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FINITE ELEMENT METHODS FOR AIR POLLUTION PROBLEMS

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Suranaree University of Technology has approved this thesis submitted in partial fulfillment of the requirements for a Doctoral Degree.

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ขั้นตอนวิธีเชิงตัวเลข/วิธีสมาชิกจำกัด/มลพิษทางอากาศ

ในการวิจัยครั้งนี้ เราใช้ตัวแบบเชิงคณิตศาสตร์เพื่อศึกษาความเข้มข้นของมลพิษทางอากาศซึ่งถูกปล่อยจากแหล่งกำเนิดที่เป็นเส้นสู่บรรยากาศที่อยู่ใต้ทิศทางลม ความเข้มข้นเริ่มแรกเป็นฟังก์ชันเดลตาที่มีอัตรากระจายคงที่ สัมประสิทธิ์ของการพาและการแพร่เป็นฟังก์ชันของ z ในการคำนวณหาความเข้มข้นในแนวดิ่งใกล้แหล่งกำเนิดใช้ขนาดของช่วงที่ไม่คงที่ โดยอาศัยเทคนิคการกระจายเกาส์เซียนช่วยในการคำนวณขนาดของช่วงในแนวดิ่ง ในกรณีสถานะอยู่ตัว ได้ประยุกต์ใช้วิธีสมาชิกจำกัด ส่วนในกรณีสถานะไม่อยู่ตัวได้ใช้วิธีผลต่างจำกัดแบบลากรานจ์ และวิธีสมาชิกจำกัดกับส่วนการพาและส่วนการแพร่ตามลำดับ

ได้เสนอตัวอย่างข้อมูลการจำลองเชิงตัวเลขโดยใช้ค่าพารามิเตอร์ที่แตกต่างกัน และใช้โปรแกรมแมทแลบในการคำนวณผลเฉลยของระบบสมการเชิงเส้น ในกรณีสถานะอยู่ตัว ผลการคำนวณได้เปรียบเทียบกับผลเฉลยที่แท้จริง ปรากฏว่าได้ผลลัพธ์ใกล้เคียงกันเป็นที่น่าพอใจ สำหรับกรณีสถานะไม่อยู่ตัว ผลการคำนวณได้เปรียบเทียบกับผลการคำนวณของงานวิจัยอื่นที่ใช้วิธีแยกส่วน ปรากฏว่าผลลัพธ์ทั้งสองวิธีที่แสดงโดยกราฟไม่มีความแตกต่างกัน นอกจากนี้ ได้กล่าวถึงรายละเอียดของการลู่เข้าและความคลาดเคลื่อนของผลเฉลยเชิงตัวเลขไว้ด้วย

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NUMERICAL ALGORITHM / FINITE ELEMENT METHODS / AIR POLLUTION

In this research we used mathematical models to study propagation of an air pollutant which is released from a line source downwind into the atmosphere. The initial condition is assumed to be the δ-function of the steady emission rate. The coefficients of the advection and diffusion are assumed to be function of z. The concentration profile near the source was calculated at the variable step sizes using the Gaussian distribution in the vertical grid intervals. We then applied the finite element method to the steady state case, and in the unsteady state case we used the Lagrangian finite difference and finite element method on the advection part and the diffusion part respectively.

The examples of numerical data simulation with varied parameters were presented. MatLab software was used to calculate solutions of linear systems. In the case of steady state, the results were compared with the existing analytical results and they show satisfactory agreement. In the unsteady state case, the computed solution is graphically well agreed with the results of other work by using the fractional step method. Besides, the convergence and error estimate of the approximate solution are also discussed.

School of Mathematics	Signature of Student__________________________
Academic Year 2002	Signature of Advisor__________________________
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Supot Witayangkurn

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Chapter I

Introduction

1.1 Mathematical models of air pollution system

Air pollution refers to an air condition in which there are contaminant substances in a higher quantity than normal for a time long enough to harm humans, animals, plants or property. It can naturally exist, for instance, dust or aerosol from wind or storms, exploded volcanoes, earthquakes, fire, or pollutant air from bikes and industrial factories.

It is the environmental problems which are easily noticed both in large communities and developing areas that are now quickly spreading in size through industrial activities. These activities include transportation, traffic, construction and also areas in which power plants are situated. Air pollutant substances which are a main problem and over standard that are still important problems for the future such as carbon-monoxide gas, dust, especially the dust in communities with heavy traffic, will have a higher concentration than standard value, about 3-5 times, while other substances such as lead, sulfur-dioxide and nitrogen-dioxide are at standard quality air criteria in the atmosphere.

These polluted substances ventilate from various sources in the community, both from vehicles, building construction or even road reconstructions and road surface repairing and also industrial factories. These substances will not only directly affect people's health but also other crises like changes in the earth's temperature and the destruction of the ozone layer.

The government is now working to solve air pollution problems by setting air quality standard from sources, oil fuel and lubricating oil quality standards, and encouraging people to use unleaded gasoline. Even setting special filter accessories for air pollution from cars, checking the polluted condition of vehicles before lengthening car licenses, controlling the air pollution quantity from industrial factories, and increasing and improving air pollution standards can help us handle such problems while still at the beginning stage. This is because there is still a lack of unique air pollution controls, as there are many firms that are in charge but the cooperation mission is not efficient, the examination staff or departments do not have enough equipment or experienced teams who can check and organize data base systems, and while the testing and traffic checking have no standards, the research and technology development for decreasing air pollution through innovations like the electric-tricycle, bus and motor bike, are not yet developed in business. Furthermore, there are neither campaigns nor continual public relations working in order to change people and drivers' habits in decreasing air pollution.

There are two main air pollution sources; one is traffic and the other is industrial factories. While the former forms air pollution problems in main communities like Bangkok or neighboring provinces, the latter forms the problems in scattered areas in the country, both in towns and villages.

The sudden economic growth of the country from agricultural section to industrial influenced Bangkok, which is the business and civilization center, leading to an increasing population, and to more traveling and transportation needs. This will affect the traffic jam crisis and cause low driving speed, and more starts and stops which burns up more fuel. The more the fuel combustion is not completed , the more air pollutant venting. Then the area near the traffic jam will have more serious problems than in a normal area. The air pollutants which ventilate into the atmosphere and come from transportation are carbon monoxide, nitrogen-oxide, hydrocarbon forming compound, tiny dust of 10 micron size, lead and sulfur dioxide.

The main goal of this research is to study a solution in two space dimensions of an air pollutant released into the atmosphere from a chimney at height h above the ground in the presence of an inversion layer (see Figure 1.1)

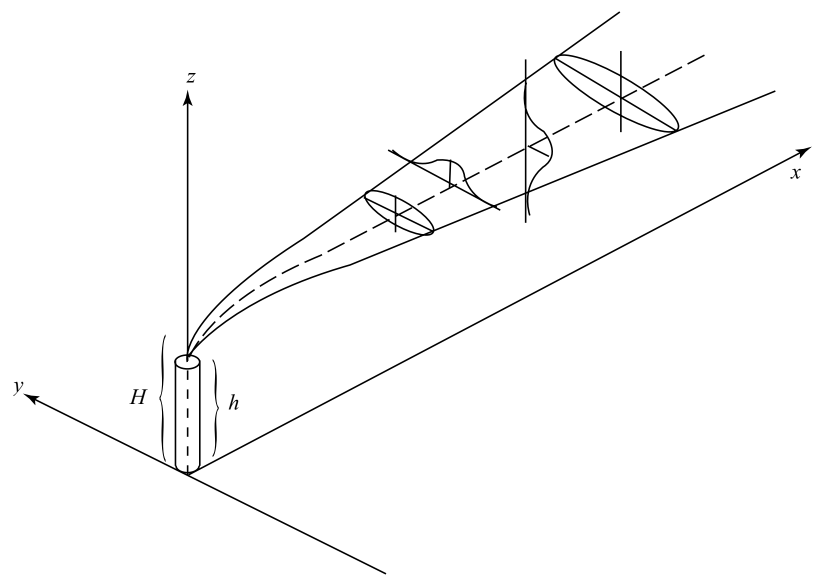


Figure 1.1 : Concentration distributions form a continuous point source. (Adapted from Seinfeld, J. H. (1975))

The well known process of diffusion of pollutants downwind from a source is assumed to be governed by the differential equation (Runca, E. and Sardei, F. (1975))

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

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 for eddy 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

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

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

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

This equation has been widely applied to describe air pollution advection-diffusion phenomena.

Rounds, M. Jr. (1955) found the analytic solution of equation

$$u(z)\frac{\partial c}{\partial x} = \frac{\partial}{\partial z}\left(K(z)\frac{\partial c}{\partial z}\right), \tag{1.3}$$

with the following boundary condition:

- The boundary condition on the z-axis is

$$c(0, z) = \frac{\delta(z-h)}{u(h)} \quad \text{for all } 0 < z < 1, \tag{1.4}$$

where h is the height of the source.

- The boundary condition on the ground and at the inversion rate

$$K(z)\frac{\partial c(x,0)}{\partial z} = 0 \quad \text{for all} \quad 0 < x, \tag{1.5}$$

and

$$K(z)\frac{\partial c(x,1)}{\partial z} = 0 \quad \text{for all} \quad 0 < x. \tag{1.6}$$

The analytic solution of case

$$u(z) = z^{\alpha}, K(z) = z, \qquad 0 \le \alpha \le 1 \tag{1.7}$$

is

$$c(x,z) = (1+\alpha)\sum_{j=0}^{\infty}\frac{J_0\left(\sigma_j z^{(1+\alpha)/2}\right)\cdot J_0\left(\sigma_j h^{(1+\alpha)/2}\right)\exp\left[-\sigma_j^2 x(1+\alpha)^2/4\right]}{\left[J_0\left(\sigma_j\right)\right]^2}. \tag{1.8}$$

Here J_0 is the Bessel function of the first kind of order zero, σ_j is the *j*th root of J_1 is the Bessel function of the first kind of order one, $\sigma_0 = 0$ and $J_0(0) = 1$.

Runca, E. and Sardei, F. (1975) carried out a numerical treatment of time dependent advection and diffusion of air pollutants equation

$$\frac{\partial c(x,z,t)}{\partial t} + u(z)\frac{\partial c}{\partial x} = \frac{\partial}{\partial z}\left(K(z)\frac{\partial c}{\partial z}\right) \text{ for all } 0 < t, 0 < x, 0 < z < 1. \tag{1.9}$$

The initial condition is

$$c(x,z,0) = 0 \text{ for all } 0 < t, 0 < x, \tag{1.10}$$

The boundary conditions are needed to define the source and to specify the vertical diffusion range. The concentration at the source is assumed to be a δ-function:

$$c(0,z,t) = \frac{\delta(z-h)}{u(h)} \text{ for all } 0 < t, \tag{1.11}$$

where h is the height of the source. Boundary conditions for the vertical diffusion are given at the ground and at the inversion layer. The latter condition is determined by considering the fact that the base of an elevated inversion layer tends to act as a lid on the upward diffusion of matter. Assuming that the ground and the inversion layer base completely reflect the diffusing material, we have

$$K(z)\frac{\partial c(x,z,t)}{\partial z}=0, \qquad z=0,1 \tag{1.12}$$

Equation (1.9) is solved with the method of fractional step (see, e.g. Yanenko, N. N. (1971)). According to this technique, the concentration field at the time $t+\Delta t$ is obtained from that at the time t by separating the contributions due to the advection and diffusion terms of equation (1.9) as follows:

In the first steps, the advection equation

$$\frac{\partial c}{\partial t}+u(z)\frac{\partial c}{\partial x}=0. \tag{1.13}$$

is solved in the whole *x*-*z* integration region over the time interval $[t,t+\Delta t]$ with the concentration field at the time t as the initial condition and the relation (1.11) as the boundary condition. The diffusion equation

$$\frac{\partial c}{\partial t}-\frac{\partial}{\partial z}\left(K(z)\frac{\partial c}{\partial z}\right)=0, \tag{1.14}$$

is 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 (1.12). The solution of (1.14) is an approximation of the concentration field at the time $t+\Delta t$.

For equation (1.13) a Lagrangian technique is used in order to avoid artificial diffusion errors associated with the advection step. The diffusion equation (1.14) is solved with a conventional Eulerian finite-difference scheme.

The mathematical models for air pollutant dynamics in the atmosphere, as it is known, and the process of pollutant transport and diffusion in the atmosphere is described by the partial differential equation (Dang Quang A. and Ngo Van Luoc. (1991))

$$\frac{\partial\varphi}{\partial t}+u\frac{\partial\varphi}{\partial x}+v\frac{\partial\varphi}{\partial y}+(w-w_g)\frac{\partial\varphi}{\partial z}-\mu\Delta\varphi-\frac{\partial}{\partial z}\left(\nu\frac{\partial\varphi}{\partial z}\right)+\sigma\varphi=f. \tag{1.15}$$

Where φ is the concentration of pollutants, t is time, x, y and z are the space coordinates, u, v and w are the components of the wind velocity, f is the power of the source, w_g is a positive constant, the falling velocity of pollutants by gravity, σ is a positive constant, the transformation coefficient of pollutants, μ, ν are the diffusion coefficients, and Δ denotes the Laplace operator, i.e. $\Delta=\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}$.

Dang Quang A. and Ngo Van Luoc. (1991) have found the exact solution of the stationary problem of the equation (1.15) under the following assumptions:

1. The source is concentrated in point (0,0,h) and has a constant power Q, i.e. $f=Q\delta(x)\delta(y)\delta(z-h)$, where $\delta(x)$ is the Dirac delta function.
2. The process of pollutant dispersion is stationary, i.e. $\frac{\partial\varphi}{\partial t}=0$.
3. The wind direction coincides with the positive direction of the axis Ox, namely $u=u(z)>0$, $v=w=0$.

Under the above assumptions the diffusion term in the direction of Ox can be neglected so that the equation (1.15) takes the form

$$u\frac{\partial\varphi}{\partial x}-w_g\frac{\partial\varphi}{\partial z}-\mu\frac{\partial^2\varphi}{\partial y^2}-\frac{\partial}{\partial z}\left(\nu\frac{\partial\varphi}{\partial z}\right)+\sigma\varphi=Q\delta(x)\delta(y)\delta(z-h). \tag{1.16}$$

This equation will be investigated together with the following boundary conditions

$$\varphi=0,\qquad x,y\to\pm\infty, \tag{1.17}$$

$$\varphi=0,\qquad z\to+\infty, \tag{1.18}$$

$$\frac{\partial \varphi}{\partial z} = \alpha\varphi, \qquad z = 0. \tag{1.19}$$

Here α = const ≥ 0 is a coefficient characterizing the reflection and absorption of the bedding surface.

The solution of the problem (1.16)-(1.19) in the case when u = const > 0, $\mu = k_0 u$, k_0 = const > 0, ν = const > 0 is

$$\varphi(x,y,z) = \frac{Q}{4\sqrt{\pi\nu\mu x}} e^{-uy^2/(4\mu x)} \left\{ \frac{1}{\sqrt{\pi x}} \left(e^{-a^2(z+h)^2/(4x)} + e^{-a^2(z-h)^2/(4x)} \right) \right.$$

$$\left. - \frac{2\alpha}{a} e^{\alpha^2 x/a^2 + \alpha(z+h)} erfc\left(\frac{a(z+h)}{2\sqrt{x}} + \frac{\alpha\sqrt{x}}{a} \right) \right\}, \quad x > 0$$

$$\varphi(x,y,z) = 0, \qquad x < 0,$$

where $a = \sqrt{\frac{u}{\nu}}$.

In 1992 Dang Quang A. and Ngo Van Luoc. (1992) proposed a numerical method for solving the problem

$$u\frac{\partial \varphi}{\partial x} - w_g \frac{\partial \varphi}{\partial z} - \frac{\partial}{\partial z}\left(\nu \frac{\partial \varphi}{\partial z} \right) + \sigma\varphi = 0, \quad x > 0, \tag{1.20}$$

$$u\varphi = Q\delta(z-h), \qquad x = 0, \tag{1.21}$$

$$\varphi = 0, \qquad z \to \infty, \tag{1.22}$$

$$\frac{\partial \varphi}{\partial z} = \alpha\varphi, \qquad z = 0. \tag{1.23}$$

For the considered problem an implicit difference scheme is constructed and investigated from the view point of an infinite system of difference equations. In order to find the solution of this infinite system they use a truncation method which allows them to determine the accuracy of the approximate solution.

The objective of this thesis is to use the finite element methods for the approximations of the two model problems.

Problem 1 The steady state problem

This thesis is concerned namely with the numerical solution of the equation (1.15) under the following assumptions :

1. The concentration at the source is assumed to be a δ -function :

$$\varphi(0,z)=\frac{Q}{u(h)}\delta(z-h),$$

where h is the height of the source and Q is the emission rate.

2. The process of pollutant dispersion is stationary, i.e. $\dfrac{\partial\varphi}{\partial t}=0.$

3. The wind direction coincides with the positive direction of the axis Ox, namely $u = u(z) > 0$, $v = w = 0$.

4. The horizontal advection by the wind dominates the horizontal diffusion.

Under the above assumptions the diffusion term in the direction Ox can be neglected. In order to eliminate the y-dependence of the problem, we assume that we have a uniform line source along the y-axis. We assume zero flux at ground level $z = 0$ and at height $z = H$ the height of the bottom of the inversion layer that acts as a barrier to the flux of the pollutant. Thus, we solve the problem in the semi-infinite strip

$\{x\in\mathbb{R} \mid x>0\}\times\{z\in\mathbb{R} \mid 0<z<H\}$. Then the equation (1.15) takes this form.

$$u(z)\frac{\partial\varphi}{\partial x}-w_g\frac{\partial\varphi}{\partial z}-\frac{\partial}{\partial z}\left(\nu(z)\frac{\partial\varphi}{\partial z}\right)+\sigma\varphi=0 \text{ for all } 0<x, 0<z<H. \tag{1.24}$$

The boundary condition on the z-axis is

$$\varphi(0,z)=\frac{Q}{u(h)}\delta(z-h) \text{ for all } 0<z<H. \tag{1.25}$$

where h is the height of the source and Q is the emission rate.

The boundary condition on the ground and at the inversion layer are

$$\nu(0)\frac{\partial\varphi(x,0)}{\partial z}=0 \text{ for all } 0<x, \tag{1.26}$$

and

$$\nu(H)\frac{\partial\varphi(0,H)}{\partial z}=0 \text{ for all } 0<x, \tag{1.27}$$

respectively.

Problem 2 The unsteady state problem

This thesis is concerned namely with the numerical solution of the equation (1.15) under the following assumptions:

1. The concentration at the source is assumed to be a δ-function :

$$\varphi(0,z,t)=\frac{Q}{u(h)}\delta(z-h), \text{ for all } 0<t,$$

   where h is the height of the source and Q is the emission rate.

2. The wind direction coincides with the positive direction of the axis Ox, namely $u = u(z) > 0$, $v = w = 0$.
3. The horizontal advection by the wind dominates the horizontal diffusion.

Under the above assumptions the diffusion term in the direction Ox can be neglected. In order to eliminate the y-dependence of the problem, we assume that we have a uniform line source along the y-axis. We consider a δ-function source at height h on the z-axis. We assume zero flux at ground level $z = 0$ and at height $z = H$- the height of the bottom of the inversion layer that acts as a barrier to the flux of the pollutant. Thus, we solve the problem for all $t > 0$ in the semi-infinite strip

$\{x\in\mathbb{R} \mid 0<x\}\times\{z\in\mathbb{R} \mid 0<z<H\}$. Then the equation (1.15) takes this form.

$$\frac{\partial \varphi}{\partial t}+u(z)\frac{\partial \varphi}{\partial x}-w_g\frac{\partial \varphi}{\partial z}-\frac{\partial}{\partial z}\left(\nu(z)\frac{\partial \varphi}{\partial z}\right)+\sigma\varphi=0 \text{ for all } 0<t, 0<x, 0<z<H. \quad (1.28)$$

We assume that the initial concentration is zero everywhere and gives the initial condition

$$\varphi(x,z,0)=0 \text{ for all } 0<x, 0<z<H. \quad (1.29)$$

The boundary condition on the z-axis is

$$\varphi(0,z,t)=\frac{Q}{u(h)}\delta(z-h) \text{ for all } 0<t, 0<z<H, \quad (1.30)$$

where h is the height of the source and Q is the emission rate.

The boundary conditions on the ground and at the inversion layer are

$$\nu(0)\frac{\partial \varphi(x,0,t)}{\partial z}=0 \text{ for all } 0<t, 0<x, \quad (1.31)$$

and

$$\nu(H)\frac{\partial \varphi(x,H,t)}{\partial z}=0 \text{ for all } 0<t, 0<x, \quad (1.32)$$

respectively.

1.2 Research objectives

We are interested in using the finite element methods to model problem 1 and problem 2 and with the following procedure: first we will develop a finite element method to the steady state problem and then we will consider the unsteady state case. The convergence of the approximated problems will be investigated. The goals of the research are as follows:

- To review and choose the finite element methods for two-dimensional steady and unsteady state problems, problem 1 and problem 2.

- To develop computer programs for two-dimensional steady and unsteady state problems, problem 1 and problem 2.
- To compare the computational solution with the known solutions of the problems.

1.3 Scope and limitations of the study

We will consider the finite element methods applicable to the problem in both steady and unsteady cases. This problem is concerned with the numerical solution of the equation (1.15) under the following assumptions.

- The wind direction coincides with the positive direction of the axis Ox and the wind velocity $\vec{V}$ = $(u,0,0)$, where $u = u(z) > u_0 > 0$, u_0 = constant.
- The concentration at the source is assumed to be a δ-function:

$$\varphi = \frac{Q}{u(h)}\delta(z-h),$$

where h is the height of the source and Q is the emission rate.

1.4 Survey of the thesis

Numerical methods which are called Finite Element Methods were used to solve the process of pollutant transport and diffusion. We performed the calculation upon the steady state and the unsteady state cases.

The standard definitions, notations from functional analysis and fundamental concepts of finite element method are defined and presented in Chapter II. In Chapter III, the stationary problem is solved by using the finite element method. We assume that the wind direction coincides with the positive direction x-axis. The advection and diffusion coefficients are of the function of z. The corresponding schemes are solved using MatLab software. The computational techniques in the numerical experiment enable the study to determine the realistic estimate of error constant and the order of convergence of numerical algorithms developed in this thesis. We have compared this solution with the analytical solution.

The finite element algorithms for approximate solution of the unsteady state problem are proposed in Chapter IV. The calculations are performed in two steps. In the first step we find the auxiliary solution $\varphi*$ and find the true solution φ from second step, using the $\varphi*$ as an initial data. By this algorithm, we assumed that the pollutant moves by transportation and then diffusion. The numerical schemes were performed and solved by MatLab software. The concentration contour line obtained from the computer programs are reasonably in accordance with the former results, using the fractional step method in the reference. Then the thesis is briefly reviewed and the conclusions are presented in Chapter V.

Chapter II

Preliminaries

In this chapter we will give some information from functional analysis, some definitions of finite element method and some definitions which we use in this thesis to make itself sufficient about. In our explanation, we are following the results from the handbook. [Brenner, S. C. and Scotf, L. R. (1940), Becker, E. B., Carey, G. F. and Oden J. T. (1981)]

2.1 Notations and definitions

Let Ω be a domain in $\mathbb{R}^n$. The notation $C(\Omega)$ denotes the set of continuous functions on the domain Ω. Similarly, for any domain, $C^k(\Omega)$ denotes the set of functions which together with all derivatives up to and including the *k*-th derivative are continuous. We use the notation $L^p(\Omega)$ to denote the set of all functions for which

$$\|f\|_p = \left(\int_\Omega |f(x)|^p \, dx \right)^{1/p} < \infty. \tag{2.1}$$

Definition 2.1.1 Given a linear (vector) space *V*, a **norm**, $\|\cdot\|$, is a function on *V* with values in the non-negative reals having the following properties:

i) $\|v\| \geq 0$ for all $v \in V$

ii) $\|v\| = 0$ iff $v = 0$

iii) $\|\alpha \cdot v\| = |\alpha| \cdot \|v\|$ for all $\alpha \in \mathbb{R}$, $v \in V$

iv) $\|v + w\| \leq \|v\| + \|w\|$ for all $v, w \in V$

Given a multi-index $\alpha = (\alpha_1, \cdots, \alpha_n) \in \mathbb{N}^n$, we use the following notation:

$$\left.\begin{aligned} |\alpha| &= \sum_{i=1}^{n} \alpha_i \\ \partial^\alpha &= \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_n}} \end{aligned}\right\} \tag{2.2}$$

Definition 2.1.2 Let Ω be a domain in $\mathbb{R}^n$. Denote by $D(\Omega)$ or $C_0^\infty(\Omega)$ the set of $C^\infty(\Omega)$ functions with compact support in Ω.

Definition 2.1.3 Given a domain Ω, the set of **locally integrable** functions is denoted by

$$L_{loc}^1(\Omega) = \{ f : f \in L^1(K) \text{ for all compact } K \subset \text{interior } \Omega \}.$$

Definition 2.1.4 We say that a given function $f \in L_{loc}^1(\Omega)$ has a **weak derivative**, $\partial_w^\alpha f$, provided there exits a function $g \in L_{\log}^1(\Omega)$ such that

$$\int_\Omega g(x)\phi(x)dx = (-1)^{|\alpha|} \int f(x)\phi^{(\alpha)}(x)dx \text{ for all } \phi \in D(\Omega).$$

If such a g exist, we define $\partial_w^\alpha f = g$.

Definition 2.1.5 Let k be a non-negative integer, and let $f \in L_{loc}^1(\Omega)$. Suppose that the weak derivatives $\partial_w^\alpha f$ exist for all $|\alpha| \leq k$. Define the **Sobolev norm**

$$\|f\|_{W_p^k(\Omega)} = \left(\sum_{|\alpha| \leq k} \|\partial_w^\alpha f\|_{L^p(\Omega)}^p \right)^{1/p},$$

in the case $1 \leq p < \infty$, and in the case $p = \infty$

$$\|f\|_{W^p_\infty(\Omega)} = \max_{|\alpha|\le k} \|\partial^\alpha_w f\|_{L^\infty(\Omega)}.$$

In either case, we define the **Sobolev spaces** via

$$W^k_p(\Omega) = \left\{ f \in L^1_{loc}(\Omega) : \|f\|_{W^k_p(\Omega)} < \infty \right\}.$$

Notation 2.1.1

$$H^k(\Omega) = W^k_2(\Omega).$$

Definition 2.1.6 For k a non-negative integer and $f \in W^k_p(\Omega)$, let

$$|f|_{W^k_p(\Omega)} = \left(\sum_{|\alpha|\le k} \|\partial^\alpha_w f\|^p_{L^p(\Omega)} \right)^{1/p},$$

in the case $1 \le p < \infty$, and in the case $p = \infty$

$$|f|_{W^k_\infty(\Omega)} = \max_{|\alpha|=k} \|\partial^\alpha_w f\|_{L^\infty(\Omega)}.$$

Definition 2.1.7 A **bilinear form**, $b(\cdot,\cdot)$, on a linear space V is a mapping $b: V \times V \to \mathbb{R}$ such that each of the maps $v \mapsto b(v,w)$ and $w \mapsto b(v,w)$ is a linear form on V. It is **symmetric** if $b(v,w) = b(w,v)$ for all $v, w \in V$. A (real) **inner product**, denoted by $(\cdot,\cdot)$, is a symmetric bilinear form on a linear space V that satisfies

i) $(v,v) \ge 0$ for all $v \in V$

ii) $(v,v) = 0$ iff $v = 0$

Definition 2.1.8 A linear space V together with an inner product defined on it is called an **inner-product space** and is denoted by $(V,(\cdot,\cdot))$.

Definition 2.1.9 Let $(V,(\cdot,\cdot))$ be an inner-product space. If the associated normed linear space $(V,\|\cdot\|)$ is complete, then $(V,(\cdot,\cdot))$ is called a **Hilbert space**.

Definition 2.1.10 The δ-function, often called **Dirac's delta function** or just **the Dirac function** $\delta(x)$ is defined to be zero when $x \neq 0$, and infinite at $x = 0$ in such a way that the area under the function is unity.

A concise definition is the following:

$$\int_{-\infty}^{\infty} \delta(x)dx = 1,$$

$$\delta(x) = 0 \quad \text{for} \quad x \neq 0,$$

The generalized function $\delta(x)$ has the following properties.

$$\begin{aligned}
\delta(-x) &= \delta(x), \\
x\delta(x) &= 0, \\
\int_{-\infty}^{\infty} f(x)\delta(x-\xi)\,dx &= f(\xi), \\
\int_{-\infty}^{\infty} f(x)\delta(x)\,dx &= f(0), \\
\int_{-\infty}^{\infty} \delta(\xi-x)\delta(x-\eta)\,dx &= \delta(\xi-\eta), \\
\delta'(x) &= -\delta'(x), \\
x\delta'(x) &= \delta(x), \\
\int_{-\infty}^{\infty} f(x)\delta'(x-\xi)\,dx &= -f'(\xi), \\
\delta(ax) &= a^{-1}\delta(x)
\end{aligned}$$

$$\delta(x^2-a^2) \quad = \quad \frac{1}{2}a^{-1}\left[\delta(x-a)+\delta(x+a)\right].$$

2.2 Weak formulation of problem with linear second order partial differential equation

The general form of a linear second order partial differential equation in n variable $x_1,\ldots,x_n$ is

$$\sum_{i,j=1}^{n} a_{ij}u_{x_ix_j} + \sum_{i=1}^{n} b_i u_{x_i} + cu = f, \tag{2.3}$$

where the coefficients a_{ij}, b_j, c and f are real constants or function of $x_1,\ldots,x_n$.

