

APPLYING QUASILINEARIZATION TECHNIQUE TO
AIR POLLUTION AND BIOENGINEERING SYSTEMS MODELING

by

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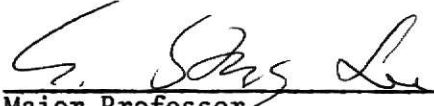
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CHAPTER 1

INTRODUCTION

Recently developed modeling and optimization techniques are used to study the modeling and control of environmental and bioengineering systems. One purpose of this work is to apply the quasilinearization technique to the air pollution modeling. By using quasilinearization technique, the parameters of the air pollution models can be estimated fairly easily. Two bioengineering modeling problems were also solved by the quasilinearization technique. It is found that the quasilinearization technique appears to be a fairly powerful tool for the modeling of these systems. Another purpose of this work is directed toward revising Tillman and Lee's dynamic decomposition model [16]. This model is used to represent an air pollution control system which is optimized by using linear programming. Experimental data from St. Louis were used. An optimal control scheme is obtained by solving the model.

Many investigations have done on pollutants mixing and distribution. Pollutant concentrations are a function of emission source and meteorological factors, such as source strength, stack height, wind speed, wind direction, turbulence and stability. In order to relate the pollutants concentration with source and meteorological factors, mathematical equations are used to represent diffusion model. Since the meteorological factors are very unstable and complex, a perfect diffusion model cannot be obtained due to computer limitation. Several models have been derived under different assumptions and simplifications. Most of the previous models

were developed only for one point source or some simple pattern of stack allocation. Practical configurations of emission sources are much more complex. Some of the complicating factors are topography, buildings, and other obstructions. So, the above mentioned simplified models cannot be applied easily to air pollution control. Recently, more complicated models have been derived. In general, there are two ways to approach this complicated modeling problem. One is the statistical approach and the other is physical approach.

Martin [3] proposed a diffusion model designed to permit calculation of seasonal average concentrations of air pollutants, in particular, Sulfur Dioxide. The calculations can encompass multiple sources and multiple receptors. For each receptor location, the model sums the effect of all sources over a wide range of meteorological conditions. Input data include source pollutant emissions, source configuration and location, receptor location, and meteorological data expressed as a joint frequency distribution of wind direction, wind speed, and stability. Thus, the long-term average concentration can be obtained.

Pooler [1] developed an empirical diffusion equation by using the wind direction and speed frequencies obtained by Nashville Weather Bureau Station. Clark [7] derived a simple diffusion model for calculating point concentration from multiple sources. Two kinds of pollutants, NO_x and SO_2 , were estimated. Bowe [2] presented a different approach to the modeling of large-scale atmosphere processes. The mathematical model formulated is fairly general.

Turner [9] proposed a working model for the diffusion of gases from

multiple sources in an urban area. A diffusion equation using area instead of point sources was established. 24-hr concentrations at 1-mile intervals were calculated for sulfur dioxide emissions. Wind velocity and stability were averaged by 2-hr periods. By averaging twelve 2-hr calculated concentrations, 24-hr concentrations were determined.

Miller and Holzworth [11] developed an atmospheric model for metropolitan areas. The main simplifying assumptions are that the continuous pollutant sources are uniformly distributed over the urban area and vertical diffusion occurs only when the effluent from each line source reaches the top of the mixing layer.

Koogler [10] proposed a mathematical model to describe the dispersion of atmospheric pollutants. The model was compiled in Fortran and can be used for both gaseous and particulates. The variant nature of meteorological parameters and emission rates are also considered.

The other approach is the use of a physical or theoretical model. The equations representing the flow, diffusion, and reaction of pollutants are very complicated. Furthermore, the parameters in the equations such as turbulent diffusivity, wind velocity, reaction rates, and even pollutant emission rates are changing constantly with time. Efficient computational techniques must be found to up-date these parameters. Recently, fairly efficient techniques for the up-dating of parameters have been developed by the use of quasilinearization, invariant imbedding, and the optimization techniques [12, 14, 20-23]. Seinfeld [12] proposed a method to estimate unknown parameters of a diffusion model. He assumed that a physical process can be represented by a system of nonlinear hyperbolic or parabolic partial differential equations of known form but containing unknown

parameters. The parameters may present in the equations themselves or in the boundary conditions. A steep decent algorithm is used to estimate these unknown parameters.

Singer [13] proposed a method to estimate atmospheric diffusion parameters based on the various combination of meteorological instruments that might be available. The technique is suitable only for obtaining rough estimates of downwind concentrations. It can be useful in assessing potential problem. The distances should be confined to 10-15 km. Lee [14] proposed two techniques, mainly quasilinearization and invariant imbedding, to up-date the parameters of the diffusion model.

Based on the diffusion model, various control techniques can be devised by using modern optimization methods. One of the frequently used control technique is mathematical programming. It employs available information on control costs, the behavior of air pollution, and the nature of air quality standards, so that these standards are implemented while pollution abatement costs are minimized. The abatement model minimizes control costs while ensuring that pollutant concentrations do not exceed air quality standards. Numerical solution procedures for an optimal pollution abatement model had appeared in the literature in various forms.

Kohn [15] used linear programming technique to solve a static model which selects the fuels to be used on a least cost basis. Shepard [6] developed a load shifting model for air pollution control in the electric power industry. The model involves transferring the generating load from one power plant to another according to meteorological conditions. This is a mathematical model incorporating an atmospheric dispersion model.

The optimization technique used is mixed-integer programming.

The control techniques discussed above, whether they are long term or short term, do not include the dynamic nature of the problem. To establish a model for online control, the dynamic aspect must be included and the time period must be stated in fraction of a day. Tillman and Lee [16] developed a dynamic decomposition model which is optimized by using linear programming. The time period they used is one hour. Since the basic linear programming algorithm can solve very large problems with a large number of inequality constraints, this approach of linearly decomposing the nonlinear dynamic system appears to be a very powerful tool for the optimization of air pollution distribution in a large metropolitan area. The pollutant concentrations are assumed constant within each region and within each time period in the model. The disadvantage of this model is that the total amount of pollutants removed during a specific time period are difficult to obtain.

CHAPTER 2

QUASILINEARIZATION

2.1 INTRODUCTION

The quasilinearization technique, also known as the generalized Newton-Raphson method, was developed by Bellman and Kalaba [4,5,8]. This technique has been applied to various chemical engineering problems by Lee [20-23, 26] for obtaining numerical solutions of two-point or multi-point nonlinear boundary-value problems. Lee and his co-workers have also applied this technique to various problems in the field of industrial management systems [18, 32], applied mechanics [27], and water resources research [28], etc. In this work, this technique will be applied to air pollution and Bioengineering problems.

Generally speaking, most engineering problems belong to nonlinear boundary-value problems whose numerical solutions are difficult to obtain. So, a method which can solve this kind of problem efficiently is desirable. As we know, there are no severe difficulties in solving linear boundary-value problems, so whenever a nonlinear boundary-value problem is encountered, there is a natural temptation to try to linearize the nonlinear problem. However, the approximate linearized equations are often unsatisfactory for many application purposes. By using quasilinearization technique, not only the original nonlinear equations can be linearized, but even more important, a sequence of functions which converges rapidly to the solution of the original nonlinear equations can be provided. For most practical problems, an initial approximation for the unknown function

can be obtained from engineering experience and intuition. With this initial approximation, the solution of the original equations can be obtained through a sequence of functions.

