = \frac{1}{0.033} e^{-A_2(z_k-0.2)^2}, \qquad let \qquad A_2 = \alpha$$

$$\triangle z_{k-1} = 0.033 e^{\alpha(z_k-0.2)^2}$$

$$\begin{aligned} \triangle z_5 &= 0.033 e^{\alpha(z_6-0.2)^2} = 0.033 e^{\alpha(0.2-0.2)^2} = 0.033 \\ \triangle z_4 &= 0.033 e^{\alpha(z_5-0.2)^2} = 0.033 e^{\alpha(z_6-\triangle z_5-0.2)^2} = 0.033 e^{\alpha(0.033)^2} \\ \triangle z_3 &= 0.033 e^{\alpha(z_4-0.2)^2} \\ &= 0.033 e^{\alpha(z_6-\triangle z_5-\triangle z_4-0.2)^2} = 0.033 e^{\alpha(0.033+\triangle z_4)^2} \\ \triangle z_2 &= 0.033 e^{\alpha(z_3-0.2)^2} \\ &= 0.033 e^{\alpha(z_6-\triangle z_5-\triangle z_4-\triangle z_3-0.2)^2} = 0.033 e^{\alpha(0.033+\triangle z_4+z_3)^2} \\ \triangle z_1 &= 0.033 e^{\alpha(z_2-0.2)^2} \\ &= 0.033 e^{\alpha(z_6-\triangle z_5-\triangle z_4-\triangle z_3-\triangle z_2-0.2)^2} = 0.033 e^{\alpha(0.033-\triangle z_4+\triangle z_3+\triangle z_2)^2} \end{aligned}$$

and find α *by solve*

$$\triangle z_1 + \triangle z_2 + \triangle z_3 + \triangle z_4 + \triangle z_5 + \triangle z_6 = 0.2.$$

For grid above the source

$$z_k \geqslant h \quad \text{i.e.} \quad v = k, i = 1, k = 7,8,9,....20$$

from (3.9) and (3.10),

$$\frac{1}{\triangle z_k} = \frac{1}{0.033} e^{-A_1(z_k-0.2)^2}, \qquad let \qquad A_1 = \beta$$

$$\triangle z_k = 0.033 e^{\beta(z_k - 0.2)^2}$$

$$\begin{aligned}
\triangle z_7 &= 0.033 e^{\beta(z_7-0.2)^2} \\
&= 0.033 e^{\beta(z_6+\triangle z_6-0.2)^2} = 0.033 e^{\beta(0.033)^2} \\
\triangle z_8 &= 0.033 e^{\beta(z_8-0.2)^2} \\
&= 0.033 e^{\beta(z_6+\triangle z_6+\triangle z_7-0.2)^2} = 0.033 e^{\alpha(0.033+\triangle z_7)^2} \\
\triangle z_9 &= 0.033 e^{\beta(z_9-0.2)^2} \\
&= 0.033 e^{\beta(z_6+\triangle z_6+\triangle z_7+\triangle z_8-0.2)^2} = 0.033 e^{\alpha(0.033+\triangle z_7+\triangle z_8)^2} \\
&\quad - - - - - - - - - - - - \\
\triangle z_{20} &= 0.033 e^{\beta(z_{20}-0.2)^2} \\
&= 0.033 e^{\beta(z_6+\triangle z_6+...+\triangle z_{19}-0.2)^2} = 0.033 e^{\alpha(0.033+\triangle z_7+...+\triangle z_{19})^2}
\end{aligned}$$

and find β *by solve*

$$\triangle z_7 + \triangle z_8 + ... + \triangle z_{20} = 0.8.$$

The finally, take all of intervals in equation (3.10), then we get vertical grid $z_1, z_2, ..., z_{21}$.

3.4 Handling of the Method

In this section we give some details concerning the practical use of the method.
The input parameters are:

1. Physical quantities : $u(z), K(z), h$.
2. Numerical quantities : $\triangle t, q, \triangle z_s, n$.

The size of the vertical interval $\triangle z_k$ is variable and is determined by given values of $\triangle z_s$ and n. Both $\triangle z_k$ and z_k as well as A_1 and A_2 are calculated by iteration, from the relations (3.9) and (3.10).

The step function u_k approximating the given velocity profiles $u(z)$ is obtained as follows, The mean values of the velocity $\overline{u_k}$ are calculated over any two adjacent vertical half intervals from

$$\overline{u_k} = \frac{2}{\triangle z_{k-1} + \triangle z_k} \int_{z_k - \frac{\triangle z_{k-1}}{2}}^{z_k + \frac{\triangle z_k}{2}} u(z) dz. \qquad (3.11)$$

Applying equation (3.4) to the $\overline{u_k}$ we get non-integer estimates for p_k. The p_k are then obtained as the nearest integers to these estimates. Finally, the step function u_k is calculated back by substituting p_k into the relation (3.4).

The concentration profile at the source, expressed as a $\delta-$function in the boundary condition (1.10), is approximated numerically by a one-step function centered at the source and having width $\triangle z_s$. Its amplitude is determined by requiring the same emission rate as in (1.10) :

$$\left.\begin{aligned} c(0,z,t) = 0 \quad \text{for} \quad & \left\{ \begin{array}{l} 0 \le z < h - \dfrac{\triangle z_s}{2} \\ h + \dfrac{\triangle z_s}{2} < z \le 1 \end{array} \right. \\ c(0,z,t) = \frac{1}{u_s \triangle z_s} \quad \text{for} \quad & h - \frac{\triangle z_s}{2} \le z \le h + \frac{\triangle z_s}{2} \end{aligned}\right\} \tag{3.12}$$

where $u_s = u_k$ at the source.

The advection-diffusion process is calculated starting at the source and following the "real" advection motion of the pollutant. At any time step the concentration field is first translated to the variable distances $\triangle x_k = u_k \triangle t$, according to the Lagrangian equation (3.3). Then the contaminant is diffused according to equation (3.2). The calculations are carried out only inside the region of the $x - t$ plane where the concentration is time dependent (Figure 3.2). The moving boundaries of this region are given by the characteristics $x = u_{\max} t$ and $x = u_{\min} t$. In fact, no pollutant can move with a velocity larger than $u_{\max}$ or lower than $u_{\min}$. Therefore no pollutant can exist "on the right" of the characteristic $x = u_{\max} t$. Time independent conditions that $c = c(x,z)$ only are established "on the left" of the characteristic $x = u_{\min} t$, provided the emission rate is constant in time.

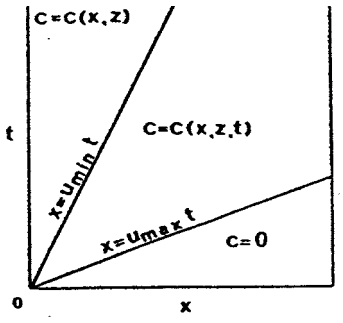


Figure:3.2 Characteristics $x = u_{\max} t$ and $x = u_{\min} t$, separating the region where the concentration is time dependent from the two regions where the pollutant has not yet arrived and steady-state conditions are established.

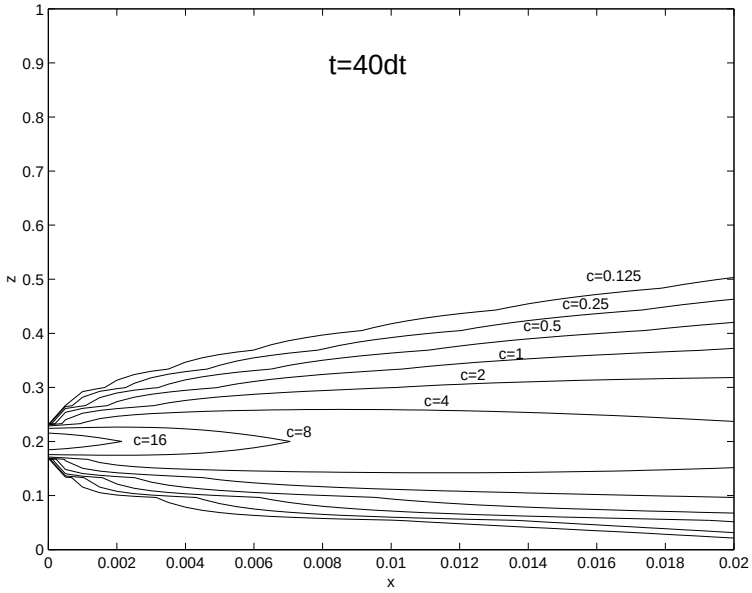
Chapter IV
Numerical Solution

If we attempt to solve the hyperbolic problems involved in the advection steps by a standard numerical method, it is well known that large artificial diffusion errors may occur. To avoid this source of error we replace the wind velocity u by a piecewise constant approximation of u on a suitable chosen mesh in the $z-$direction. We then solve the resulting set of equations with constant coefficients on appropriate $z-$subdomains by a Lagrangian method. The mesh in the $z-$direction is chosen so that all mesh values of c at time level $t + \triangle t$ are transported from mesh values of c at time level t. This means that we can eliminate the artificial diffusion errors completely, however, in approximating $u(z)$ we introduce a new source of errors.

4.1 Computer Implementation of The Numerical Method

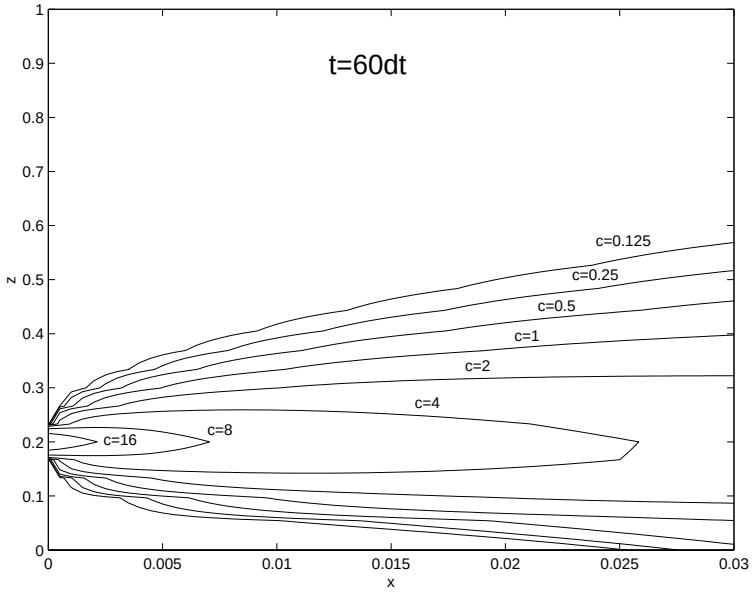
Typical examples of the time evolution of the described advection-diffusion process for constant and variable velocity profiles are shown in Figure 4.1-4.5. The plots represent, by means of concentration isolines, time sequences of the pollutant distribution in the $x - z$ plane for $u = 1$, $u = z^{0.1}$, $u = z^{0.2}$, $u = z^{0.5}$, $u = z$. In the first case (Fig 4.1) the "clean" and the polluted regions are seperated by a sharp front moving with the wind velocity and located at $x = ut$. Since for $u =$ constant steady-state conditions are immediately established behind this front corresponding isolines have the same locations in the $x - z$ planes of Figure (4.1). On the other hand, if a variable velocity $u(z)$ is given (Figure 4.2-4.5), a time dependent concentration region exists behind the front $x = u_{\max}t$ as aready mentioned in the section 3.4. Comparing the picture in Figure 4.1 with the picture in Figure 4.2-4.5, we can immediately conclude that the wind shear is responsible (Figure 4.1) for a strong vertical diffusion of material into high regions above the source and (Figure 4.2-4.5) for a fast accumulation of material near the ground.