Let

$$L \equiv \sum_{i,j}^{n} a_{ij}\frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i=1}^{n} b_i \frac{\partial}{\partial x_i} + c, \tag{2.4}$$

be a second order linear differential operator.

Given an open and bounded region Ω in $\mathbb{R}^n$ with polygonal boundary $\Gamma = \Gamma_1 \cup \Gamma_2$ such that Γ_1 and Γ_2 are nonoverlapping, then if L is a second order linear differential operator we consider the problem

$$\begin{gathered} Lu = f \quad \text{in } \Omega \\ u = 0 \text{ on } \Gamma_1, \quad \frac{\partial u}{\partial \mathbf{n}} = 0 \text{ on } \Gamma_2 \end{gathered} \tag{2.5}$$

where f is a source term and $\frac{\partial u}{\partial \mathbf{n}}$ refers to differentiation in the direction of the outward normal.

Let $H^k(\Omega)$ denote the Sobolev space of functions with derivatives up to order k being square integrable over the region Ω. We suppose that there exists a unique, continuous linear mapping $\gamma : H^1(\Omega) \to L^2(\Gamma_1)$ such that for each $v \in H^1(\Omega)$, γv is the restriction of v to Γ_1. We define

$$H_0^1 = \left\{ v \in H^1\left(\Omega\right) \mid \gamma v = 0 \text{ on } \Gamma_1 \right\}.$$

The **weak formulation** of problem (2.5) is :

Find $u \in H_0^1(\Omega)$ such that

$$b(u,v) = (f,v) \text{ for all } v \in H_0^1(\Omega),$$

where $(f,v) = \int_\Omega fv\, d\Omega$ is the L^2 inner product and $b(u,v)$ is the bilinear form resulting the second order terms of the inner product (Lu, v) is integration by parts, so that only derivatives of first order remain.

The solution of this **weak formulation** is said to be the **weak solution** of equation (2.5). It is not true however that the weak solution is also the classical solution of equation (2.5). For this to be the case we need the weak solution u to be sufficiently regular so that Lu is well-defined in the classical sense. So for example if L is an nth-order differential operator then the classical solution is C^n continuous. The advantage of using **weak solutions** if they are unique is that it is easier to prove the existence of weak solutions than the existence of classical solutions. Moreover, since all strong solutions are also weak solutions, if we have a unique weak solution then there must be no more than one strong solution.

2.3 Conforming finite element methods

The process of pollutant transport and diffusion in the atmosphere is described by the partial differential equation

$$\frac{\partial \varphi}{\partial t} + \mathbf{U} \cdot \nabla \varphi - \nabla \cdot \mathbf{K} \nabla \varphi - \mu \Delta \varphi + \sigma \varphi = f, \tag{2.6}$$

where φ and $\mathbf{U}$ are the pollutant concentration and the wind field respectively, t is time, $\mathbf{K}$ is the eddy-diffusivity tensor, μ is the diffusion coefficient, σ is the transformation coefficient of pollutants, Δ denotes the Laplace operator, i.e. $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ and f is source.

The standard weak form of the equation (2.6) is: find $\varphi \in H_0^1(\Omega)$ such that

$$a(\varphi, v) + c(\varphi, v) - d(\varphi, v) - e(\varphi, v) + h(\varphi, v) = (f, v) \quad \text{for all } v \in H_0^1(\Omega) \qquad (2.7)$$

where

$$
\begin{aligned}
a(\varphi, v) &= \int_\Omega \frac{\partial \varphi}{\partial t} v \, d\Omega, \\
c(\varphi, v) &= \int_\Omega (\mathbf{U} \cdot \nabla \varphi) v \, d\Omega, \\
d(\varphi, v) &= \int_\Omega (\nabla \cdot \mathbf{K} \nabla \varphi) v \, d\Omega, \\
e(\varphi, v) &= \int_\Omega (\mu \Delta \varphi) v \, d\Omega, \\
h(\varphi, v) &= \int_\Omega (\sigma \varphi) v \, d\Omega, \\
(f, v) &= \int_\Omega f v \, d\Omega,
\end{aligned}
$$

and $H_0^1(\Omega)$ is the usual Sobolev space.

Let us suppose that we are given an infinite set of functions $\{\phi_1, \phi_2, \phi_3, \ldots\}$ in H_0^1 which have the property that each test function v in H_0^1 can be represented as a linear combination of the ϕ_i by a series of the type

$$v = \sum_{i=1}^{\infty} \beta_i \phi_i, \qquad (2.8)$$

where the β_i are constants and the series converges in a sense appropriate for the space H_0^1 of (2.7). A set of function $\{\phi_i\}$ with these properties is said to provide a basis for H_0^1 and the functions ϕ_i are called **basis functions**.

It is clear that if we take only a finite number N of terms in the series (2.8), then we will obtain only an approximation v_N of v :

$$v_N = \sum_{i=1}^{N} \beta_i \phi_i \tag{2.9}$$

The N basis functions $\{\phi_1, \phi_2, \ldots, \phi_N\}$ define an N-dimensional subspace $H_0^{(N)}$ of H_0^1. The subspace $H_0^{(N)}$ is of only finite dimension N because each function v_N in $H_0^{(N)}$ is determined by a linear combination of only the N functions $\phi_1, \ldots, \phi_N$ by (2.9). $H_0^{(N)}$ is subspace of H_0^1 because each ϕ_i, $i = 1, 2, \ldots, N$, is, by definition, a member of H_0^1.

We consider Galerkin's method for constructing approximate solutions to the variational boundary-value problem (2.7). Galerkin's method consists of seeking an approximate solution to (2.7) in a finite-dimensional subspace $H_0^{(N)}$ of the space H_0^1 of admissible functions rather than in the whole space H_0^1. Thus, instead of tackling the infinite-dimensional problem (2.7), we seek an approximate solution φ_N in $H_0^{(N)}$ of the form

$$\varphi_N = \sum_{i=1}^{N} \alpha_i \phi_i, \tag{2.10}$$

which satisfies (2.7) with H_0^1 replaced by $H_0^{(N)}$. In other words , the variational statement of the approximate problem is this : find $u_N \in H_0^{(N)}$ such that

$$a(\varphi_N, v_N) + c(\varphi_N, v_N) - d(\varphi_N, v_N) - e(\varphi_N, v_N) + h(\varphi_N, v_N) = (f, v_N) \text{ for all } v_N \in H_0^{(N)}. \tag{2.11}$$

Since the ϕ_i are known, φ_N will be completely determined once the N coefficients α_i in (2.10) are determined. The α_i in (2.10) are referred to as the degrees of freedom of the approximation.

We first observe that all of the test functions v_N are linear combinations of the basis function ϕ_i of the form (2.10), β_i being the arbitrary constant. Note again that v_N in (2.9) can take on the values of any function in $H_0^{(N)}$ through a proper choice of the constant β_i.

The Petrov-Galerkin method for problem (2.7) consists of choosing two finite dimensional spaces $V, W \subset H_0^1$ such that $\dim(V) = \dim(W)$, and solving

find $\varphi \in V$ such that

$$a(\varphi, w) + c(\varphi, w) - d(\varphi, w) - e(\varphi, w) + h(\varphi, w) = (f, w) \text{ for all } w \in W.$$

The space V is known as the **trial space** and W is known as the **test space**. The finite element Petrov-Galerkin method consists of producing V and W to contain piecewise functions (usually continuous piecewise polynomials) defined over a mesh.

2.4 Non-dimensional form

We now non-dimensionalize the problem 1 and 2 in section 1.1. The non-dimensional expressions of variables $x, z, t, h, \varphi, u, v, w_g$ and σ are

$$x^* = \frac{x \cdot v(H)}{H^2 u(H)},$$

$$z^* = \frac{z}{H},$$

$$t^* = \frac{t \cdot \nu(H)}{H^2},$$

$$h^* = \frac{h}{H},$$

$$\varphi^* = \frac{\varphi \cdot u(H) \cdot H}{Q},$$

$$u^* = \frac{u}{u(H)},$$

$$\nu^* = \frac{\nu}{\nu(H)},$$

$$w_g^* = \frac{w_g \cdot H}{\nu(H)},$$

$$\sigma^* = \frac{\sigma \cdot H^2}{\nu(H)}.$$

Thus

$$\frac{\partial \varphi^*}{\partial t^*} = \frac{u(H) \cdot H^3}{Q \cdot \nu(H)} \frac{\partial \varphi}{\partial t}. \tag{2.12}$$

From the above definitions we get

$$u^*(z^*)\frac{\partial \varphi^*}{\partial x^*} = \frac{u(H) \cdot H^3}{Q \cdot \nu(H)} u\left(\frac{z}{H}\right)\frac{\partial \varphi}{\partial x} \tag{2.13}$$

$$w_g^* \frac{\partial \varphi^*}{\partial z^*} = \frac{u(H) \cdot H^3}{Q \cdot \nu(H)} w_g \frac{\partial \varphi}{\partial z} \tag{2.14}$$

$$\frac{\partial}{\partial z^*}\left(\nu^*(z^*)\frac{\partial \varphi^*}{\partial z^*}\right) = \frac{u(H) \cdot H^3}{Q \cdot \nu(H)} \frac{\partial}{\partial z}\left(\nu(z^*)\frac{\partial \varphi}{\partial z}\right) \tag{2.15}$$

$$\sigma^* \varphi^* = \frac{u(H) \cdot H^3}{Q \cdot \nu(H)} \sigma \varphi \tag{2.16}$$

2.4.1 Steady state problem

In steady case, we have

$$u^*(z^*)\frac{\partial\varphi^*}{\partial x^*}-w_g\frac{\partial\varphi^*}{\partial z^*}-\frac{\partial}{\partial z^*}\left(\nu^*(z^*)\frac{\partial\varphi^*}{\partial z^*}\right)+\sigma^*\varphi^*$$

$$=\frac{u(H)\cdot H^3}{Q\cdot\nu(H)}\left[u\left(\frac{z}{H}\right)\frac{\partial\varphi}{\partial x}-w_g\frac{\partial\varphi}{\partial z}-\frac{\partial}{\partial z}\left(\nu\left(\frac{z}{H}\right)\frac{\partial\varphi}{\partial z}\right)+\sigma\varphi\right],$$

but from (1.24)

$$u\left(\frac{z}{H}\right)\frac{\partial\varphi}{\partial x}-w_g\frac{\partial\varphi}{\partial z}-\frac{\partial}{\partial z}\left(\nu\left(\frac{z}{H}\right)\frac{\partial\varphi}{\partial z}\right)+\sigma\varphi=0,$$

so we have

$$u^*(z^*)\frac{\partial\varphi^*}{\partial x^*}-w_g\frac{\partial\varphi^*}{\partial z^*}-\frac{\partial}{\partial z^*}\left(\nu^*(z^*)\frac{\partial\varphi^*}{\partial z^*}\right)+\sigma^*\varphi^*=0 \text{ for all } 0<x^*, 0<z^*<1, \tag{2.17}$$

and

$$\varphi^*(0,z^*) = \frac{u(H)\cdot H}{Q}\varphi(0,z^*),$$

$$= \frac{u(H)\cdot H}{Q}\frac{Q}{u(h)}\delta(z^*-h),$$

$$= \frac{H\cdot\delta(z^*-h)}{\dfrac{u(h)}{u(H)}},$$

$$= \frac{H\cdot\delta(z^*-h)}{u^*(h^*)},$$

$$= \frac{\delta\left(z^*-\dfrac{h}{H}\right)}{u^*(h^*)},$$

$$\varphi^*(0,z^*)=\frac{\delta(z^*-h^*)}{u^*(h^*)} \text{ for all } 0<z^*<1 \tag{2.18}$$

since

$$v^*(z^*)\frac{\partial\varphi^*(x^*,z^*)}{\partial z^*}=\frac{u(H)\cdot H^2}{Q\cdot v(H)}v(z^*)\frac{\partial\varphi(x^*,z^*)}{\partial z},$$

Let $z^*=0$ then

$$v^*(0)\frac{\partial\varphi^*(x^*,0)}{\partial z^*}=\frac{u(H)\cdot H^2}{Q\cdot v(H)}v(0)\frac{\partial\varphi(x^*,0)}{\partial z},$$

since

$$v(0)\frac{\partial\varphi^*(x^*,0)}{\partial z}=0,$$

so we have

$$v(0)\frac{\partial\varphi^*(x^*,0)}{\partial z^*}=0 \text{ for all } 0<x^*, \tag{2.19}$$

Let $z^*=1$ then

$$v^*(1)\frac{\partial\varphi^*(x^*,1)}{\partial z^*}=\frac{u(H)\cdot H^2}{Q\cdot v(H)}v(H)\frac{\partial\varphi(x^*,H)}{\partial z},$$

since

$$v(H)\frac{\partial\varphi^*(x^*,H)}{\partial z}=0,$$

so we have

$$v^*(1)\frac{\partial\varphi^*(x^*,1)}{\partial z^*}=0 \text{ for all } 0<x^* \tag{2.20}$$

2.4.2 Unsteady state problem

In the unsteady case, we have

$$\frac{\partial \varphi^*}{\partial t^*}+u^*(z^*)\frac{\partial \varphi^*}{\partial x^*}-w_g^*\frac{\partial \varphi^*}{\partial z^*}-\frac{\partial}{\partial z^*}\left(\nu^*(z^*)\frac{\partial \varphi^*}{\partial z^*}\right)+\sigma^*\varphi^*$$

$$=\frac{u(H)\cdot H^3}{Q\cdot \nu(H)}\left[\frac{\partial \varphi}{\partial t}+u\left(\frac{z}{H}\right)\frac{\partial \varphi}{\partial x}-w_g\frac{\partial \varphi}{\partial z}-\frac{\partial}{\partial z}\left(\nu\left(\frac{z}{H}\right)\frac{\partial \varphi}{\partial z}\right)+\sigma\varphi\right],$$

but from (1.28)

$$\frac{\partial \varphi}{\partial t}+u\left(\frac{z}{H}\right)\frac{\partial \varphi}{\partial x}-w_g\frac{\partial \varphi}{\partial z}-\frac{\partial}{\partial z}\left(\nu\left(\frac{z}{H}\right)\frac{\partial \varphi}{\partial z}\right)+\sigma\varphi=0,$$

so we have

$$\frac{\partial \varphi^*}{\partial t^*}+u^*\left(z^*\right)\frac{\partial \varphi^*}{\partial x^*}-w_g^*\frac{\partial \varphi^*}{\partial z^*}-\frac{\partial}{\partial z^*}\left(\nu^*(z^*)\frac{\partial \varphi^*}{\partial z^*}\right)+\sigma^*\varphi^*=0 \tag{2.21}$$

$$\text{for all } 0<t^*, 0<x^*, 0<z^*<1,$$

since

$$\varphi^*(x^*,z^*,0)=\frac{u(H)\cdot H}{Q}\varphi(x^*,z^*,0),$$

but from (1.29)

$$\varphi(x^*,z^*,0)=0,$$

so we have

$$\varphi^*(x^*,z^*,0)=0 \text{ for all } 0<x^*, 0<z^*<1, \tag{2.22}$$

and

$$\begin{aligned}
\varphi^*(0,z^*,t^*) &= \frac{u(H)\cdot H}{Q}\varphi(0,z^*,t^*),\\
&= \frac{u(H)\cdot H}{Q}\frac{Q}{u(h)}\delta(z^*-h),\\
&= \frac{H\cdot\delta(z^*-h)}{\frac{u(h)}{u(H)}},
\end{aligned}$$

$$= \qquad \frac{H \cdot \delta(z^* - h)}{u^*(h^*)},$$

$$= \qquad \frac{\delta(z^* - \frac{h}{H})}{u^*(h^*)},$$

$$\varphi^*(0, z^*, t^*) = \frac{\delta(z^* - h^*)}{u^*(h^*)} \text{ for all } 0 < t^*, 0 < z^* < 1, \tag{2.23}$$

since

$$\nu^*(z^*)\frac{\partial \varphi^*(x^*, z^*, t^*)}{\partial z^*} = \frac{u(H) \cdot H^2}{Q \cdot \nu(H)} \nu(z^*) \frac{\partial \varphi(x^*, z^*, t^*)}{\partial z}$$

Let $z^* = 0$ then

$$\nu^*(0)\frac{\partial \varphi^*(x^*, 0, t^*)}{\partial z^*} = \frac{u(H) \cdot H^2}{Q \cdot \nu(H)} \nu(0) \frac{\partial \varphi(x^*, 0, t^*)}{\partial z},$$

but from (1.31)

$$\nu(0)\frac{\partial \varphi(x^*, 0, t^*)}{\partial z} = 0,$$

so we have

$$\nu^*(0)\frac{\partial \varphi^*(x^*, 0, t^*)}{\partial z^*} = 0 \text{ for all } 0 < t^*, 0 < x^*. \tag{2.24}$$

Let $z^* = 1$ then

$$\nu^*(1)\frac{\partial \varphi^*(x^*, 1, t^*)}{\partial z^*} = \frac{u(H) \cdot H^2}{Q \cdot \nu(H)} \nu(H) \frac{\partial \varphi(x^*, H, t^*)}{\partial z},$$

but from (1.32)

$$\nu(H)\frac{\partial \varphi(x^*, H, t^*)}{\partial z} = 0,$$

so we have

$$\nu^*(1)\frac{\partial \varphi^*(x^*, 1, t^*)}{\partial z^*} = 0 \text{ for all } 0 < t^*, 0 < x^*. \tag{2.25}$$

2.5 Approximations of the boundary conditions on a non-uniform grid

We have a non-uniform grid $\{z_i : i = 1, 2, \cdots, n\}$ where $\begin{array}{l} z_1 = 0 \\ z_k = \sum_{i=1}^{k-1} \Delta z_i, \quad k = 2, 3, \cdots, n-1 \\ z_n = 1 \end{array}$.

At the lower boundary, since

$$\frac{\partial \varphi}{\partial z} = 0 \quad \text{at} \quad z = 0.$$

Let

$$\begin{aligned}
\varphi'(z_1) &\approx a\varphi(z_1) + b\varphi(z_2) + c\varphi(z_3) \\
&= a\varphi(z_1) + b\varphi(z_1 + \Delta z_1) + c\varphi(z_1 + (\Delta z_1 + \Delta z_2)) \\
&= a\varphi(z_1) + b\left[\varphi(z_1) + \Delta z_1 \varphi'(z_1) + \frac{(\Delta z_1)^2}{2}\varphi''(z_1) + \cdots\right] + \\
&\quad + c\left[\varphi(z_1) + (\Delta z_1 + \Delta z_2)\varphi'(z_1) + \frac{\left(\Delta z_1 + \Delta z_2\right)^2}{2}\varphi''(z_1) + \cdots\right] \\
&= (a + b + c)\varphi_1(z_1) + \left[b\Delta z_1 + c\left(\Delta z_1 + \Delta z_2\right)\right]\varphi'(z_1) + \\
&\quad + \left[b\frac{\left(\Delta z_1\right)^2}{2} + c\frac{\left(\Delta z_1 + \Delta z_2\right)^2}{2}\right]\varphi''(z_1) + \cdots
\end{aligned}$$

By comparison of the coefficients of $\varphi(z_1), \varphi'(z_1)$ and $\varphi''(z_1)$, we have;

$$a + b + c = 0, \tag{2.26}$$

$$b\Delta z_1 + c\left(\Delta z_1 + \Delta z_2\right) = 1, \tag{2.27}$$

$$b\frac{\left(\Delta z_1\right)^2}{2}+c\frac{\left(\Delta z_1+\Delta z_2\right)^2}{2}=0. \tag{2.28}$$

Solving these equations for a, b and c gives

$$\begin{aligned} a &= -\frac{2\Delta z_1+\Delta z_2}{\Delta z_1\left(\Delta z_1+\Delta z_2\right)}, \\ b &= \frac{\Delta z_1+\Delta z_2}{\Delta z_1\Delta z_2}, \\ c &= -\frac{\Delta z_1}{\Delta z_2\left(\Delta z_1+\Delta z_2\right)}. \end{aligned}$$

So that

$$\varphi'(z_1)=\left[-\frac{2\Delta z_1+\Delta z_2}{\Delta z_1\left(\Delta z_1+\Delta z_2\right)}\right]\varphi(z_1)+\left[\frac{\Delta z_1+\Delta z_2}{\Delta z_1\Delta z_2}\right]\varphi(z_2)+\left[-\frac{\Delta z_1}{\Delta z_2\left(\Delta z_1+\Delta z_2\right)}\right]\varphi(z_3).$$

At the upper boundary, since

$$\frac{\partial\varphi}{\partial z}=0 \quad \text{at} \quad z=1.$$

Let

$$\begin{aligned} \varphi'(z_n) &\approx p\varphi(z_n)+q\varphi(z_{n-1})+r\varphi(z_{n-2}) \\ &= p\varphi(z_n)+q\varphi(z_n-\Delta z_{n-1})+r\varphi(z_n-(\Delta z_{n-1}+\Delta z_{n-2})) \\ &= p\varphi(z_n)+q\left[\varphi(z_n)-\Delta z_{n-1}\varphi'(z_n)+\frac{\left(\Delta z_{n-1}\right)^2}{2}\varphi''(z_n)+\cdots\right]+ \\ &\quad +r\left[\varphi(z_n)-\left(\Delta z_{n-1}+\Delta z_{n-2}\right)\varphi'(z_n)+\frac{\left(\Delta z_{n-1}+\Delta z_{n-2}\right)^2}{2}\varphi''(z_n)+\cdots\right] \\ &= (p+q+r)\varphi(z_n)+\left[-q\Delta z_{n-1}-r\left(\Delta z_{n-1}+\Delta z_{n-2}\right)\right]\varphi'(z_n)+ \end{aligned}$$

$$+\left[q\frac{\left(\Delta z_{n-1}\right)^2}{2}+r\frac{\left(\Delta z_{n-1}+\Delta z_{n-2}\right)^2}{2}\right]\varphi''(z_n)+\cdots$$

By comparison of the coefficients of $\varphi(z_n),\varphi'(z_n)$ and $\varphi''(z_n)$, we have;

$$p+q+r=0, \tag{2.29}$$

$$-q\Delta z_{n-1}-r\left(\Delta z_{n-1}+\Delta z_{n-2}\right)=1, \tag{2.30}$$

$$q\frac{\left(\Delta z_{n-1}\right)^2}{2}+r\frac{\left(\Delta z_{n-1}+\Delta z_{n-2}\right)^2}{2}=0. \tag{2.31}$$

Solving these equations we get

$$p = \frac{2\Delta z_{n-1}+\Delta z_{n-2}}{\Delta z_{n-1}\left(\Delta z_{n-1}+\Delta z_{n-2}\right)},$$

$$q = -\frac{\Delta z_{n-1}+\Delta z_{n-2}}{\Delta z_{n-1}\Delta z_{n-2}},$$

$$r = \frac{\Delta z_{n-1}}{\Delta z_{n-2}\left(\Delta z_{n-1}+\Delta z_{n-2}\right)}.$$

So that

$$\varphi'(z_n)=\left[\frac{2\Delta z_{n-1}+\Delta z_{n-2}}{\Delta z_{n-1}\left(\Delta z_{n-1}+\Delta z_{n-2}\right)}\right]\varphi(z_n)+\left[-\frac{\Delta z_{n-1}+\Delta z_{n-2}}{\Delta z_{n-1}\Delta z_{n-2}}\right]\varphi(z_{n-1})+$$
$$+\left[\frac{\Delta z_{n-1}}{\Delta z_{n-2}\left(\Delta z_{n-1}+\Delta z_{n-2}\right)}\right]\varphi(z_{n-2}).$$

Chapter III

Approximate Solution of Steady State Problem

3.1 Introduction

The main goal of this chapter is to study the time independent solution in two-dimensional space of an air pollutant released into the atmosphere from the chimney at height h above the ground in the presence of an inversion layer, which acts as an impermeable barrier to flux of the pollutant to higher levels of the atmosphere. 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 chimney is assumed to be presented as a δ-function, which gives rise to a steady emission rate Q of pollutant from the chimney. The resulting discrete problem is then solved by the Petrov-Galerkin finite element method.

3.2 Mathematical formulation

We will study the steady state problem (1.24) - (1.27). We use the same notation for the non-dimensionalized variables. In these new variables, the resulting system is

$$u(z)\frac{\partial \varphi}{\partial x} - w_g \frac{\partial \varphi}{\partial z} - \frac{\partial}{\partial z}\left(v(z)\frac{\partial \varphi}{\partial z} \right) + \sigma\varphi = 0 \quad \text{for all } \; 0 < x, 0 < z < 1, \qquad (3.1)$$

the boundary conditions are

$$\varphi(0,z) = \frac{\delta(z-h)}{u(h)} \text{ for all } 0 < z < 1, \tag{3.2}$$

$$\nu(0)\frac{\partial\varphi(x,0)}{\partial z} = 0 \text{ for all } 0 < x, \tag{3.3}$$

$$\nu(1)\frac{\partial\varphi(x,1)}{\partial z} = 0 \text{ for all } 0 < x. \tag{3.4}$$

3.3 Finite element approximation

Let $\Omega = \left\{(x,z) \in \mathbb{R}^2 \mid 0 < x, 0 < z < 1\right\}$ be a domain and let

$$L(\varphi) \equiv u(z)\frac{\partial\varphi}{\partial x} - w_g\frac{\partial\varphi}{\partial z} - \frac{\partial}{\partial z}\left(\nu(z)\frac{\partial\varphi}{\partial z}\right) + \sigma\varphi = 0. \tag{3.5}$$

For $(x,z) \in \Omega$, we have

$$\varphi(x,z) \approx \hat{\varphi}(x,z) = \sum_{j=1}^{n}\varphi_j(x)\phi_j(z). \tag{3.6}$$

In this presentation of trial function $\hat{\varphi}$ is the parameters φ_j depend upon x and basis functions ϕ_j are only functions of z .When this trial function is substituted into (3.5), we have

$$L(\hat{\varphi}) = R, \tag{3.7}$$

where R is a residual arising from the fact that (3.6) does not identically satisfy (3.5). According to the Galerkin approach, we require that the residual is orthogonal to the weighting functions $\omega_i(z)$, $i = 1,\ldots,n.$ Thus the approximating integral equations have the form

$$\int_0^1 L(\hat{\varphi})\omega_i(z)dz = 0, \qquad i = 1,2,\cdots,n. \tag{3.8}$$

Therefore integrating (3.8) by parts gives

$$\int_0^1 \left(u(z)\frac{\partial \hat{\varphi}}{\partial x} - w_g \frac{\partial \hat{\varphi}}{\partial z} - \frac{\partial}{\partial z}\left(\nu(z)\frac{\partial \hat{\varphi}}{\partial z} \right) + \sigma\hat{\varphi} \right)\omega_i\left(z\right) dz = 0, \quad i = 1,2,\ldots n. \qquad (3.9)$$

$$\int_0^1 u(z)\frac{\partial \hat{\varphi}}{\partial z}\omega_i(z)\,dz - w_g \int_0^1 \frac{\partial \hat{\varphi}}{\partial z}\omega_i(z)\,dz - \int_0^1 \frac{\partial}{\partial z}\left(\nu(z)\frac{\partial \hat{\varphi}}{\partial z} \right)\omega_i(z)\,dz + \int_0^1 \sigma\hat{\varphi}\omega_i(z)\,dz = 0$$

$$\int_0^1 u(z)\frac{\partial \hat{\varphi}}{\partial z}\omega_i(z)\,dz - w_g \int_0^1 \frac{\partial \hat{\varphi}}{\partial z}\omega_i(z)\,dz - \nu(z)\frac{\partial \hat{\varphi}}{\partial z}\omega_i(z)\Big|_0^1$$
$$+ \int_0^1 \nu(z)\frac{\partial \hat{\varphi}}{\partial z}\frac{\partial \omega_i(z)}{\partial z}\,dz + \int_0^1 \sigma\hat{\varphi}\omega_i(z)\,dz = 0$$

since

$$\nu(0)\frac{\partial \hat{\varphi}(x,0)}{\partial z} = 0 \quad \text{and} \quad \nu(1)\frac{\partial \hat{\varphi}(x,1)}{\partial z} = 0$$

so

$$\int_0^1 u(z)\frac{\partial \hat{\varphi}}{\partial x}\omega_i(z)\,dz - w_g \int_0^1 \frac{\partial \hat{\varphi}}{\partial z}\omega_i(z)\,dz + \int_0^1 \nu(z)\frac{\partial \hat{\varphi}}{\partial z}\frac{\partial \omega_i(z)}{\partial z}\,dz + \int_0^1 \sigma\hat{\varphi}\omega_i(z)\,dz = 0.$$

(3.10)

To determine the functional form of $\omega_i(z)$, let us consider the element of Figure 3.1, where, for convenience, we have selected the origin to coincide with $z = 0$. Because integrations are performed elementwise, this does not result in any loss of generality. The basis functions in this case have the form

$$\phi_j(z) = 1 - \frac{z}{k} \qquad (0 \le z \le k), \qquad (3.11)$$

$$\phi_{j+1}(z) = \frac{z}{k} \qquad (0 \le z \le k). \qquad (3.12)$$

Let the weighting functions ω_j and ω_{j+1} be expressed in the form (see, e.g. Lapidus, L. and Pinderm, G. F.(1982))

$$\omega_j(z) = \phi_j(z) - F(z), \qquad (3.13)$$

$$\omega_{j+1}(z) = \phi_{j+1}(z) + F(z), \tag{3.14}$$

$$F(z) = a\frac{z^2}{k^2} + b\frac{z}{k} + c, \tag{3.15}$$

where $F(z)$ is a piecewise quadratic function with undetermined coefficients a, b and c. To determine the values of a, b and c we impose the following

$$F(0) = 0, \tag{3.16}$$

$$F(k) = 0. \tag{3.17}$$

Substitution of (3.16) and (3.17) into (3.15) yields

$$F(z) = a\left(-\frac{z^2}{k^2} + \frac{z}{k}\right), \tag{3.18}$$

where a is the remaining undetermined parameter. For convenience, we define $\theta = a/3$. The complete weighting functions can now be written as

$$\omega_j(z) = \phi_j(z) + 3\theta\frac{z^2}{k^2} - 3\theta\frac{z}{k}, \tag{3.19}$$

$$\omega_{j+1}(z) = \phi_{j+1}(z) - 3\theta\frac{z^2}{k^2} + 3\theta\frac{z}{k}. \tag{3.20}$$

The parameter θ lies between zero and 1 and dictates the degree of upstream weighing to be employed. The maximum degree $(\theta = 1)$ is the case illustrated in Figure 3.1. For $\theta = 0$, the weighting function obviously reduces to the basis function and the method becomes identical to Galerkin's approximation. The sign of the θ parameter must be consistent with the direction of flow [$\theta > 0$ when $b(z) > 0$].