2.2 GENERALIZED NEWTON-RAPHSON FORMULA

To apply quasilinearization technique, consider the following general system of nonlinear differential equations:

$$\frac{dX_i}{dt} = f_i(X_1, X_2, \dots, X_M; t) \quad i = 1, 2, \dots, M \quad (2.1)$$

where X_i represents the dependent variables and t is the independent variable. In vector form, this system of equations can be written as

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t) \quad (2.2)$$

where $\mathbf{x}$ and $\mathbf{f}$ represent M -dimensional vectors with component $X_1, X_2, \dots, X_M$ and $f_1, f_2, \dots, f_M$, respectively. Eq. (2.2) can be linearized by the recurrence vector equations [8, 20-23],

$$\frac{d\mathbf{x}_{k+1}}{dt} = \mathbf{f}(\mathbf{x}_k, t) + \mathbf{J}(\mathbf{x}_k)(\mathbf{x}_{k+1} - \mathbf{x}_k) \quad (2.3)$$

where $\mathbf{x}_{k+1}$ and $\mathbf{x}_k$ represent M -dimensional vectors with components $X_{1,k+1}, X_{2,k+1}, \dots, X_{M,k+1}$ and $X_{1,k}, X_{2,k}, \dots, X_{M,k}$ respectively. The Jacobian matrix $\mathbf{J}(\mathbf{x}_k)$ is:

$$J(\underline{X}_k) = \begin{pmatrix} \frac{\partial f_1}{\partial X_{1,k}} & \frac{\partial f_1}{\partial X_{2,k}} & \cdots & \frac{\partial f_1}{\partial X_{M,k}} \\ \frac{\partial f_2}{\partial X_{1,k}} & \frac{\partial f_2}{\partial X_{2,k}} & \cdots & \frac{\partial f_2}{\partial X_{M,k}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_M}{\partial X_{1,k}} & \frac{\partial f_M}{\partial X_{2,k}} & \cdots & \frac{\partial f_M}{\partial X_{M,k}} \end{pmatrix} \quad (2.4)$$

Note that Eq. (2.3) is essentially the Taylor series expansion with the second and higher order terms neglected. $\underline{X}_k$ is assumed to be the known value and is obtained from previous calculations and $\underline{X}_{k+1}$ is the unknown value, Eq. (2.3) is always linear.

2.3. PRINCIPLE OF SUPERPOSITION

Generally speaking, it is difficult to solve a two-point or multipoint nonlinear boundary-value problem. However, if the performance equations are linear, the superposition principle can be used [20-21].

Assume that the boundary conditions for Eq. (4) are

$$X_{j,k+1}(t_f) = X_j^f, \quad j = 1, 2, \dots, M \quad (2.5a)$$

$$X_{L,k+1}(t_0) = X_L^0, \quad L = M+1, M+2, \dots, M \quad (2.5b)$$

Now, consider the system represented by Eqs. (2.3) and (2.5). In general, the system cannot be solved in closed form. However, since Eq. (2.3) is linear, the system can be solved numerically by the use of

superposition principle: and a well-known numerical integration technique such as the Runge-Kutta integration scheme [20, 31] for initial value problems can be used. It is known that for M simultaneous linear equations, their general solutions can be represented by one set of particular solutions and M sets of homogeneous solutions [20-21]. So, the general solutions of Eq. (2.3) are

$$\tilde{X}_{k+1}(t) = \tilde{X}_{p,k+1}(t) + \sum_{j=1}^M a_{j,k+1} \tilde{X}_{hj,k+1}(t) \quad (2.6)$$

$$t_0 \leq t \leq t_f$$

where $\tilde{X}_{p,k+1}(t)$ and $\tilde{X}_{hj,k+1}(t)$ are M -dimensional column vectors with components $X_{1p,k+1}(t)$, $X_{2p,k+1}(t)$, ..., $X_{Mp,k+1}(t)$ and $X_{1hj,k+1}(t)$, $X_{2hj,k+1}(t)$, ..., $X_{Mhj,k+1}(t)$, respectively. The $a_{j,k+1}$, $j = 1, 2, \dots, M$, represent the M scalar integration constants to be determined from the boundary conditions.

The one set of particular solutions and M sets of homogeneous solutions must be obtained numerically. However, since they can be any solutions of Eq. (2.3) as long as the homogeneous solutions are nontrivial and distinct, any set of initial conditions can be used to obtain the particular solutions; any M sets of initial conditions, as long as they are nontrivial and distinct, can be used to obtain the M sets of homogeneous solutions. Furthermore, if these $M+1$ sets of initial conditions are chosen in such a way that they satisfy the given initial conditions as given in Eq. (2.5b), only m sets of homogeneous solutions are needed with m integration constants, $a_{j,k+1}$, $j = 1, 2, \dots, m$. Thus, Eq. (2.6) can be reduced to

$$\tilde{x}_{k+1}(t) = \tilde{x}_{p,k+1}(t) + \sum_{j=1}^m a_{j,k+1} \tilde{x}_{hj,k+1}(t). \quad (2.7)$$

$$t_0 \leq t \leq t_f$$

In vector form, the set of algebraic equations (2.7) can be represented by

$$\tilde{x}_{k+1}(t) = \tilde{x}_{p,k+1}(t) + \tilde{x}_{h,k+1}(t) a_{k+1} \quad (2.8)$$

where a_{k+1} is the m -dimensional integration constant vector with components $a_{1,k+1}, a_{2,k+1}, \dots, a_{m,k+1}$. The symbol $\tilde{x}_{h,k+1}(t)$ represents the homogeneous solution matrix

$$\tilde{x}_{h,k+1}(t) = \begin{pmatrix} x_{1h1,k+1}(t) & x_{1h2,k+1}(t) & \dots & x_{1hm,k+1}(t) \\ x_{2h1,k+1}(t) & x_{2h2,k+1}(t) & \dots & x_{2hm,k+1}(t) \\ & & \vdots & \\ x_{mh1,k+1}(t) & x_{mh2,k+1}(t) & \dots & x_{mhm,k+1}(t) \end{pmatrix} \quad (2.9)$$

Once the particular and homogeneous solutions are obtained, the integration constants, a_{k+1} can be obtained from Eq. (2.8). Once a_{k+1} is known, the general solution $\tilde{x}_{k+1}(t)$ of Eq. (2.3) can be obtained. Once $\tilde{x}_{k+1}(t)$, $t_0 \leq t \leq t_f$, is obtained, an improved solution vector x_{k+2} can be obtained. The procedure is continued until the process converges and the desired accuracy is obtained.

CHAPTER 3

AIR POLLUTION MODELING AND
ESTIMATION BY QUASILINEARIZATION TECHNIQUE

3.1 INTRODUCTION

Brock and Hewson [17] proposed an analog computing technique to solve the diffusion equation for the case of a continuous point source. It is assumed that the source is located between an inversion layer and the ground. Furthermore, the wind speed and eddy diffusivity are assumed constant over the diffusing region. The factor of the presence of wind direction shear in the diffusing layers was also considered.

For the purpose of identifying the model, the parameters, wind direction shear, must be estimated first. Since this parameter is a function of height, it is desirable to estimate this parameter at different heights. The purpose of this chapter is to apply the quasilinearization technique to estimate the parameters at different heights.