The Matlab codes and Maple codes used to generate the figures shown in this thesis. In the computations in this section we took $n = 21, h = 0.2, \triangle t = .0005, K(z) = z, \triangle z_s = 0.033$.



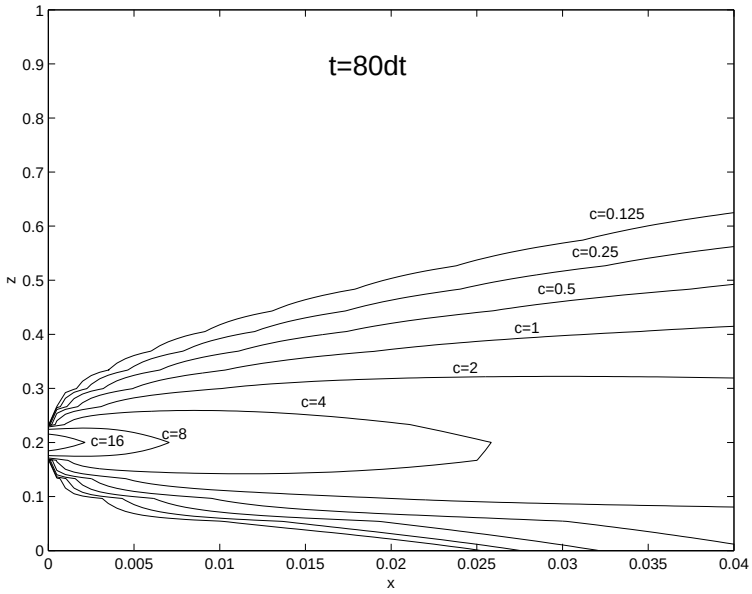
(a) $t = 40 \triangle t$.

Figure:4.1 The contour lines of concentration at different time, calculated for $u = 1$ with $K = z$, $h = 0.2$ and $t = 40 \triangle t$, $t = 60 \triangle t$, $t = 80 \triangle t$, $t = 100 \triangle t$, $t = 120 \triangle t$ and $t = 140 \triangle t$,respectively, $\triangle t = .0005$.



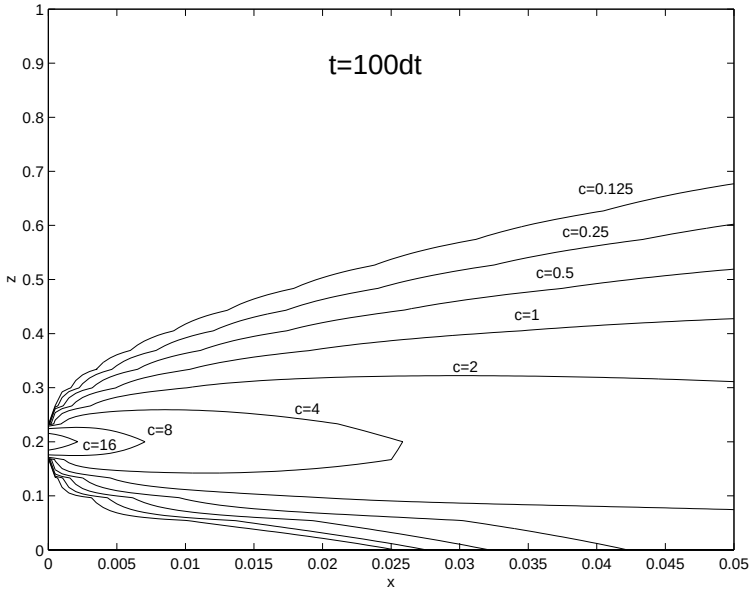
(b) $t = 60 \triangle t$.

Figure:4.1 (continued)



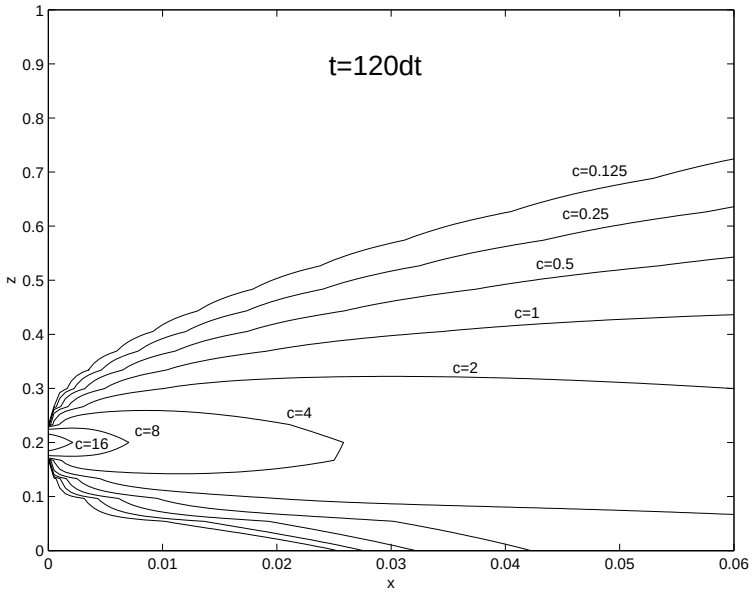
(c) $t = 80 \triangle t$.

Figure:4.1 (continued)



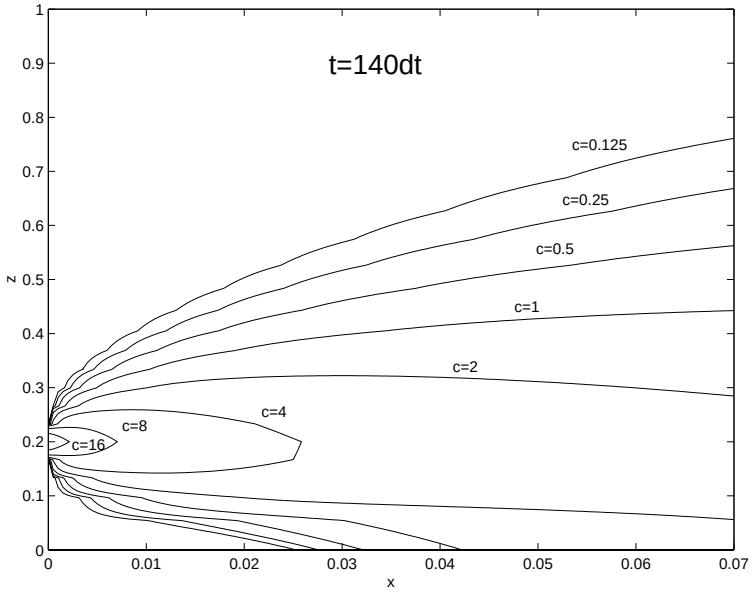
(d)$t = 100 \triangle t$.

Figure:4.1 (continued)



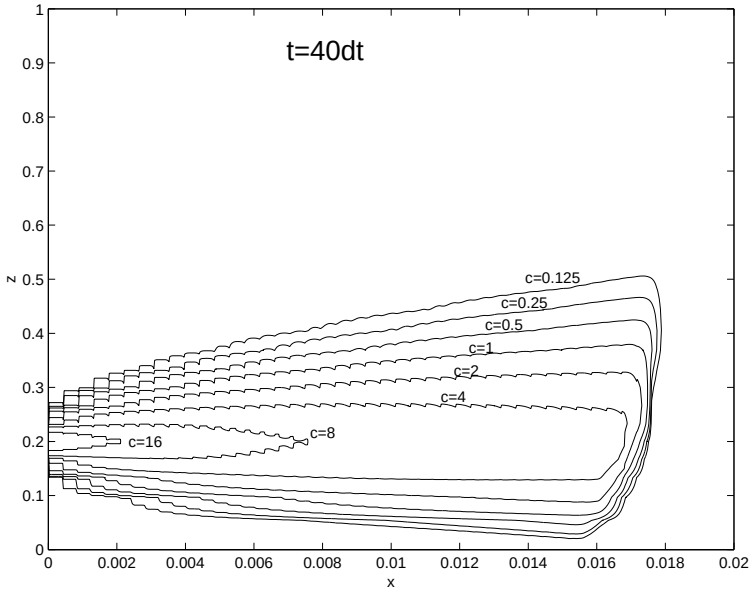
(e) $t = 120 \triangle t$.

Figure:4.1 (continued)



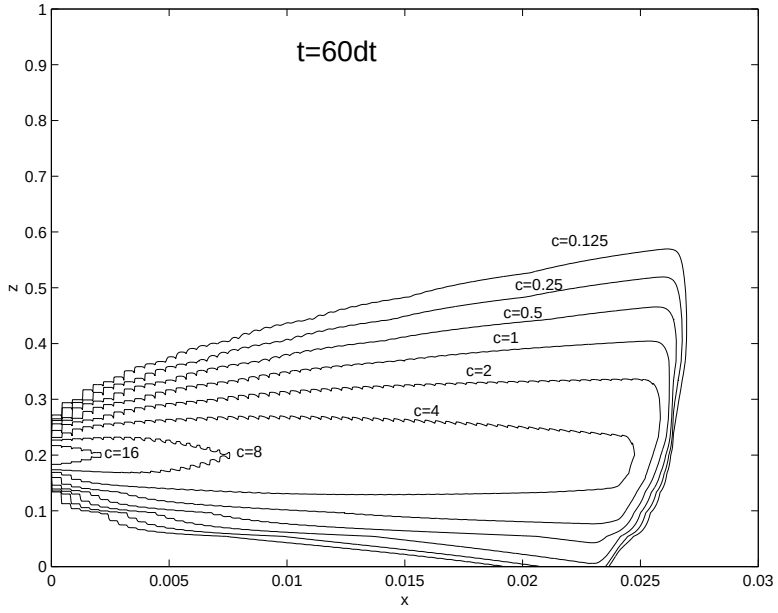
(f) $t = 140 \triangle t$.