The local z-coordinate system presented above is related to be the more commonly encountered η system though the relationship

$$\frac{z}{k} = \frac{\eta + 1}{2}, \qquad -1 \le \eta \le 1 \tag{3.21}$$

Thus we can write (3.11), (3.12), (3.19) and (3.20) in the alternative form

$$\phi_j(\eta) = \frac{1}{2}(1-\eta), \tag{3.22}$$

$$\phi_{j+1}(\eta) = \frac{1}{2}(1+\eta), \tag{3.23}$$

$$\omega_j(\eta) = \frac{1}{4}\left[(1+\eta)(3\theta\eta - 3\theta - 2) + 4\right], \tag{3.24}$$

$$\omega_{j+1}(\eta) = \frac{1}{4}\left[(1+\eta)(-3\theta\eta + 3\theta + 2)\right]. \tag{3.25}$$

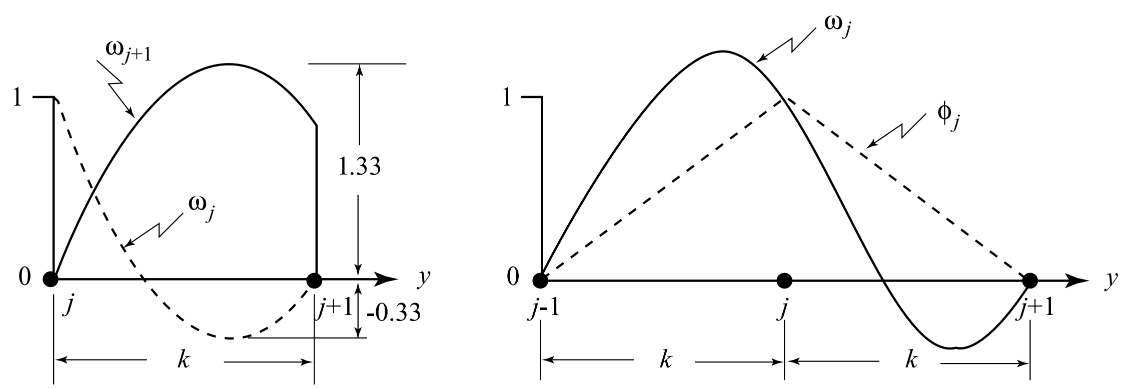


Figure 3.1: Weighting function ω_j and basis functions ϕ_j for the asymmetric weighting function approximation.(Adapted from Lapidus, L. and Pinderm, G. F. (1982))

Since this result is valid for every closed interval, the integration of (3.10) can take place in every element. Thus, it can be written as

$$\int_{-1}^{1}\left[u(\eta)\frac{\partial\hat{\varphi}}{\partial x}\omega_i(\eta) - w_g\frac{\partial\hat{\varphi}}{\partial z}\omega_i(\eta) + v(\eta)\frac{\partial\hat{\varphi}}{\partial z}\frac{\partial\omega_i(\eta)}{\partial z} + \sigma\hat{\varphi}\omega_i(\eta)\right]\frac{k}{2}d\eta = 0, \tag{3.26}$$

where

$$\frac{\partial\hat{\varphi}}{\partial z} = \sum_{j=1}^{n}\varphi_j(x)\frac{d\phi_j(\eta)}{d\eta}\frac{d\eta}{dz} = \frac{2}{k}\sum_{j=1}^{n}\varphi_j(x)\frac{d\phi_j(\eta)}{d\eta}. \tag{3.27}$$

Equation (3.26) describes a set of n ordinary differential equations. This is readily apparent when (3.26) is written in matrix form.

$$[A]\left\{\frac{d\varphi}{dx}\right\}+[B]\{\varphi\}=0. \tag{3.28}$$

Where $A_{ij}=\int_{-1}^{1}u(\eta)\phi_j(\eta)\omega_i(\eta)\frac{k}{2}d\eta$ and

$$B_{ij}=-w_g\int_{-1}^{1}\frac{d\phi_j(\eta)}{d\eta}\omega_i(\eta)\,d\eta+\int_{-1}^{1}v(\eta)\frac{d\phi_j(\eta)}{d\eta}\frac{d\omega_i(\eta)}{d\eta}d\eta+\int_{-1}^{1}\sigma\phi_j(\eta)\omega_i(\eta)\frac{k}{2}d\eta$$

This scheme is the logical extension of the backward approximation described above for the linear system of equation. The only modification involves the recognition of the dependence of matrices $[A]$ and $[B]$ and their explicit evaluation at the m th level. Thus the algorithm is written

$$[A]_m\left\{\frac{\varphi_{m+1}-\varphi_m}{\Delta x}\right\}+[B]_m\{\varphi_{m+1}\}=0, \tag{3.29}$$

or, alternatively,

$$\left([A]_m+\Delta x[B]_m\right)\{\varphi_{m+1}\}=[A]_m\{\varphi_m\}. \tag{3.30}$$

3.4 Numerical algorithm for computing of $[A]_m$ and $[B]_m$

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 density, centered at the source location, as expressed by (Runca, E. and Sardei, F.(1975))

$$\frac{1}{\Delta z_v}=\frac{1}{\Delta z_s}\exp\left[-A_i(z_k-h)^2\right],\begin{matrix}v=k,i=1\text{ for }z_k>h\\ v=k-1,i=2\text{ for }z_k\le h\end{matrix},k=2,3,\ldots,n-1 \tag{3.31}$$

with

$$z_1 = 0$$
$$z_k = \sum_{i=1}^{k-1} \Delta z_i \,, \qquad k = 2,3,\ldots,n-1 \qquad (3.32)$$
$$z_n = 1$$

Δz_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. Δz_s and n are taken as independent parameters. For given values of Δz_s and n, A_1 and A_2 are determined so that they satisfy the relations ((3.31) and (3.32)), being as close as possible to each other. For a given number of grid points *n*, a smaller value of Δz_k means a lesser uniformity of the distribution, that is, a higher concentration of grid points near the source. From a parametric numerical study Runca, E. and Sardei (1975) arrived to the empirical conclusion that the best accuracy of the overall results including regions for downwind is achieved by choosing Δz_s within the range $1/2(n-1) < \Delta z_s < 1/(n-1)$.

The size of the vertical interval Δz_k is variable and is determined by the given values of Δz_s and n. Both Δz_k and z_k as well as A_1 and A_2 are calculated by iteration, from the relation ((3.31) and (3.32)).

Suppose that in case $n = 21, h = 0.2$ we choose Δz_s in the range

$$\frac{1}{2(21-1)} \quad < \quad \Delta z_s \quad < \quad \frac{1}{(21-1)}$$

$$0.025 \quad < \quad \Delta z_s \quad < \quad 0.05$$

if we choose $\Delta z_s = 0.033$ and choose the point of source $z_6 = h = 0.2$ then $\Delta z_5 = \Delta z_6 = 0.033$.

For grid below the source form (3.31) and (3.32),

$$\frac{1}{\Delta z_{k-1}} = \frac{1}{0.033}\exp\left[-A_2(z_k-0.2)^2\right]$$

then

$$\Delta z_{k-1} = 0.033\exp\left[A_2(z_k-0.2)^2\right]$$

we have

$$\Delta z_5 = 0.033\exp\left[A_2(z_6-0.2)^2\right]$$

$$= 0.033\exp\left[A_2(0.2-0.2)^2\right]$$

$$= 0.033$$

$$\Delta z_4 = 0.033\exp\left[A_2(z_5-0.2)^2\right]$$

$$= 0.033\exp\left[A_2(z_6-\Delta z_5-0.2)^2\right]$$

$$= 0.033\exp\left[A_2(0.033)^2\right]$$

$$\Delta z_3 = 0.033\exp\left[A_2(z_4-0.2)^2\right]$$

$$= 0.033\exp\left[A_2(z_6-\Delta z_5-\Delta z_4-0.2)^2\right]$$

$$= 0.033\exp\left[A_2(0.033+\Delta z_4)^2\right]$$

$$\Delta z_2 = 0.033\exp\left[A_2(z_3-0.2)^2\right]$$

$$= 0.033\exp\left[A_2(z_6-\Delta z_5-\Delta z_4-\Delta z_3-0.2)^2\right]$$

$$= 0.033\exp\left[A_2(0.033+\Delta z_4+\Delta z_3)^2\right]$$

$$\Delta z_1 = 0.033\exp\left[A_2(z_2-0.2)^2\right]$$

$$= 0.033\exp\left[A_2(z_6-\Delta z_5-\Delta z_4-\Delta z_3-\Delta z_2-0.2)^2\right]$$

$$= \quad 0.033\exp\left[A_2(0.033+\Delta z_4+\Delta z_3+\Delta z_2)^2\right]$$

and find A_2 by solve

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

For grid above the source form (3.31) and (3.32),

$$\frac{1}{\Delta z_k} \quad = \quad \frac{1}{0.033}\exp\left[-A_1(z_k-0.2)^2\right]$$

then

$$\Delta z_k \quad = \quad 0.033\exp\left[A_1(z_k-0.2)^2\right]$$

we have

$$\Delta z_7 \quad = \quad 0.033\exp\left[A_1(z_7-0.2)^2\right]$$

$$= \quad 0.033\exp\left[A_1(z_6+\Delta z_6-0.2)^2\right]$$

$$= \quad 0.033\exp\left[A_1(0.033)^2\right]$$

$$\Delta z_8 \quad = \quad 0.033\exp\left[A_1(z_8-0.2)^2\right]$$

$$= \quad 0.033\exp\left[A_1(z_6+\Delta z_6+\Delta z_7-0.2)^2\right]$$

$$= \quad 0.033\exp\left[A_1(0.033+\Delta z_7)^2\right]$$

$$\Delta z_9 \quad = \quad 0.033\exp\left[A_1(z_9-0.2)^2\right]$$

$$= \quad 0.033\exp\left[A_1(z_6+\Delta z_6+\Delta z_7+\Delta z_8-0.2)^2\right]$$

$$= \quad 0.033\exp\left[A_1(0.033+\Delta z_7+\Delta z_8)^2\right]$$

$$\vdots$$

$$\Delta z_{19} \quad = \quad 0.033\exp\left[A_1(z_{19}-0.2)^2\right]$$

$$= \quad 0.033\exp\left[A_1(0.033+\Delta z_7+\Delta z_8+\cdots+\Delta z_{18})^2\right]$$

$$\Delta z_{20} \quad = \quad 0.033\exp\left[A_1(z_{20}-0.2)^2\right]$$

$$= \quad 0.033\exp\left[A_1(0.033+\Delta z_7+\Delta z_8+\cdots+\Delta z_{18}+\Delta z_{19})^2\right]$$

and find A_1 by solve

$$\Delta z_{20}+\Delta z_{19}+\cdots+\Delta z_8+\Delta z_7=0.8 .$$

Finally, take all intervals in equation (3.32), we get vertical grid $z_1, z_2, \ldots, z_{21}$.

The concentration profile at the source, expressed as a δ-function in the boundary condition (3.2), is approximated numerically by a one-step function centered at the source and having the width Δz_s. Its amplitude is determined by requiring the same emission as in (3.2) :

$$\varphi(0,z)=\begin{cases} 0 & \text{for } 0\le z<h-\dfrac{\Delta z_s}{2}, \\ \dfrac{1}{u_s\Delta z_s} & \text{for } h-\dfrac{\Delta z_s}{2}\le z\le h+\dfrac{\Delta z_s}{2}, \\ 0 & \text{for } h+\dfrac{\Delta z_s}{2}<z\le 1, \end{cases} \tag{3.33}$$

where $u_s = u_k$ at the source.

Suppose that $n = 21$ so A and B (in equation (3.30)) are 21×21 matrices. We have , first row

$$A_{1,1} \quad = \quad -\frac{2\Delta z_1+\Delta z_2}{\Delta z_1(\Delta z_1+\Delta z_2)},$$

$$A_{1,2} \quad = \quad \frac{\Delta z_1+\Delta z_2}{\Delta z_1\Delta z_2},$$

$$A_{1,3} \quad = \quad -\frac{\Delta z_1}{\Delta z_2(\Delta z_1+\Delta z_2)},$$

$$A_{1,j} = 0 \quad \text{for} \quad j = 4,5,\dots,21,$$

and last row

$$A_{21,19} = \frac{\Delta z_{20}}{\Delta z_{19}(\Delta z_{20} + \Delta z_{19})},$$

$$A_{21,20} = -\frac{\Delta z_{20} + \Delta z_{19}}{\Delta z_{20}\Delta z_{19}},$$

$$A_{21,21} = \frac{2\Delta z_{20} + \Delta z_{19}}{\Delta z_{20}(\Delta z_{20} + \Delta z_{19})},$$

$$A_{21,j} = 0 \quad \text{for} \quad j = 1,2,\dots,18.$$

In the case $u(z) = 1$ (see appendix B)

$$\left.\begin{aligned} A_{k,k} &= \left(-\frac{1}{4}\theta + \frac{1}{3}\right)\Delta z_k + A_{k-1,k-1}, \\ A_{k,k+1} &= \left(-\frac{1}{4}\theta + \frac{1}{6}\right)\Delta z_k, \\ A_{k+1,k} &= \left(\frac{1}{4}\theta + \frac{1}{6}\right)\Delta z_k, \\ A_{k+1,k+1} &= \left(\frac{1}{4}\theta + \frac{1}{3}\right)\Delta z_k, \end{aligned}\right\} \text{for } k = 2,3,\dots,20,$$

$$\left.\begin{aligned} B_{1,j} &= 0, \\ B_{21,j} &= 0, \end{aligned}\right\} \text{for } j = 1,2,3,\dots,21,$$

$$\left.\begin{aligned} B_{k,k} &= \left(-\frac{1}{2}\theta + \frac{1}{2}\right)w_g - \frac{1}{2}\theta + \frac{1}{2} + \left(-\frac{1}{4}\theta + \frac{1}{3}\right)\sigma\Delta z_k + B_{k-1,k-1} \\ B_{k,k+1} &= \left(\frac{1}{2}\theta - \frac{1}{2}\right)w_g + \frac{1}{2}\theta - \frac{1}{2} + \left(-\frac{1}{4}\theta + \frac{1}{6}\right)\sigma\Delta z_k, \\ B_{k+1,k} &= \left(\frac{1}{2}\theta + \frac{1}{2}\right)w_g + \frac{1}{2}\theta - \frac{1}{2} + \left(\frac{1}{4}\theta + \frac{1}{6}\right)\sigma\Delta z_k, \\ B_{k+1,k+1} &= \left(-\frac{1}{2}\theta - \frac{1}{2}\right)w_g - \frac{1}{2}\theta + \frac{1}{2} + \left(\frac{1}{4}\theta + \frac{1}{3}\right)\sigma\Delta z_k, \end{aligned}\right\} \text{for } k = 2,3,\dots,20.$$

In the case $u(z) = z^{0.5}$ (see appendix B)

$$\left.\begin{aligned} A_{k,k} &= \left(-\frac{16}{105}\theta+\frac{16}{105}\right)(\Delta z_k)^{3/2}+A_{k-1,k-1},\\ A_{k,k+1} &= \left(-\frac{16}{105}\theta+\frac{16}{105}\right)(\Delta z_k)^{3/2},\\ A_{k+1,k} &= \left(-\frac{4}{21}\theta+\frac{4}{35}\right)(\Delta z_k)^{3/2},\\ A_{k+1,k+1} &= \left(\frac{4}{21}\theta+\frac{2}{7}\right)(\Delta z_k)^{3/2}, \end{aligned}\right\} \text{for } k=2,3,\ldots,20,$$

$$\left.\begin{aligned} B_{1,j} &= 0,\\ B_{21,j} &= 0, \end{aligned}\right\} \text{for } \quad j=1,2,3,\ldots,21,$$

$$\left.\begin{aligned} B_{k,k} &= \left(-\frac{1}{2}\theta+\frac{1}{2}\right)w_g-\frac{1}{2}\theta+\frac{1}{2}+\left(-\frac{1}{4}\theta+\frac{1}{3}\right)\sigma\Delta z_k+B_{k-1,k-1}\\ B_{k,k+1} &= \left(\frac{1}{2}\theta-\frac{1}{2}\right)w_g+\frac{1}{2}\theta-\frac{1}{2}+\left(-\frac{1}{4}\theta+\frac{1}{6}\right)\sigma\Delta z_k,\\ B_{k+1,k} &= \left(\frac{1}{2}\theta+\frac{1}{2}\right)w_g+\frac{1}{2}\theta-\frac{1}{2}+\left(\frac{1}{4}\theta+\frac{1}{6}\right)\sigma\Delta z_k,\\ B_{k+1,k+1} &= \left(-\frac{1}{2}\theta-\frac{1}{2}\right)w_g-\frac{1}{2}\theta+\frac{1}{2}+\left(\frac{1}{4}\theta+\frac{1}{3}\right)\sigma\Delta z_k, \end{aligned}\right\} \text{for } k=2,3,\ldots,20.$$

3.5 Comparison and convergence of numerical solutions

3.5.1 Comparison of numerical solutions with analytical solutions

In this section, we obtain the numerical solution for the test problem (3.1) - (3.4) by using the finite element method presented in section 3.4. Then performing a rigorous comparison of approximate and exact solutions.

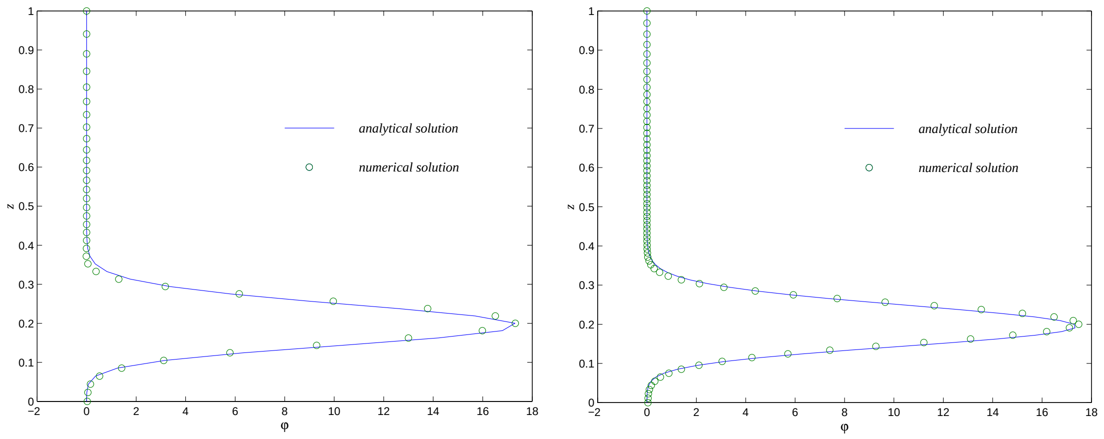
To construct a test problem (3.1) - (3.4) with the known solution, we use the results of Rounds (1955).

$$\varphi(x,z)=(1+\alpha)\sum_{j=0}^{\infty}\frac{J_0(\sigma_j z^{(1+\alpha)/2})\cdot J_0(\sigma_j h^{(1+\alpha)/2})\exp\left[-\sigma_j^2 x(1+\alpha)^2/4\right]}{\left[J_0(\sigma_j)\right]^2}, \quad (3.34)$$

where J_0 is the Bessel function of the first kind of order zero, σ_j is the j th root of J_1 is the Bessel function of the first kind of order one, $\sigma_0 = 0$ and $J_0(0) = 1$. In our calculations we used 51 terms of the series.

Analytical and computational results for steady-state conditions with the parameters $v(z) = z, h = 0.2, w_g = 0.0, \sigma = 0.0, \Delta x = 10^{-4}$ are presented in Figure 3.2 – 3.5. In the pictures, the numerical results are reported for two different numbers of grid on z-axis, namely $n = 41$ and $n = 81$. Figure 3.2 and 3.3 shows vertical concentration profiles two different numbers of grid on z-axis at distances from the source $x = 0.003$ and $x = 0.01$ with $u(z) = z^{0.5}$. Figure 3.4 and 3.5 shows vertical concentration profiles two different numbers of grid on z-axis at distances from the source $x = 0.003$ and $x = 0.01$ with $u(z) = z^{0.2}$.

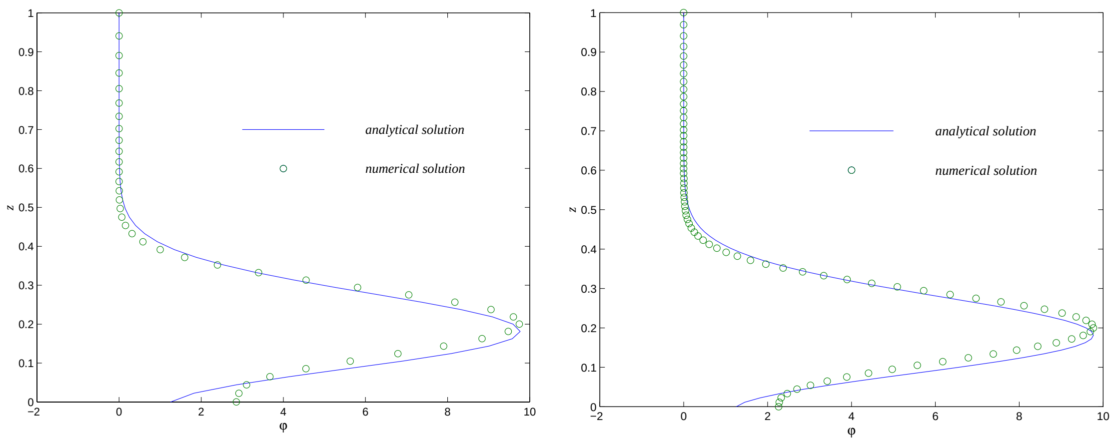
The approximations are evidently sufficient to give good agreement between theory and numerical calculations. The graphics presented in Figure 3.2-3.5 are also indicated that the approximate solutions near to the source seems more accurate than those far from the sources.



$(a)\quad n = 41$

$(b)\quad n = 81$

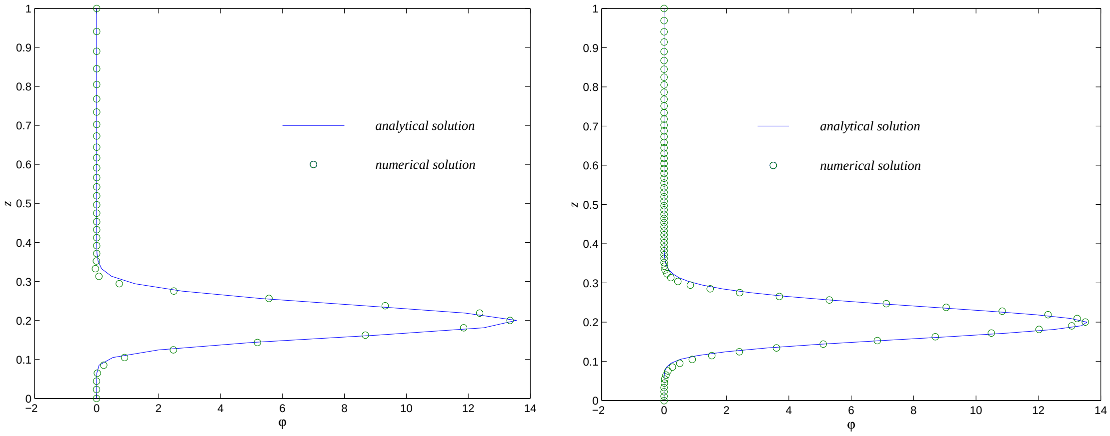
Figure 3.2: A comparison of the analytical and numerical solution at distances $x = 0.003$ from the source, $u(z) = z^{0.5}$, Analytical solution —, approximate solution $\circ$.



$(a)\quad n = 41$

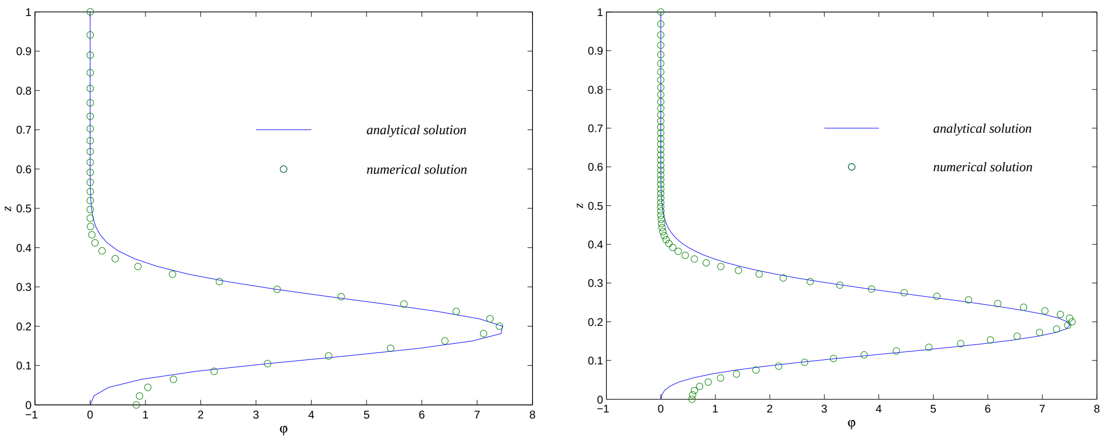
$(b)\quad n = 81$

Figure 3.3: A comparison of the analytical and numerical solution at distances $x = 0.01$ from the source, $u(z) = z^{0.5}$, Analytical solution —, approximate solution $\circ$.



$(a)\quad n = 41$ $(b)\quad n = 81$

Figure 3.4: A comparison of the analytical and numerical solution at distances $x = 0.003$ from the source, $u(z) = z^{0.2}$, Analytical solution —, approximate solution $\circ$.



$(a)\quad n = 41$ $(b)\quad n = 81$

Figure 3.5: A comparison of the analytical and numerical solution at distances $x = 0.01$ from the source, $u(z) = z^{0.2}$, Analytical solution —, approximate solution $\circ$.

3.5.2 Estimation of the errors

A criterion for assessing the quality of a numerical method is a theoretical error estimate.

Let Ω_h be finite dimensional subspaces of domain Ω.There exist a positive constant h_0, $C = C(h_0)$ and $m = m(h_0)$, all are independent of h, such that for all $h \le h_0$

$$\left\| u^h - P_h(u) \right\|_{\Omega_h} \le Ch^m, \tag{3.35}$$

where $P_h(u)$ is a projection of the exact solution of the differential problem onto a set of grid functions given on Ω_h, u^h is a solution of a finite element scheme on the mesh Ω_h and h is a parameter of grid Ω_h. In case of $h \to 0$, it means that the distance between two neighboring grid points tends to zero.

Numerical methods are usually applied to problems for which the exact solution is unknown, which is the usual situation. This means that the error, $u^h - P_h(u)$, in the numerical solution, u^h, can not be determined directly, and therefore an indirect estimate of its magnitude has to be used. We follow the results of J. Miller *et al*. (1996) and use two algorithms to estimate C and m in equation (3.35).