3.2 AIR POLLUTION MODEL

Turbulent diffusion from an elevated point source is of primary concern in air pollution meteorology. But atmospheric diffusion is such an intricate mechanism that no one model can satisfy all demands. One model which is fairly general is the following parabolic diffusion equation [17].

$$\frac{dC}{dt} = \frac{\partial}{\partial x} [K_x \frac{\partial C}{\partial x}] + \frac{\partial}{\partial y} [K_y \frac{\partial C}{\partial y}] + \frac{\partial}{\partial z} [K_z \frac{\partial C}{\partial z}] \quad (3.1)$$

where

$$\frac{dC}{dt} = u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} + w \frac{\partial C}{\partial z} + \frac{\partial C}{\partial t}$$

and

C = average concentration

x, y, z = space coordinates

u, v, w = average wind components

K_1 = coefficient of eddy diffusivity in the i -direction

t = time

In this work, the problems are based on the case of diffusion in the steady state. A point source is located half-way between the surface of the ground and the base of an inversion. Wind speed and eddy diffusivity are constant over the diffusion region. The case of wind direction shear with height in the diffusion region is added to basic model. The model is arranged so that the origin is at the source, the x -axis oriented downwind, the y -axis crosswind, and the z -axis vertical. According to above assumptions, Eq. (3.1) can be simplified to [17]

$$u \frac{\partial C}{\partial x} = K \frac{\partial^2 C}{\partial y^2} + K \frac{\partial^2 C}{\partial z^2} - v \frac{\partial C}{\partial y} \quad (3.2)$$

It is convenient to state Eq. (3.2) in nondimensional form

$$\frac{\partial S}{\partial \bar{x}} = \frac{\partial^2 S}{\partial \bar{y}^2} + \frac{\partial^2 S}{\partial \bar{z}^2} - v \frac{\partial S}{\partial \bar{y}} \quad (3.3)$$

Where

$$S = C/C_0$$

$$Y = y/H$$

$$Z = z/H$$

$$\bar{x} = Kx/uH^2$$

$$V = Hv/K$$

By applying finite difference technique, we obtain [17]

$$\begin{aligned} \frac{\partial^2 S}{\partial Y^2} \Big|_m &= \frac{1}{\Delta Y(m)} \left(\frac{S(m+1) - S(m)}{\Delta Y(m + \frac{1}{2})} - \frac{S(m) - S(m-1)}{\Delta Y(m - \frac{1}{2})} \right) \\ \frac{\partial S}{\partial Y} \Big|_m &= \frac{S(m+1) - S(m-1)}{2\Delta Y(m)} \end{aligned} \quad (3.4)$$

$$\frac{\partial^2 S}{\partial Z^2} \Big|_n = \frac{S(n+1) - 2S(n) + S(n-1)}{\Delta Z^2}$$

Eq. (3.3) can now be reduced into a set of ordinary differential equations [17]

$$\begin{aligned} \frac{dS}{d\bar{x}} \Big|_{m,n} &= \frac{1}{\Delta Y(m)} \left(\frac{S(m+1,n) - S(m,n)}{\Delta Y(m + \frac{1}{2})} - \frac{S(m,n) - S(m-1,n)}{\Delta Y(m - \frac{1}{2})} \right) \\ &+ \frac{S(m,n+1) - 2S(m,n) + S(m,n-1)}{\Delta Z^2} \\ &- V_n \frac{S(m+1,n) - S(m-1,n)}{2\Delta Y(m)} \end{aligned} \quad (3.5)$$

where m and n are the grid sizes in Y and Z respectively.

The presence of wind direction shear in the diffusion layers causes

the plume cross section to be skewed. The amount of skewness can be determined by inserting terms in the diffusion equation for cross wind components. Eq. (3.5) contains the nondimensional parameter $V = Hv/k$ for these cross wind components. A 25-cell model [17] is used as shown in Figure 1. The source is in cell (0,3). Since the concentrations of cells (-2, 1), (-2, 2), (-2, 3), (-2, 4), (-2, 5), (+2, 1), (+2, 2), (+2, 3), (+2, 4), and (+2, 5) are assumed zero, there are only 15 active cells in the model. Eq. (3.5) may be written as [17]

$$\begin{aligned} \frac{dS}{dX} \Big|_{m,n} = & \frac{1}{25\Delta Y(m)} \left(\frac{S(m+1,n) - S(m,n)}{\Delta Y(m + \frac{1}{2})} - \frac{S(m,n) - S(m-1,n)}{\Delta Y(m - \frac{1}{2})} \right. \\ & - \frac{V_n}{50\Delta Y(m)} [S(m+1,n) - S(m-1,n)] \\ & \left. + [S(m,n+1) - 2S(m,n) + S(m,n-1)] \right] \end{aligned} \quad (3.6)$$

where

$X = 25 \bar{x}$ and boundary conditions are

$$S(-2, n) = 0$$

$$S(2, n) = 0$$

$$S(m, 0) = S(m, 1)$$

$$S(m, 5) = S(m, 6)$$

$$S(0, 3) \Big|_0 = 1$$

There are 15 cells with $m = 0, 1, 2$; $n = 1, 2, 3, 4, 5$. Let $S(m, n)$ represents the concentration of cell (m, n) , and also let

$$\begin{array}{lll}
S(0, 1) = x_1 & S(1, 1) = x_6 & S(-1, 1) = x_{11} \\
S(0, 2) = x_2 & S(1, 2) = x_7 & S(-1, 2) = x_{12} \\
S(0, 3) = x_3 & S(1, 3) = x_8 & S(-1, 3) = x_{13} \\
S(0, 4) = x_4 & S(1, 4) = x_9 & S(-1, 4) = x_{14} \\
S(0, 5) = x_5 & S(1, 5) = x_{10} & S(-1, 5) = x_{15}
\end{array}$$

According to Figure 1, we have

$$\begin{aligned}
\Delta Y(m) &= 0.2 \text{ EXP } [0.917m/(2-m)] \\
\Delta Y(0.5) &= 0.2 \text{ EXP } [0.917 \times 0.5/(2-0.5)] = 0.2714 \\
\Delta Y(1.5) &= 0.2 \text{ EXP } [0.917 \times 1.5/(2-1.5)] = 3.12
\end{aligned}$$

Let

$$\begin{aligned}
A &= 0.2 / \Delta Y(0.5) = 0.7369 \\
A_6 &= 0.08 / \Delta Y(0.5) = 0.2948 \\
B &= 0.08 / \Delta Y(1.5) = 0.0256
\end{aligned} \tag{3.6.1}$$

Substituting Eq. (3.6.1) into Eq. (3.6), we have

$$\begin{aligned}
\frac{dS(0,1)}{dX} &= \frac{dx_1}{dX} = \frac{1}{25\Delta Y(0)} \left(\frac{S(1,1) - S(0,1)}{\Delta Y(0,5)} - \frac{S(0,1) - S(-1,1)}{\Delta Y(-0.5)} \right) \\
&\quad - \frac{V_1}{50\Delta Y(0)} [S(1,1) - S(-1,1)] + [S(0,2) - 2S(0,1) + S(0,0)] \\
&= \frac{1}{25 \times 0.2} \left(\frac{x_6 - x_1}{0.2714} - \frac{x_1 - x_{11}}{0.2714} \right) \\
&\quad - \frac{V_1}{50 \times 0.2} [x_6 - x_{11}] + [x_2 - 2x_1 + x_1] \\
&= \frac{0.2}{0.2714} [x_6 - 2x_1 + x_{11}] - 0.1 V_1 [x_6 - x_{11}] \\
&\quad + [x_2 - x_1]
\end{aligned} \tag{3.7}$$

$$= (A - 0.1 V_1) x_6 - 2.4738 x_1 + (A + 0.1 V_1) x_{11} + x_2$$

The following equations can be obtained in the same way

$$\frac{dS(0,2)}{dX} = \frac{dx_2}{dX} = (A - 0.1 V_2) x_7 - 3.4738 x_2 + (A + 0.1 V_2) x_{12} + x_3 + x_1 \quad (3.8)$$

$$\frac{dS(0,3)}{dX} = \frac{dx_3}{dX} = (A - 0.1 V_3) x_8 - 3.4738 x_3 + (A + 0.1 V_3) x_{13} + x_4 + x_2 \quad (3.9)$$

$$\frac{dS(0,4)}{dX} = \frac{dx_4}{dX} = (A - 0.1 V_4) x_9 - 3.4738 x_4 + (A + 0.1 V_4) x_{14} + x_5 + x_3 \quad (3.10)$$