Figure:4.1 (continued)



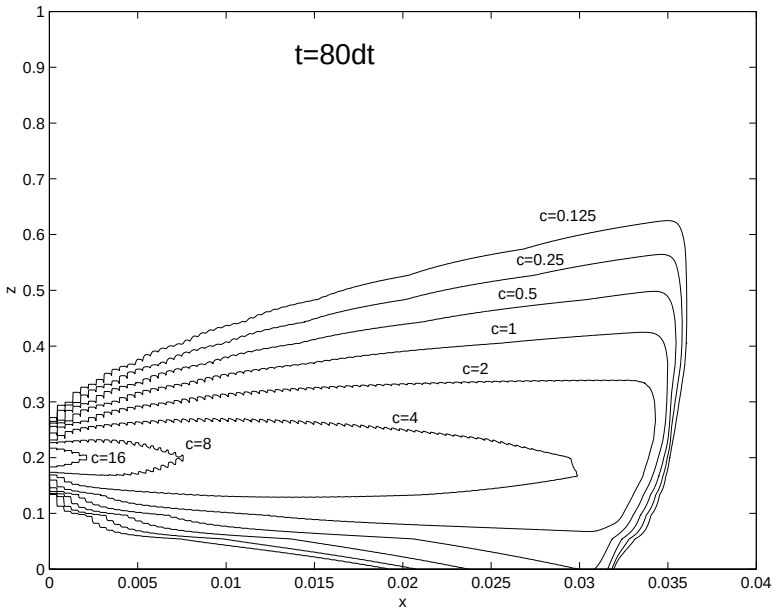
(a) $t = 40 \triangle t$.

Figure:4.2 The contour lines of concentration at different time, calculated for $u = z^{0.1}$ with $K = z$, $h = 0.2$ and $t = 40 \triangle t$, $t = 60 \triangle t$, $t = 80 \triangle t$, $t = 100 \triangle t$, $t = 120 \triangle t$ and $t = 140 \triangle t$,respectively, $\triangle t = .0005$.



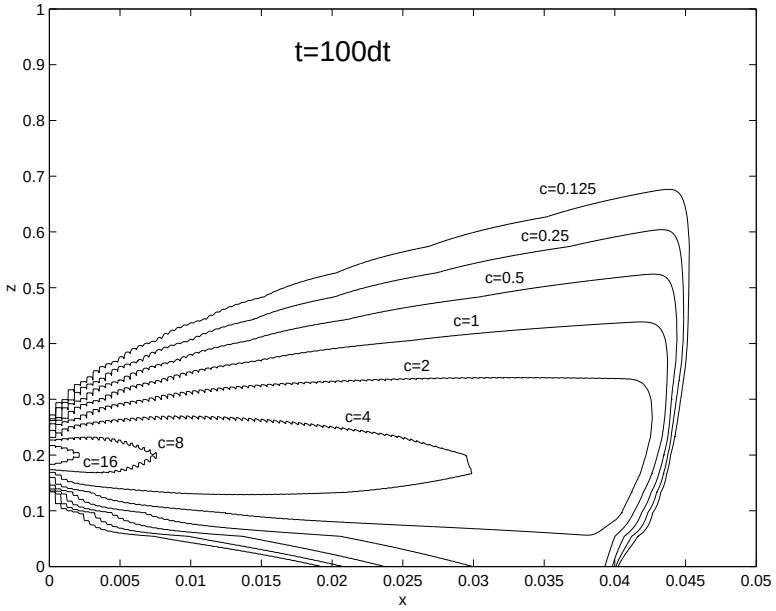
(b) $t = 60 \triangle t$.

Figure:4.2 (continued)



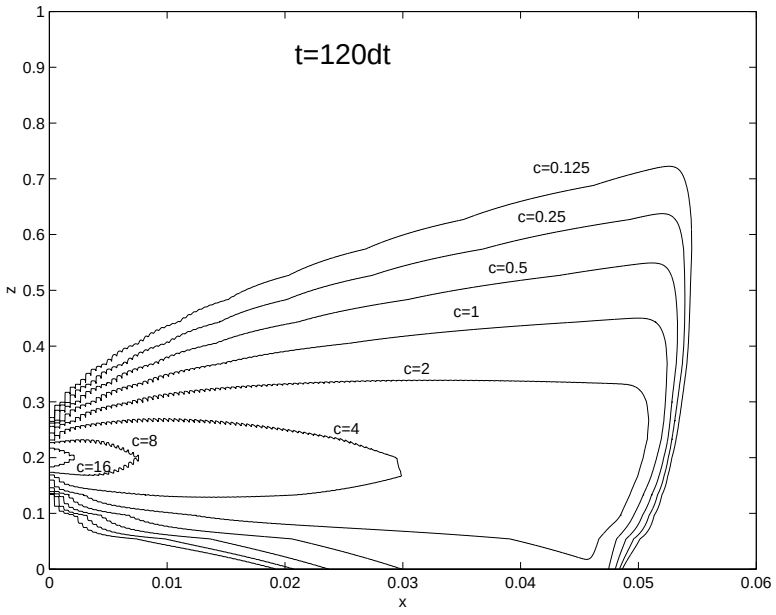
(c) $t = 80 \triangle t$.

Figure:4.2 (continued)



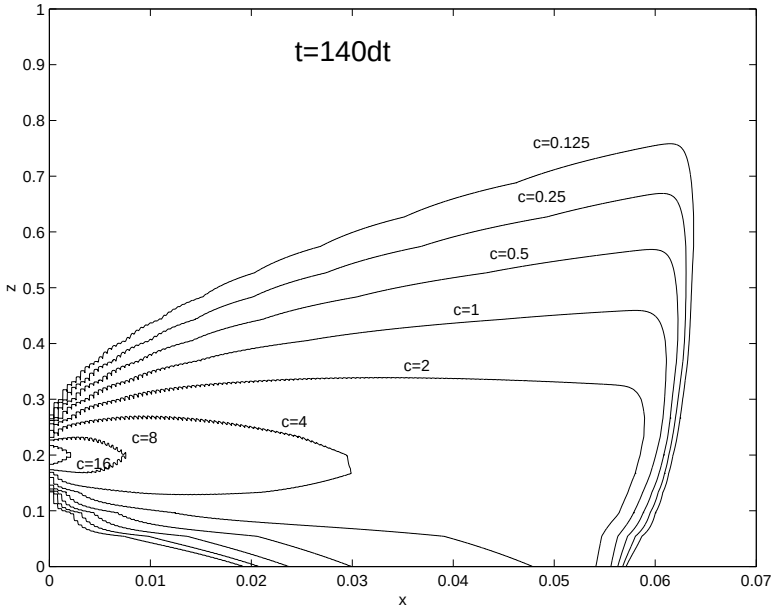
(d) $t = 100 \triangle t$.

Figure:4.2 (continued)



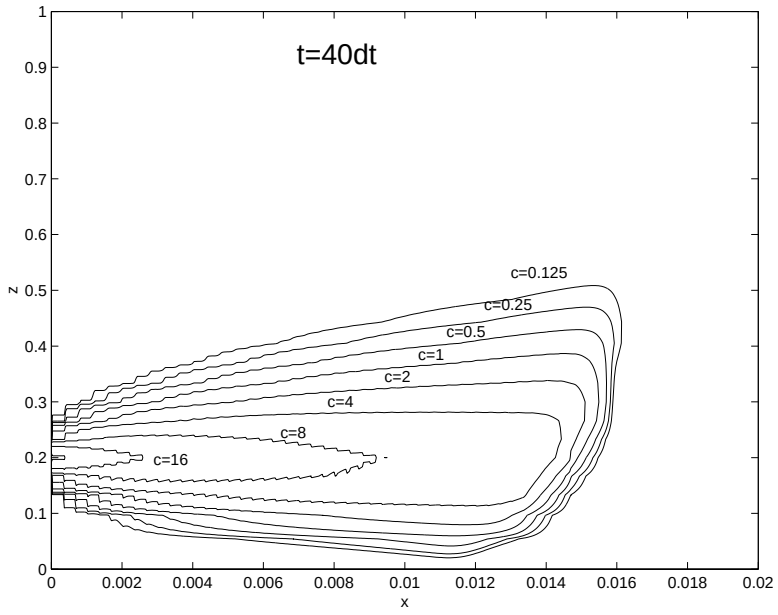
(e) $t = 120 \triangle t$.

Figure:4.2 (continued)



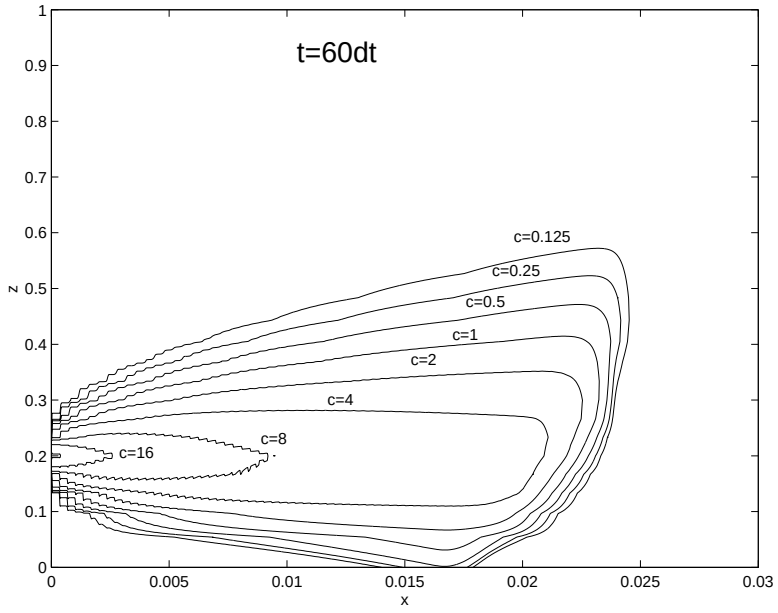
(f) $t = 140 \triangle t$.

Figure:4.2 (continued)



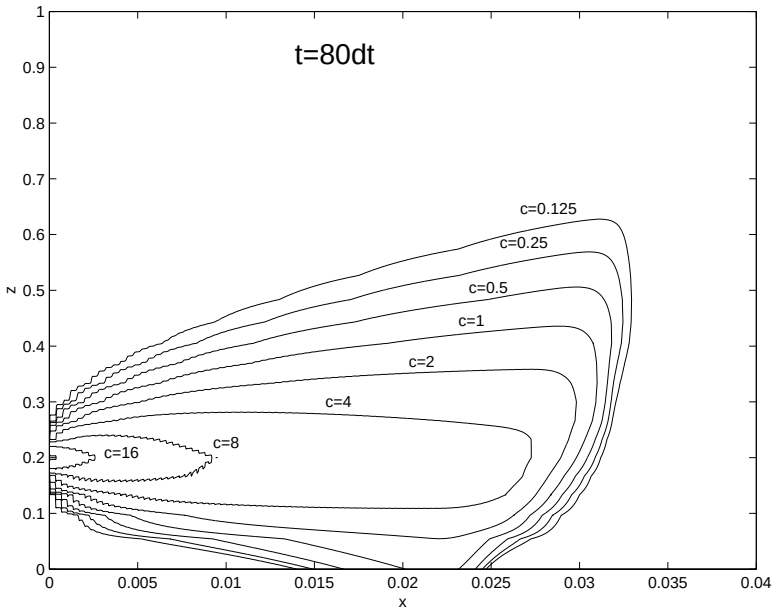
(a) $t = 40 \triangle t$.