The first algorithm is useful in a case when two numerical solutions can be computed on two different grids. It is assumed that the order of convergence is known to be approximately m. The algorithm then provides an approximate value for the error constant C. Let u denote the exact solution of the problem and $h \in R^h$, $R^h = \left\{ h : \underline{h} \le h \le \overline{h} \right\}$, R^h is the range of h in which numerical solution can be computed. Choose any convenient value h_1 such that $h_1, h_1/4 \in R^h$. The first step is to use the numerical method to compute the two numerical solutions of the problem for the two grids Ω_{h_1} and $\Omega_{h_1/4}$. Denoting these approximate solutions by u^{h_1} and $u^{h_1/4}$ respectively, we compute the norm of difference on the grid Ω_{h_1} between u^{h_1} and the linear interplant $\tilde{u}^{h_1/4}$, namely

$$D = \left\| u^{h_1} - u^{h_1/4} \right\|_{\Omega_{h_1}} = \max_{i,j \in \Omega_{h_1}} \left| u_{ij}^{h_1} - \tilde{u}_{ij}^{h_1/4} \right|. \tag{3.36}$$

Using the triangle inequality and equation (3.36), we obtain

$$D \geq \left\| u^{h_1} - u \right\|_{\Omega_{h_1}} - \left\| \tilde{u}^{h_1/4} - u \right\|_{\Omega_{h_1}} \geq \left\| u^{h_1} - u \right\|_{\Omega_{h_1}} - C_m \left(\frac{h_1}{4} \right)^m \approx C_m (1 - 4^{-m}) h_1^m.$$

We can set

$$C_m^* = \frac{D h_1^{-m}}{1 - 4^{-m}}, \tag{3.37}$$

to be the computed approximation to the unknown error constant.

The second algorithm is useful in a case where three numerical solutions can be computed on three different grids. It provides us with approximations of both the order of convergence m and the error constant C_m. A computed estimate of m is obtained the first by computing the three numerical solutions $u^{h_1}, u^{h_1/2}$ and $u^{h_1/4}$ on the grid $\Omega_{h_1}, \Omega_{h_1/2}$ and $\Omega_{h_1/4}$ respectively, where h_1 is chosen so that $h_1/2, h_1/4 \in R^h$. Let $\tilde{u}^{h_1/2}, \tilde{u}^{h_1/4}$ denote the piecewise linear interpolation of $u^{h_1/2}, u^{h_1/4}$ on Ω_{h_1}. We compute the norms of differences

$$D_1 = \left\| u^{h_1} - \tilde{u}^{h_1/2} \right\|_{\Omega_{h_1}}, D_2 = \left\| \tilde{u}^{h_1/2} - \tilde{u}^{h_1/4} \right\|_{\Omega_{h_1/2}}, D = \left\| \tilde{u}^{h_1} - \tilde{u}^{h_1/4} \right\|_{\Omega_{h_1}}.$$

on the appropriate grids. Using the triangle inequality, equation (3.35), we obtain

$$\frac{D_1}{D_2} \approx \frac{Ch_1^m(1-2^{-m})}{C\left(\frac{h_1}{2}\right)^m(1-2^{-m})} \approx 2^m.$$

We can set

$$m^* = \log_2 \frac{D_1}{D_2},$$

to be the computed approximation to the unknown value of the order of convergence. Using this computed value of m and the above value of D, we apply the previous algorithm to obtain from equation (3.37) the computed approximation

$$C_{m^*}^* = \frac{Dh_1^{-m^*}}{1-4^{-m^*}}. \tag{3.38}$$

Without computing further numerical solutions of the problem, it is now possible to test the sensitivity, relative to changes in h, of the computed error constant $C_{m^*}^*$. Using the analogous argument to the one which is used to obtain equation (3.37) from equation (3.35), we see that each of the quantities

$$C_1^* = \frac{D_1h_1^{-m^*}}{1-2^{-m^*}} \quad \text{or} \quad C_2^* = \frac{D_2(h_1/2)^{-m^*}}{1-2^{-m^*}},$$

may be taken as computed approximates to the error constant. The values C_1^* or C_2^* may not be close to the value C_m^* in equation (3.38), but if $C_1^* \approx C_{m^*}^*$ or $C_2^* \approx C_{m^*}^*$ then it can be concluded, that m^* and $C_{m^*}^*$ are insensitive to variations in h between h_1 and $h_1/4$.

We now use these two algorithms to find approximations to error parameters m and C for finite element scheme applied to the air pollution problem. We choose

$h_1 = 10^{-3}$ in case $u(z) = 1$ and $h_1 = 10^{-4}$ in case $u(z) = z^{0.5}$, respectively, to estimate the quantities D, D_1, D_2.

Table 3.1 : Computed error parameters, sensitivity.

	$u(z) = 1$	$u(z) = z^{0.5}$
D	0.0498740000000026	0.0315680000000000
D_1	0.0332860000000004	0.0210729999999995
D_2	0.0165880000000023	0.0104950000000006
$m*$	1.0047755589478900	1.0056935474790000
C_m^*	137.6109585385730000	87.6745889241680000
C_1^*	137.6109585385730000	87.6745889241680000
C_2^*	137.6109585385730000	87.6745889241681000

The algorithm developed in section 3.3 is then implemented to the equation (3.1) with boundary conditions (3.2)-(3.4). The results of our computations are summarized in Table 3.1. In Table 3.1, we analyze the data for boundary conditions (3.2)-(3.4) with parameters $w_g = 0.0, \sigma = 0.0, h = 0.2, v(z) = z$. The first column of the table refers to the quantities whose computed values are shown in the corresponding rows. The analysis of results in Table 3.1 illustrates the convergence of the finite element method under consideration. So, we have $m \approx m* = 1.004$ for $u(z) = 1$ and $m* = 1.005$ for $u(z) = z^{0.5}$.

3.6 Numerical results

In this section we will present contour lines of concentration which characterize some general views.

3.6.1 The contour lines of concentrations

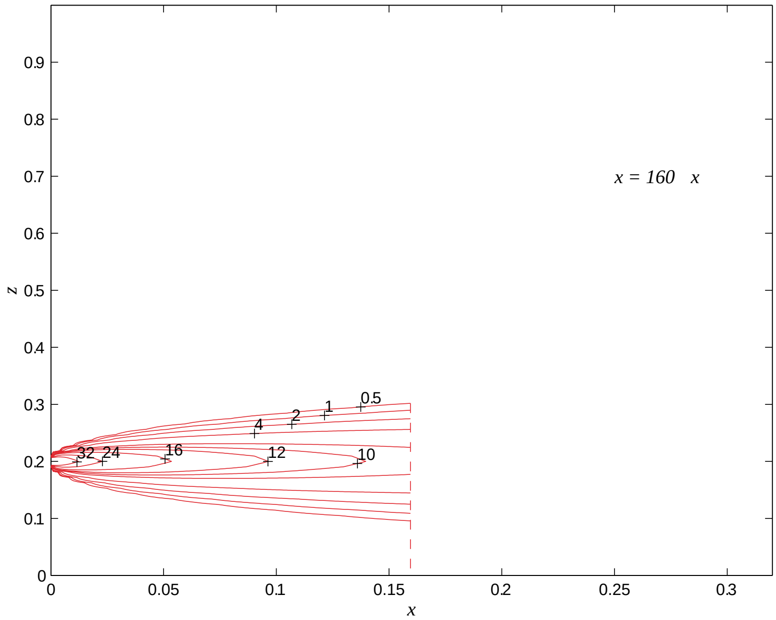
The parameters used in this study were : n = 81, Δz_s = 0.009375, h = 0.2, $v(z) = z, \theta = 0.125$. The results are used to solve computer program 1 in appendix C.

The results are illustrated in Figures 3.6-3.11. From Figures 3.6-3.8 are the contour lines of concentration at different falling velocity of pollutants by gravity, transformation coefficient of pollutants and distances x from the source with $u(z) = 1, x = 160\Delta x, x = 320\Delta x, \Delta x = 0.001$.

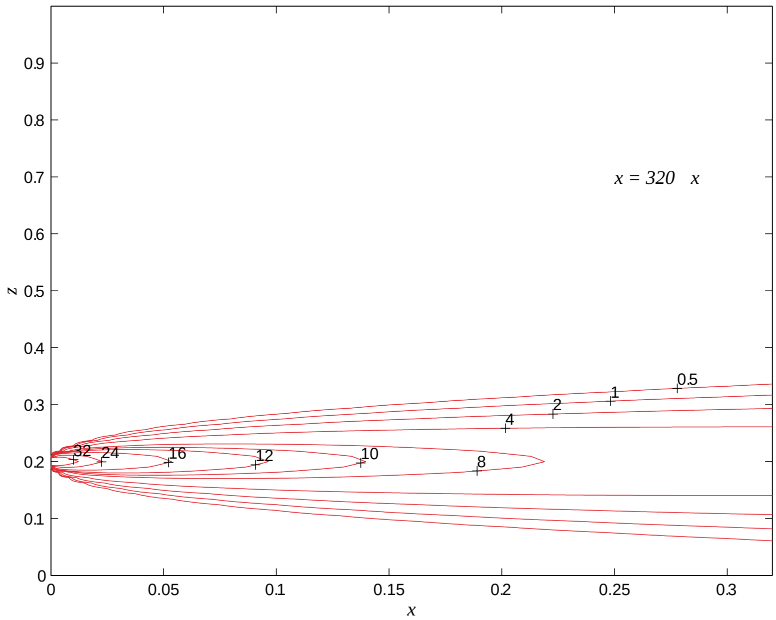
Figures 3.9-3.11 are the contour lines of concentration at different falling velocity of pollutants by gravity, transformation coefficient of pollutants and distances x from the source with $u(z) = z^{0.5}, x = 160\Delta x, x = 320\Delta x, \Delta x = 10^{-4}$

It can be observed that the falling velocity of pollutants by gravity has more strong effect on fall of pollutants than the transformation coefficient. The wind velocity has significant effect on fall of pollutants so that, if velocity is $u(z) = z^{0.5}$ pollutants fall down faster than in the case velocity is $u(z) = 1$.

We note that the results from the examples give different contour lines, depend on the values of the coefficients of the advection and diffusion terms.

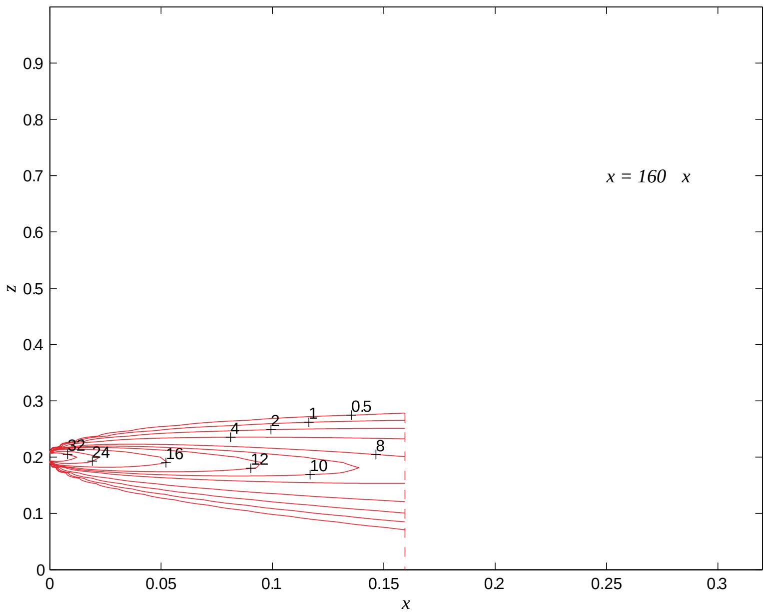


$(a) \quad x = 160\Delta x$

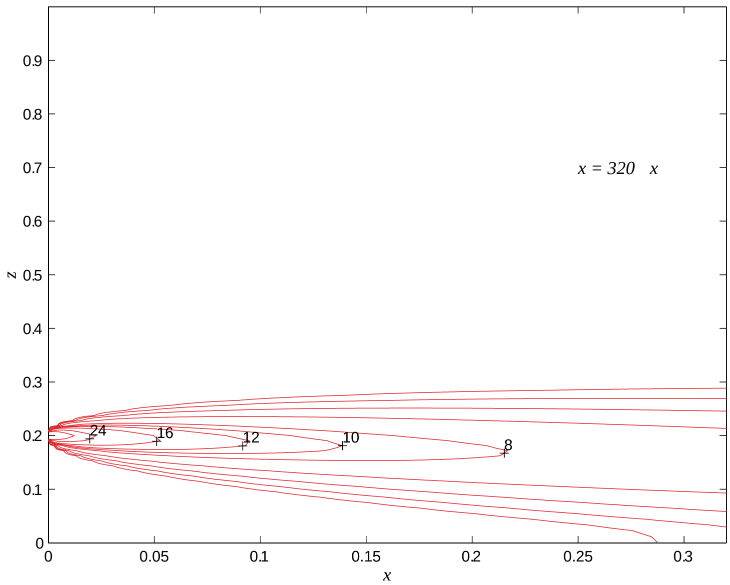


$(b) \quad x = 320\Delta x$

Figure 3.6: The contour lines of concentration at different distances x from the source, calculated for $u(z)=1, v(z)=z, \Delta x=10^{-3}, w_g=0.0$ and $\sigma=0.0$.

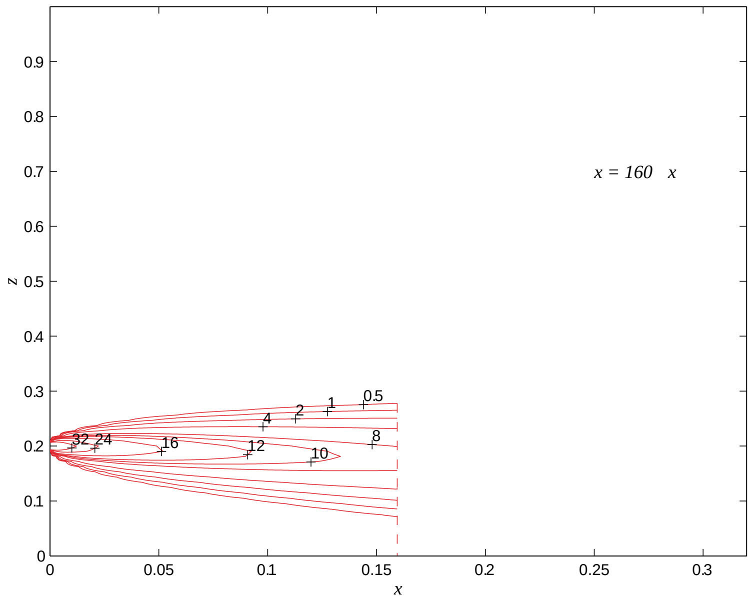


$(a) \quad x = 160\Delta x$

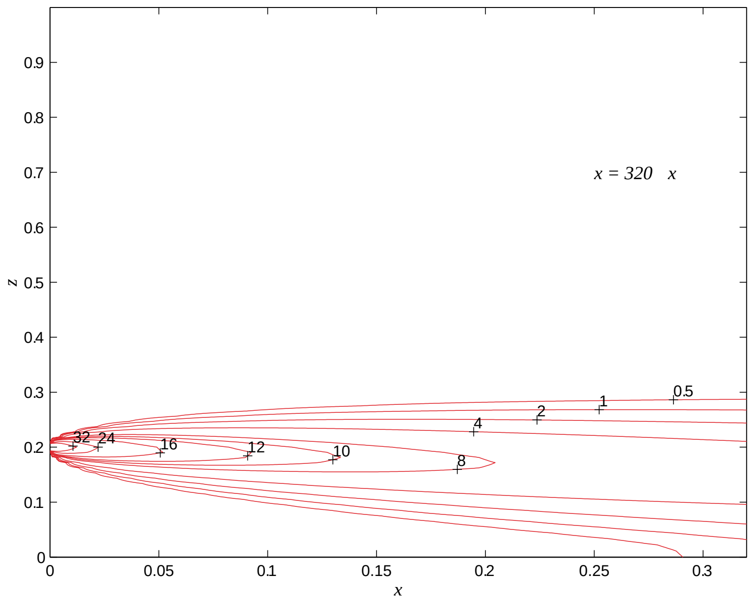


$(b) \quad x = 320\Delta x$

Figure 3.7: The contour lines of concentration at different distances x from the source, calculated for $u(z)=1, v(z)=z, \Delta x = 10^{-3}, w_g = 0.125$ and $\sigma = 0.0$.

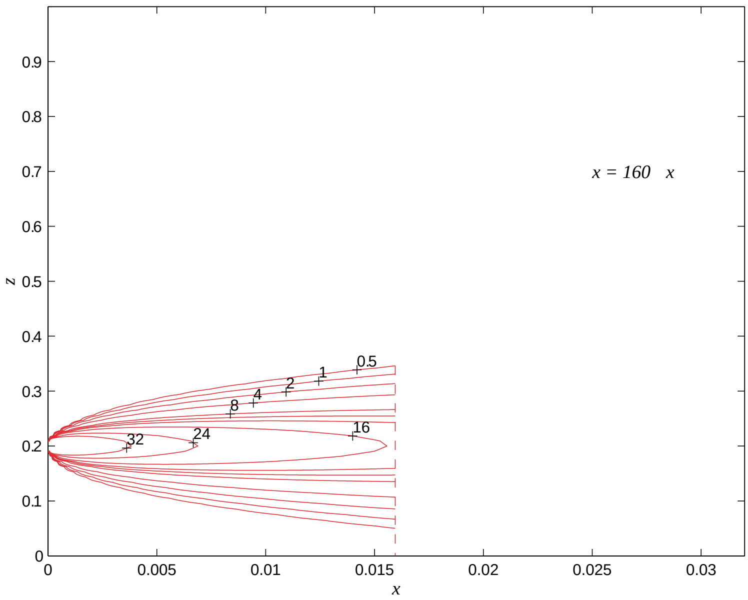


$(a)\quad x = 160\Delta x$

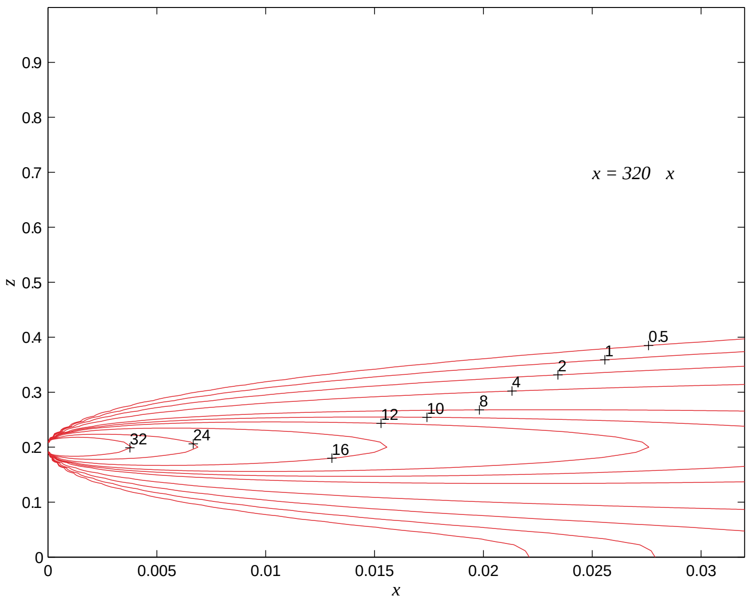


$(b)\quad x = 320\Delta x$

Figure 3.8: The contour lines of concentration at different distances x from the source, calculated for $u(z) = 1, v(z) = z, \Delta x = 10^{-3}, w_g = 0.125$ and $\sigma = 0.125$.

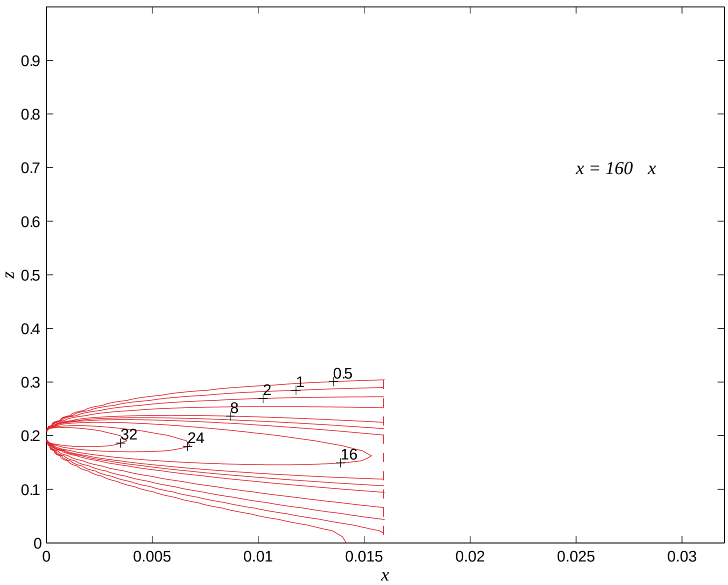


$(a) \quad x = 160\Delta x$

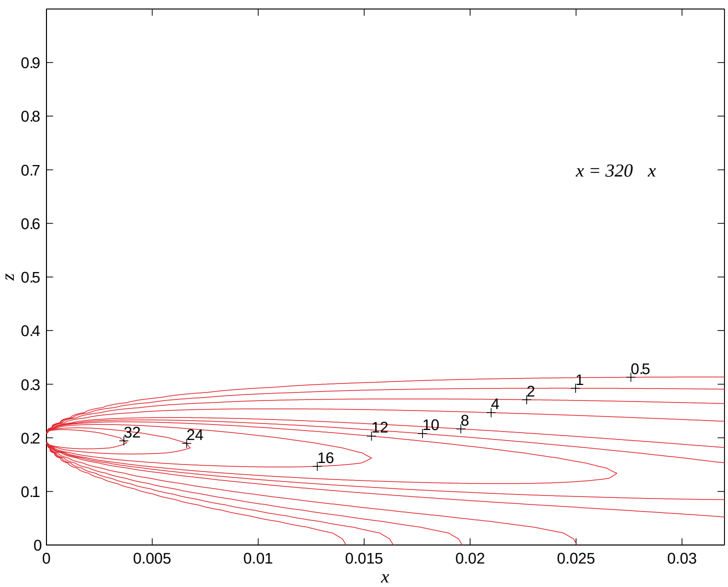


$(b) \quad x = 320\Delta x$

Figure 3.9: The contour lines of concentration at different distances x from the source, calculated for $u(z) = z^{0.5}, v(z) = z, \Delta x = 10^{-4}, w_g = 0.0$ and $\sigma = 0.0$.

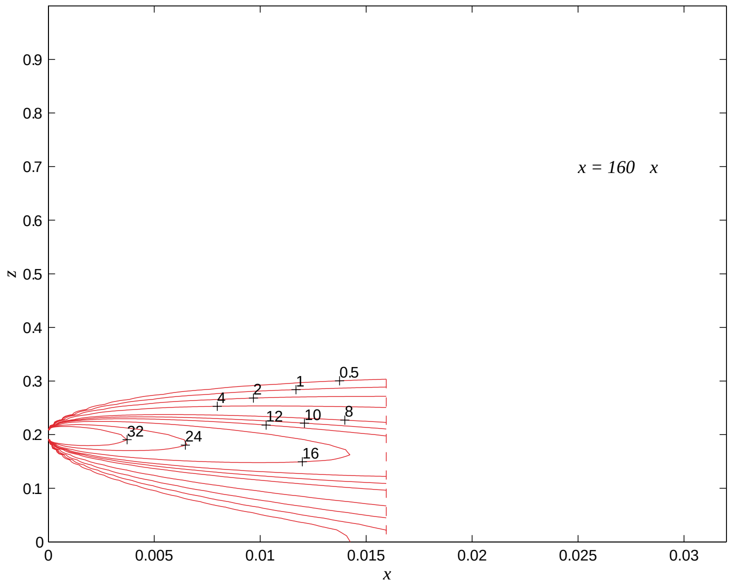


(a) $x = 160\Delta x$

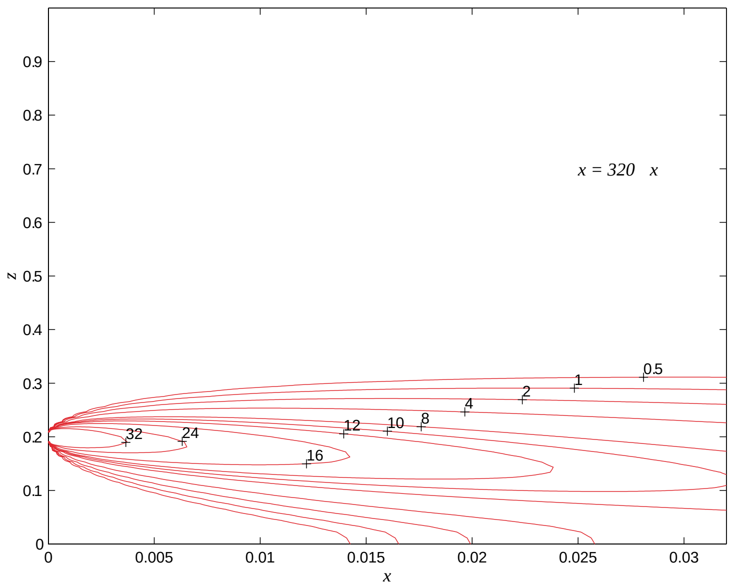


(b) $x = 320\Delta x$

Figure 3.10: The contour lines of concentration at different distances x from the source, calculated for $u(z) = z^{0.5}, \nu(z) = z, \Delta x = 10^{-4}, w_g = 0.125$ and $\sigma = 0.0$.



$(a) \quad x = 160\Delta x$



$(b) \quad x = 320\Delta x$

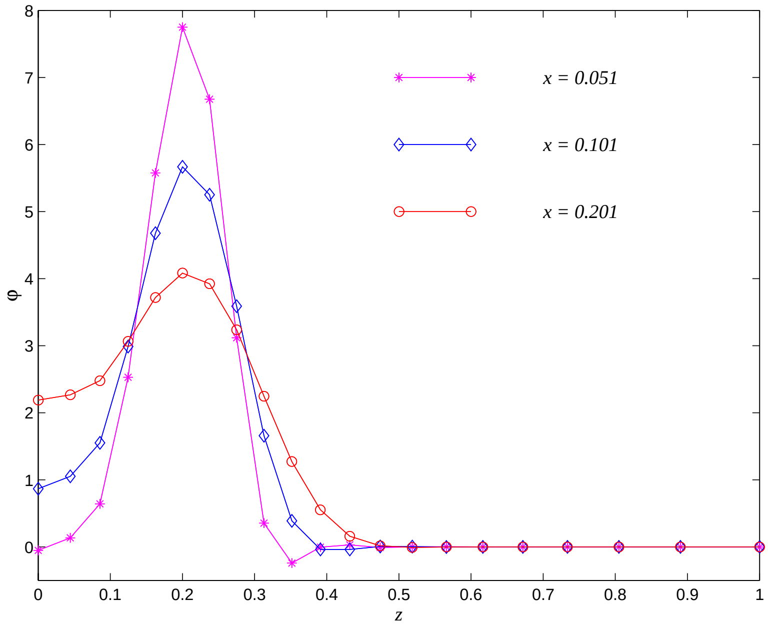
Figure 3.11: The contour lines of concentration at different distances x from the source, calculated for $u(z) = z^{0.5}, \nu(z) = z, \Delta x = 10^{-4}, w_g = 0.125$ and $\sigma = 0.125$.

3.6.2 The concentrations at different z for fixed x

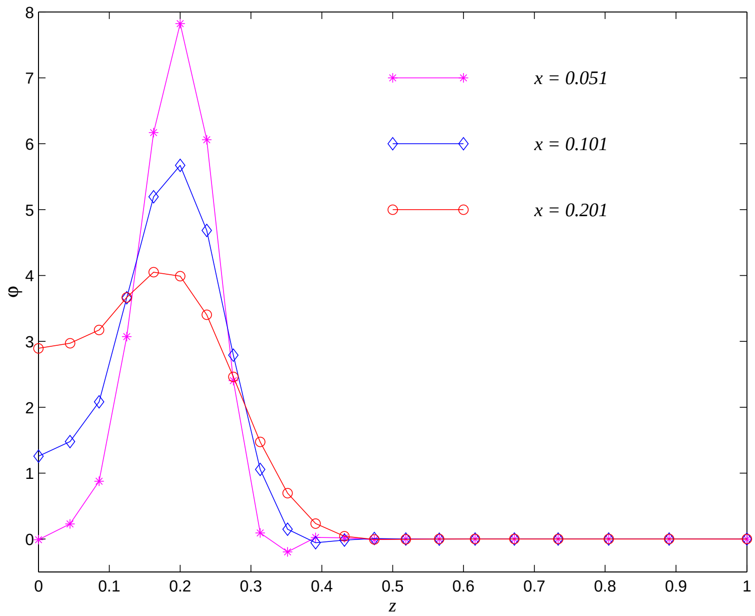
We now show the results of the computed solution of concentrations at different z for a fixed distance x. The parameters used in this study were: $n = 21$, $\Delta z_s = 0.033, h = 0.2, \nu(z) = z, \theta = 0.125$. In Figures 3.12-3.13 present some profiles of concentration field at different falling velocity of pollutants by gravity, the transformation coefficient of pollutants.