$$\frac{dS(0,5)}{dX} = \frac{dx_5}{dX} = (A - 0.1 V_5) x_{10} - 3.4738 x_5 + (A + 0.1 V_5) x_{15} + x_4 \quad (3.11)$$

$$\frac{dS(1,1)}{dX} = \frac{dx_6}{dX} = -1.3204 x_6 + (A_6 + 0.04 V_1) x_1 + x_7 \quad (3.12)$$

$$\frac{dS(1,2)}{dX} = \frac{dx_7}{dX} = -2.3204 x_7 + (A_6 + 0.04 V_2) x_2 + x_8 + x_6 \quad (3.13)$$

$$\frac{dS(1,3)}{dX} = \frac{dx_8}{dX} = -2.3204 x_8 + (A_6 + 0.04 V_3) x_3 + x_9 + x_7 \quad (3.14)$$

$$\frac{dS(1,4)}{dX} = \frac{dx_9}{dX} = -2.3204 x_9 + (A_6 + 0.04 V_4) x_4 + x_{10} + x_8 \quad (3.15)$$

$$\frac{dS(1,5)}{dX} = \frac{dx_{10}}{dX} = -1.3204 x_{10} + (A_6 + 0.04 V_5) x_5 + x_9 \quad (3.16)$$

$$\frac{dS(-1,1)}{dX} = \frac{dx_{11}}{dX} = (A_6 - 0.04 V_1) x_1 - 1.3204 x_{11} + x_{12} \quad (3.17)$$

$$\frac{dS(-1,2)}{dX} = \frac{dx_{12}}{dX} = (A6 - 0.04 V_2) x_2 - 2.3204 x_{12} + x_{13} + x_{11} \quad (3.18)$$

$$\frac{dS(-1,3)}{dX} = \frac{dx_{13}}{dX} = (A6 - 0.04 V_3) x_3 - 2.3204 x_{13} + x_{14} + x_{12} \quad (3.19)$$

$$\frac{dS(-1,4)}{dX} = \frac{dx_{14}}{dX} = (A6 - 0.04 V_4) x_4 - 2.3204 x_{14} + x_{15} + x_{13} \quad (3.20)$$

$$\frac{dS(-1,5)}{dX} = \frac{dx_{15}}{dX} = (A6 - 0.04 V_5) x_5 - 1.3204 x_{15} + x_{14} \quad (3.21)$$

The given initial conditions are:

$$\begin{array}{lll} x_1(0) = 0 & x_6(0) = 0 & x_{11}(0) = 0 \\ x_2(0) = 0 & x_7(0) = 0 & x_{12}(0) = 0 \\ x_3(0) = 1 & x_8(0) = 0 & x_{13}(0) = 0 \\ x_4(0) = 0 & x_9(0) = 0 & x_{14}(0) = 0 \\ x_5(0) = 0 & x_{10}(0) = 0 & x_{15}(0) = 0 \end{array} \quad (3.22)$$

3.3 PARAMETER ESTIMATION

The purpose of this section is to illustrate how the quasilinearization technique can be applied to the estimation problems in air pollution modeling. One example is solved to illustrate the technique.

3.3.1 The estimation problem

To illustrate this approach, a finite difference model proposed by Brock and Hewson [17], described in Eq. (3.6), will be considered.

In actual experimental situations, the wind direction shear constants (V_n) can not be measured directly. Only concentrations of different

regions $[S (m,n)]$ can be measured at various downwind distances (X) . The wind direction shear constants must be estimated from these experiment values. The estimation of these wind direction shear constants from the experimental data becomes very difficult when closed form solutions for the equations representing the process cannot be obtained. Furthermore, even if closed form solutions for the process model could be obtained, the present approach of directly estimating the parameters from the differential equations still has distinct advantages. The parameters (or wind direction shear constants) appear nonlinearly in the resulting analytical solutions of Eq. (3.6). The estimation of parameters from nonlinear algebraic equations is not easy. The quasilinearization technique appears to be much more powerful than the commonly used nonlinear regression or nonlinear least square estimation techniques.

The problem now can be stated as follows: Estimate the wind direction shear constants, V_n (where $n = 1, 2, 3, 4$, and 5), for Eq. (3.6) with the following measured or experimental data

$$\begin{aligned}
 x1^{(exp)}(X_s) &= x1_s, & s &= 1, 2, \dots, S \\
 x2^{(exp)}(X_\gamma) &= x2_\gamma, & \gamma &= 1, 2, \dots, R \\
 &\vdots & & \\
 x15^{(exp)}(X_q) &= x15_q, & q &= 1, 2, \dots, Q
 \end{aligned} \tag{3.23}$$

where

$$S + R + \dots + Q \geq 5$$

and

$$X_0 \leq X_s \leq X_f, X_0 \leq X_\gamma \leq X_f, \dots, X_0 \leq X_q \leq X_f$$

The quantities $x1_s, x2_\gamma, \dots, x15_q$ are known values and are obtained by measuring $x1, x2, \dots, x15$ at various value of X . The number of the experimental values must be greater than or equal to the number of the unknown constant parameters. The superscript, (exp), means that the values of $x1, x2, \dots, x15$ are experimental values.

3.3.2 Computational consideration

First, the case in which $S + R + \dots + Q = 5$ is considered. It is assumed that only the following five data points are available for estimating the wind direction shear parameters

$$\begin{aligned} x1^{(exp)}(X_1) &= x1_1; x2^{(exp)}(X_2) = x2_2, \\ x3^{(exp)}(X_1) &= x3_1; x4^{(exp)}(X_3) = x4_3; \\ x5^{(exp)}(X_4) &= x5_4 \end{aligned} \tag{3.24}$$

In here, we have assumed that the experimental errors resulting from the experimental data are very small and thus these experimental values can be regarded as the true values of $x1, x2, x3, x4$, and $x5$ at the given values of X . To consider the estimation of the wind direction shear constants, it is convenient to consider the unknown parameters $V1, V2, V3, V4$, and $V5$ as dependent variables parallel to $x1, x2, \dots$, and $x15$, and as functions of the independent variable X . Since V_1, V_2, V_3, V_4 , and V_5 do not change with downwind distance X , they can be written as:

$$\frac{dV_1}{dX} = 0 \tag{3.25}$$

$$\frac{dV_2}{dX} = 0 \quad (3.26)$$

$$\frac{dV_3}{dX} = 0 \quad (3.27)$$

$$\frac{dV_4}{dX} = 0 \quad (3.28)$$

$$\frac{dV_5}{dX} = 0 \quad (3.29)$$

Now, the system has twenty simultaneous differential equations, Eqs. (3.7) - (3.21) and (3.25) - (3.29). The twenty eqs. can be solved by using the boundary conditions given in Eq. (3.22) with $X_0 = 0$ and

$$\begin{aligned} x1(X_1) &= x1_1 \\ x2(X_2) &= x2_2 \\ x3(X_1) &= x3_1 \\ x4(X_3) &= x4_3 \\ x5(X_4) &= x5_4 \end{aligned} \quad (3.30)$$

where X_1 , X_2 , X_3 , and X_4 are four discrete values of X within the interval $0 \leq X \leq X_f$. Note that the experimental data are used as the boundary conditions. Since these boundary conditions are not all given at one point, the problem is therefore a multipoint boundary-value problem. And, since both the wind direction shear constants V_1 , V_2 , V_3 , V_4 , and V_5 , and the original variables $x1$, $x2$, ..., and $x15$ are considered as unknown functions, Eqs. (3.7) - (3.21) are nonlinear

equations. So, the system represented by Eqs. (3.7) - (3.21) and (3.25) - (3.29) is a multipoint nonlinear boundary-value problem.