Figure:4.3 The contour lines of concentration at different time, calculated for $u = z^{0.2}$ with $K = z$, $h = 0.2$ and $t = 40 \triangle t$, $t = 60 \triangle t$, $t = 80 \triangle t$, $t = 100 \triangle t$, $t = 120 \triangle t$ and $t = 140 \triangle t$,respectively, $\triangle t = .0005$.



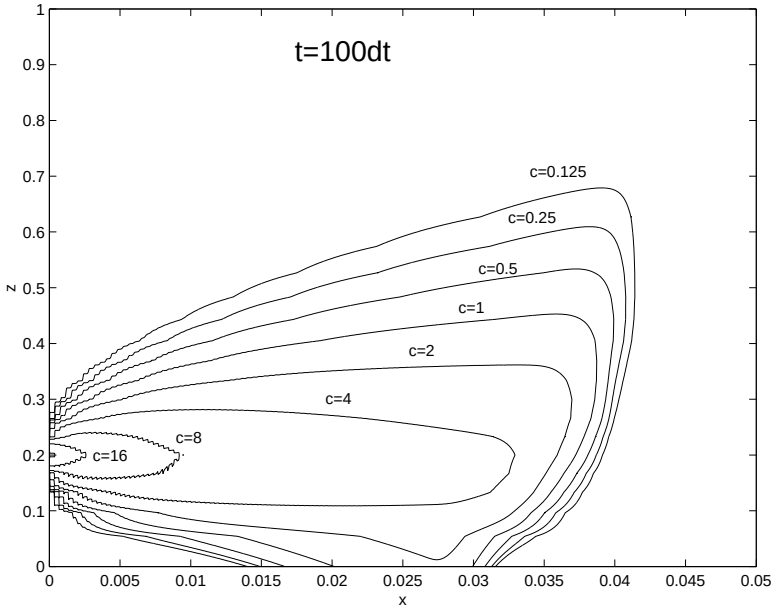
(b) $t = 60 \triangle t$.

Figure:4.3 (continued)



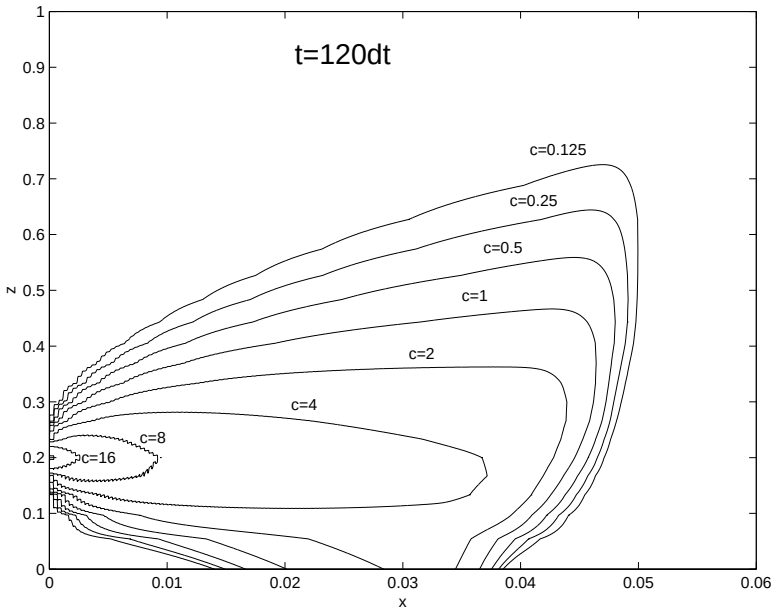
(c) $t = 80 \triangle t$.

Figure:4.3 (continued)



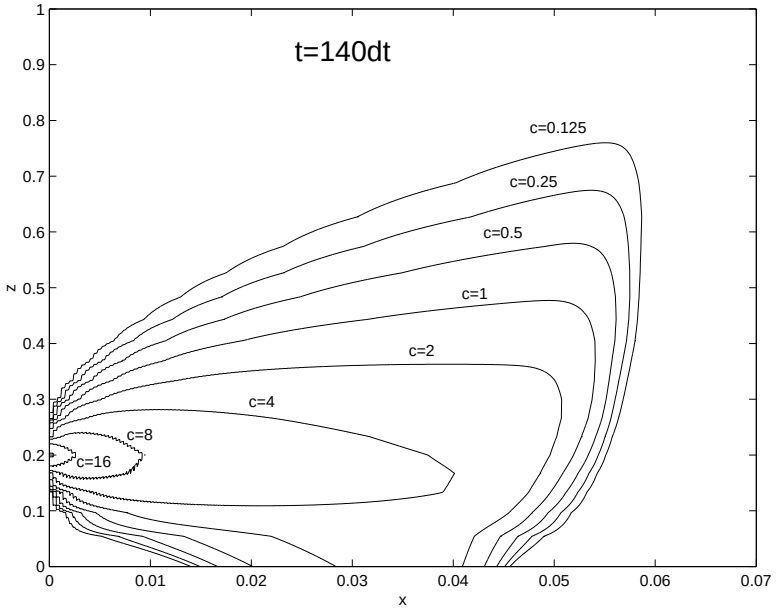
(d) $t = 100 \triangle t$.

Figure:4.3 (continued)



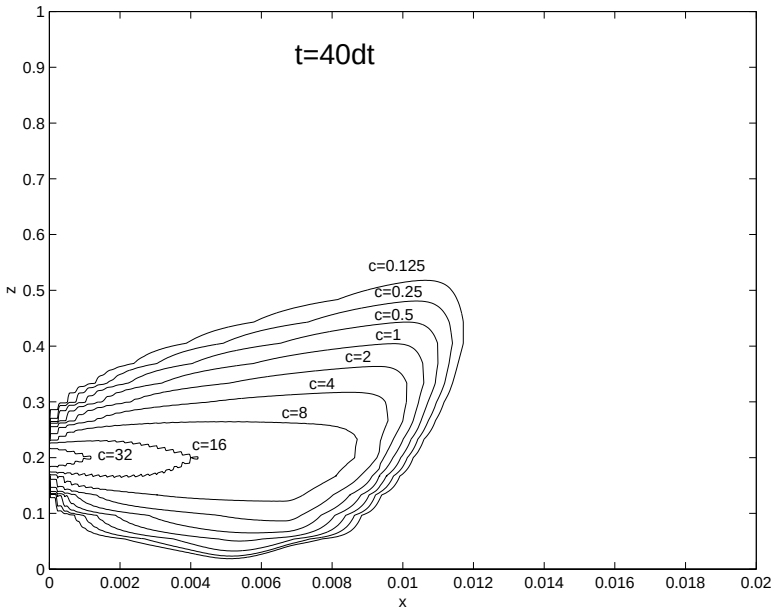
(e) $t = 120 \triangle t$.

Figure:4.3 (continued)



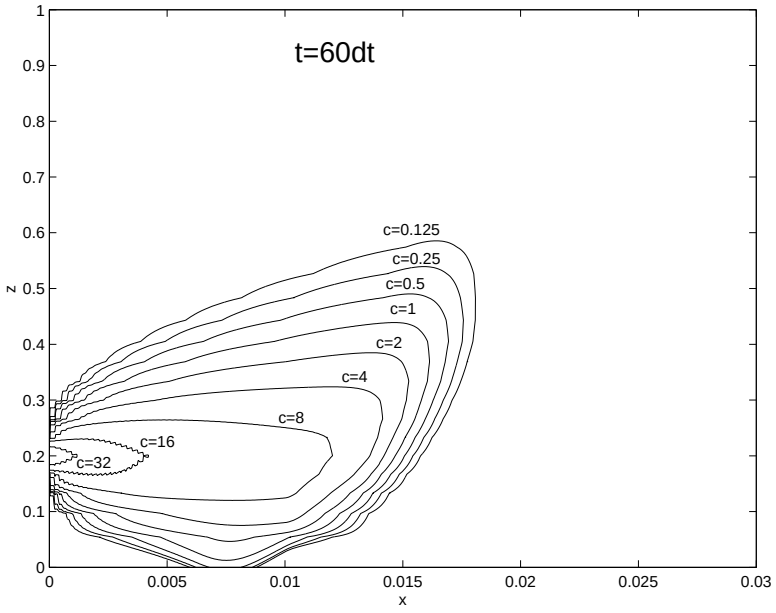
(f) $t = 140 \triangle t$.

Figure:4.3 (continued)



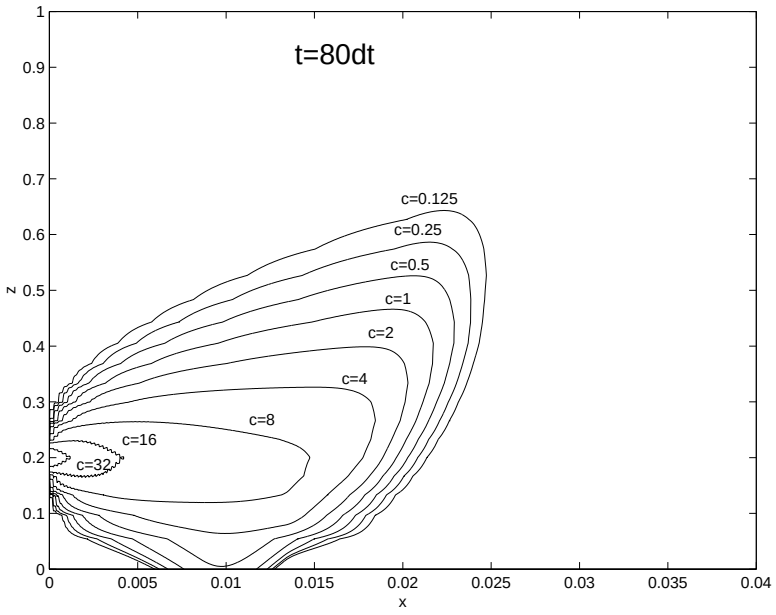
(a) $t = 40 \triangle t$.

Figure:4.4 The contour lines of concentration at different time, calculated for $u = z^{0.5}$ with $K = z$, $h = 0.2$ and $t = 40 \triangle t$, $t = 60 \triangle t$, $t = 80 \triangle t$, $t = 100 \triangle t$, $t = 120 \triangle t$ and $t = 140 \triangle t$,respectively, $\triangle t = .0005$.