In Figures 3.12 shows concentration profiles $\varphi(z)$ at different falling velocity of pollutants by gravity, the transformation coefficient of pollutants and distances x from the source with $u(z) = 1, \Delta x = 0.001$, $x = 0.051, x = 0.101, x = 0.201$. In Figures 3.13 shows concentration profiles $\varphi(z)$ at different falling velocity of pollutants by gravity, the transformation coefficient of pollutants and distances x from the source with $u(z) = z^{0.5}, \Delta x = 0.0001$, $x = 0.0051, x = 0.0101, x = 0.0201$.

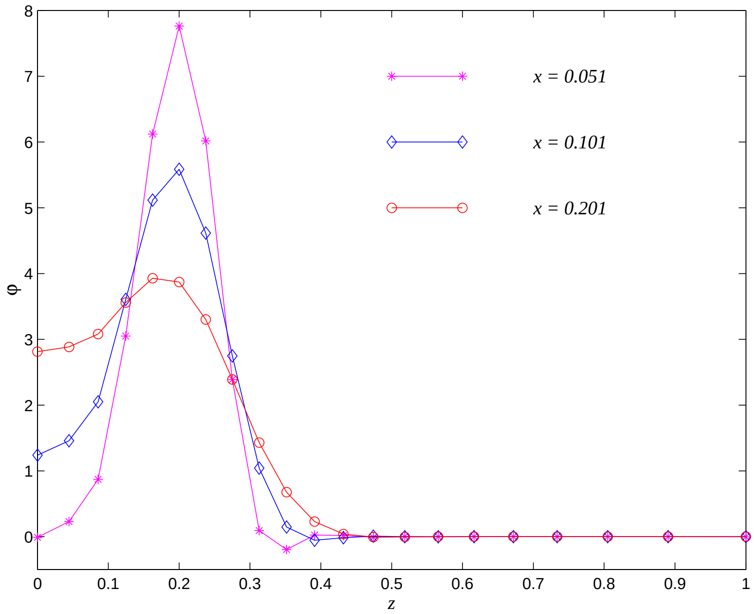
From Figures 3.12 and 3.13, we can see concentration profiles $\varphi(z)$ which is the highest at $z = 0.2$, and equal zero at $z \geq 0.5$ all distance x. If the falling velocity of pollutants by gravity is different the graph has a little difference. Yet, the graph is not different if the transformation coefficient is different.



(a) $w_g = 0.0$ and $\sigma = 0.0$

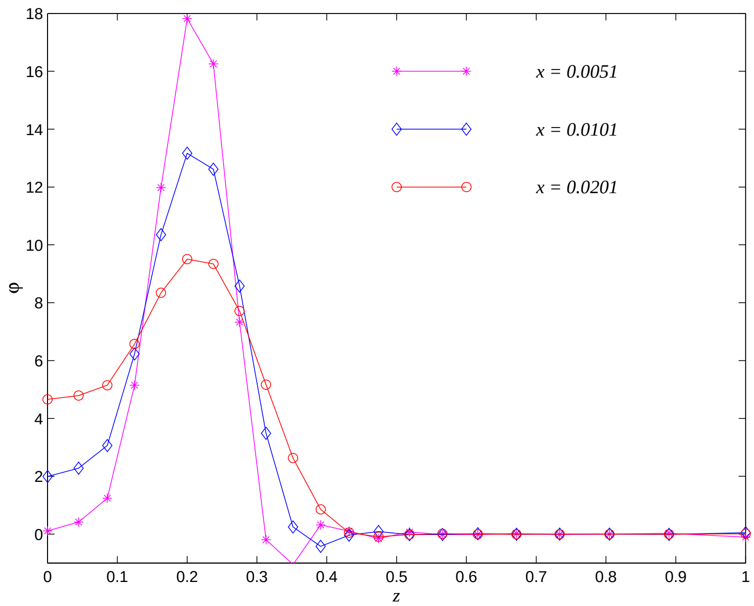


(b) $w_g = 0.125$ and $\sigma = 0.0$

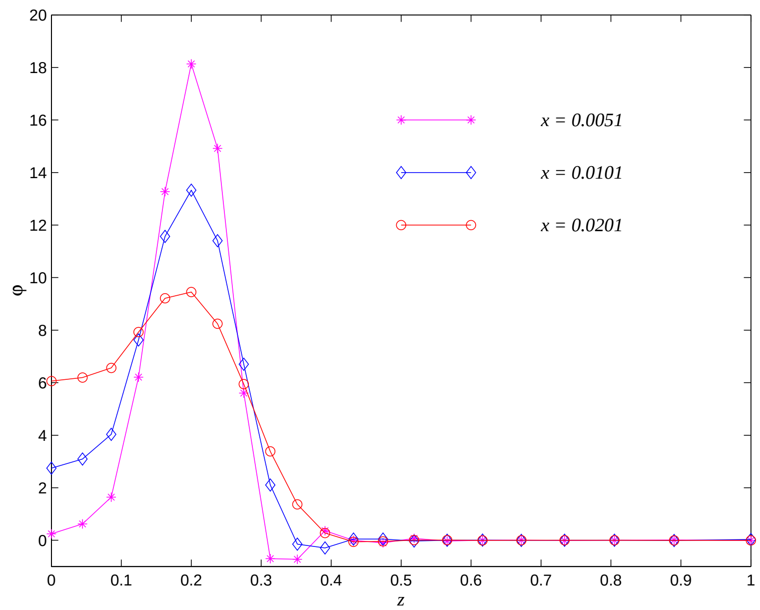


$(c)\ w_g = 0.125$ and $\sigma = 0.125$

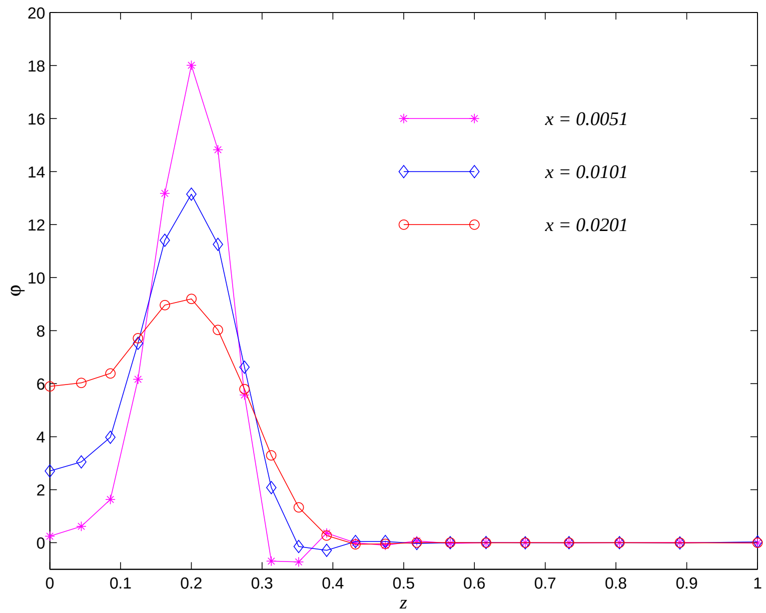
Figure 3.12: Concentration profiles $\varphi(z)$ at different distances x from the source, calculated for $\Delta x = 0.001$ and $u(z) = 1$ respectively, with $n = 21, v(z) = z, h = 0.2$.



$(a)\ w_g = 0.0$ and $\sigma = 0.0$



$(b)\ \ w_g = 0.125$ and $\sigma = 0.0$



$(c)\ \ w_g = 0.125$ and $\sigma = 0.125$

Figure 3.13: Concentration profiles $\varphi(z)$ at different distances x from the source, calculated for $\Delta x = 0.0001$ and $u(z) = z^{0.5}$ respectively, with $n = 21, v(z) = z, h = 0.2$.

Chapter IV

Approximate Solution of Unsteady State Problem

4.1 Introduction

The main goal of this chapter is to study the time dependent behavior in two-dimensional space of an air pollutant given in the equations (1.28) - (1.32).

4.2 Mathematical formulation

In order to solve the unsteady state problem equation, we use the same notations for the non-dimensionalized variables. In these new variables the resulting system can be written in the form :

$$\frac{\partial\varphi}{\partial t}+u(z)\frac{\partial\varphi}{\partial x}-w_g\frac{\partial\varphi}{\partial z}-\frac{\partial}{\partial z}\left(\nu(z)\frac{\partial\varphi}{\partial z}\right)+\sigma\varphi=0 \text{ for all } 0<t,\ 0<x,\ 0<z<1, \quad (4.1)$$

with the initial and boundary conditions

$$\varphi(x,z,0)=0 \text{ for all } 0<x, 0<z<1, \quad (4.2)$$

$$\varphi(0,z,t)=\frac{\delta(z-h)}{u(h)} \text{ for all } 0<t,\ 0<z<1, \quad (4.3)$$

$$\nu(0)\frac{\partial\varphi(x,0,t)}{\partial z}=0 \text{ for all } 0<t, 0<x, \quad (4.4)$$

$$\nu(1)\frac{\partial\varphi(x,1,t)}{\partial z}=0 \text{ for all } 0<t, 0<x. \quad (4.5)$$

4.3 Splitting the problem into convection and convection-diffusion equations

We construct uniform meshes in the x-and t-directions with mesh widths Δx and Δt, respectively, and a non--uniform mesh in the z-direction. For each time level t we obtain the value of φ at time $t+\Delta t$ from its value at t by first taking a first step to obtain an auxiliary value φ^* followed by a second step to obtain the required value.

Given φ at time level t, we obtain the auxiliary value φ^* at time level $t+\Delta t$ by solving the following hyperbolic equation in the time sub-interval $(t, t+\Delta t]$

$$\frac{\partial \varphi^*}{\partial t} + u(z)\frac{\partial \varphi^*}{\partial x} = 0 \text{ for all } [t, t+\Delta t],\ 0 < x,\ 0 < z < 1, \tag{4.6}$$

with the initial condition at $t = t$

$$\varphi^*(x,z,t) = \varphi(x,z,t) \quad \text{for all} \quad 0 < x,\ 0 < z < 1. \tag{4.7}$$

and the boundary conditions at $x = 0$

$$\varphi^*(0,z,t) = \frac{\delta(z-h)}{u(h)} \text{ for all } [t, t+\Delta t],\ 0 < z < 1, \tag{4.8}$$

given φ^* we obtain the required value φ at time level $t+\Delta t$ by solving the following parabolic equation in the time sub-interval $[t, t+\Delta t]$

$$\frac{\partial \varphi}{\partial t} - w_g\frac{\partial \varphi}{\partial z} - \frac{\partial}{\partial z}\left(v(z)\frac{\partial \varphi}{\partial z}\right) + \sigma\varphi = 0 \quad \text{for all} \quad [t, t+\Delta t],\ 0 < x,\ 0 < z < 1, \tag{4.9}$$

with the initial condition at $t = t$

$$\varphi(x,z,t) = \varphi^*(x,z,t+\Delta t] \text{ for all } 0 < x,\ 0 < z < 1, \tag{4.10}$$

and the boundary conditions at $z = 0$, $z = 1$

$$\nu(0)\frac{\partial\varphi(x,0,t)}{\partial z}=0 \quad \text{for all} \quad [t,t+\Delta t],\ 0<x, \tag{4.11}$$

$$\nu(1)\frac{\partial\varphi(x,1,t)}{\partial z}=0 \quad \text{for all} \quad [t,t+\Delta t],\ 0<x. \tag{4.12}$$

The concentration field at the time $t+\Delta t$ is obtained from that at the time t by separating the contributions due to terms as follows :

In the first step the convection equation

$$\frac{\partial\varphi}{\partial t}+u(z)\frac{\partial\varphi}{\partial x}=0, \tag{4.13}$$

is solved in the whole $x-z$ integration region over the time interval $[t,t+\Delta t]$ with the concentration field at the time t as initial conditions (4.7) and (4.8) as boundary condition. In the second step convection-diffusion equation

$$\frac{\partial\varphi}{\partial t}-w_g\frac{\partial\varphi}{\partial z}-\frac{\partial}{\partial z}\left(\nu(z)\frac{\partial\varphi}{\partial z}\right)+\sigma\varphi=0, \tag{4.14}$$

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 (4.10) and the boundary conditions by the relation (4.11) and (4.12). Let us show that the solution of (4.13) and (4.14) is an approximation of the concentration field at the time $t+\Delta t$.

If we denote

$$L_1\varphi\equiv -u(z)\frac{\partial\varphi}{\partial x},$$

$$L_2\varphi\equiv w_g\frac{\partial\varphi}{\partial z}+\frac{\partial}{\partial z}\left(\nu(z)\frac{\partial\varphi}{\partial z}\right)-\sigma\varphi.$$

The Cauchy problem for equation (4.1) is

$$\begin{cases} \dfrac{\partial \varphi}{\partial t} = (L_1 + L_2)\varphi, \\ \\ \varphi(x,z,0) = \varphi_0(x,z) \end{cases}$$

We can split into two problems

$$\begin{cases} \dfrac{\partial \varphi^*}{\partial t} = L_1\varphi^*, \\ \\ \varphi^*(x,z,t_n) = \varphi(x,z,t_n), \end{cases}$$

and

$$\begin{cases} \dfrac{\partial \tilde{\varphi}}{\partial t} = L_2\tilde{\varphi}, \\ \\ \tilde{\varphi}(x,z,t_n) = \varphi^*(x,z,t_n + \tau). \end{cases}$$

By Taylor series, we have

$$\begin{aligned} \varphi(x,z,t_n+\tau) &= \varphi(x,z,t_n) + \tau\frac{\partial \varphi}{\partial t} + O(\tau^2) \\ &= \varphi(x,z,t_n) + \tau(L_1+L_2)\varphi(x,z,t_n) + O(\tau^2) \\ &= \left[E + \tau(L_1+L_2)\right]\varphi(x,z,t_n) + O(\tau^2) \end{aligned}$$

Where E is the identity operator, in the same way, we get

$$\begin{aligned} \varphi^*(x,z,t_n+\tau) &= \varphi^*(x,z,t_n) + \tau\frac{\partial \varphi^*}{\partial t} + O(\tau^2) \\ &= \varphi^*(x,z,t_n) + \tau L_1\varphi^*(x,z,t_n) + O(\tau^2) \\ &= \left[E + \tau L_1\right]\varphi^*(x,z,t_n) + O(\tau^2) \\ &= \left[E + \tau L_1\right]\varphi(x,z,t_n) + O(\tau^2) \end{aligned}$$

since $\varphi^*(x,z,t_n) = \varphi(x,z,t_n)$

So

$$\begin{aligned}
\tilde{\varphi}(x,z,t_n+\tau) &= \tilde{\varphi}(x,z,t_n)+\tau\frac{\partial\tilde{\varphi}}{\partial t}+O(\tau^2) \\
&= \tilde{\varphi}(x,z,t_n)+\tau L_2\tilde{\varphi}(x,z,t_n)+O(\tau^2) \\
&= \left[E+\tau L_2\right]\tilde{\varphi}(x,z,t_n)+O(\tau^2) \\
&= \left[E+\tau L_2\right]\varphi^*(x,z,t_n)+O(\tau^2) \\
&= \left[E+\tau L_2\right]\left[E+\tau L_1\right]\varphi(x,z,t_n)+O(\tau^2) \\
&= \left[E+\tau(L_1+L_2)\right]\varphi(x,z,t_n)+O(\tau^2) \\
&= \varphi(x,z,t_n+\tau)+O(\tau^2)
\end{aligned}$$

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

$$\tilde{\varphi}(x,z,t_n+\tau)=\varphi(x,z,t_n+\tau).$$

4.3.1 Numerical algorithm of convection equation problem

The equation (4.13) in the Lagrangian form is

$$\frac{\partial\varphi(\xi,z,t)}{\partial t}=0 \quad \text{with} \quad \xi=x+ut \tag{4.15}$$

Equation (4.15) simply means that in a reference frame moving with the velocity u the concentration does not change in time. Thus equation (4.13) is exactly satisfied by translating the concentration field at any time step Δt to the distance $u\Delta t$.

If the wind velocity is constant in space and time, equation (4.15) can directly be represented in the Eulerian frame use for equation (4.14) simply by choosing $\Delta x=u\Delta t$. A further simplification is provided by the fact that for $u=$constant equation (4.13) and (4.14) can be integrated separately not only over a single time interval, but over the whole integration time. In fact, the equation (4.1) can be transformed by introduction Lagrangian coordinates to a equation (4.14) valid in frame moving with the velocity u.

If the wind velocity is not constant, the described Lagrangian treatment of equation (4.13) becomes problematic in connection with Petrov-Galerkin finite element method used for equation (4.14). In fact, for constants Δt and a variable u, the condition $\frac{u \cdot \Delta t}{\Delta x} = 1$ means a variable Δx. Thus, positions which are not coincident with grid point will be reached by all particles whose velocity is different from the chosen ratio $\frac{\Delta x}{\Delta t}$. In other words, equation (4.13) cannot be satisfied by translating the whole concentration field to the next grid points of an Eulerian frame.

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 $u_{\max}$:

$$u_k = \frac{p_k}{q} u_{\max}, \quad p_k \leq q, \quad k = 1, 2, \ldots, n, \tag{4.16}$$

where p_k and q are positive integers and n is the number of vertical grid point. For a given distribution of the vertical intervals Δz_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 (4.16) as the best approximations to the mean values of $u(z)$ over any vertical step. Figure 4.1 shows as an example, how the velocity profile $u(z) = z^{0.5}$ is approximated for a constant interval $\Delta z = 0.05$ and $q = 5$. For sufficiently small Δz

and sufficiently large $q = 5$, the approximation error of step function is arbitrarily small.

The horizontal interval Δx is defined as

$$\Delta x = \frac{u_{\max}}{q} \Delta t. \tag{4.17}$$

Consequently, the pollutant moving with the velocity u_k is translated at any time step to the distance $p_k \Delta x$, that is, to positions coincident with grid points. In particular, the pollutant with the maximum velocity $u_{\max}$ is translated to a distance $q\Delta x$. 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. 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 (4.16). The parameters $u_{\max}$ and q can still be taken as constant. Equation (4.17) shows that the horizontal interval Δx 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.(see Runca, E. and Sardei, F. (1975))

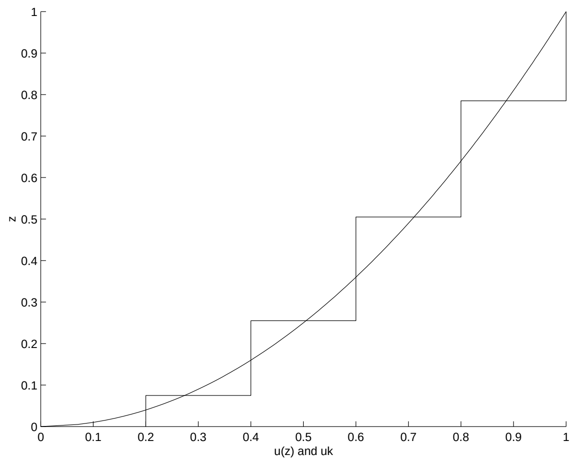


Figure 4.1: Wind profile $u(z)=z^{0.5}$ and approximating step function u_k for $q=5$ and uniform vertical grid spacing $\Delta z = 0.05$.

4.3.2 Numerical algorithm of convection-diffusion equation problem

Equations (4.9)-(4.12) are solved by Petrov-Galerkin finite element method. Let $\Omega=\{(z,t)\in \mathbb{R}^2 \mid 0<t,\ 0<z<1\}$ be domain and let

$$L(\varphi)\equiv \frac{\partial \varphi}{\partial t}-w_g\frac{\partial \varphi}{\partial z}-\frac{\partial}{\partial z}\left(\nu(z)\frac{\partial \varphi}{\partial z}\right)+\sigma\varphi=0. \tag{4.18}$$

Consider the finite element which is subdivided the domain Ω into the a rectangular K with four nodes, we defined the trial function $\hat{\varphi}$ by

$$\begin{aligned}\varphi\big|_K=\hat{\varphi}_K &= C_1+C_2 z+C_3 t+C_4 zt\\ &= \sum_{j=1}^{4}\varphi_j\phi_j(z,t)\end{aligned}$$

For $(z,t)\in\Omega$, we have

$$\varphi(z,t)\approx\hat{\varphi}(z,t)=\sum_j \varphi_j\phi_j(z,t). \tag{4.19}$$

When this trial function $\hat{\varphi}$ is substituted into (4.18), we have

$$L(\hat{\varphi})=R, \tag{4.20}$$

where R is a residual arising from the fact that (4.19) does not identically satisfy (4.18). According to the Petrov-Galerkin approach, we require that residual be orthogonal to the weighing function $\omega_i(z,t)$. Thus the approximating integral equations have the form

$$\iint_{\Omega} L(\hat{\varphi})\omega_i(z,t)\,dz\,dt = 0. \tag{4.21}$$

Therefore integration (4.21) by parts gives

$$\iint_{\Omega}\left(\frac{\partial\hat{\varphi}}{\partial t} - w_g\frac{\partial\hat{\varphi}}{\partial z} - \frac{\partial}{\partial z}\left(\nu(z)\frac{\partial\hat{\varphi}}{\partial z}\right) + \sigma\hat{\varphi}\right)\omega_i(z,t)\,dz\,dt = 0. \tag{4.22}$$

$$\iint_{\Omega}\frac{\partial\hat{\varphi}}{\partial t}\omega_i(z,t)\,dz\,dt - w_g\iint_{\Omega}\frac{\partial\hat{\varphi}}{\partial z}\omega_i(z,t)\,dz\,dt$$

$$-\iint_{\Omega}\frac{\partial}{\partial z}\left(\nu(z)\frac{\partial\hat{\varphi}}{\partial z}\right)\omega_i(z,t)\,dz\,dt + \iint_{\Omega}\sigma\hat{\varphi}\omega_i(z,t)\,dz\,dt = 0. \tag{4.23}$$

If the integration is assumed to be in the closed region Ω_C with the boundary $\partial\Omega_C$, a closed conservative system with no change in energy, then by using Green's theorem, we have

$$\iint_{\Omega_C}\frac{\partial\hat{\varphi}}{\partial t}\omega_i(z,t)\,dz\,dt - w_g\iint_{\Omega_C}\frac{\partial\hat{\varphi}}{\partial z}\omega_i(z,t)\,dz\,dt - \int_{\partial\Omega_C}\nu(z)\frac{\partial\hat{\varphi}}{\partial z}\omega_i(z,t)dt$$

$$+\iint_{\Omega_C}\nu(z)\frac{\partial\hat{\varphi}}{\partial z}\frac{\partial\omega_i(z,t)}{\partial z}\,dz\,dt + \iint_{\Omega_C}\sigma\hat{\varphi}\omega_i(z,t)\,dz\,dt = 0.$$

i.e.

$$\begin{aligned}&\iint_{\Omega_C}\frac{\partial\hat{\varphi}}{\partial t}\omega_i(z,t)\,dz\,dt - w_g\iint_{\Omega_C}\frac{\partial\hat{\varphi}}{\partial z}\omega_i(z,t)\,dz\,dt\\ &+\iint_{\Omega_C}\nu(z)\frac{\partial\hat{\varphi}}{\partial z}\frac{\partial\omega_i(z,t)}{\partial z}\,dz\,dt + \iint_{\Omega_C}\sigma\hat{\varphi}\omega_i(z,t)\,dz\,dt = 0.\end{aligned} \tag{4.24}$$

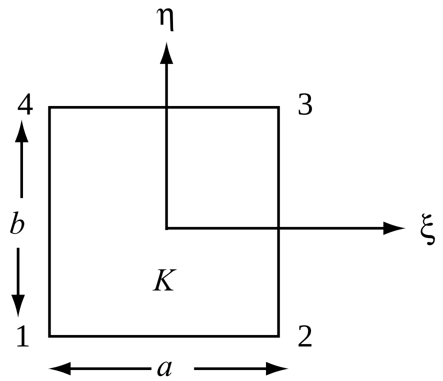


Figure 4.2: Linear plane isoparametric element.

The local (z,t) coordinate system is related to more commonly encountered (ξ,η) system through the relationship

$$\frac{t}{a}=\frac{\xi+1}{2}, \quad \frac{z}{b}=\frac{\eta+1}{2} \tag{4.25}$$

The basis functions in this case have the form

$$\left.\begin{array}{ll} \phi_1(\xi,\eta)=\frac{1}{4}(1-\xi)(1-\eta) \;, & \phi_2(\xi,\eta)=\frac{1}{4}(1+\xi)(1-\eta) \\ \phi_3(\xi,\eta)=\frac{1}{4}(1+\xi)(1+\eta) \;, & \phi_4(\xi,\eta)=\frac{1}{4}(1-\xi)(1+\eta) \end{array}\right\} \tag{4.26}$$

To perform the calculation (4.24) we use the linear plane isoparametric element transformation. Since this result is valid for every closed region Ω_C, the integration of (4.24) can take place in every element. Thus, it can be written as

$$\int_{-1}^{1}\int_{-1}^{1}\left[\frac{\partial\hat{\varphi}}{\partial t}\omega_i(\xi,\eta)-w_g\frac{\partial\hat{\varphi}}{\partial z}\omega_i(\xi,\eta)+v(\eta)\frac{\partial\hat{\varphi}}{\partial z}\frac{\partial\omega_i(\xi,\eta)}{\partial z}+\sigma\hat{\varphi}\omega_i(\xi,\eta)\right]|J|\,d\xi\,d\eta=0. \tag{4.27}$$

where

$$\frac{\partial\hat{\varphi}}{\partial t}=\sum_{j=1}^{4}\varphi_j\frac{\partial\phi_j}{\partial\xi}\frac{\partial\xi}{\partial t}=\frac{2}{a}\sum_{j=1}^{4}\varphi_j\frac{\partial\phi_j(\xi,\eta)}{\partial\xi}, \tag{4.28}$$

$$\frac{\partial \hat{\varphi}}{\partial z} = \sum_{j=1}^{4} \varphi_j \frac{\partial \phi_j}{\partial \eta} \frac{\partial \eta}{\partial z} = \frac{2}{b} \sum_{j=1}^{4} \varphi_j \frac{\partial \phi_j(\xi,\eta)}{\partial \eta}, \tag{4.29}$$

$$|J| = \begin{vmatrix} \frac{\partial t}{\partial \xi} & \frac{\partial t}{\partial \eta} \\ \frac{\partial z}{\partial \xi} & \frac{\partial z}{\partial \eta} \end{vmatrix} = \frac{ab}{4}. \tag{4.30}$$

Let the weighting functions $\omega_i(\xi,\eta)$ be the two dimension asymmetric form, which can be expressed in the form (see Lapidus, L. and Pinderm, G. F. (1982))

$$\left.\begin{aligned} \omega_1(\xi,\eta) &= G_1(\xi,\alpha_1)H_1(\eta,\beta_2), \\ \omega_2(\xi,\eta) &= G_2(\xi,\alpha_1)H_1(\eta,\beta_1), \\ \omega_3(\xi,\eta) &= G_2(\xi,\alpha_2)H_2(\eta,\beta_1), \\ \omega_4(\xi,\eta) &= G_1(\xi,\alpha_2)H_2(\eta,\beta_2), \end{aligned}\right\} \tag{4.31}$$

where

$$G_1(\xi,\alpha_1) = \frac{1}{4}\left[(1+\xi)(3\alpha_1\xi - 3\alpha_1 - 2) + 4\right], \tag{4.32}$$

$$G_2(\xi,\alpha_1) = \frac{1}{4}\left[(1+\xi)(-3\alpha_1\xi + 3\alpha_1 + 2)\right], \tag{4.33}$$

$$G_1(\xi,\alpha_2) = \frac{1}{4}\left[(1+\xi)(3\alpha_2\xi - 3\alpha_2 - 2) + 4\right], \tag{4.34}$$

$$G_2(\xi,\alpha_2) = \frac{1}{4}\left[(1+\xi)(-3\alpha_2\xi + 3\alpha_2 + 2)\right], \tag{4.35}$$

$$H_1(\eta,\beta_1) = \frac{1}{4}\left[(1+\eta)(3\beta_1\eta - 3\beta_1 - 2) + 4\right], \tag{4.36}$$

$$H_2(\eta,\beta_1) = \frac{1}{4}\left[(1+\eta)(-3\beta_1\eta + 3\beta_1 + 2)\right], \tag{4.37}$$

$$H_1(\eta,\beta_2)=\frac{1}{4}\left[(1+\eta)(3\beta_2\eta-3\beta_2-2)+4\right], \tag{4.38}$$

$$H_2(\eta,\beta_2)=\frac{1}{4}\left[(1+\eta)(-3\beta_2\eta+3\beta_2+2)\right], \tag{4.39}$$

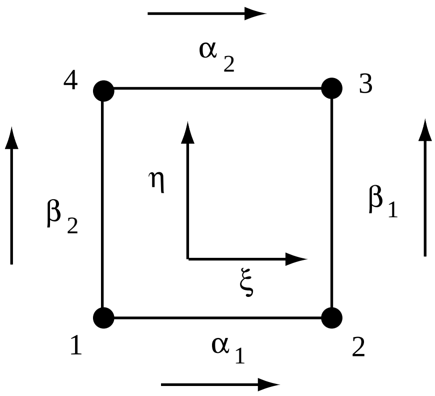


Figure 4.3: Asymmetric weighting function for four nodes defined in (ξ,η) coordinates. (Adapted from Lapidus, L. and Pinderm, G. F. (1982))

From the equations (4.31)- (4.39)we have :

$$\left.\begin{aligned}
\omega_1(\xi,\eta)&=\frac{1}{16}\left[(1+\xi)(3\alpha_1\xi-3\alpha_1-2)+4\right]\left[(1+\eta)(3\beta_2\eta-3\beta_2-2)+4\right],\\
\omega_2(\xi,\eta)&=\frac{1}{16}\left[(1+\xi)(-3\alpha_1\xi+3\alpha_1+2)\right]\left[(1+\eta)(3\beta_1\eta-3\beta_1-2)+4\right],\\
\omega_3(\xi,\eta)&=\frac{1}{16}\left[(1+\xi)(-3\alpha_2\xi+3\alpha_2+2\right]\left[(1+\eta)(-3\beta_1\eta+3\beta_1+2)\right],\\
\omega_4(\xi,\eta)&=\frac{1}{16}\left[(1+\xi)(3\alpha_2\xi-3\alpha_2-2)+4\right]\left[(1+\eta)(-3\beta_2\eta+3\beta_2+2)\right].
\end{aligned}\right\} \tag{4.40}$$

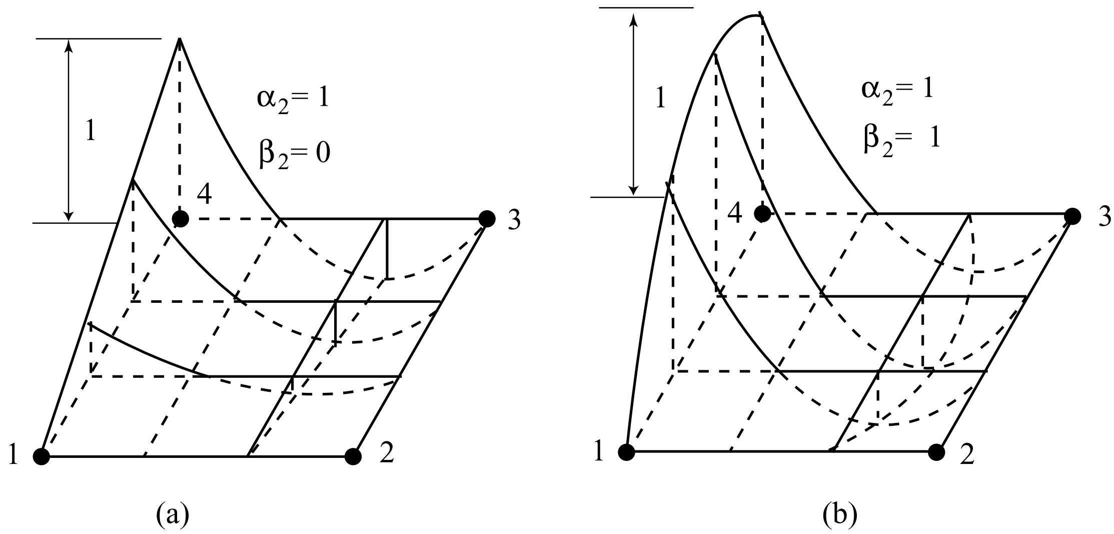


Figure 4.4: Asymmetric weighting function for node 4 defined in η_i coordinates. In (a) $\alpha_2 = 1, \beta_2 = 0$ and in (b) $\alpha_2 = 1, \beta_2 = 0$.(Adapted from Lapidus, L. and Pinderm, G. F. (1982))

It is apparent from Figure 4.4 and (4.40) that there are two α-type factors in each coordinate direction. Thus the variation in α from one side of an element to the other can be taken into account. The sense of the direction of flow velocity corresponding to a positive α (or β) is also indicated in Figure 4.4.