3.3.3 The least squares approach

In practical situations, the experimental data are not exact. They have experimental or measurement errors. It is therefore desirable to obtain large amount of data instead of just five data points. For, $S + R + \dots + Q > 5$, the classical least squares criterion can be used. The object is to determine the constant parameters so that the sum of the squares of the deviations is minimized. Instead of using boundary conditions (3.30), one can obtain these five conditions by minimizing the following least square expression

$$Q = \sum_{s=1}^S [x1(X_s) - x1_s]^2 + \sum_{\gamma=1}^R [x2(X_\gamma) - x2_\gamma]^2 + \dots + \sum_{q=1}^Q [x15(X_q) - x15_q]^2 \quad (3.31)$$

where the minimizing is over the constant parameters, V_1, V_2, V_3, V_4 , and V_5 . The values of $x1(X_s), x2(X_\gamma), \dots, x15(X_q)$ are obtained by solving Eqs. (3.7) - (3.21).

3.3.4 Computational procedures

The estimation procedure for air pollution model can now be solved by quasilinearization technique. The Eqs. (3.7) - (3.21) and (3.25) - (3.29) can be linearized by using the generalized Newton-Raphson formula, Eq. (2.3), with $M = 20$. These linearized equations are

$$\begin{aligned}
\frac{dx1_{k+1}}{dX} = & -2.4738 \, x1_{k+1} + x2_{k+1} + (A - 0.1 \, v_{1,k}) \, x6_{k+1} \\
& + (A + 0.1 \, v_{1,k}) \, x11_{k+1} + (0.1x11_k - 0.1x6_k) \, v_{1,k+1} \quad (3.32) \\
& - (0.1 \, x11_k - 0.1 \, x6_k) \, v_{1,k}
\end{aligned}$$

$$\begin{aligned}
\frac{dx2_{k+1}}{dX} = & -3.4738 \, x2_{k+1} + x1_{k+1} + x3_{k+1} + (A - 0.1 \, v_{2,k}) \, x7_{k+1} \\
& + (A + 0.1 \, v_{2,k}) \, x12_{k+1} + (0.1 \, x12_k - 0.1x7_k) \, v_{2,k+1} \quad (3.33) \\
& - (0.1 \, x12_k - 0.1 \, x7_k) \, v_{2,k}
\end{aligned}$$

$$\begin{aligned}
\frac{dx3_{k+1}}{dX} = & -3.4738 \, x3_{k+1} + x2_{k+1} + x4_{k+1} + (A - 0.1 \, v_{3,k}) \, x8_{k+1} \\
& + (A + 0.1 \, v_{3,k}) \, x13_{k+1} + (0.1 \, x13_k - 0.1 \, x8_k) \, v_{3,k+1} \quad (3.34) \\
& - (0.1 \, x13_k - 0.1 \, x8_k) \, v_{3,k}
\end{aligned}$$

$$\begin{aligned}
\frac{dx4_{k+1}}{dX} = & -3.4738 \, x4_{k+1} + x3_{k+1} + x5_{k+1} + (A - 0.1 \, v_{4,k}) \, x9_{k+1} \\
& + (A + 0.1 \, v_{4,k}) \, x14_{k+1} + (0.1 \, x14_k - 0.1 \, x9_k) \, v_{4,k+1} \quad (3.35) \\
& - (0.1 \, x14_k - 0.1 \, x9_k) \, v_{4,k}
\end{aligned}$$

$$\begin{aligned}
\frac{dx5_{k+1}}{dX} = & -2.4738 \, x5_{k+1} + x4_{k+1} + (A - 0.1 \, v_{5,k}) \, x10_{k+1} \\
& + (A + 0.1 \, v_{5,k}) \, x15_{k+1} + (0.1 \, x15_k - 0.1 \, x10_k) \, v_{5,k+1} \quad (3.36) \\
& - (0.1 \, x15_k - 0.1 \, x10_k) \, v_{5,k}
\end{aligned}$$

$$\begin{aligned}\frac{dx6_{k+1}}{dX} &= (A6 + 0.04 v_{1,k}) x1_{k+1} - 1.3204 x6_{k+1} + x7_{k+1} \\ &+ (0.04 x1_k) v_{1,k+1} - (0.04 x1_k) v_{1,k}\end{aligned}\quad (3.37)$$

$$\begin{aligned}\frac{dx7_{k+1}}{dX} &= (A6 + 0.04 v_{2,k}) x2_{k+1} + x6_{k+1} - 2.3204 x7_{k+1} + x8_{k+1} \\ &+ (0.04 x2_k) v_{2,k+1} - (0.04 x2_k) v_{2,k}\end{aligned}\quad (3.38)$$

$$\begin{aligned}\frac{dx8_{k+1}}{dX} &= (A6 + 0.04 v_{3,k}) x3_{k+1} + x7_{k+1} - 2.3204 x8_{k+1} + x9_{k+1} \\ &+ (0.04 x3_k) v_{3,k+1} - (0.04 x3_k) v_{3,k}\end{aligned}\quad (3.39)$$

$$\begin{aligned}\frac{dx9_{k+1}}{dX} &= (A6 + 0.04 v_{4,k}) x4_{k+1} + x8_{k+1} - 2.3204 x9_{k+1} + x10_{k+1} \\ &+ (0.04 x4_k) v_{4,k+1} - (0.04 x4_k) v_{4,k}\end{aligned}\quad (3.40)$$

$$\begin{aligned}\frac{dx10_{k+1}}{dX} &= (A6 + 0.04 v_{5,k}) x5_{k+1} + x9_{k+1} - 1.3204 x10_{k+1} \\ &+ (0.04 x5_k) v_{5,k+1} - (0.04 x5_k) v_{5,k}\end{aligned}\quad (3.41)$$

$$\begin{aligned}\frac{dx11_{k+1}}{dX} &= (A6 - 0.04 v_{1,k}) x1_{k+1} - 1.3204 x11_{k+1} + x12_{k+1} \\ &- (0.04 x1_k) v_{1,k+1} + (0.04 x1_k) v_{1,k}\end{aligned}\quad (3.42)$$

$$\begin{aligned}\frac{dx12_{k+1}}{dX} &= (A6 - 0.04 v_{2,k}) x2_{k+1} - 2.3204 x12_{k+1} + x11_{k+1} + x13_{k+1} \\ &- (0.04 x2_k) v_{2,k+1} + (0.04 x2_k) v_{2,k}\end{aligned}\quad (3.43)$$

$$\begin{aligned} \frac{dx_{13,k+1}}{dX} &= (A6 - 0.04 v_{3,k}) x_{3,k+1} - 2.3204 x_{13,k+1} + x_{12,k+1} + x_{14,k+1} \\ &\quad - (0.04 x_{3,k}) v_{3,k+1} + (0.04 x_{3,k}) v_{3,k} \end{aligned} \quad (3.44)$$

$$\begin{aligned} \frac{dx_{14,k+1}}{dX} &= (A6 - 0.04 v_{4,k}) x_{4,k+1} - 2.3204 x_{14,k+1} + x_{13,k+1} + x_{15,k+1} \\ &\quad - (0.04 x_{4,k}) v_{4,k+1} + (0.04 x_{4,k}) v_{4,k} \end{aligned} \quad (3.45)$$

$$\begin{aligned} \frac{dx_{15,k+1}}{dX} &= (A6 - 0.04 v_{5,k}) x_{5,k+1} - 1.3204 x_{15,k+1} + x_{14,k+1} \\ &\quad - (0.04 x_{5,k}) v_{5,k+1} + (0.04 x_{5,k}) v_{5,k} \end{aligned} \quad (3.46)$$