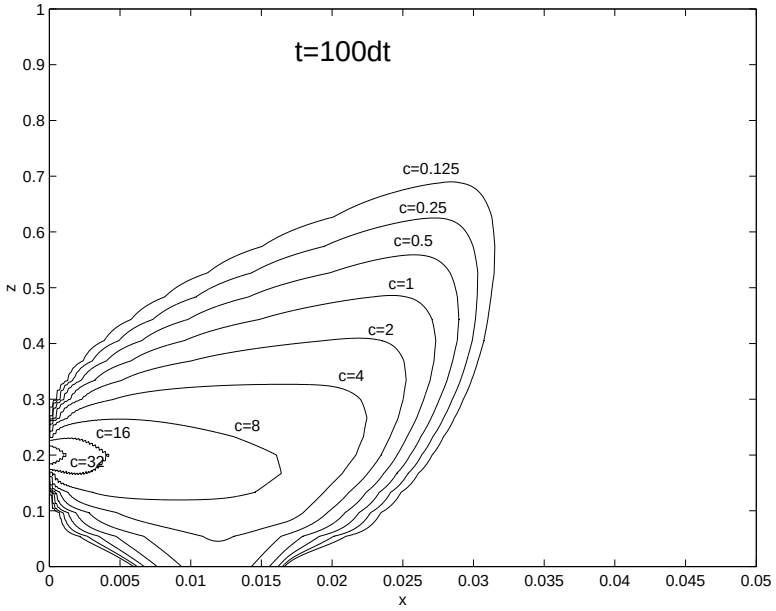
(b) $t = 60 \triangle t$.

Figure:4.4 (continued)



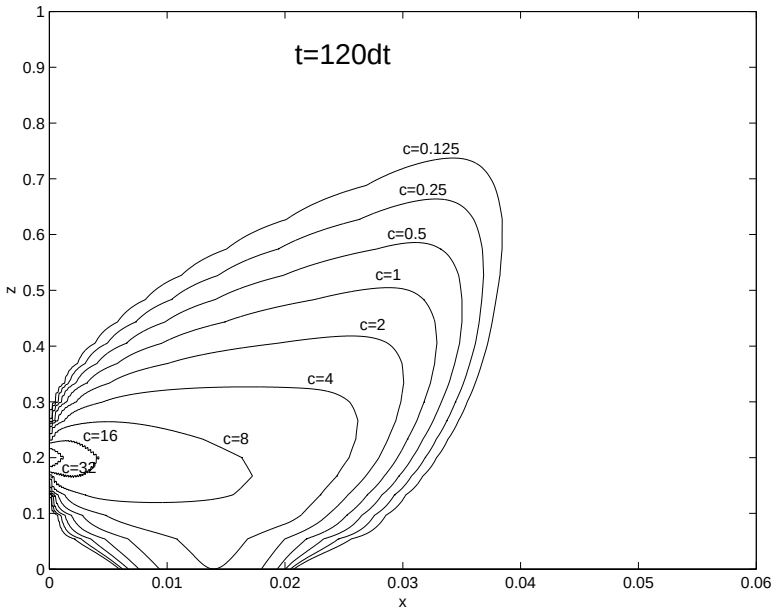
(c) $t = 80 \triangle t$.

Figure:4.4 (continued)



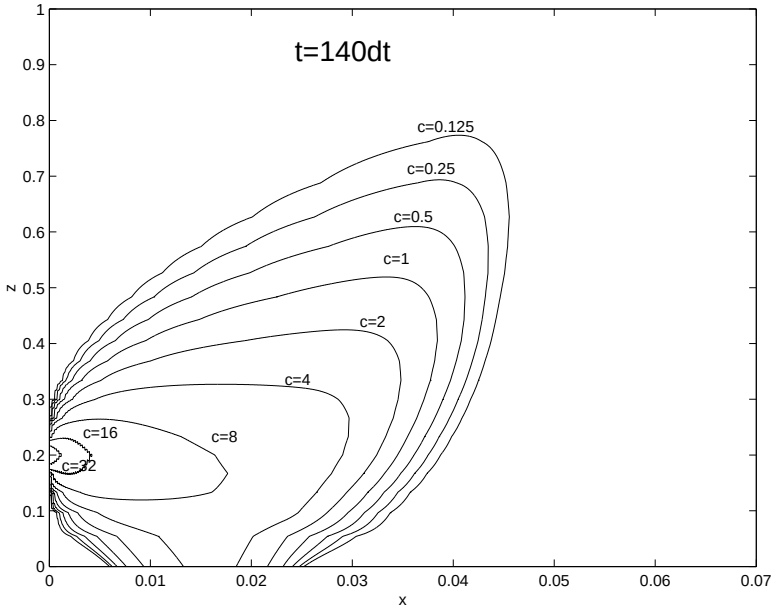
(d) $t = 100 \triangle t$.

Figure:4.4 (continued)



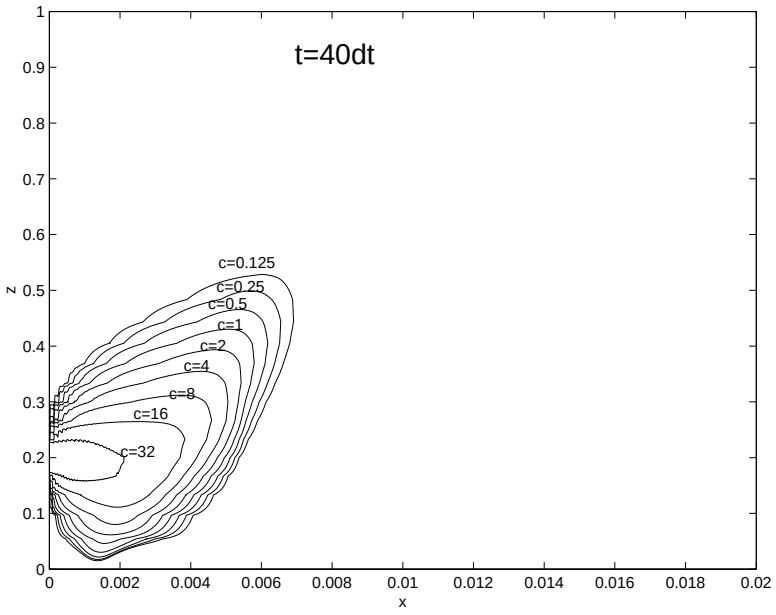
(e) $t = 120 \triangle t$.

Figure:4.4 (continued)



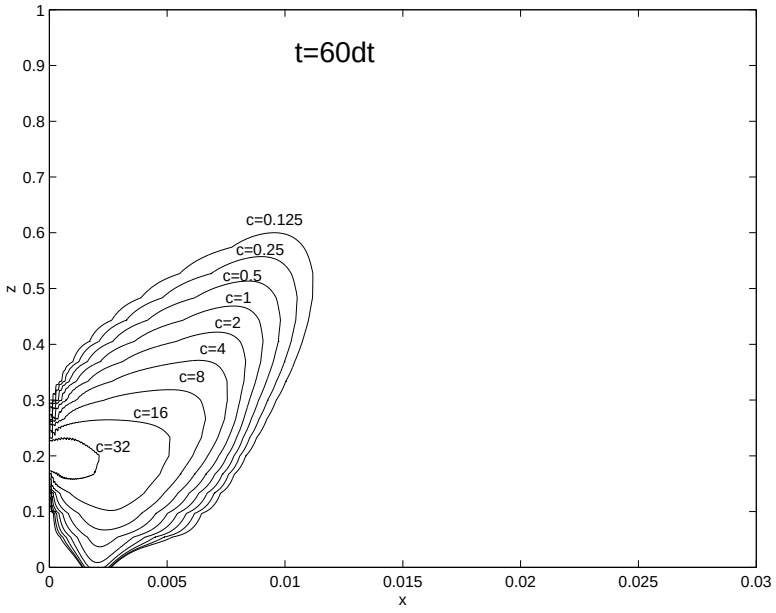
(f) $t = 140 \triangle t$.

Figure:4.4 (continued)



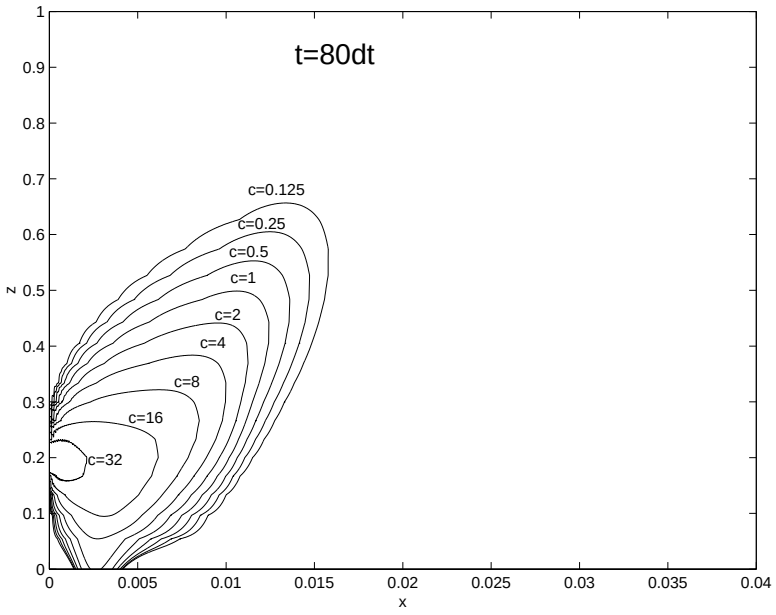
(a) $t = 40 \triangle t$.

Figure:4.5 The contour lines of concentration at different time, calculated for $u = z$ with $K = z$, $h = 0.2$ and $t = 40 \triangle t$, $t = 60 \triangle t$, $t = 80 \triangle t$, $t = 100 \triangle t$, $t = 120 \triangle t$ and $t = 140 \triangle t$,respectively, $\triangle t = .0005$.



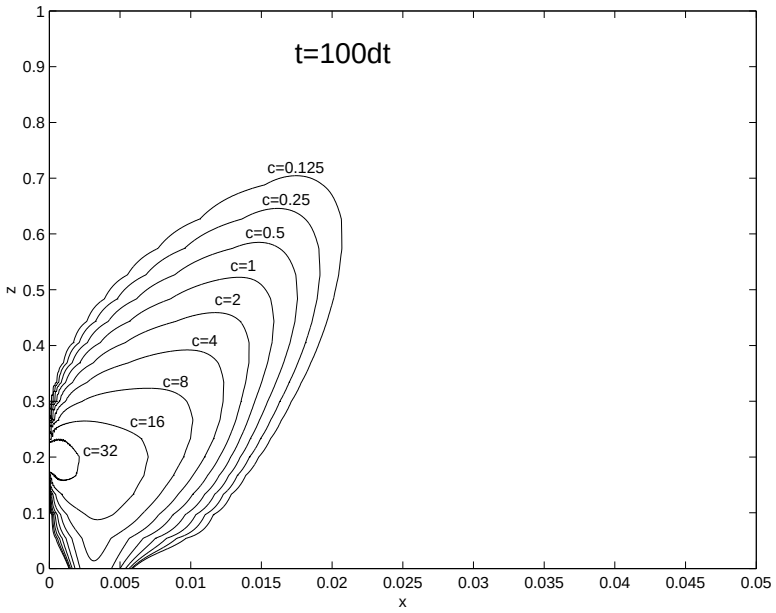
(b) $t = 60 \triangle t$.