For every element, the integration (4.27) leads to the equation

$$\sum_{j=1}^{4} M_j^{(k)} \varphi_j^{(k)} = 0, \qquad k = 1,2,3,4 \tag{4.41}$$

where

$$M_j^{(k)} = A_j^{(k)} - B_j^{(k)} + C_j^{(k)} + D_j^{(k)}$$

$$A_j^{(k)} = \frac{\Delta z_k}{2} \int_{-1}^{1}\int_{-1}^{1} \frac{\partial \phi_j(\xi,\eta)}{\partial \xi} \omega_k(\xi,\eta)\, d\xi\, d\eta,$$

$$B_j^{(k)} = w_g \frac{\Delta t}{4} \int_{-1}^{1}\int_{-1}^{1} \frac{\partial \phi_j(\xi,\eta)}{\partial \eta} \omega_k(\xi,\eta)\, d\xi\, d\eta,$$

$$C_j^{(k)} \quad = \quad \frac{\Delta t}{4}\int_{-1}^{1}\int_{-1}^{1} \nu(\eta)\frac{\partial \phi_j(\xi,\eta)}{\partial \eta}\frac{\partial \omega_k(\xi,\eta)}{\partial \eta}\, d\xi\, d\eta,$$

$$D_j^{(k)} \quad = \quad \sigma\frac{\Delta t \Delta z_k}{8}\int_{-1}^{1}\int_{-1}^{1} \phi_j(\xi,\eta)\omega_k(\xi,\eta)\, d\xi\, d\eta.$$

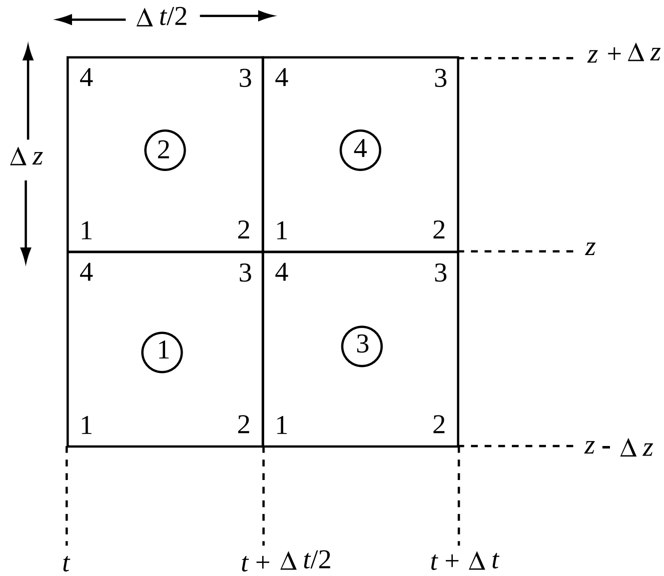


Figure 4.5: Group of 4 elements.

The totality of these finite element equations for the four elements is now represented in molecular form by Figure 4.6. If these elements are suitably chosen to be within the i th, $(i+\frac{1}{2})$ th and $(i+1)$ th time-levels and the $(j-1)$ th, j th and $(j+1)$ th horizontal space-lines, we can obtain from (4.27) the following relationship, which can be regarded as a grouped finite element equation centred at the point $(i+\frac{1}{2}, j)$

$$M_1^{(1)}\varphi_{i,j-1} + \left(M_2^{(1)} + M_1^{(3)}\right)\varphi_{i+1/2,j-1} + M_2^{(3)}\varphi_{i+1,j-1}$$

$$+\left(M_4^{(1)} + M_1^{(2)}\right)\varphi_{i,j} + \left(M_3^{(1)} + M_2^{(2)} + M_4^{(3)} + M_1^{(4)}\right)\varphi_{i+1/2,j} + \left(M_3^{(3)} + M_2^{(4)}\right)\varphi_{i+1,j}$$

$$+M_4^{(2)}\varphi_{i,j+1} + \left(M_3^{(2)} + M_4^{(4)}\right)\varphi_{i+1/2,j+1} + M_3^{(4)}\varphi_{i+1,j+1} = 0. \qquad (4.42)$$

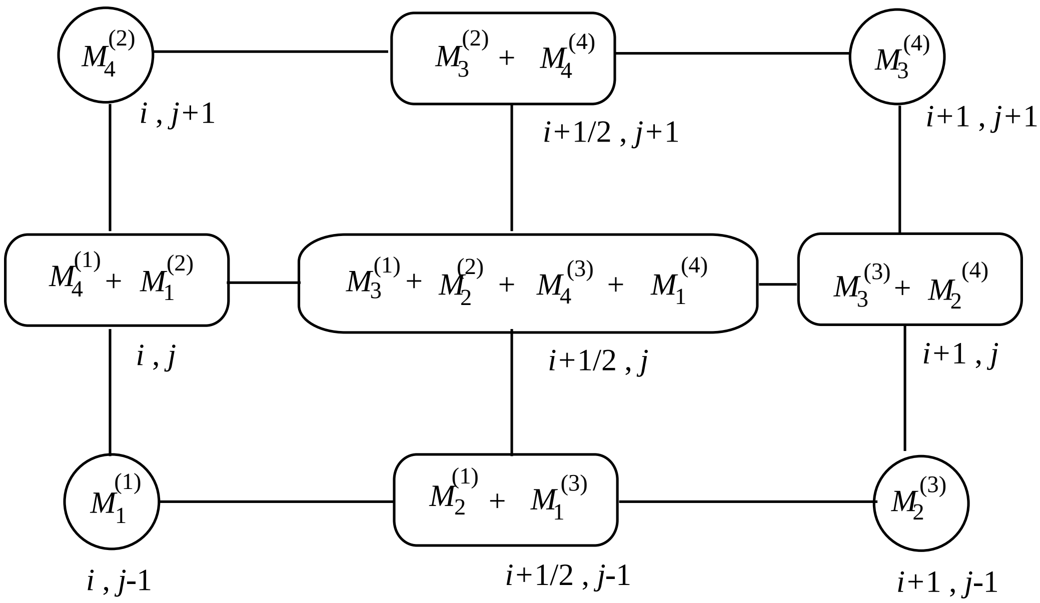


Figure 4.6: The group finite element equation.

The formula (4.42) will be meaningful if the component on the $(i+\frac{1}{2})$th line are weighted with factors θ and $(1-\theta)$ to the $(i+1)$th and ith time-levels, respectively, which will then produce the six-point formula (see, e.g. Evans, D. J. and Abdullah, A. R. (1986)), i.e.

$$\left(M_2^{(3)}+\theta\left(M_2^{(1)}+M_1^{(3)}\right)\right)\varphi_{i+1,j-1}+\left(\left(M_3^{(3)}+M_2^{(4)}\right)+\theta\left(M_3^{(1)}+M_2^{(2)}+M_4^{(3)}+M_1^{(4)}\right)\right)\varphi_{i+1,j}$$

$$+\left(M_3^{(4)}+\theta\left(M_3^{(2)}+M_4^{(4)}\right)\right)\varphi_{i+1,j+1}=-\left(M_1^{(1)}+(1-\theta)\left(M_2^{(1)}+M_1^{(3)}\right)\right)\varphi_{i,j-1}-\left(\left(M_4^{(1)}+M_1^{(2)}\right)\right.$$

$$\left.+(1-\theta)\left(M_3^{(1)}+M_2^{(2)}+M_4^{(3)}+M_1^{(4)}\right)\right)\varphi_{i,j}-\left(M_4^{(2)}+(1-\theta)\left(M_3^{(2)}+M_4^{(4)}\right)\right)\varphi_{i,j+1}. \quad (4.43)$$

Therefore, the six-point formula (4.43) which is obtained from the integration (4.27) in any four adjacent elements can be regarded as a finite element system for approximating the solution to equation (4.14). This system will lead to a tridiagonal system of equations which is easily solved by any of the standard algorithms for solving banded linear systems.

We can write (4.43) in the form

$$X\begin{bmatrix}\varphi_1^{t+\Delta t}\\ \varphi_2^{t+\Delta t}\\ \vdots\\ \varphi_n^{t+\Delta t}\end{bmatrix}=Y\begin{bmatrix}\varphi_1^{t}\\ \varphi_2^{t}\\ \vdots\\ \varphi_n^{t}\end{bmatrix}$$

where X is diagallydominant tridiagonal matrix, which guarantee the exist of X^{-1}, then

$$\begin{bmatrix}\varphi_1^{t+\Delta t}\\ \varphi_2^{t+\Delta t}\\ \vdots\\ \varphi_n^{t+\Delta t}\end{bmatrix}=X^{-1}Y\begin{bmatrix}\varphi_1^{t}\\ \varphi_2^{t}\\ \vdots\\ \varphi_n^{t}\end{bmatrix} \tag{4.44}$$

Now we will show how to create matrices X and Y. The concentration profile at the source, expressed as a δ-function in the boundary condition (4.3), is approximated numerically by a one-step function centered at the source and having the width Δz_s. Its amplitude is determined by requiring the same emission as in (4.3):

$$\varphi(0,z,t)=\begin{cases}0 & \text{for } 0\le z<h-\dfrac{\Delta z_s}{2},\\ \dfrac{1}{u_s\Delta z_s} & \text{for } h-\dfrac{\Delta z_s}{2}\le z\le h+\dfrac{\Delta z_s}{2},\\ 0 & \text{for } h+\dfrac{\Delta z_s}{2}<z\le 1,\end{cases} \tag{4.45}$$

where $u_s=u_k$ at the source.

The step function u_k approximating the give velocity profile $u(z)$ is obtained as follows :

The mean values of the velocity $\bar{u}_k$ are calculated over any two adjacent vertical half intervals from

$$\bar{u}_k = \frac{2}{\Delta z_{k-1} + \Delta z_k} \int_{z_k - \Delta z_{k-1}/2}^{z_k + \Delta z_k/2} u(z)\, dz. \tag{4.46}$$

Applying equation (4.16) to the $\bar{u}_k$ 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 relation (4.16). (see Runca, E. and Sardei, F. (1975))

In particular case, suppose that $n = 81$ so X and Y are 81×81. We have first row

$$X_{1,1} = -\frac{2\Delta z_1 + \Delta z_2}{\Delta z_1(\Delta z_1 + \Delta z_2)},$$

$$X_{1,2} = \frac{\Delta z_1 + \Delta z_2}{\Delta z_1 \Delta z_2},$$

$$X_{1,3} = -\frac{\Delta z_1}{\Delta z_2(\Delta z_1 + \Delta z_2)},$$

$$X_{1,j} = 0 \quad \text{for} \quad j = 4, 5, \ldots, 81,$$

and last row

$$X_{81,79} = \frac{\Delta z_{80}}{\Delta z_{70}\left(\Delta z_{80} + \Delta z_{79}\right)}$$

$$X_{81,80} = -\frac{\Delta z_{80} + \Delta z_{79}}{\Delta z_{80} \Delta z_{79}},$$

$$X_{81,81} = \frac{2\Delta z_{80} + \Delta z_{79}}{\Delta z_{80}\left(\Delta z_{80} + \Delta z_{79}\right)},$$

$$X_{81,j} = 0 \quad \text{for} \quad j = 1, 2, \ldots, 78.$$

For $j = 1,2,3,4$ and $k = 1,2,3,4$

$$M_j^{(k)} = A_j^{(k)} - B_j^{(k)} + C_j^{(k)} + D_j^{(k)}$$

$$A_j^{(k)} = \frac{\Delta z_k}{2}\int_{-1}^{1}\int_{-1}^{1}\frac{\partial \phi_j(\xi,\eta)}{\partial \xi}\omega_k(\xi,\eta)\,d\xi\,d\eta,$$

$$B_j^{(k)} = w_g\frac{\Delta t}{4}\int_{-1}^{1}\int_{-1}^{1}\frac{\partial \phi_j(\xi,\eta)}{\partial \eta}\omega_k(\xi,\eta)\,d\xi\,d\eta,$$

$$C_j^{(k)} = \frac{\Delta t}{4}\int_{-1}^{1}\int_{-1}^{1}\nu(\eta)\frac{\partial \phi_j(\xi,\eta)}{\partial \eta}\frac{\partial \omega_k(\xi,\eta)}{\partial \eta}\,d\xi\,d\eta,$$

$$D_j^{(k)} = \sigma\frac{\Delta t\Delta z_k}{8}\int_{-1}^{1}\int_{-1}^{1}\phi_j(\xi,\eta)\omega_k(\xi,\eta)\,d\xi\,d\eta.$$

The calculation of matrices X and Y at the point (i, j), $i = 1,2,3,$ $j = 1,2,3$ from the Figure 4.6, we let

$$XP(1,1) = M(1,1),$$

$$XP(1,2) = M(1,2) + M(3,1),$$

$$XP(1,3) = M(3,2),$$

$$XP(2,1) = M(1,4) + M(2,1),$$

$$XP(2,2) = M(1,3) + M(2,2) + M(3,4) + M(4,1),$$

$$XP(2,3) = M(3,3) + M(4,2),$$

$$XP(3,1) = M(2,4),$$

$$XP(3,2) = M(2,3) + M(4,4)$$

$$XP(3,3) = M(4,3),$$

$$\left.\begin{aligned} X_{k,k-1} &= XP(1,3) + \theta XP(1,2), \\ X_{k,k} &= XP(2,3) + \theta XP(2,2), \\ X_{k,k+1} &= XP(3,3) + \theta XP(3,2), \end{aligned}\right\} \text{ for } k = 2,3,\ldots,80,$$

$$\left.\begin{aligned} Y_{1,j} &= 0, \\ Y_{81,j} &= 0, \end{aligned}\right\} \text{ for } j = 1,2,3,\ldots,81,$$

$$\left.\begin{aligned} Y_{k,k-1} &= -\left[XP(1,1) + (1-\theta)XP(1,2)\right], \\ Y_{k,k} &= -\left[XP(2,1) + (1-\theta)XP(2,2)\right], \\ Y_{k,k+1} &= -\left[XP(3,1) + (1-\theta)XP(3,2),\right] \end{aligned}\right\} \text{ for } k = 2,3,\ldots,80.$$

4.4 Numerical results

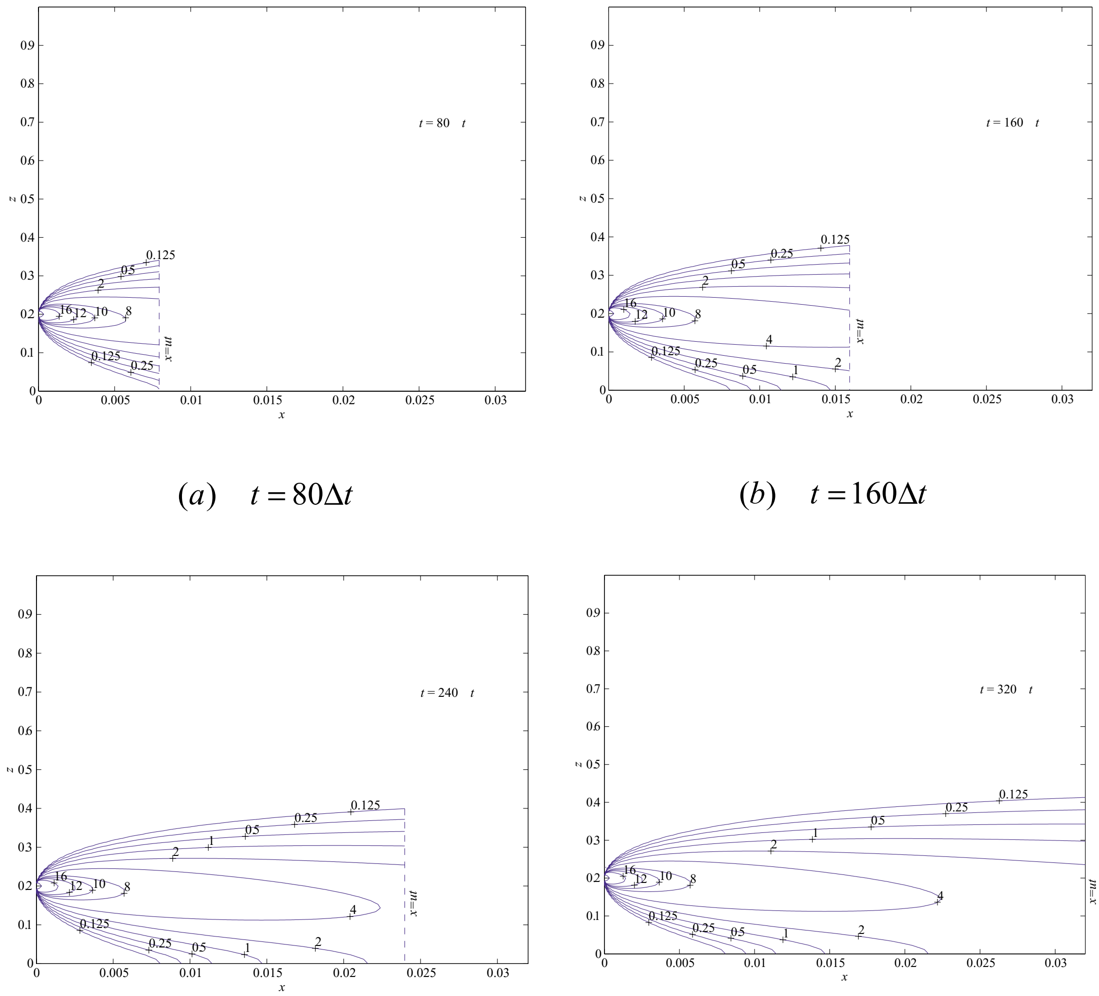
Typical examples of the time evolution of the described transport and diffusion process for constant and variable velocity profiles are shown in Figures 4.7 - 4.12. The plots represent, time sequences of the pollutant distribution in the XZ plane for $u(z) = 1$ and $u(z) = z^{0.5}$.

In the cases (Figures 4.7-4.9) the "clean" and the polluted regions are separated 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 XZ planes of Figures 4.10-4.12. On the other hand, if a variable velocity $u(z)$ is given (Figures 4.10-4.12), a time dependent concentration region exists behind the front $x = u_{\max}t$ as already mentioned in section 4.3. Comparing the picture in Figures 4.7-4.9 with the picture in Figures 4.10-4.12, we can immediately conclude that the wind shear is responsible (Figures 4.7-4.9) for a strong vertical diffusion of material into high regions above the source and (Figures 4.10-4.12) for a fast accumulation of material near the ground.

The parameters used in this study were : $n = 81, \Delta z_s = 0.009375, h = 0.2,$ $\theta = 0.125, \alpha_1 = 0.125, \alpha_2 = 1.0, \beta_1 = 0.125, \beta_2 = 0.0$.

In Figures 4.7-4.9 show time sequences of the contour lines of concentration at different the falling velocity of pollutants by gravity w_g, the transformation coefficient of pollutants σ with $u(z) = 1$, $t = 80\Delta t$, $t = 160\Delta t$, $t = 240\Delta t$, $t = 320\Delta t$, $\Delta t = 10^{-4}$ where $w_g = 0.0, \sigma = 0.0$, $w_g = 0.5, \sigma = 0.0$ and $w_g = 0.5, \sigma = 10.0$. The results are used to solve computer program 2 in appendix C.

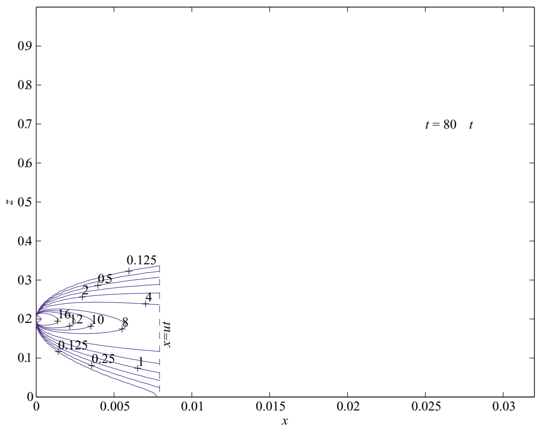
Figures 4.10-4.12 show time sequences of the contour lines of concentration at different the falling velocity of pollutants by gravity, the transformation coefficient of pollutants and distances x from the source with $u(z) = z^{0.5}$, $t = 80\Delta t$, $t = 160\Delta t$, $t = 240\Delta t$, $t = 320\Delta t$, $\Delta t = 10^{-4}$ where $w_g = 0.0, \sigma = 0.0$, $w_g = 0.5, \sigma = 0.0$ and $w_g = 0.5, \sigma = 10.0$. The results are used to solve computer program 3 in appendix C.



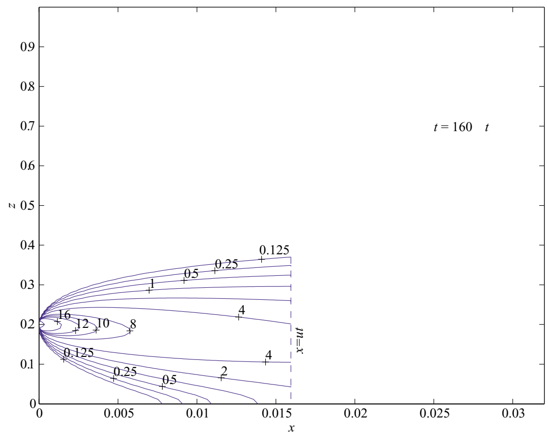
$(a)\quad t = 80\Delta t$ $(b)\quad t = 160\Delta t$

$(c)\quad t = 240\Delta t$ $(d)\quad t = 320\Delta t$

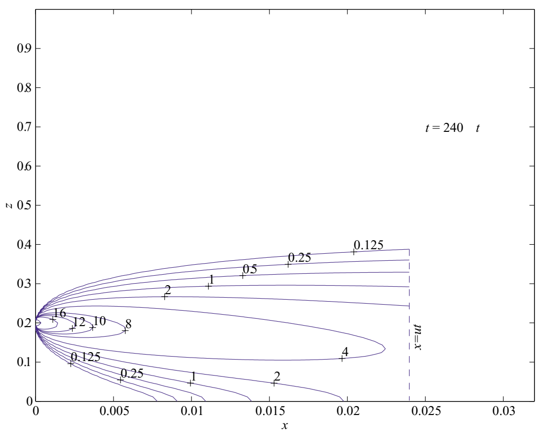
Figure 4.7: Time sequences of the contour line of concentration distribution in the XZ plane, calculated for $u(z) = 1, v(z) = z, \Delta t = 10^{-4}, w_g = 0.0$ and $\sigma = 0.0$.



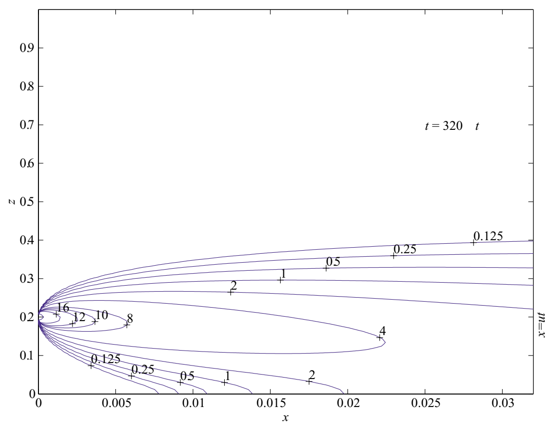
$(a)\quad t = 80\Delta t$



$(b)\quad t = 160\Delta t$

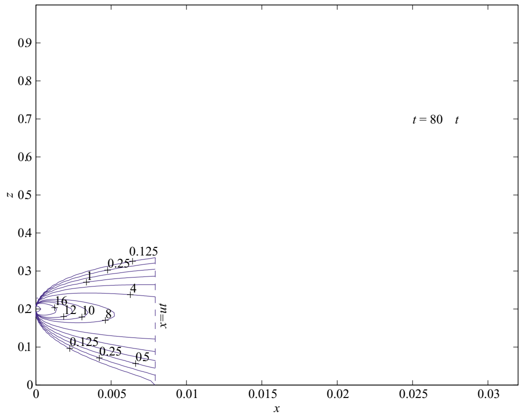


$(c)\quad t = 240\Delta t$

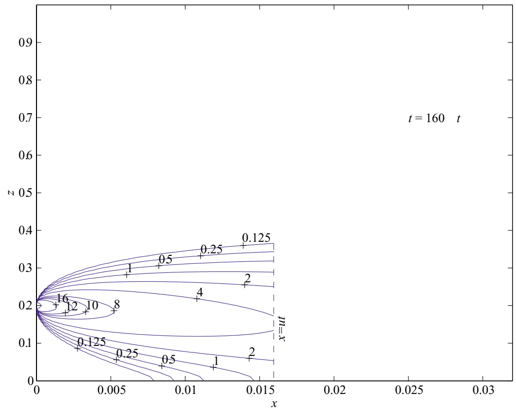


$(d)\quad t = 320\Delta t$

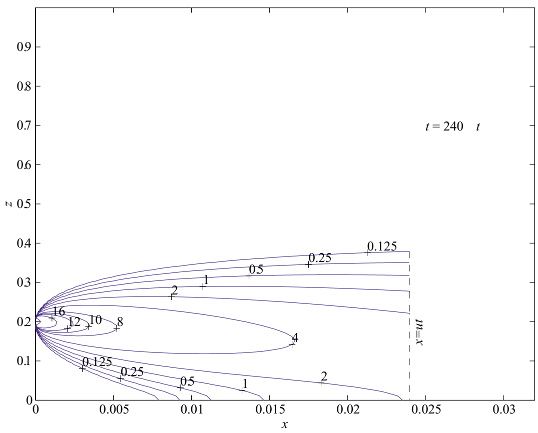
Figure 4.8: Time sequences of the contour line of concentration distribution in the XZ plane, calculated for $u(z)=1, v(z)=z, \Delta t = 10^{-4}, w_g = 0.5$ and $\sigma = 0.0$.