$$\frac{dv_{1,k+1}}{dX} = 0 \quad (3.47)$$

$$\frac{dv_{2,k+1}}{dX} = 0 \quad (3.48)$$

$$\frac{dv_{3,k+1}}{dX} = 0 \quad (3.49)$$

$$\frac{dv_{4,k+1}}{dX} = 0 \quad (3.50)$$

$$\frac{dv_{5,k+1}}{dX} = 0 \quad (3.51)$$

The fifteen given boundary conditions are

$$x1_{k+1}(0) = x1^0 \quad (3.52)$$

$$x2_{k+1}(0) = x2^0 \quad (3.53)$$

$$x3_{k+1}(0) = x3^0 \quad (3.54)$$

$$x4_{k+1}(0) = x4^0 \quad (3.55)$$

$$x5_{k+1}(0) = x5^0 \quad (3.56)$$

$$x6_{k+1}(0) = x6^0 \quad (3.57)$$

$$x7_{k+1}(0) = x7^0 \quad (3.58)$$

$$x8_{k+1}(0) = x8^0 \quad (3.59)$$

$$x9_{k+1}(0) = x9^0 \quad (3.60)$$

$$x10_{k+1}(0) = x10^0 \quad (3.61)$$

$$x11_{k+1}(0) = x11^0 \quad (3.62)$$

$$x12_{k+1}(0) = x12^0 \quad (3.63)$$

$$x13_{k+1}(0) = x13^0 \quad (3.64)$$

$$x14_{k+1}(0) = x14^0 \quad (3.65)$$

$$x15_{k+1}(0) = x15^0 \quad (3.66)$$

The other five boundary conditions can be obtained either by solving Eq. (3.30) or by minimizing the least squares expression Eq. (3.31). Since almost all practical problem has experimental errors, the case of minimizing Eq. (3.31) used in this report.

Eqs. (3.32) - (3.51) are linear equations with variable coefficients. They cannot be solved in closed form. However, since they are linear, the principle of superposition can be used. The general solution vector equation for the system of equations, Eqs. (3.32) through (3.51), can be represented by

$$\tilde{x}_{k+1}(X) = \tilde{x}_{p,k+1}(X) + \tilde{x}_{h,k+1}(X) \quad (3.67)$$

where

$$0 \leq X \leq X_f.$$

The state vector $\tilde{x}_{k+1}(X)$ and the particular solution vector $\tilde{x}_{p,k+1}(X)$ are defined as

$$\tilde{x}_{k+1}(X) = \begin{pmatrix} x1_{k+1}(X) \\ x2_{k+1}(X) \\ \vdots \\ x15_{k+1}(X) \end{pmatrix} \quad (3.68)$$

and

$$\tilde{x}_{p,k+1}(X) = \begin{pmatrix} x1_{p,k+1}(X) \\ x2_{p,k+1}(X) \\ \vdots \\ x15_{p,k+1}(X) \end{pmatrix} \quad (3.69)$$

The integration constant vector is

$$\tilde{a}_{k+1} = \begin{pmatrix} a_{1,k+1} \\ a_{2,k+1} \\ a_{3,k+1} \\ a_{4,k+1} \\ a_{5,k+1} \end{pmatrix} \quad (3.70)$$

The homogeneous solution matrix is defined by

$$\tilde{x}_{h,k+1}(X) = \begin{pmatrix} x_{h1,k+1}^1(X) & x_{h2,k+1}^1(X) & \dots & x_{h5,k+1}^1(X) \\ x_{h1,k+1}^2(X) & x_{h2,k+1}^2(X) & \dots & x_{h5,k+1}^2(X) \\ \vdots & & & \vdots \\ x_{h1,k+1}^{15}(X) & x_{h2,k+1}^{15}(X) & \dots & x_{h5,k+1}^{15}(X) \end{pmatrix} \quad (3.71)$$

The particular and homogeneous solutions are chosen in such a way that they satisfy the fifteen given initial conditions in Eqs. (3.21) - (3.66). Thus, only five sets of homogeneous solutions and five integration constants are needed. In actual calculations, the set of particular solutions are obtained by integrating Eqs. (3.32) - (3.51) with the following initial values

$$\tilde{x}_{p,k+1}(0) = \begin{pmatrix} x_1^0 \\ x_2^0 \\ \vdots \\ x_{15}^0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (3.72)$$

The homogeneous forms of Eqs. (3.32) through (3.51) are

$$\begin{aligned} \frac{dx1_{k+1}}{dX} = & -2.4738 x1_{k+1} + x2_{k+1} + (A - 0.1 v_{1,k}) x6_{k+1} \\ & + (A + 0.1 v_{1,k}) x11_{k+1} + (0.1 x11_k - 0.1 x6_k) v_{1,k+1} \end{aligned} \quad (3.73)$$

$$\begin{aligned} \frac{dx2_{k+1}}{dX} = & -3.4738 x2_{k+1} + x1_{k+1} + x3_{k+1} + (A - 0.1 v_{2,k}) x7_{k+1} \\ & + (A + 0.1 v_{2,k}) x12_{k+1} + (0.1 x12_k - 0.1 x7_k) v_{2,k+1} \end{aligned} \quad (3.74)$$

$$\begin{aligned} \frac{dx3_{k+1}}{dX} = & -3.4738 x3_{k+1} + x2_{k+1} + x4_{k+1} + (A - 0.1 v_{3,k}) x8_{k+1} \\ & + (A + 0.1 v_{3,k}) x13_{k+1} + (0.1 x13_k - 0.1 x8_k) v_{3,k+1} \end{aligned} \quad (3.75)$$

$$\begin{aligned} \frac{dx4_{k+1}}{dX} = & -3.4738 x4_{k+1} + x3_{k+1} + x5_{k+1} + (A - 0.1 v_{4,k}) x9_{k+1} \\ & + (A + 0.1 v_{4,k}) x14_{k+1} + (0.1 x14_k - 0.1 x9_k) v_{4,k+1} \end{aligned} \quad (3.76)$$

$$\begin{aligned} \frac{dx5_{k+1}}{dX} = & -2.4738 x5_{k+1} + x4_{k+1} + (A - 0.1 v_{5,k}) x10_{k+1} \\ & + (A + 0.1 v_{5,k}) x15_{k+1} + (0.1 x15_k - 0.1 x10_k) v_{5,k+1} \end{aligned} \quad (3.77)$$

$$\begin{aligned} \frac{dx6_{k+1}}{dX} = & (A6 + 0.04 v_{1,k}) x1_{k+1} - 1.3204 x5_{k+1} + x7_{k+1} + (0.04 x1_k) v_{1,k+1} \end{aligned} \quad (3.78)$$

$$\begin{aligned}\frac{dx7_{k+1}}{dX} &= (A6 + 0.04 v_{2,k}) x2_{k+1} + x6_{k+1} - 2.3204 x7_{k+1} + x8_{k+1} \\ &+ (0.04 x2_k) v_{2,k+1}\end{aligned}\quad (3.79)$$

$$\begin{aligned}\frac{dx8_{k+1}}{dX} &= (A6 + 0.04 v_{3,k}) x3_{k+1} + x7_{k+1} - 2.3204 x8_{k+1} + x9_{k+1} \\ &+ (0.04 x3_k) v_{3,k+1}\end{aligned}\quad (3.80)$$

$$\begin{aligned}\frac{dx9_{k+1}}{dX} &= (A6 + 0.04 v_{4,k}) x4_{k+1} + x8_{k+1} - 2.3204 x9_{k+1} + x10_{k+1} \\ &+ (0.04 x4_k) v_{4,k+1}\end{aligned}\quad (3.81)$$

$$\begin{aligned}\frac{dx10_{k+1}}{dX} &= (A6 + 0.04 v_{5,k}) x5_{k+1} + x9_{k+1} - 1.3204 x10_{k+1} \\ &+ (0.04 x5_k) v_{5,k+1}\end{aligned}\quad (3.82)$$

$$\begin{aligned}\frac{dx11_{k+1}}{dX} &= (A6 - 0.04 v_{1,k}) x1_{k+1} - 1.3204 x11_{k+1} + x12_{k+1} \\ &- (0.04 x1_k) v_{1,k+1}\end{aligned}\quad (3.83)$$