Figure:4.5 (continued)



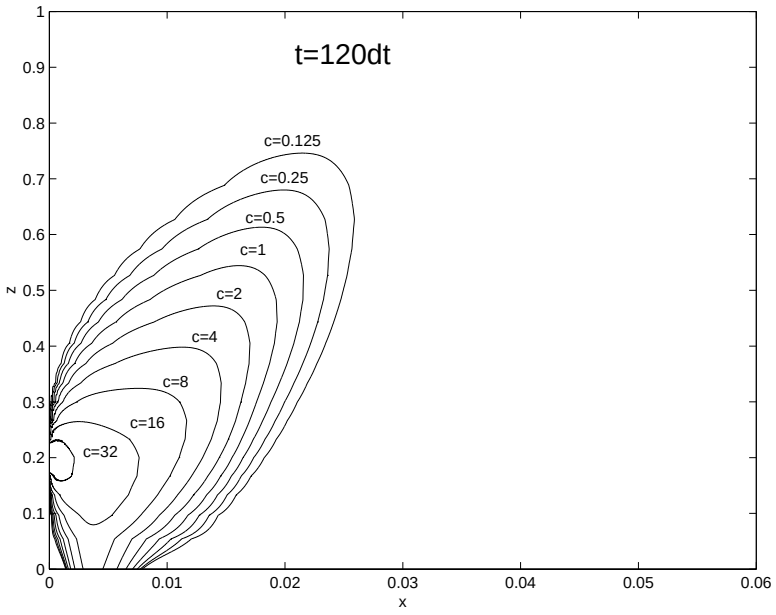
(c) $t = 80 \triangle t$.

Figure:4.5 (continued)



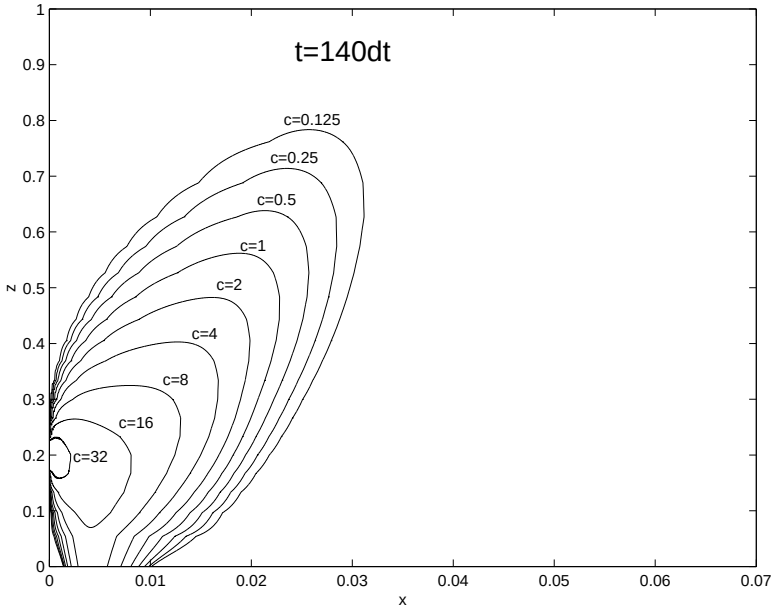
(d) $t = 100 \triangle t$.

Figure:4.5 (continued)



(e) $t = 120 \triangle t$.

Figure:4.5 (continued)



(f) $t = 140 \triangle t$.

Figure:4.5 (continued)

Chapter V
Conclusion

The mathematical model of advection diffusion equation for an air pollutant was solved by the numerical method which is called the Fractional Step method. We performed the calculation into two step using the Lagrangian and Eulerian methods. We find the auxiliary solution c^* from the advection part and then find the true solution c from the diffusion part, using the c^* as an initial data. By this method, we assumed that the pollutant move by convection and then by diffusion. In the case of the constant and variable coefficients of advection and diffusion, the numerical schemes were developed and solved by Matlab and Maple codes. The concentration line contours obtained from the computer programs are reasonably agreed with the former researches, for example in (Runca, Sardei 1975).

In the application of this programs to the real problem in some regions of an industrial area, we need to know the field data of the wind velocity and the diffusion coefficients.

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Appendix A
The Taylor Series

A power series in power of x is a series of the form

$$\sum_{n=0}^{\infty} a_n x^n = a_0 + a_1 x + a_2 x^2 + ... \qquad (A\_1)$$

A power series in powers of $(x - x_0)$ is given by

$$\sum_{n=0}^{\infty} a_n (x - x_0)^n = a_0 + a_1 (x - x_0) + a_2 (x - x_0)^2 + ... \qquad (A\_2)$$

Within its radius of convergence r, any continuous function $f(x)$ can be represented exactly by a power series. Thus,

$$f(x) = \sum_{n=0}^{\infty} a_n (x - x_0)^n \qquad (A\_3)$$

is continuous for $(x_0 - r) < x < (x_0 + r)$.

A.1 Taylor Series in One Independent Variable

If the coefficients a_n in equation(A_3) are given by the rule

$$a_0 = f(x_0), \quad a_1 = \frac{1}{1!} f'(x_0), \quad a_2 = \frac{1}{2!} f''(x_0), ... \qquad (A\_4)$$

then equation(A_3) becomes the *Taylor series* of $f(x)$ at $x = x_0$. Thus,

$$f(x) = f(x_0) = \frac{1}{1!} f'(x_0)(x - x_0) + \frac{1}{2!} f''(x_0)(x - x_0)^2 + ... \qquad (A\_5)$$

Equation(A_5) can be written in the simpler from

$$f(x) = f_i + f' \Big|_i \triangle x + \frac{1}{2} f'' \Big|_i \triangle x^2 + ... + + \frac{1}{n!} f^{(n)} \Big|_i \triangle x^n + ... \qquad (A\_6)$$

where $f^{(n)} = \dfrac{df^n}{dx^n}$ and $\triangle x = (x - x_0)$. Equation(A_5) can be written in the compressed form

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(a_n)(x - x_0)^n \qquad (A\_7)$$

when $x_0 = 0$, the Taylor series is known as the *Maclaurin's series.* In that case, equation(A_5) and (A_7) become

$$f(x) = f(0) = f^{'}(0)x + \frac{1}{2}f^{''}(0)x^2 + ... \qquad \text{(A\_8)}$$

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(0)x^n \qquad \text{(A\_9)}$$

It is, of course, impractical to evaluate an infinite Taylor series term by term. The Taylor series can be written as the finite Taylor series, also known as the *Taylor formula* or *polynomial* with *remainder*, as follows:

$$f(x) = f(x_0) = f^{'}(x_0)(x - x_0) + \frac{1}{2!}f^{''}(x_0)(x - x_0)^2 + ...$$

$$+\frac{1}{n!}f^{(n)}(x_0)(x - x_0)^n + R^{n+1} \qquad \text{(A\_10)}$$

where the term R^{n+1} is the remainder term given by

$$R^{n+1} = \frac{1}{(n+1)!} f^{(n+1)}(\xi)(x - x_0)^{n+1} \qquad \text{(A\_11)}$$

where ξ lies between x_0 and x. Equation(A_10) is quite useful in numerical analysis, where as approximation of $f(x)$ is obtained by neglecting the remainder term.

A.2 Taylor Series in Two Independent Variable

Power series can also be written for functions of more than one independent variable. For a function of two independent variables, $f(x, y)$, the Taylor series of $f(x, y)$ at (x_0, y_0) is given by

$$f(x,y) = f_0 + \left.\frac{\partial f}{\partial x}\right|_0 (x - x_0) + \left.\frac{\partial F}{\partial y}\right|_0 (y - y_0).$$

$$+\frac{1}{2!}\left(\left.\frac{\partial^2 f}{\partial x^2}\right|_0 (x - x_0)^2 + 2\left.\frac{\partial^2 f}{\partial x \partial y}\right|_0 (x - x_0)(y - y_0) + \left.\frac{\partial^2 f}{\partial y^2}\right|_0 (y - y_0)^2\right) + ... \qquad \text{(A\_12)}$$

Equation(A_12) can be written in the general form

$$f(x,y) = \sum_{n=0}^{\infty} \frac{1}{n!}\left((x - x_0)\frac{\partial}{\partial x} + (y - y_0)\frac{\partial}{\partial y}\right)^n f(x_0, y_0) \qquad \text{(A\_13)}$$

where the term $(....)^n$ is expanded by the binomial expansion and the resulting expansion operates on the function $f(x, y)$ and it is evaluated at (x_0, y_0).

The Taylor formula with remainder for a function of two independent variables is obtained by evaluating the derivatives in the $(n+1)st$ term at the point (x^*, y^*), where (x^*, y^*) lies in the region between points (x_0, y_0) and (x, y).

Appendix B
The Notation

Table B_1 : Notations Used in This Thesis

Symbol	Brief description	Units in English	Units in SI
c	concentration	$(lbm \text{ or } lbmol)/ft^3$	$(kg \text{ or } mol)/m^3$
H	height of inversion layer	ft	m
h	height of source (above the ground)	ft	m
K_x, K_y, K_z	coefficients of diffusion along the- $x-, y-, z-$directions, respectively	-	–
Q	emission rate	lbm/s	g/s
t	time	s	s
u	horizaotal conponent of the wind velocity	ft/s	m/s
w	vertical conponent of the wind velocity	ft/s	m/s
x, y, z	coordinate directions or lengths	ft	m