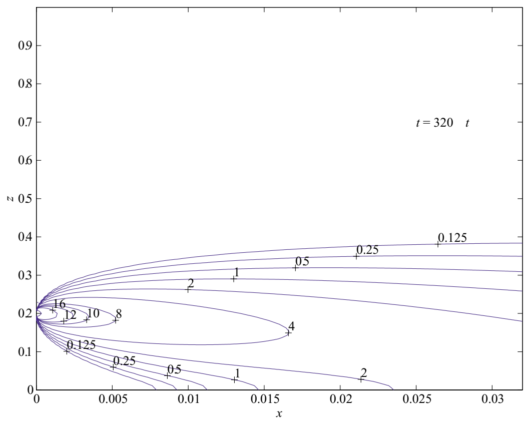
$(a)\quad t = 80\Delta t$



$(b)\quad t = 160\Delta t$



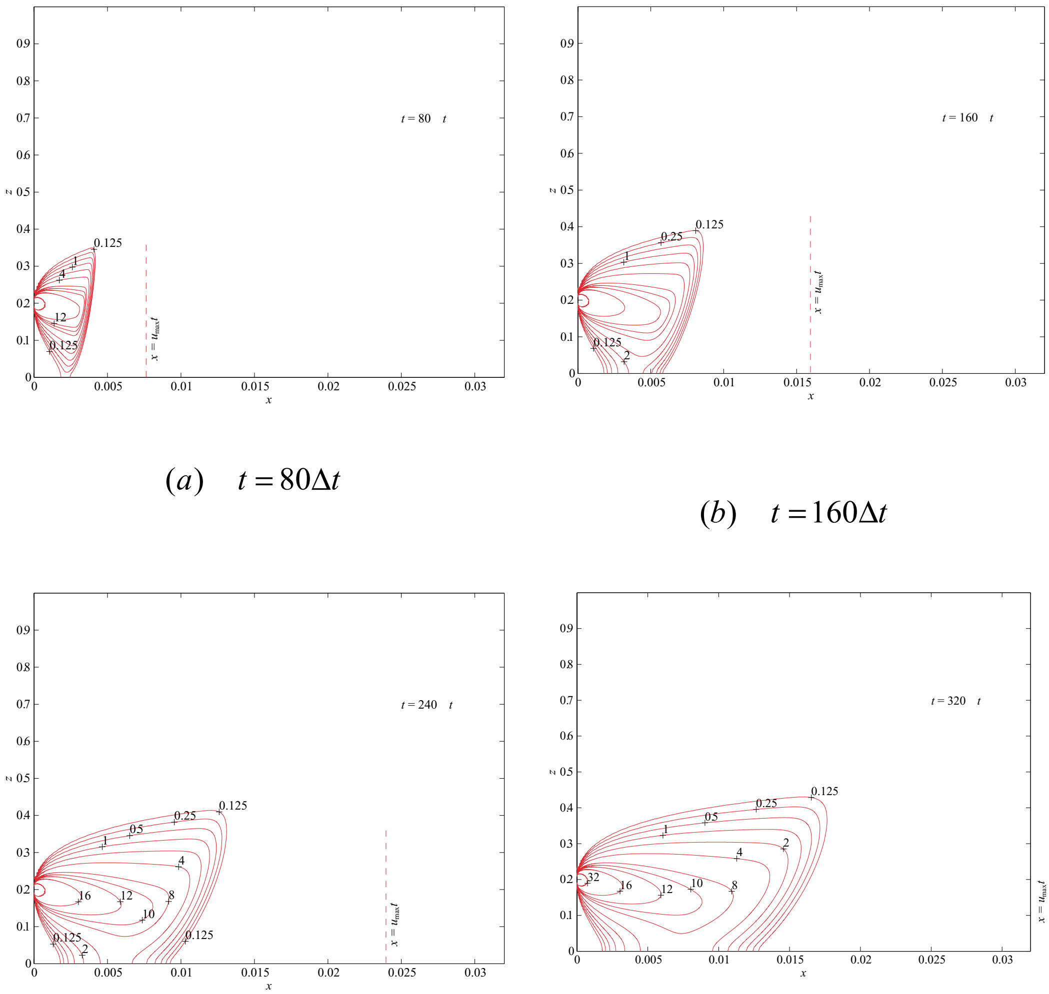
$(c)\quad t = 240\Delta t$



$(d)\quad t = 320\Delta t$

Figure 4.9: Time sequences of the contour line of concentration distribution in the XZ plane, calculated for $u(z)=1, v(z)=z, \Delta t=10^{-4}, w_g=0.5$ and $\sigma=10.0$

Figures 4.10-4.12 illustrate time sequences of the contour lines of concentration at different w_g and σ calculated for $u(z)=z^{0.5}$. In the computations, we take of $n=81$, $h=0.2$, $v(z)=z$, $\Delta z_s = 0.009375$, $\Delta t = 10^{-4}$, $\theta = 0.125$, $\alpha_2 = 1.0$, $\beta_1 = 0.125$ and $\beta_2 = 0.0$.



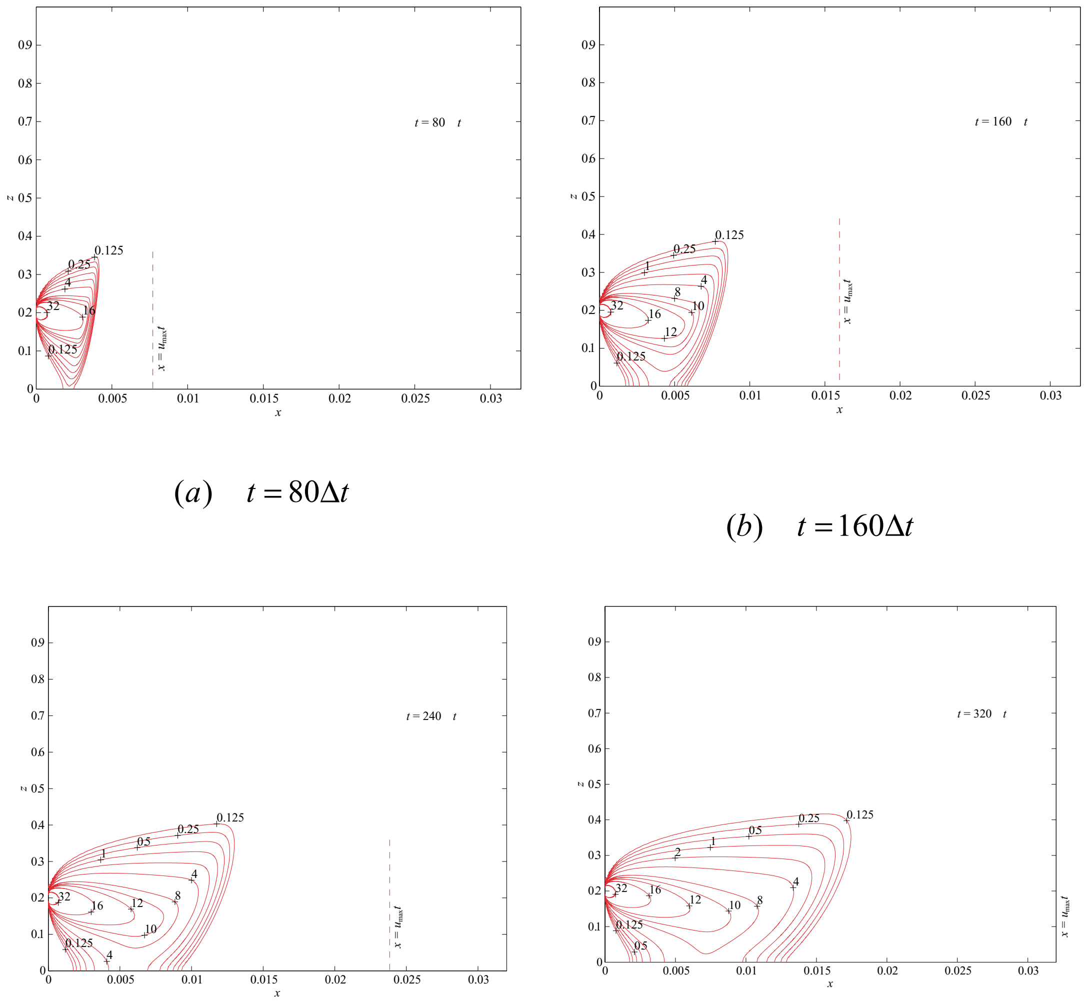
$(a) \quad t = 80\Delta t$

$(b) \quad t = 160\Delta t$

$(c) \quad t = 240\Delta t$

$(d) \quad t = 320\Delta t$

Figure 4.10: Time sequences of the contour line of concentration distribution in the XZ plane, calculated for $u(z) = z^{0.5}, v(z) = z, \Delta t = 10^{-4}, w_g = 0.0$ and $\sigma = 0.0$.



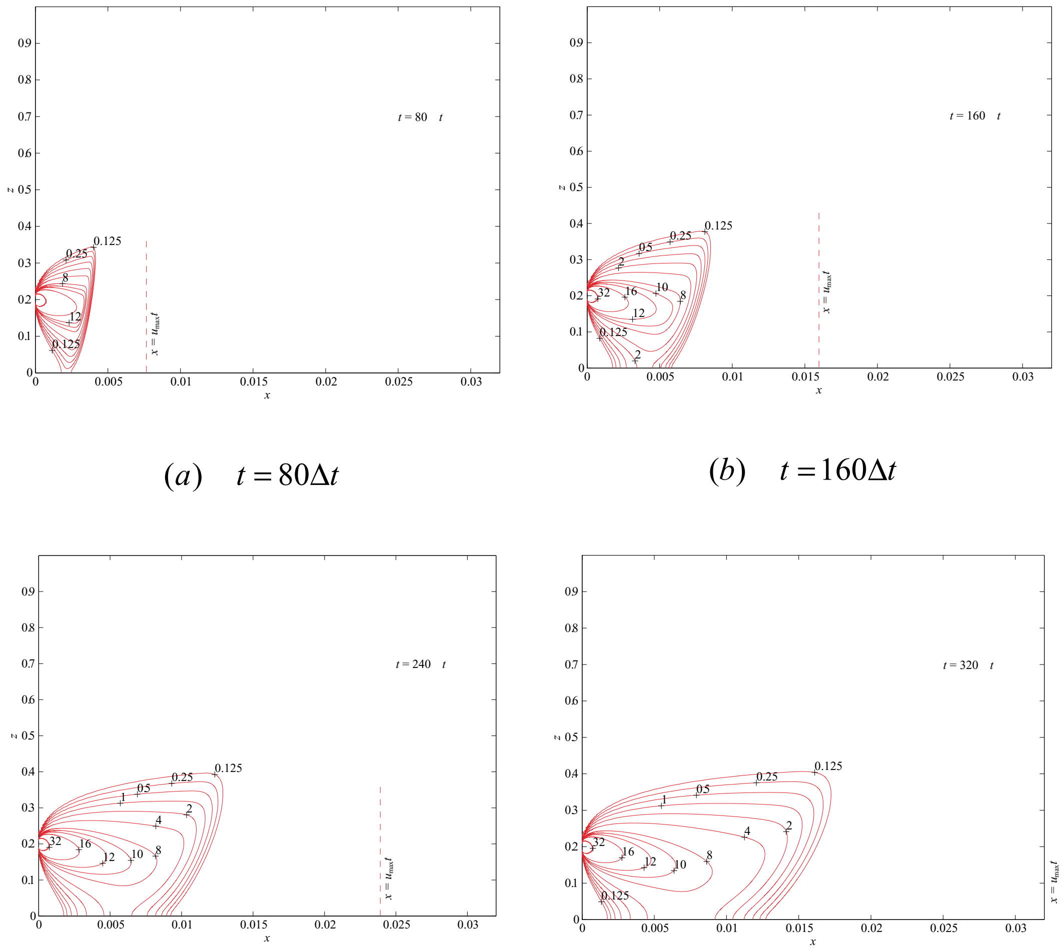
$(a)\quad t = 80\Delta t$

$(b)\quad t = 160\Delta t$

$(c)\quad t = 240\Delta t$

$(d)\quad t = 320\Delta t$

Figure 4.11: Time sequences of the contour line of concentration distribution in the XZ plane, calculated for $u(z) = z^{0.5}, v(z) = z, \Delta t = 10^{-4}, w_g = 0.5$ and $\sigma = 0.0$.



(a) $t = 80\Delta t$ (b) $t = 160\Delta t$

(c) $t = 240\Delta t$ (d) $t = 320\Delta t$

Figure 4.12: Time sequences of the contour line of concentration distribution in the XZ plane, calculated for $u(z) = z^{0.5}, \nu(z) = z, \Delta t = 10^{-4}, w_g = 0.5$ and $\sigma = 10.0$.

4.5 Comparison of the numerical results of the finite element method and of the fractional step method

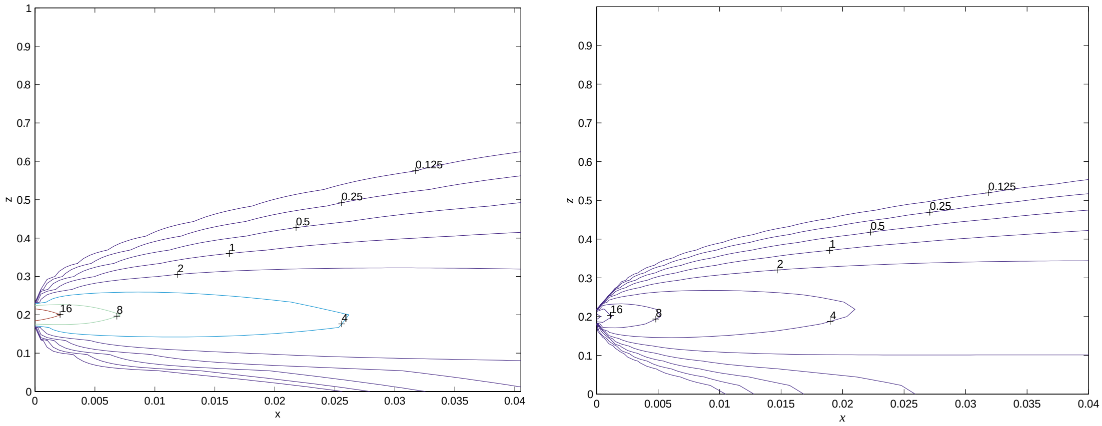
In this section, the numerical solution for the test problem using the finite element method (prescribed in the section 4.3) is presented. The numerical results are compared with the numerical result by the fractional step method (Areeraksakul, S. (2001)). The results are illustrated in Figure 4.13 and 4.14, with the parameter $n = 21$, $v(z) = z$, $\Delta z_s = 0.033$, $h = 0.2$ and $\theta = 0.125$.

In Figure 4.13, we use $u(z) = 1$ and compare between the numerical solution by the two method with $\Delta t = 0.0005$, $\alpha_1 = 0.125$, $\alpha_2 = 1.0$, $\beta_1 = 0.125$ and $\beta_2 = 0.2$ at $t = 80\Delta t$ and $t = 120\Delta t$.

The numerical results of the contour line of concentrations are plotted. They show no significant difference in the contour line of concentrations by both methods, for example at $x = 0.02$ and $t = 80\Delta t$, the $\max\left|C_f - C_{\bar{f}}\right| = 1.0858$,where C_f and $C_{\bar{f}}$ represent the concentrations by the finite element method and fractional step method respectively. While at $x = 0.025$ and $t = 120\Delta t$, the $\max\left|C_f - C_{\bar{f}}\right| = 0.9999$.

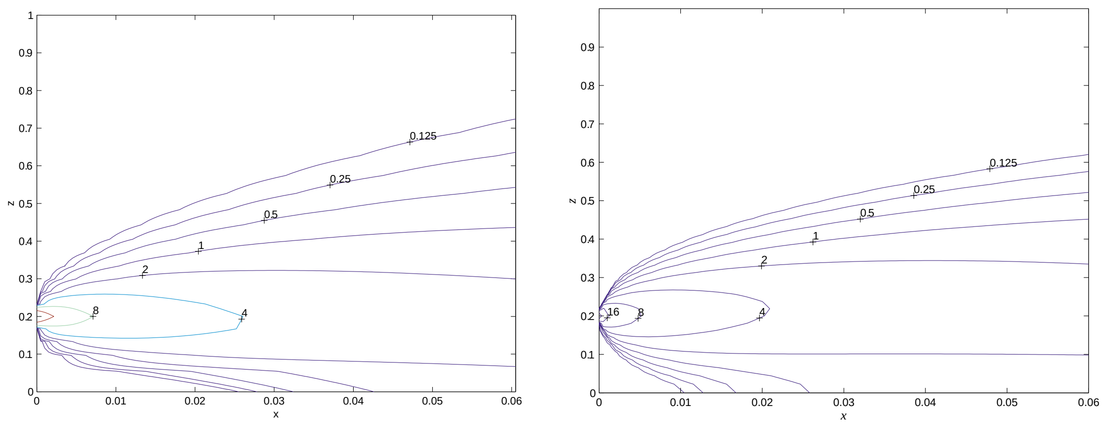
In Figure 4.14, we use $u(z) = z^{0.5}$ and compare between the numerical solution by the two method with $\Delta t = 0.0001$, $\alpha_1 = 0.125$, $\alpha_2 = 1.0$, $\beta_1 = 0.125$ and $\beta_2 = 0.2$ at $t = 80\Delta t$ and $t = 120\Delta t$.

The numerical results of the contour line of concentrations are plotted. They show no significant difference in the contour line of concentrations by both methods, for example at $x = 0.10$ and $t = 80\Delta t$, the $\max\left|C_f - C_{\bar{f}}\right| = 0.6812$, While at $x = 0.15$ and $t = 120\Delta t$, the $\max\left|C_f - C_{\bar{f}}\right| = 0.7114$.



(a) (b)

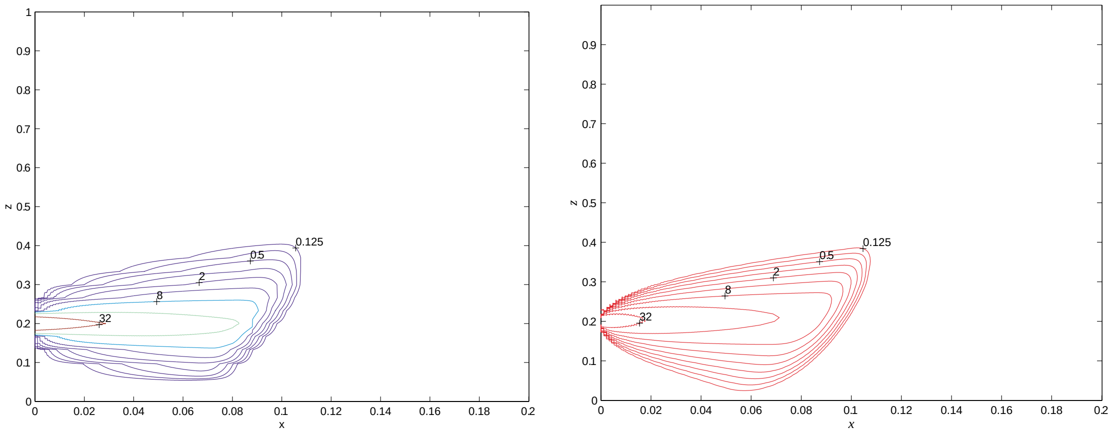
Figure 4.13: (i) $t = 80\Delta t$



(a) (b)

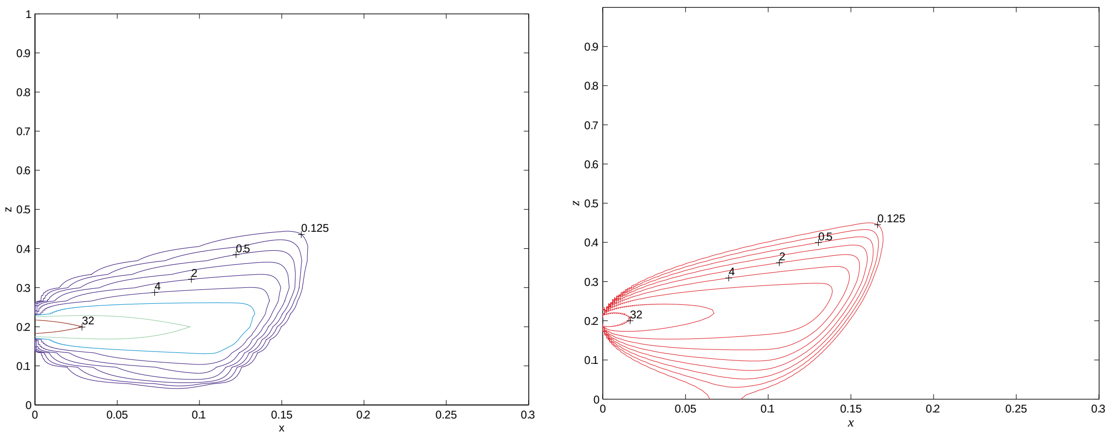
Figure 4.13: (ii) $t = 120\Delta t$

Figure 4.13: Comparison between the numerical solution by (a) using the fractional step method and (b) using the finite element method for $u(z) = 1, v(z) = z, h = 0.2, w_g = 0.0$ and $\sigma = 0.0$.



(*a*) (*b*)

Figure 4.14: (i) $t = 80\Delta t$



(*a*) (*b*)

Figure 4.14: (ii) $t = 120\Delta t$

Figure 4.14: Comparison between the numerical solution by (a) using the fractional step method and (b) using the finite element method for $u(z) = z^{0.5}, v(z) = z, h = 0.2, w_g = 0.0$ and $\sigma = 0.0$.

Chapter V

Conclusion

The mathematical model for air pollutant dynamics in the atmosphere, as it is known, the process of pollutant transport and diffusion in the atmosphere were solved by numerical method which is called Finite Element Methods. We performed the calculation into the steady state and the unsteady state cases. The goal of this research is to use the finite element methods to solve air pollution problems. The research are performed into four chapters as followings :

Chapter I consists of air pollution system, some review of literatures and survey of the articles.

Chapter II, are the standard definitions, notations from functional analysis and fundamental concepts of finite element method.

In Chapter III, the finite element method is used to solve the stationary problem. We assume that the wind direction coincides with the positive direction x-axis. The advection and diffusion coefficients are of the function of vertical direction z. The corresponding schemes are solved by using MathLab. The computational techniques in the numerical experiment enable the study to determine the realistic estimate of error constant and the order of convergence of numerical algorithms developed in this thesis. We have compared this solution with another analytical solution.

In Chapter IV, the finite element algorithms for approximate solution of unsteady state problem are proposed. The calculations are performed into two steps. The first step we find the auxiliary solution φ^* and find the true solution φ from second step, using the φ^* as an initial data. By this algorithms, we assumed that the pollutant move by transportation and then diffusion. The numerical schemes were performed and solved by MatLab. The concentration contour line obtained from the computer programs are reasonably agreed with the former results, using fractional step method in the reference.

The final remark of the research is that finite element methods are intended to be used as tools for studying flow phenomena and helping design of studying the model of an air pollutant in the complicated regions or domains.

Recommendations for further study are as follows:

1) Study the effect of varying the non-uniform z-mesh.
2) Solve using a space-time finite element method.
3) Try different approximations of the flux (Neumann) boundary conditions.
4) Determine the error caused by the approximation of $u(z)$ by step function.
5) Solve the similar 3 dimension problem using an appropriate coordinate system.

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Appendix

Appendix A

The Notation

Table A.1 : Notation Used in this Thesis

Symbol	**Brief description**	**Units in English**	**Units in SI**
φ	concentration	(*lbm* or *lbmol*)/*ft*^{3}	(*kg* or *mol*)/*m*^{3}
t	Time	s	s
u, v, w	components of the wind velocity	*ft/s*	*m/s*
w_g	The falling velocity of pollutants by gravity	*ft/s*	*m/s*
μ, ν	The diffusion coefficients	$ft^2 s^{-1}$	$m^2 s^{-1}$
σ	The transformation coefficient of pollutants	s^{-1}	s^{-1}
H	height of inversion layer	*ft*	*m*
h	height of source	*ft*	*m*
Q	emission rate	*lbm/s*	*kg/s*
x, y, z	coordinate directions or lengths	*ft*	*m*
f	The power of the source	(*lbm* or *lbmol*)/(*ft*^{3}.*s*)	(*kg* or *mol*)/(*m*^{3}.*s*)

Appendix B

Example of Computation of A_{ij}, B_{ij}

By equation (3.26), we have

$$P(i,j) = \frac{\Delta z_k}{2}\int_{-1}^{1} u(\eta)\phi_j(\eta)\omega_i(\eta)\,d\eta$$

$$Q(i,j) = -w_g\int_{-1}^{1}\frac{d\phi_j(\eta)}{d\eta}\omega_i(\eta)\,d\eta + \frac{2}{\Delta z_k}\int_{-1}^{1} v(\eta)\frac{d\phi_j(\eta)}{d\eta}\frac{d\omega_i(\eta)}{d\eta}\,d\eta$$

$$+\frac{\Delta z_k}{2}\sigma\int_{-1}^{1}\phi_j(\eta)\omega_i(\eta)\,d\eta$$

where $i = 1,2,\quad j = 1,2.$

Case $u(z) = 1, v(z) = z$, we have

$$P(1,1) = \frac{\Delta z_k}{2}\int_{-1}^{1} u(\eta)\phi_1(\eta)\omega_1(\eta)\,d\eta$$

$$= \frac{\Delta z_k}{16}\int_{-1}^{1}(1-\eta)\left[(1+\eta)(3\theta\eta-3\theta-2)+4\right]d\eta$$

$$Q(1,1) = -w_g\int_{-1}^{1}\frac{d\phi_1(\eta)}{d\eta}\omega_1(\eta)\,d\eta + \frac{2}{\Delta z_k}\int_{-1}^{1} v(\eta)\frac{d\phi_1(\eta)}{d\eta}\frac{d\omega_1(\eta)}{d\eta}\,d\eta$$

$$+\frac{\Delta z_k}{2}\sigma\int_{-1}^{1}\phi_1(\eta)\omega_1(\eta)\,d\eta$$

$$= \frac{w_g}{2}\int_{-1}^{1}\left[(1+\eta)(3\theta\eta-3\theta-2)+4\right]d\eta + \frac{1}{2}\int_{-1}^{1}(1+\eta)(3\theta\eta-1)\,d\eta$$

$$+\frac{\Delta z_k}{16}\sigma\int_{-1}^{1}(1-\eta)\left[(1+\eta)(3\theta\eta-3\theta-2)+4\right]d\eta$$

Case $u(z)=z^{0.5}, v(z)=z$, we have

$$P(1,1) = \left(\frac{\Delta z_k}{2}\right)^{3/2}\int_{-1}^{1}(1+\eta)^{1/2}\phi_1(\eta)\omega_1(\eta)\,d\eta$$

$$= \frac{1}{8}\left(\frac{\Delta z_k}{2}\right)^{3/2}\int_{-1}^{1}(1+\eta)^{1/2}(1-\eta)\left[(1+\eta)(3\theta\eta-3\theta-2)+4\right]d\eta$$

$$Q(1,1) = \frac{w_g}{2}\int_{-1}^{1}\left[(1+\eta)(3\theta\eta-3\theta-2)+4\right]d\eta+\frac{1}{2}\int_{-1}^{1}(1+\eta)(3\theta\eta-1)\,d\eta$$

$$+\frac{\Delta z_k}{16}\sigma\int_{-1}^{1}(1-\eta)\left[(1+\eta)(3\theta\eta-3\theta-2)+4\right]d\eta$$

so, we have

$$A_{k,k} = P(1,1)+A_{k-1,k-1}$$

$$A_{k,k+1} = P(1,2)$$

$$A_{k+1,k} = P(2,1)$$

$$A_{k+1,k+1} = P(2,2)$$

$$B_{k,k} = Q(1,1)+B_{k-1,k-1}$$

$$B_{k,k+1} = Q(1,2)$$

$$B_{k+1,k} = Q(2,1)$$

$$B_{k+1,k+1} = Q(2,2)$$

Appendix C

Computer Program

Computer programs use program MatLab version 6.1. Program 1 is MatLab program which can find numerical solutions of steady state problem with the finite element method, including graphs the contour lines concentration at different distances. Program 2 and 3 are MatLab programs which help you find numerical solution of unsteady state problem with constant wind velocity and function of z wind velocity respectively, including graphs of contour lines concentration at different times. Program 4 shows the graphs of analytic solution of steady state problem.