$$\begin{aligned}\frac{dx12_{k+1}}{dX} &= (A6 - 0.04 v_{2,k}) x2_{k+1} - 2.3204 x12_{k+1} + x11_{k+1} + x13_{k+1} \\ &- (0.04 x2_k) v_{2,k+1}\end{aligned}\quad (3.84)$$

$$\begin{aligned} \frac{dx_{13,k+1}}{dX} &= (A6 - 0.04 V_{3,k}) x_{3,k+1} - 2.3204 x_{13,k+1} + x_{12,k+1} + x_{14,k+1} \\ &\quad - (0.04 x_{3,k}) V_{3,k+1} \end{aligned} \quad (3.85)$$

$$\begin{aligned} \frac{dx_{14,k+1}}{dX} &= (A6 - 0.04 V_{4,k}) x_{4,k+1} - 2.3204 x_{14,k+1} + x_{13,k+1} + x_{15,k+1} \\ &\quad - (0.04 x_{4,k}) V_{4,k+1} \end{aligned} \quad (3.86)$$

$$\begin{aligned} \frac{dx_{15,k+1}}{dX} &= (A6 - 0.04 V_{5,k}) x_{5,k+1} - 1.3204 x_{15,k+1} + x_{14,k+1} \\ &\quad - (0.04 x_{5,k}) V_{5,k+1} \end{aligned} \quad (3.87)$$

$$\frac{dV_{1,k+1}}{dX} = 0 \quad (3.88)$$

$$\frac{dV_{2,k+1}}{dX} = 0 \quad (3.89)$$

$$\frac{dV_{3,k+1}}{dX} = 0 \quad (3.90)$$

$$\frac{dV_{4,k+1}}{dX} = 0 \quad (3.91)$$

$$\frac{dV_{5,k+1}}{dX} = 0 \quad (3.92)$$

The initial values used to obtain the homogeneous solutions are

$$\tilde{x}_{h,k+1}^{(0)} = \begin{pmatrix} \tilde{A} \\ - \tilde{A} \\ \tilde{B} \end{pmatrix} \quad (3.93)$$

where

$$\tilde{A} = \tilde{0}$$

$$\tilde{B} = \tilde{I}$$

$\tilde{A}$ is a (15 x 5) zero matrix, and $\tilde{B}$ is a (5 x 5) identity matrix.

Note that the initial values in Eqs. (3.72) and (3.93) are chosen in such a way that at $t = 0$, the general solutions of $x_1, x_2, \dots, x_{15}$ in Eq. (3.67) satisfy the given initial conditions (3.52) - (3.66). So, only five sets of homogeneous solutions are needed. Note also that five simple linear relationships between the integration constants, $a_{j,k+1}$ ($j = 1, 2, 3, 4$, and 5), and the constant parameters, $V_{j,k+1}$ ($j = 1, 2, 3, 4$, and 5), can be obtained from the general solutions of V_1, V_2, V_3, V_4 , and V_5 in Eq. (3.67) and the initial conditions (3.72) and (3.93). These linear relationships are as follows

$$V_{1,k+1}(X) = a_{1,k+1} \quad (3.94)$$

$$V_{2,k+1}(X) = a_{2,k+1} \quad (3.95)$$

$$V_{3,k+1}(X) = a_{3,k+1} \quad (3.96)$$

$$V_{4,k+1}(X) = a_{4,k+1} \quad (3.97)$$

$$V_{5,k+1}(X) = a_{5,k+1} \quad (3.98)$$

Since the fifteen given boundary conditions, Eqs. (3.52) - (3.66), have already been used in choosing the initial conditions for obtaining

the particular and homogeneous solutions, the remaining five integration constants, $a_{j,k+1}$ ($j = 1, 2, 3, 4, 5$), can be obtained from the remaining five boundary conditions. For the case $S + R + \dots + Q > 5$, these five conditions can be obtained by minimizing Eq. (3.31). At various positions of $X_s, X_\gamma, \dots, X_q$ ($s = 1, 2, \dots, S; \gamma = 1, 2, \dots, R; \dots; q = 1, 2, \dots, Q$), the following $S + R + \dots + Q$ equations can be obtained from the general solutions of $X_1, X_2, \dots, X_{15}$ in vector equation (3.67)

$$x_{1,k+1}(X_s) = x_{1,p,k+1}(X_s) + \sum_{j=1}^5 a_{j,k+1} x_{1,hj,k+1}(X_s) \quad (3.99)$$

$$x_{2,k+1}(X_\gamma) = x_{2,p,k+1}(X_\gamma) + \sum_{j=1}^5 a_{j,k+1} x_{2,hj,k+1}(X_\gamma) \quad (3.100)$$

$$\vdots$$

$$x_{15,k+1}(X_q) = x_{15,p,k+1}(X_q) + \sum_{j=1}^5 a_{j,k+1} x_{15,hj,k+1}(X_q) \quad (3.113)$$

Substitution of the above fifteen equations into Eq. (3.31), yields

$$\begin{aligned} Q_{k+1} = & \sum_{s=1}^S [x_{1,p,k+1}(X_s) + \sum_{j=1}^5 a_{j,k+1} x_{1,hj,k+1}(X_s) - x_{1s}]^2 + \\ & \sum_{\gamma=1}^R [x_{2,p,k+1}(X_\gamma) + \sum_{j=1}^5 a_{j,k+1} x_{2,hj,k+1}(X_\gamma) - x_{2\gamma}]^2 + \\ & \vdots \\ & \sum_{q=1}^Q [x_{15,p,k+1}(X_q) + \sum_{j=1}^5 a_{j,k+1} x_{15,hj,k+1}(X_q) - x_{15q}]^2 \end{aligned} \quad (3.114)$$

Since the particular and homogeneous solutions at the various positions of X are known and are obtained numerically by using the initial values in Eqs. (3.72) and (3.93), the only unknowns on the right-hand side of Eq. (3.114) are the five integration constants, $a_{j,k+1}$ ($j = 1, 2, 3, 4, 5$). Thus, the problem is now changed into an optimization problem of determining the values of these five integration constants such that the value of Q_{k+1} is minimized.

There are many techniques which can be used to minimize Eq. (3.114). However, for this work, partial differentiation will be used to obtain the extreme values. By differentiating Eq. (3.114) with respect to $a_{j,k+1}$ ($j = 1, 2, 3, 4, 5$) respectively, and setting the results equal to zeros, the following five algebraic equations are obtained

$$\begin{aligned}
 \frac{\partial Q_{k+1}}{\partial a_{i,k+1}} = & 2 \sum_{s=1}^S x1_{hj,k+1} (X_s) [x1_{p,k+1} (X_s) + \sum_{j=1}^5 a_{j,k+1} x1_{hj,k+1} (X_s) - x1_s] + \\
 & 2 \sum_{\gamma=1}^R x2_{hj,k+1} (X_\gamma) [x2_{p,k+1} (X) + \sum_{j=1}^5 a_{j,k+1} x2_{hj,k+1} (X_\gamma) - x2_\gamma] + \\
 & \vdots \\
 & 2 \sum_{q=1}^Q x15_{hj,k+1} (X_q) [x15_{p,k+1} (X_q) + \sum_{j=1}^5 a_{j,k+1} x15_{hj,k+1} (X_q) - x15_q] \\
 & = 0
 \end{aligned}
 \tag{3.115}$$

$i = 1, 2, 3, 4, \text{ and } 5$

These five equations form the remaining five boundary conditions.