Appendix C
Computer Program

C.1 Matlab Code

```
%Step I . Compute vertical grid geometry. ( z(k) ; k=1..21 )
%choose point source=0.2 at z(6) and choose delta_z(s)=.033=d(5)=d(6)
% I.1 Lowbisection Compute alpha and d(1),d(2),...,d(5)
n=21;
min=0;
max=100;
tot=10^(-6);
while (max-min) > tot
    d=1:5
    d(5)=0.033;
    tempsum=0.033;
    for k=1:4
        d(5-k)=0.033*exp((.5*(max+min))*(tempsum)^2);
        tempsum=tempsum+d(5-k);
    end
    dd=sum(d)-0.2;
    if sign(dd)==1
        max=(max+min)/2;
    else
        min=(max+min)/2;
    end
end
alpha=(max+min)/2;
downd=d;
% I.2 Upbisection Compute beta and d(6),d(7),...,d(20)
minn=0;
maxx=100;
tott=10^(-6);
while (maxx-minn) > tott
    d=1:15
```

```
        d(1)=0.033;
        tempsum = 0.033;
    for k = 2:15
        d(k)=0.033*exp((.5*(maxx+minn))*(tempsum)^2);
        tempsum=tempsum+d(k);
    end
    dd=sum(d)-0.8;
    if sign(dd)==1
        maxx=(maxx+minn)/2;
    else
        minn=(maxx+minn)/2;
    end
end
beta=(maxx+minn)/2;
upd=d;
% I.3 Compute dz
dz=1:20
for i=1:5
    dz(i)=downd(i);
end
for i=6:20
    dz(i)=upd(i-5);
end
% I.4 Compute meash z
z(1)=0;
z(21)=1;
for k=2:20
    z(k)=z(k-1)+dz(k-1);
end
n
alpha
beta
dz
z
%Step II . The advection step : to solve by a Lagrangian technique.
% II.1 Compute step function ubar=pbar/q , calculated p(k)
n=21;
```

```
q=15; % choose q=15 for u=z^ 0.2 and u=z^ 0.5 and choose q=25 for u=z^ 0.1 and u=z
dt=0.001/2;
u=z.^ .2;
pk=1:21
pk(1)=round(q*(2/dz(1))*quad('z.^ .2',0,dz(1)/2)));
uk(1)=pk(1)/q;
for k=2:n-1
    pk(k)=round(q*(2/(dz(k-1)+dz(k)))*quad('z.^ .2',(z(k)-(dz(k-1)/2)),(z(k)+(dz(k)/2))));
uk(k)=pk(k)/q;
end
pk(n)=round(q*(2/dz(n-1))*quad('z.^ .2',(1-(dz(n-1)/2)),1));
uk(n)=pk(n)/q;
pk
uk
i=1
for x=0:0.005:1
    if 0<= x <=(1/2)*dz(1)
        ukb(i)=0;
    elseif z(2)-(1/2)*dz(2) <= x <= z(2)+(1/2)*dz(2)
        ukb(i)=uk(1);
    elseif z(3)-(1/2)*dz(3) <= x <= z(3)+(1/2)*dz(3)
        ukb(i)=uk(2);
    elseif z(4)-(1/2)*dz(4) <= x <= z(4)+(1/2)*dz(4)
        ukb(i)=uk(3);
    elseif z(5)-(1/2)*dz(5) <= x <= z(5)+(1/2)*dz(5)
        ukb(i)=uk(4);
    elseif z(6)-(1/2)*dz(6) <= x <= z(6)+(1/2)*dz(6)
        ukb(i)=uk(5);
    elseif z(7)-(1/2)*dz(7) <= x <= z(7)+(1/2)*dz(7)
        ukb(i)=uk(6);
    elseif z(8)-(1/2)*dz(8) <= x <= z(8)+(1/2)*dz(8)
        ukb(i)=uk(7);
    elseif z(9)-(1/2)*dz(9) <= x <= z(9)+(1/2)*dz(9)
        ukb(i)=uk(8);
    elseif z(10)-(1/2)*dz(10) <= x <= z(10)+(1/2)*dz(10)
        ukb(i)=uk(9);
    elseif z(11)-(1/2)*dz(11) <= x <= z(11)+(1/2)*dz(11)
```

```
        ukb(i)=uk(10);
    elseif z(12)-(1/2)*dz(12) <= x <= z(12)+(1/2)*dz(12)
        ukb(i)=uk(11);
    elseif z(13)-(1/2)*dz(13) <= x <= z(13)+(1/2)*dz(13)
        ukb(i)=uk(12);
    elseif z(14)-(1/2)*dz(14) <= x <= z(14)+(1/2)*dz(14)
        ukb(i)=uk(13);
    elseif z(15)-(1/2)*dz(15) <= x <= z(15)+(1/2)*dz(15)
        ukb(i)=uk(14);
    elseif z(16)-(1/2)*dz(16) <= x <= z(16)+(1/2)*dz(16)
        ukb(i)=uk(15);
    elseif z(17)-(1/2)*dz(17) <= x <= z(17)+(1/2)*dz(17)
        ukb(i)=uk(16);
    elseif z(18)-(1/2)*dz(18) <= x <= z(18)+(1/2)*dz(18)
        ukb(i)=uk(17);
    elseif z(19)-(1/2)*dz(19) <= x <= z(19)+(1/2)*dz(19)
        ukb(i)=uk(18);
    elseif z(20)-(1/2)*dz(20) <= x <= z(20)+(1/2)*dz(20)
        ukb(i)=uk(19);
    else
        ukb(i)=1;
    end
    i=i+1;
end
uk
figure(1)
hold on;
plot(u,z,'b')
stairs(uk,z,'r')
xlabel('u(z) and uk')
ylabel('z')
hold off;
%step III . The diffusion step : to solve an implicit central-space
%difference scheme allowing for a variable vertical grid spacing.
%implicit central-space difference scheme allowing
%for a variable vertical grid spacingn=21
for k=2:n-1
```

```
    U(k)=(dz(k-1)+dz(k))/dt;
    Q(k)=(1/U(k))*((z(k)+z(k-1))/(2*dz(k-1)));
    R(k)=(1/U(k))*(((z(k)+z(k-1))/(2*dz(k-1)))+((z(k)+z(k+1))/(2*dz(k))));
    S(k)=(1/U(k))*((z(k)+z(k+1))/(2*dz(k)));
end
for i=1:n
    for j=1:n
        M(i,j)=0;
        A(i,j)=0;
    end
end
M=zeros(n,n);
A=zeros(n,n);
M(1,1)=-(2*dz(1)+dz(2))/(dz(1)*(dz(1)+dz(2)));
M(1,2)=(dz(1)+dz(2))/(dz(1)*dz(2));
M(1,3)=-(dz(1))/(dz(2)*(dz(1)+dz(2))) ;
M(21,19)=(dz(20))/(dz(19)*(dz(20)+dz(19)));
M(21,20)=-(dz(20)+dz(19))/(dz(20)*dz(19));
M(21,21)=(2*dz(20)+dz(19))/(dz(20)*(dz(20)+dz(19)));
for i=2:n-1
    M(i,i-1)=-Q(i);
    M(i,i)=1+R(i);
    M(i,i+1)=-S(i);
    A(i,i-1)=Q(i);
    A(i,i)=1-R(i);
    A(i,i+1)=S(i);
end
IMA=inv(M)*A
M
A
IMA
%step IV . Time sequences of pollutant distribution in xz plane
%calculate for u(z)=1 , h=0.2 , K(z)=z , t=.001 , delta_t=delta_x.
t=40;
source= 1/(1*.033);
C=zeros(n,t+1);
C(:,1)=[0;0;0;0;0;source;0;0;0;0;0;0;0;0;0;0;0;0;0;0;0];
```

```
for i=2:t+1
    C(:,i)=IMA*C(:,i-1);
end
C
figure(2)
xx=linspace(0, n*10^(-3),t+1);
[X,Z]=meshgrid(xx,z);
cvals=[.125, .25, .5, 1, 2, 4, 8, 16, 32];
C_graph=contour(X,Z,C, cvals);
%clable(C_graph,'manual')
xlabel('x')
ylabel('z')
%step V . Time sequences of pollutant distribution in xz plane
%calculate for u(z), h=0.2, K(z)=z, t=.001, delta_t=5*delta_x.
t=40;
source=1/(((0.2)^(0.2))*.033);
CC=zeros(n,(q*t)+1);
CC(:,1)=[0;0;0;0;0;source;0;0;0;0;0;0;0;0;0;0;0;0;0;0;0];
for k=2:n-1
    for i=2:pk(k)+1
        CC(k,i)=CC(k,1);
    end
end
for j=2:q+1
    CC(:,j)=IMA*CC(:,j);
end
for k=2:t
    for i=1:n-1
        for j=(q*k)+1:-1:pk(i)+1
            CC(i,j)=CC(i,j-pk(i));
        end
        for j=pk(i)+1:-1:2
            CC(i,j)=CC(i,1);
        end
    end
    for j=2:(q*k)+1
        CC(:,j)=IMA*CC(:,j);
```

```
    end
end
CC
figure(3)
xx=linspace(0, n*10^ (-3),(q*t)+1);
[X,Z]=meshgrid(xx,z);
cvals=[.125, .25, .5, 1, 2, 4, 8, 16, 32];
CC_graph=contour(X,Z,CC, cvals);
%clable(CC_graph,'manual')
xlabel('x');
ylabel('z');
%plot concentration for fix time t=.0005*t_1
t_1=30; %choose t_1<=t
c_fixt=CC(:,q*t_1);
figure(4)
plot(z,c_fixt);
xlabel('z');
ylabel('concentration');
```

C.2 Maple Code

```
Numerical Treatment of Time Dependent Advection-Diffusion of An Air Pollutant.
(Computer Implementation of the Numerical Method )
Solve for u(z)=z^0.5 , h=0.2 ,delta_t=.001 , K(z)=z


Step I . Compute vertical grid geometry. ( z(k) ; k=1..21)
Start.
% define delta_z(k)=d[k]%
%choose point source=0.2 at z[6 ] and choose delta_z[s]=.033=d[5]=d[6]%

n:=21;q:=15.;dt:=.001;uz:=z^0.5;
z:=array(1..21):d:=array(1..21):
low:=0:up:=100:tot:=10^(-6.):
% choose q=15 for u=z^0.2 and u=z^0.5 and choose q=25 for u=z^0.1 and u=z


%lowbisection% compute alpha and d[1],d[2],...,d[5]%

while (up-low) > tot do
d[5]:=.033;tempsum:=.033;
for k from 1 to 4 do
d[5-k]:=.033*exp((.5*(up+low))*(tempsum)^2);
tempsum:=tempsum+d[5-k];
od;
dd:=sum('d[j]', 'j'=1..5)-0.2;
if (sign(dd)=1) then
up:=(up+low)/2;
else
low :=(up+low)/2;
end if;
od:
alpha:=(up+low)/2.;


% compute beta and d[6],d[7],...,d[20]%

l:=0:u:=100:t:=10^(-6.):
while (u-l) > t do
d[6]:=.033;tsum:=.033;
```

```
for j from 7 to 20 do
d[j]:=.033*exp((.5*(u+l))*(tsum)^2);
tsum:=tsum+d[j]
od;
ff:=sum('d[i]', 'i'=6..20)-0.8;
if (sign(ff)=1) then
u:=(u+l)/2;
else
l :=(u+l)/2;
end if;
od:
beta:=(u+l)/2.;
```

% compute vertical grids z(k), k=1...21%

```
z[1]:=0;z[21]:=1;
for k from 2 to 20 do
z[k]:=z[k-1]+d[k-1];
od;
```

Step II . The advection step : to solve by a Lagrangian technique.
%compute step function u_bar=p_bar /q , calculated p(k) by $$ p(k)=q*u(k) $$ and $$ u(k)= 2/(d(k-1)+d(k))*(integral(u(z)dz), z = z(k)-(d(k-1))/2.. to .. z(k)+(d(k))/2) $$ %

```
p:=array(1..n):u:=array(1..n):
p[1]:=round(q*(2/d[1])*int(uz,z=0..(d[1]/2))):
u[1]:=p[1]/q:
for k from 2 to n-1 do
p[k]:=round(q*(2/(d[k-1]+d[k]))*int(uz,z=(z[k]-(d[k-1]/2))..(z[k]+(d[k]/2)))):
u[k]:=p[k]/q;
od:
p[n]:=round(q*(2/d[n-1])*int(uz,z=(1-(d[n-1]/2))..1)):
u[n]:=p[n]/q:
```