Program 1

```
%Program Finite Element Method of Steady State Problem of Air Pollution Problem.
%By Mr. Supot  Witayangkrun Department of Mathematics, Faculty of Science,
% Khon Kean University.
%u(z) = z^alpha  where 0 < alpha < 1
clear all
syms  eta
n=81
Delta_zs = ((1/(2*(n-1)))+(1/(n-1)))/2
```

```
alpha = 0.0
m=320  %number of step of length Delta_x
mm=320
varphi=zeros(n,mm)
Delta_x=10^(-3)
h=0.2
theta=0.125
wg=0.0
semga=0.0
%bisection follows
lo1=0
up1=100
tol=10^(-10)
while up1-lo1 > tol
  d=1:(n-1)/4
    d((n-1)/4)=Delta_zs
    tempsum=Delta_zs
    for k=1:(n-1)/4-1
      d((n-1)/4-k)=Delta_zs*exp(0.5*(lo1+up1)*(tempsum)^2)
      tempsum=tempsum+d((n-1)/4-k)
    end
    dd=sum(d)-0.2
    if sign(dd)==1
      up1=(up1+lo1)/2
```

```
        else
           lo1=(up1+lo1)/2
        end
end
A1=(up1+lo1)/2
downd=d
%upbisection dollows
lo2=0
up2=100
while up2-lo2 > tol
    d=1:3*(n-1)/4
    d(1)=Delta_zs
    tempsum = Delta_zs
    for k = 2:3*(n-1)/4
        d(k)=Delta_zs*exp(0.5*(lo2+up2)*(tempsum)^2)
        tempsum=tempsum+d(k)
    end
    dd=sum(d)-0.8
          if sign(dd)==1
           up2=(up2+lo2)/2
        else
           lo2=(up2+lo2)/2
        end
end
```

```
A2=(lo2+up2)/2
upd=d
%mesh subintervals Delta_z follow
Delta_z=1:(n-1)
for k=1:(n-1)/4
   Delta_z(k)=downd(k)
end
for k=(n-1)/4+1:n-1
   Delta_z(k)=upd(k-(n-1)/4)
end
%mesh points z follow
z=1:n
z(1)=0
z(n)=1
for k=2:n
   z(k)=z(k-1)+Delta_z(k-1)
end
for k=1:n
   if z(1,k)<= h-(Delta_zs/2)
      varphi(k,1)=0
   elseif z(1,k)<=h+(Delta_zs/2)
      varphi(k,1)=1/(z(k)^(alpha)*Delta_zs)
   else
      varphi(k,1)=0
```

```
    end
end
phi(1)=0.5*(1-eta)
phi(2)=0.5*(1+eta)
omega(1)=(1/4)*((1+eta)*(3*theta*eta-3*theta-2)+4)
omega(2)=(1/4)*(1+eta)*(-3*theta*eta+3*theta+2)
dphi_deta(1)=diff(phi(1),eta)
dphi_deta(2)=diff(phi(2),eta)
domega_deta(1)= diff(omega(1),eta)
domega_deta(2)= diff(omega(2),eta)
M=zeros(n,n)
A=zeros(n,n)
B=zeros(n,n)
D=zeros(n,n)
PP=zeros(2,2)
QQ=zeros(2,2)
RR=zeros(2,2)
SS=zeros(2,2)
for i=1:2
    for j=1:2
        PP(i,j)=int((eta+1)^(alpha)*phi(j)*omega(i),eta,-1,1);
        QQ(i,j)=-wg*int(dphi_deta(j)*omega(i),eta,-1,1);
        RR(i,j)=int((eta+1)*dphi_deta(j)*dphi_deta(i),eta,-1,1);
        SS(i,j)=semga*int(phi(j)*omega(i),eta,-1,1);
```

```
   end
end
M(1,1)= -((2*Delta_z(1)+Delta_z(2))/(Delta_z(1)*(Delta_z(1)+Delta_z(2))));
M(1,2)=(Delta_z(1)+Delta_z(2))/(Delta_z(1)*Delta_z(2));
M(1,3)= -(Delta_z(1))/(Delta_z(2)*(Delta_z(1)+Delta_z(2)));
M(n,n-2)=(Delta_z(n-1))/(Delta_z(n-2)*(Delta_z(n-1)+Delta_z(n-2)));
M(n,n-1)=-((Delta_z(n-1)+Delta_z(n-2))/(Delta_z(n-1)*Delta_z(n-2)));
M(n,n)=(2*Delta_z(n-1)+Delta_z(n-2))/(Delta_z(n-1)*(Delta_z(n-1)
          +Delta_z(n-2)));
for k=2:n-1
   p1(k)= (Delta_z(k)/2)^(1+alpha)*PP(1,1);
   p2(k)=(Delta_z(k)/2)^(1+alpha)*PP(1,2);
   p3(k)=(Delta_z(k)/2)^(1+alpha)*PP(2,1);
   p4(k)=(Delta_z(k)/2)^(1+alpha)*PP(2,1);
   q1(k)=QQ(1,1)+RR(1,1)+(Delta_z(k)/2)*SS(1,1);
   q2(k)=QQ(1,2)+RR(1,2)+(Delta_z(k)/2)*SS(1,2);
   q3(k)=QQ(2,1)+RR(2,1)+(Delta_z(k)/2)*SS(2,1);
   q4(k)=QQ(2,2)+RR(2,2)+(Delta_z(k)/2)*SS(2,2);
end for k=2:n-1
   M(k,k)=p1(k)+M(k,k);
   M(k,k+1)=p2(k);
   M(k+1,k)=p3(k);
   M(k+1,k+1)=p4(k);
   A(k,k)=q1(k)+A(k,k);
```

```
   A(k,k+1)=q2(k);
   A(k+1,k)=q3(k);
   A(k+1,k+1)=q4(k);
end
B=M.*(1/Delta_x)
D=A+B S=inv(D)*B
for k=2:m
   varphi(:,k)=S*varphi(:,k-1);
end
figure(1)
xx=linspace(0, mm*Delta_x, mm);
[X,Z]=meshgrid(xx,z);
cvals=[0.5, 1, 2, 4, 8, 10, 12, 16, 24, 32];
pl=contour(X,Z,varphi, cvals,'r-');
xlabel('x');
ylabel('z')
xlabel('x','FontName','Times','FontAngle','italic','FontSize',12);
ylabel('z','FontName','Times','FontAngle','italic','FontSize',12);
text(0.25,0.7,'x = 320\Delta x','FontName','Times','FontAngle',
    'italic','FontSize',12)
clabel(pl,'manual' )
```

Program 2

```
%Program Finite Element Method of time-Dependent of Air Pollution Problem.
%By Mr. Supot  Witayangkrun Department of Mathematics, Faculty of Science,
```

```
%Khon Kean University.
%u(z) = 1
clear all
n=81
Delta_zs = ((1/(2*(n-1)))+(1/(n-1)))/2
%bisection follows
lo1=0
up1=100
tol=10^(-10)
while up1-lo1 > tol
  d=1:(n-1)/4
    d((n-1)/4)=Delta_zs
    tempsum=Delta_zs
    for k=1:(n-1)/4-1
      d((n-1)/4-k)=Delta_zs*exp(0.5*(lo1+up1)*(tempsum)^2)
      tempsum=tempsum+d((n-1)/4-k)
    end
    dd=sum(d)-0.2
    if sign(dd)==1
      up1=(up1+lo1)/2
    else
      lo1=(up1+lo1)/2
    end
end
```

```
A1=(up1+lo1)/2
downd=d
%upbisection dollows
lo2=0
up2=100
while up2-lo2 > tol
   d=1:3*(n-1)/4
   d(1)=Delta_zs
   tempsum = Delta_zs
   for k = 2:3*(n-1)/4
      d(k)=Delta_zs*exp(0.5*(lo2+up2)*(tempsum)^2)
      tempsum=tempsum+d(k)
   end
   dd=sum(d)-0.8
        if sign(dd)==1
          up2=(up2+lo2)/2
      else
          lo2=(up2+lo2)/2
      end
end
A2=(lo2+up2)/2
upd=d
%mesh subintervals Delta_z follow
Delta_z=1:(n-1)
```

```
for k=1:(n-1)/4
   Delta_z(k)=downd(k)
end
for k=(n-1)/4+1:n-1
   Delta_z(k)=upd(k-(n-1)/4)
end
%mesh points z follow
z=1:n
z(1)=0
z(n)=1
for k=2:n
   z(k)=z(k-1)+Delta_z(k-1)
end
syms xi eta
m=320
mm =320 %number of time step of length Delta_t
Delta_t= 10^(-4)
h=0.2
uk=1
alpha1=0.125
alpha2=1.0
beta1=0.125
beta2=0.0
theta=0.125
```

```
wg=0.0
semga=0.0
varphi=zeros(n,m);
for k=1:n
   if z(1,k)<= h-(Delta_zs/2)
      varphi(k,1)=0
   elseif z(1,k)<=h+(Delta_zs/2)
      varphi(k,1)=1/(uk*Delta_zs)
   else
      varphi(k,1)=0
   end
end
phi(1)=0.25*(1-xi)*(1-eta)
phi(2)=0.25*(1+xi)*(1-eta)
phi(3)=0.25*(1+xi)*(1+eta)
phi(4)=0.25*(1-xi)*(1+eta)
omega(1)=(1/16)*((1+xi)*(3*alpha1*xi-3*alpha1-2)+4)*((1+eta)
       *(3*beta2*eta-3*beta2-2)+4)
omega(2)=(1/16)*((1+xi)*(-3*alpha1*xi+3*alpha1+2))*((1+eta)
       *(3*beta1*eta-3*beta1-2)+4)
omega(3)=(1/16)*((1+xi)*(-3*alpha2*xi+3*alpha2+2))*((1+eta)
       *(-3*beta1*eta+3*beta1+2))
omega(4)=(1/16)*((1+xi)*(3*alpha2*xi-3*alpha2-2)+4)*((1+eta)
       *(-3*beta2*eta+3*beta2+2))
```

```
dphi_dxi(1)=diff(phi(1),xi)
dphi_dxi(2)=diff(phi(2),xi)
dphi_dxi(3)=diff(phi(3),xi)
dphi_dxi(4)=diff(phi(4),xi)
dphi_deta(1)=diff(phi(1),eta)
dphi_deta(2)=diff(phi(2),eta)
dphi_deta(3)=diff(phi(3),eta)
dphi_deta(4)=diff(phi(4),eta)
domega_dxi(1)= diff(omega(1),xi)
domega_dxi(2)= diff(omega(2),xi)
domega_dxi(3)= diff(omega(3),xi)
domega_dxi(4)= diff(omega(4),xi)
domega_deta(1)= diff(omega(1),eta)
domega_deta(2)= diff(omega(2),eta)
domega_deta(3)= diff(omega(3),eta)
domega_deta(4)= diff(omega(4),eta)
M=zeros(n,n)
A=zeros(n,n)
B=zeros(n,n)
D=zeros(n,n)
M(1,1)=-((2*Delta_z(1)+Delta_z(2))/(Delta_z(1)*(Delta_z(1)
    + Delta_z(2))));
M(1,2)=(Delta_z(1)+Delta_z(2))/(Delta_z(1)*Delta_z(2));
M(1,3)=-(Delta_z(1))/(Delta_z(2)*(Delta_z(1)+Delta_z(2)));
```

```
M(n,n-2)=(Delta_z(n-1))/(Delta_z(n-2)*(Delta_z(n-1)+Delta_z(n-2)));
M(n,n-1)=-((Delta_z(n-2)+Delta_z(n-2))/(Delta_z(n-2)*Delta_z(n-1)));
M(n,n)=(2*Delta_z(n-1)+Delta_z(n-2))/(Delta_z(n-1)*(Delta_z(n-1)
    + Delta_z(n-2)));
P=zeros(4,4)
Q=zeros(4,4)
R=zeros(4,4)
S=zeros(4,4)
YP=zeros(3,3)
YQ=zeros(3,3)
YR=zeros(3,3)
YS=zeros(3,3)
for i=1:4
  for j=1:4
    P(i,j)=0.5*int(int(dphi_dxi(j)*omega(i),xi,-1,1),eta,-1,1)
    Q(i,j)=-wg*Delta_t*0.25*int(int(dphi_deta(j)*omega(i)
        ,xi,-1,1),eta,-1,1)
    R(i,j)=Delta_t*0.25*int(int((eta+1)*dphi_deta(j)*domega_deta(i)
        ,xi,-1,1),eta,-1,1)
    S(i,j)=semga*Delta_t*0.125*int(int(phi(j)*omega(i),xi,-1,1)
        ,eta,-1,1)
  end
end
YP(1,1)=P(1,1)
```

YP(1,2)=P(1,2)+P(3,1)

YP(1,3)=P(3,2)

YP(2,1)=P(1,4)+P(2,1)

YP(2,2)=P(1,3)+P(2,2)+P(3,4)+P(4,1)

YP(2,3)=P(3,3)+P(4,2)

YP(3,1)=P(2,4)

YP(3,2)=P(2,3)+P(4,4)

YP(3,3)=P(4,3)

YQ(1,1)=Q(1,1)

YQ(1,2)=Q(1,2)+Q(3,1)

YQ(1,3)=Q(3,2)

YQ(2,1)=Q(1,4)+Q(2,1)

YQ(2,2)=Q(1,3)+Q(2,2)+Q(3,4)+Q(4,1)

YQ(2,3)=Q(3,3)+Q(4,2)

YQ(3,1)=Q(2,4)

YQ(3,2)=Q(2,3)+Q(4,4)

YQ(3,3)=Q(4,3)

YR(1,1)=R(1,1)

YR(1,2)=R(1,2)+R(3,1)

YR(1,3)=R(3,2)

YR(2,1)=R(1,4)+R(2,1)

YR(2,2)=R(1,3)+R(2,2)+R(3,4)+R(4,1)

YR(2,3)=R(3,3)+R(4,2)

YR(3,1)=R(2,4)

```
YR(3,2)=R(2,3)+R(4,4)

YR(3,3)=R(4,3)

YS(1,1)=S(1,1)

YS(1,2)=S(1,2)+S(3,1)

YS(1,3)=S(3,2)

YS(2,1)=S(1,4)+S(2,1)

YS(2,2)=S(1,3)+S(2,2)+S(3,4)+S(4,1)

YS(2,3)=S(3,3)+S(4,2)

YS(3,1)=S(2,4)

YS(3,2)=S(2,3)+S(4,4)

YS(3,3)=S(4,3)

for k=2:n-1

   M(k,k-1)=Delta_z(k)*(YP(1,3)+theta*YP(1,2))+(YQ(1,3)+theta
          *YQ(1,2))+(1/Delta_z(k))*(YR(1,3)+theta*YR(1,2))
          + Delta_z(k-1)*(YS(1,3)+theta*YS(1,2));

   M(k,k)=Delta_z(k)*(YP(2,3)+theta*YP(2,2))+(YQ(2,3)+theta
         *YQ(2,2))+(1/Delta_z(k))*(YR(2,3)+theta*YR(2,2))
         + Delta_z(k)*(YS(2,3)+theta*YS(2,2));

   M(k,k+1)=Delta_z(k)*(YP(3,3)+theta*YP(3,2))+(YQ(3,3)+theta
          *YQ(3,2))+(1/Delta_z(k))*(YR(3,3)+theta*YR(3,2))
          + Delta_z(k)*(YS(3,3)+theta*YS(3,2));

   A(k,k-1)=-(Delta_z(k)*(YP(1,1)+(1-theta)*YP(1,2))+(YQ(1,1)
          +(1-theta)*YQ(1,2))+(1/Delta_z(k))*(YR(1,1)+(1-theta)
          *YR(1,2))+ Delta_z(k)*(YS(1,1)+(1-theta)*YS(1,2)));
```

```
    A(k,k)=-(Delta_z(k)*(YP(2,1)+(1-theta)*YP(2,2))+(YQ(2,1)
         +(1-theta)*YQ(2,2))+(1/Delta_z(k))*(YR(2,1)+(1-theta)
         *YR(2,2))+ Delta_z(k)*(YS(2,1)+(1-theta)*YS(2,2)));
    A(k,k+1)=-(Delta_z(k)*(YP(3,1)+(1-theta)*YP(3,2))+(YQ(3,1)
          +(1-theta)*YQ(3,2))+(1/Delta_z(k))*(YR(3,1)+(1-theta)
          *YR(3,2))+ Delta_z(k)*(YS(3,1)+(1-theta)*YS(3,2)));
end
S=inv(M)*A
for k=2:mm
    varphi(:,k)=S*varphi(:,k-1);
end
xx=linspace(0, m*10^(-4), m);
[X,Z]=meshgrid(xx,z);
cvals=[0.25,0.5, 1, 2, 4, 8, 10, 12, 16, 20, 24, 28, 32];
pl=contour(X,Z,varphi, cvals,'b-');
xlabel('x','FontName','Times','FontAngle','italic','FontSize',12);
ylabel('z','FontName','Times','FontAngle','italic','FontSize',12);
text(0.003,0.7,'t = 40\Delta t','FontName','Times','FontAngle','italic','FontSize',12)
clabel(pl,'manual' )
```

Program 3

```
%Program Finite Element Method of time-Dependent of Air Pollution Problem.
%By Mr. Supot  Witayangkrun Department of Mathematics,  Faculty of Science,
% Khon Kean University.
%u(z) = z^0.5
```

```
clear all
n=81
Delta_zs = ((1/(2*(n-1)))+(1/(n-1)))/2
%bisection follows
lo1=0
up1=100
tol=10^(-10)
while up1-lo1 > tol
  d=1:(n-1)/4
    d((n-1)/4)=Delta_zs
    tempsum=Delta_zs
    for k=1:(n-1)/4-1
      d((n-1)/4-k)=Delta_zs*exp(0.5*(lo1+up1)*(tempsum)^2)
      tempsum=tempsum+d((n-1)/4-k)
    end
    dd=sum(d)-0.2
    if sign(dd)==1
      up1=(up1+lo1)/2
    else
      lo1=(up1+lo1)/2
    end
end
A1=(up1+lo1)/2
downd=d
```

```
%upbisection dollows
lo2=0
up2=100
while up2-lo2 > tol
  d=1:3*(n-1)/4
  d(1)=Delta_zs
  tempsum = Delta_zs
  for k = 2:3*(n-1)/4
    d(k)=Delta_zs*exp(0.5*(lo2+up2)*(tempsum)^2)
    tempsum=tempsum+d(k)
  end
  dd=sum(d)-0.8
     if sign(dd)==1
      up2=(up2+lo2)/2
    else
      lo2=(up2+lo2)/2
    end
end
A2=(lo2+up2)/2
upd=d
%mesh subintervals Delta_z follow
Delta_z=1:(n-1)
for k=1:(n-1)/4
  Delta_z(k)=downd(k)
```

```
end
for k=(n-1)/4+1:n-1
   Delta_z(k)=upd(k-(n-1)/4)
end
%mesh points z follow
z=1:n
z(1)=0
z(n)=1
for k=2:n
   z(k)=z(k-1)+Delta_z(k-1)
end
syms xi eta
m=25
lo=320  %number of time step of length Delta_t
Delta_t=10^(-4)
h=0.2
alpha1=0.125
alpha2=1.0
beta1=0.125
beta2=0.0
theta=0.125
wg=0.0
semga=0.0
varphi=zeros(n,lo*m+1);
```

```
pkbar=zeros(1,n);
pkbar(1,1)=m*(2/Delta_z(1)*quad('z.^0.5',0,Delta_z(1)/2));
pkbar(1,n)=m*(2/Delta_z(n-1)*quad('z.^0.5',z(n)-(Delta_z(n-1)/2)
        ,z(n)));
for k=2:(n-1)
   pkbar(1,k)=m*(2/(Delta_z(k-1)+Delta_z(k))*quad('z.^0.5',z(1,k)
           -(Delta_z(k-1)/2),z(k)+(Delta_z(k)/2)));
end
pk=round(pkbar);
for k=1:n
   if z(1,k)<= h-(Delta_zs/2)
      varphi(k,1)=0
   elseif z(1,k)<=h+(Delta_zs/2)
      varphi(k,1)=1/(z(k)^(0.5)*Delta_zs)
   else
      varphi(k,1)=0
   end
end
phi(1)=0.25*(1-xi)*(1-eta)
phi(2)=0.25*(1+xi)*(1-eta)
phi(3)=0.25*(1+xi)*(1+eta)
phi(4)=0.25*(1-xi)*(1+eta)
omega(1)=(1/16)*((1+xi)*(3*alpha1*xi-3*alpha1-2)+4)*((1+eta)
       *(3*beta2*eta-3*beta2-2)+4)
```

```
omega(2)=(1/16)*((1+xi)*(-3*alpha1*xi+3*alpha1+2))*((1+eta)
        *(3*beta1*eta-3*beta1-2)+4)
omega(3)=(1/16)*((1+xi)*(-3*alpha2*xi+3*alpha2+2))*((1+eta)
        *(-3*beta1*eta+3*beta1+2))
omega(4)=(1/16)*((1+xi)*(3*alpha2*xi-3*alpha2-2)+4)*((1+eta)
        *(-3*beta2*eta+3*beta2+2))
dphi_dxi(1)=diff(phi(1),xi)
dphi_dxi(2)=diff(phi(2),xi)
dphi_dxi(3)=diff(phi(3),xi)
dphi_dxi(4)=diff(phi(4),xi)
dphi_deta(1)=diff(phi(1),eta)
dphi_deta(2)=diff(phi(2),eta)
dphi_deta(3)=diff(phi(3),eta)
dphi_deta(4)=diff(phi(4),eta)
domega_dxi(1)= diff(omega(1),xi)
domega_dxi(2)= diff(omega(2),xi)
domega_dxi(3)= diff(omega(3),xi)
domega_dxi(4)= diff(omega(4),xi)
domega_deta(1)= diff(omega(1),eta)
domega_deta(2)= diff(omega(2),eta)
domega_deta(3)= diff(omega(3),eta)
domega_deta(4)= diff(omega(4),eta)
M=zeros(n,n)
A=zeros(n,n)
```

```
B=zeros(n,n)
D=zeros(n,n)
M(1,1)=-((2*Delta_z(1)+Delta_z(2))/(Delta_z(1)*(Delta_z(1)
    + Delta_z(2))));
M(1,2)=(Delta_z(1)+Delta_z(2))/(Delta_z(1)*Delta_z(2));
M(1,3)=-(Delta_z(1))/(Delta_z(2)*(Delta_z(1)+Delta_z(2)));
M(n,n-2)=(Delta_z(n-1))/(Delta_z(n-2)*(Delta_z(n-1)+Delta_z(n-2)));
M(n,n-1)=-((Delta_z(n-2)+Delta_z(n-2))/(Delta_z(n-2)*Delta_z(n-1)));
M(n,n)=(2*Delta_z(n-1)+Delta_z(n-2))/(Delta_z(n-1)*(Delta_z(n-1)
    + Delta_z(n-2)));
P=zeros(4,4)
Q=zeros(4,4)
R=zeros(4,4)
S=zeros(4,4)
YP=zeros(3,3)
YQ=zeros(3,3)
YR=zeros(3,3)
YS=zeros(3,3)
for i=1:4
  for j=1:4
    P(i,j)=0.5*int(int(dphi_dxi(j)*omega(i),xi,-1,1),eta,-1,1)
    Q(i,j)=-wg*Delta_t*0.25*int(int(dphi_deta(j)*omega(i)
        ,xi,-1,1),eta,-1,1)
    R(i,j)=Delta_t*0.25*int(int((eta+1)*dphi_deta(j)*domega_deta(i)
```

```
            ,xi,-1,1),eta,-1,1)
        S(i,j)=semga*Delta_t*0.125*int(int(phi(j)*omega(i) ,xi,-1,1),eta,-1,1)
    end
end
YP(1,1)=P(1,1)
YP(1,2)=P(1,2)+P(3,1)
YP(1,3)=P(3,2)
YP(2,1)=P(1,4)+P(2,1)
YP(2,2)=P(1,3)+P(2,2)+P(3,4)+P(4,1)
YP(2,3)=P(3,3)+P(4,2)
YP(3,1)=P(2,4)
YP(3,2)=P(2,3)+P(4,4)
YP(3,3)=P(4,3)
YQ(1,1)=Q(1,1)
YQ(1,2)=Q(1,2)+Q(3,1)
YQ(1,3)=Q(3,2)
YQ(2,1)=Q(1,4)+Q(2,1)
YQ(2,2)=Q(1,3)+Q(2,2)+Q(3,4)+Q(4,1)
YQ(2,3)=Q(3,3)+Q(4,2)
YQ(3,1)=Q(2,4)
YQ(3,2)=Q(2,3)+Q(4,4)
YQ(3,3)=Q(4,3)
YR(1,1)=R(1,1)
YR(1,2)=R(1,2)+R(3,1)
```

```
YR(1,3)=R(3,2)
YR(2,1)=R(1,4)+R(2,1)
YR(2,2)=R(1,3)+R(2,2)+R(3,4)+R(4,1)
YR(2,3)=R(3,3)+R(4,2)
YR(3,1)=R(2,4)
YR(3,2)=R(2,3)+R(4,4)
YR(3,3)=R(4,3)
YS(1,1)=S(1,1)
YS(1,2)=S(1,2)+S(3,1)
YS(1,3)=S(3,2)
YS(2,1)=S(1,4)+S(2,1)
YS(2,2)=S(1,3)+S(2,2)+S(3,4)+S(4,1)
YS(2,3)=S(3,3)+S(4,2)
YS(3,1)=S(2,4)
YS(3,2)=S(2,3)+S(4,4)
YS(3,3)=S(4,3)
for k=2:n-1
  M(k,k-1)=Delta_z(k)*(YP(1,3)+theta*YP(1,2))+(YQ(1,3)+theta
         *YQ(1,2))+(1/Delta_z(k))*(YR(1,3)+theta*YR(1,2))
         + Delta_z(k-1)*(YS(1,3)+theta*YS(1,2));
  M(k,k)=Delta_z(k)*(YP(2,3)+theta*YP(2,2))+(YQ(2,3)+theta
       *YQ(2,2))+(1/Delta_z(k))*(YR(2,3)+theta*YR(2,2))
       + Delta_z(k)*(YS(2,3)+theta*YS(2,2));
  M(k,k+1)=Delta_z(k)*(YP(3,3)+theta*YP(3,2))+(YQ(3,3)+theta
```

```
          *YQ(3,2))+(1/Delta_z(k))*(YR(3,3)+theta*YR(3,2))
          + Delta_z(k)*(YS(3,3)+theta*YS(3,2));
   A(k,k-1)=-(Delta_z(k)*(YP(1,1)+(1-theta)*YP(1,2))+(YQ(1,1)
          +(1-theta)*YQ(1,2))+(1/Delta_z(k))*(YR(1,1)+(1-theta)
          *YR(1,2))+ Delta_z(k)*(YS(1,1)+(1-theta)*YS(1,2)));
   A(k,k)=-(Delta_z(k)*(YP(2,1)+(1-theta)*YP(2,2))+(YQ(2,1)
        +(1-theta)*YQ(2,2))+(1/Delta_z(k))*(YR(2,1)+(1-theta)
        *YR(2,2))+ Delta_z(k)*(YS(2,1)+(1-theta)*YS(2,2)));
   A(k,k+1)=-(Delta_z(k)*(YP(3,1)+(1-theta)*YP(3,2))+(YQ(3,1)
          +(1-theta)*YQ(3,2))+(1/Delta_z(k))*(YR(3,1)+(1-theta)
          *YR(3,2))+ Delta_z(k)*(YS(3,1)+(1-theta)*YS(3,2)));
end
S=inv(M)*A
%Step 1
for k=2:n-1
   for i=1:pk(1,k)
      varphi(k,1+i)=varphi(k,1);
   end
end for k=2:m+1
   varphi(:,k)=S*varphi(:,k);
end
%Subsequent time steps
%Step 2
for r=2:lo
```

```
    for k=2:n-1
        for i=m*r+1:-1:pk(1,k)+1
            varphi(k,i)=varphi(k,i-pk(1,k));
        end
        for i=pk(1,k):-1:2
            varphi(k,i)=varphi(k,1);
        end
    end
    for i=2:r*m+1
        varphi(:,i)=S*varphi(:,i);
    end
end
xx=linspace(0, (320*m+1)*10^(-4)/m, 320*m+1);
[X,Z]=meshgrid(xx,z);
cvals=[0.0625,0.125,0.25,0.5,1, 2, 4, 8, 10, 12, 16, 20, 24, 28, 32];
pl=contour(X,Z,varphi, cvals,'r-');
xlabel('x','FontName','Times','FontAngle','italic','FontSize',12);
ylabel('z','FontName','Times','FontAngle','italic','FontSize',12);
text(0.6,0.7,'t = 320\Delta t','FontName','Times','FontAngle','italic','FontSize',12)
clabel(pl,'manual' )
```

Curriculum Vitae

Mr. Supot Witayangkurn. was born on 15 August 1956 in Lopburi, Thailand. He finished high school from Vinitusuksa School, Lopburi, in March 1974. He was a B.A.(Secondary Education) graduate, majoring in Mathematics-Physics, from Khon Kaen University, Khon Kaen in 1977. Then he started his teaching career at Kanlayanawat School from 1977-1990. Four years after he graduated his Master's Degree of Mathematics from Chiengmai University 1985, he decided to join members of the Mathematics Department'staff, Faculty of Science, Khon Kaen University. His present work involves lecturing in Mathematics for students in the Faculty of Science, Technology, Education and Engineering. In 1999, he has been granted a scholarship from Khon Kaen University to further his doctoral studies in Mathematics at Suranaree University of Technology.