%plot graph wind profile and step function u_bar. %

```
step:=x->piecewise(0<=x and x<=(d[1]/2),0,z[2]-(d[2]/2)¡=x and
x<=z[2]+(d[2]/2),u[1],z[3]-(d[3]/2)<=x and
```

```
x<=z[3]+(d[3]/2),u[2],z[4]-(d[4]/2)<=x and
x<=z[4]+(d[4]/2),u[3],z[5]-(d[5]/2)<=x and
x<=z[5]+(d[5]/2),u[4],z[6]-(d[6]/2)<=x and
x<=z[6]+(d[6]/2),u[5],z[7]-(d[7]/2)<=x and
x<=z[7]+(d[7]/2),u[6],z[8]-(d[8]/2)<=x and
x<=z[8]+(d[8]/2),u[7],z[9]-(d[9]/2)<=x and
x<=z[9]+(d[9]/2),u[8],z[10]-(d[10]/2)<=x and
x<=z[10]+(d[10]/2),u[9],z[11]-(d[11]/2)<=x and
x<=z[11]+(d[11]/2),u[10],z[12]-(d[12]/2)<=x and
x<=z[12]+(d[12]/2),u[11],z[13]-(d[13]/2)<=x and
x<=z[13]+(d[13]/2),u[12],z[14]-(d[14]/2)<=x and
x<=z[14]+(d[14]/2),u[13],z[15]-(d[15]/2)<=x and
x<=z[15]+(d[15]/2),u[14],z[16]-(d[16]/2)<=x and
x<=z[16]+(d[16]/2),u[15],z[17]-(d[17]/2)<=x and
x<=z[17]+(d[17]/2),u[16],z[18]-(d[18]/2)<=x and
x<=z[18]+(d[18]/2),u[17],z[19]-(d[19]/2)<=x and
x<=z[19]+(d[19]/2),u[18],z[20]-(d[20]/2)<=x and
x<=z[20]+(d[20]/2),u[19],1):
step(0.15):
plot({step(z),uz},z=0..1);
```

step III . The diffusion step : to solve an implicit central-space difference scheme allowing for a variable vertical grid spacing.

% implicit central-space difference scheme allowing for a variable vertical grid spacing %

```
Q:=array(2..n-1):R:=array(2..n-1):S:=array(2..n-1):U:=array(1..n):
for k from 2 to n-1 do
U[k]:=(d[k-1]+d[k])/dt;
Q[k]:=(1/U[k])*((z[k]+z[k-1])/(2*d[k-1]));
R[k]:=(1/U[k])*(((z[k]+z[k-1])/(2*d[k-1]))+((z[k]+z[k+1])/(2*d[k])));
S[k]:=(1/U[k])*((z[k]+z[k+1])/(2*d[k]));
od:
M:=array(1..n,1..n):A:=array(1..n,1..n):
for i from 1 to n do
for j from 1 to n do
M[i,j]:=0;
A[i,j]:=0;
```

```
od:
od:
M[1,1]=-(2*dz[1]+dz[2])/(dz[1]*(dz[1]+dz[2]));
M[1,2]=(dz[1]+dz[2])/(dz[1][*dz[2]);
M[1,3]=-(dz[1])/(dz[2]*(dz[1]+dz[2])) ;
M[21,19]=(dz[20])/(dz[19]*(dz[20]+dz[19]));
M[21,20]=-(dz[20]+dz[19])/(dz[20]*dz[19]);
M[21,21]=(2*dz[20]+dz[19])/(dz[20]*(dz[20]+dz[19]));
for i from 2 to n-1 do
M[i,i-1]:=-Q[i];
M[i,i]:=1+R[i];
M[i,i+1]:=-S[i];
A[i,i-1]:=Q[i];
A[i,i]:=1-R[i];
A[i,i+1]:=S[i];
od:
print(M);
print(A);
with(linalg):
IM:=inverse(M):
S:=multiply(IM,A);
```

step IV .Time sequences of pollutant distribution in xz plane calculate for u(z)=1 , h=0.2 , K(z)=z , t=.001 , delta_t=delta_x.
compute concentration data.
%uk at source =1%

```
t:=40;
source:=1/(1*.033);
c[0]:=array(1..n,1..1,[[0],[0],[0],[0],[0],[source],[0],[0],[0],[0],[0],[0],[0],[0],[0],[0],[0],[0],[0],[0],[0]]):
for i from 1 to t do
c[i]:=multiply(S,c[i-1]);
od:
C:=matrix(n,t+1);
for i from 1 to n+1 do
for j from 1 to t+1 do
C[i,j]:=c[j-1][i,1];
od;
```

```
od:
print(C)
x[1]:=0:
for j from 2 to t+1 do
x[j]:= x[j-1]+evalf(0.1/t):
od:
B:=[seq([seq([z[i],x[j],C[i,j]],i=1..n)],j=1..t+1)]:B[10,10];
```

IV.I plot graph of concentration C(21,41) for t=40*delta_t.

```
t=40
with(plots):
surfdata(B, axes=frame, labels=[z,x,y]);
```

IV.II plot graph of concentration C(21,81) for t=80*delta_t.

```
t=80
with(plots):
surfdata(B, axes=frame, labels=[z,x,y]);
```

IV.III plot graph of concentration C(21,121) for t=120*delta_t.

```
t=120
with(plots):
surfdata(B, axes=frame, labels=[z,x,y]);
```

IV.IV compare concentration at the same point (x=.06) and difference delta_t (.001 , .0005 , .00025)

(1) call concentration at x=.06 , delta_t =.001 , column 20 from C(21,41)

```
T1:=array(1..10);
for i from 1 to 10 do
T1[i]:=C[i*2,20];
od;
print(T1);
```

(2) call concentration at x=.06 , delta_t =(.001)/2=.0005 , column 40 from C(21,81)

```
T2:=array(1..10);
for i from 1 to 10 do
T2[i]:=C[i*2,40];
od;
print(T2);
```

(3) call concentration at x=.06 , delta_t =(.001)/4=.00025 , column 80 from C(21,161)

```
T3:=array(1..10);
for i from 1 to 10 do
T3[i]:=C[i*2,80];
od;
print(T3);
```

(4) call concentration at x=.06 , delta_t =(.001)/8=.000125 , column 160 from C(21,321)

```
T4:=array(1..10);
for i from 1 to 10 do
T4[i]:=C[i*2,160];
od;
print(T4);
```

(5) call concentration at x=.06 , delta_t =(.001)/16=.0000625 , column 320 from C(21,641)

```
T5:=array(1..10);
for i from 1 to 10 do
T5[i]:=C[i*2,320];
od;
print(T5);
```

(6) compare concentration at the same point (x=.06) and difference delta_t (.001 , .0005 , .00025)

```
print(delta_t=.001,T1);
print(delta_t=(.001)/2,T2);
print(delta_t=(.001)/4,T3);
```

```
print(delta_t=(.001)/8,T4);
print(delta_t=(.001)/16,T5);
```

step V . Time sequences of pollutant distribution in xz plane calculate for u(z), h=0.2, K(z)=z, t=.001, delta_t=5*delta_x.
compute concentration data.
uk at source =u(z)=z^0.5 at z=0.2

```
t:=120;
source:=1/(((0.2)^(0.5))*.033);
c[0]:=array(1..n,1..1,[[0],[0],[0],[0],[0],[source],[0],[0],[0],[0],[0],[0],[0],[0],[0],[0],[0],[0],[0],[0],[0]]):
for k from 1 to 5 do
c_b[k]:=matrix(n,1);
od:
for k from 1 to n do
for j from 1 to (5*t)+1 do
c_b[j][k,1]:=0;
od;
od:
for k from 1 to n-1 do
for i from 2 to p[k]+1 do
c_b[i][k,1]:=c[0][k,1];
od;
od:
print(c_b[1],c_b[2],c_b[3],c_b[4],c_b[5])
for i from 1 to 6 do
c[i]:=multiply(S,c_b[i]);
od:
C:=matrix(n,(5*t)+1);
for i from 2 to n do
for j from 2 to (5*t)+1 do
C[i,j]:=0;
od;
od;
for i from 2 to n-1 do
for j from 2 to p[k]+1 do
C[i,j]:=c[j-1][i,1];
od;
```

```
od;
for k from 2 to t do
for i from 2 to n-1 do
for j from (5*k)+1 by -1 to p[i]+1 do
C[i,j]:=C[i,j-p[i]];
od;
for j from p[i]+1 by -1 to 2 do
C[i,j]:=C[i,1];
od;
od;
for m from 1 to n do
for j from 2 to (5*k)+1 do
C[m,j]:=sum('S[m,n]*C[n,j]','n=1..21');
od;
od;
od;
print(C)
x[1]:=0:
for j from 2 to (5*t)+1 do
x[j]:= x[j-1]+evalf(0.05/((5*t)+1)):
od:
B:=[seq([seq([z[i],x[j],C[i,j]],i=1..n)],j=1..(5*t)+1)]:B[10,10];
```

V.I plot graph of concentration C(21,201) for t=40*delta_t.

```
t=40
with(plots):
surfdata(B, axes=frame, labels=[z,x,y]);
```

V.II plot graph of concentration C(21,401) for t=80*delta_t.

```
t=80
with(plots):
surfdata(B, axes=frame, labels=[z,x,y]);
```

V.III plot graph of concentration C(21,601) for t=120*delta_t.

```
t=120
with(plots):
```

```
surfdata(B, axes=frame, labels=[z,x,y]);
```

V.IV compare concentration at the same point (x=.06) and difference delta_t (.001 , .0005 , .00025)

(1) call concentration at x=.06 , delta_t =.001 ,column 100 from C(21,201)

```
T1:=array(1..10);
for i from 1 to 10 do
T1[i]:=C[i*2,100];
od;
print(T1);
```

(2) call concentration at x=.06 , delta_t=(.001)/2=.0005 , column 200 from C(21,401)

```
T2:=array(1..10);
for i from 1 to 10 do
T2[i]:=C[i*2,200];
od;
print(T2);
```

(3) call concentration at x=.06 , delta_t=(.001)/4=.00025 , column 400 from C(21,801)

```
T3:=array(1..10);
for i from 1 to 10 do
T3[i]:=C[i*2,400];
od;
print(T3);
```

(4) compare concentration at the same point (x=.06) and difference delta_t (.001 , .0005 , .00025)

```
print(delta_t=.001,T1);
print(delta_t=(.001)/2,T2);
print(delta_t=(.001)/4,T3);
```

Curriculum Vitae

Miss Sureerat Areeraksakul was born in Nakhonratchasima, Thailand, on April 1976. She graduated with a high school diploma from Suranaree school, Nakhonratchasima in 1993. She attended Khon Kean University from 1993 to 1997, graduating with the Bachelor of Science Degree in Mathematics. She joined the Faculty of science, department of Mathematics at Ubonratchathani University in March 1997. In 1999, she got her scholarship to study for a Master's degree at the School of Mathematics, Institute of Science, Suranaree University of Technology.