$a_{j,k+1}$, $j = 1, 2, 3, 4, 5$ can now be obtained by solving the above five algebraic equations. Once the integration constants are known, the general

solutions for $x1_{k+1}(X)$, $x2_{k+1}(X)$, ..., and $x15_{k+1}(X)$, $V_{1,k+1}(X)$, $V_{2,k+1}$, ..., and $V_{5,k+1}(X)$ can be obtained from Eq. (3.67). Since the estimated parameters $V_{1,k+1}$, $V_{2,k+1}$, $V_{3,k+1}$, $V_{4,k+1}$, and $V_{5,k+1}$ are constants, they can be obtained either from the general solutions (3.67) or by the linear relationships represented by Eqs. (3.94) - (3.98).

With $x1_{k+1}$, $x2_{k+1}$, ..., $x15_{k+1}$, $V_{1,k+1}$, $V_{2,k+1}$, $V_{3,k+1}$, $V_{4,k+1}$ and $V_{5,k+1}$ known, an improved set of values can be obtained in the same way by making $k = k+1$ in Eqs. (3.32) - (3.51). The iterative procedure is continued until the desired accuracy are obtained provided that the process converges.

The computational procedure can now be summarized as follows

1. Linearize the system of equations (3.7) - (3.21) and (3.25) - (3.29) using the generalized Newton-Raphson Equation (2.3).
2. Assume a set of reasonable initial functions for $x1(X)$, $x2(X)$, ..., $x14(X)$, $x15(X)$, $V_1(X)$, $V_2(X)$, $V_3(X)$, $V_4(X)$, and $V_5(X)$. Let these initial functions be $x1_{k=0}(X)$, $x2_{k=0}(X)$, ..., $x15_{k=0}(X)$, $V_{1,k=0}(X)$, $V_{2,k=0}(X)$, $V_{3,k=0}(X)$, $V_{4,k=0}(X)$, and $V_{5,k=0}(X)$.
3. Integrate Eqs. (3.32) - (3.51) numerically using (3.72) as the initial value with $k = 0$.
4. Integrate the homogeneous equations (3.73) - (3.92) five times using (3.93) as the initial value with $k = 0$.
5. Solve Eq. (3.115) for the integration constants $a_{j,k+1=1}$, $j = 1, 2, 3, 4$, and 5 , using the newly obtained particular and homogeneous solutions from Step 3 and 4, and using the given experimental data, $x1_s$, $x2_\gamma$, ..., $x14_p$, and $x15_q$ ($s = 1, 2, \dots, S$; $\gamma = 1, 2, \dots, R$;

- ...; $p = 1, 2, \dots, P$; $q = 1, 2, \dots, Q$).
6. Calculate $x1_{k+1=1}(X)$, $x2_{k+1=1}(X)$, ..., $x15_{k+1=1}(X)$, $v_{1,k+1=1}(X)$, $v_{2,k+1=1}(X)$, $v_{3,k+1=1}(X)$, $v_{4,k+1=1}(X)$, and $v_{5,k+1=1}(X)$ using Eq. (3.67) or obtain $v_{1,k+1=1}$, $v_{2,k+1=1}$, $v_{3,k+1=1}$, $v_{4,k+1=1}$, and $v_{5,k+1=1}$ from Eqs. (3.94) through (3.98).
 7. Repeat step 3 through 5 with $k = 1, 2, \dots$, until no further improvement on the values of $x1(X)$, $x2(X)$, ..., $x15(X)$, v_1 , v_2 , v_3 , v_4 , and v_5 can be obtained.

Note that the best available initial functions should be used for step 2.

Experimental data can be used for this purpose.

3.4 NUMERICAL RESULTS

To test the effectiveness of this approach, the constants in Eqs. (3.7) - (3.21) are estimated. The data used are obtained numerically by solving Eqs. (3.7) - (3.21) using the following numerical values

$$\begin{array}{lll}
 x1(0) = 0 & x2(0) = 0 & x3(0) = 1 \\
 x4(0) = 0 & x5(0) = 0 & x6(0) = 0 \\
 x7(0) = 0 & x8(0) = 0 & x9(0) = 0 \\
 x10(0) = 0 & x11(0) = 0 & x12(0) = 0 \\
 x13(0) = 0 & x14(0) = 0 & x15(0) = 0
 \end{array} \tag{3.116}$$

$$X_f = 5 \tag{3.117}$$

$$v_1 = 2.99$$

$$v_2 = 1.35$$

$$v_3 = 0$$

$$v_4 = -1.11$$

$$v_5 = -1.99 \tag{3.118}$$

Eqs. (3.7) - (3.21) are integrated numerically with the Runge-Kutta integration scheme. The step size which was used in this integration is $\Delta X = 0.05$. Part of the results from this integration are listed in Table 1 and plotted in Figures 4, 5, and 6. These values are used as the experimental data. Note that 11 ($S = R = \dots = Q = 11$) data points are used and $X_S = X_Y = \dots = X_Q$ for this particular problem.

3.4.1 Estimation of Five Parameters - Without Noise

Parameters V_1, V_2, V_3, V_4 , and V_5 are estimated using the value listed in Table 1 as experimental data. In other words, V_1, V_2, V_3, V_4 , and V_5 are considered as the unknown parameters which must be estimated from the given data listed in Table 1, the given model represented by Eqs. (3.7) - (3.21) and the values represented by Eqs. (3.116) and (3.117).

The system of equations for this problem is represented by Eqs. (3.7) - (3.21) and (3.25) - (3.29). These twenty equations can be linearized in the same way as before.

The initial values used to obtain the one set of particular and five sets of homogeneous solutions are listed in Table 2. Note that the initial values are chosen in such a way that they satisfy the given initial conditions listed in Eqs. (3.52) - (3.66). Thus only five sets of homogeneous solutions are needed. This problem is solved by using the same computational procedure discussed earlier. The Runge-Kutta integration scheme is used with the step size $\Delta X = 0.05$. To test the influence of the initial functions used in step 2 in the computational procedure, the following six different sets of initial functions are used for the unknown parameters V_1, V_2, V_3, V_4 , and V_5

$$\begin{array}{ll}
(1) \quad V_{1,k=0}(X) = 4 & (4) \quad V_{1,k=0}(X) = 15 \\
\quad V_{2,k=0}(X) = 2 & \quad V_{2,k=0}(X) = 10 \\
\quad V_{3,k=0}(X) = 0 & \quad V_{3,k=0}(X) = 0 \\
\quad V_{4,k=0}(X) = -1.5 & \quad V_{4,k=0}(X) = -5 \\
\quad V_{5,k=0}(X) = -3 & \quad V_{5,k=0}(X) = -10 \\
\\
(2) \quad V_{1,k=0}(X) = 6 & (5) \quad V_{1,k=0}(X) = 20 \\
\quad V_{2,k=0}(X) = 4 & \quad V_{2,k=0}(X) = 15 \\
\quad V_{3,k=0}(X) = 0 & \quad V_{3,k=0}(X) = 0 \\
\quad V_{4,k=0}(X) = -3 & \quad V_{4,k=0}(X) = -10 \\
\quad V_{5,k=0}(X) = -5 & \quad V_{5,k=0}(X) = -15 \\
\\
(3) \quad V_{1,k=0}(X) = 10 & (6) \quad V_{1,k=0}(X) = 50 \\
\quad V_{2,k=0}(X) = 6 & \quad V_{2,k=0}(X) = 40 \\
\quad V_{3,k=0}(X) = 0 & \quad V_{3,k=0}(X) = 0 \\
\quad V_{4,k=0}(X) = -5 & \quad V_{4,k=0}(X) = 30 \\
\quad V_{5,k=0}(X) = -8 & \quad V_{5,k=0}(X) = -35
\end{array} \tag{3.117}$$

for $0 \leq X \leq X_f = 5$. The experimental data listed in Table 1 are used as the initial functions for $x_1, x_2, \dots, x_{15}$ for all the calculations.

The problem converges rapidly to the correct solutions for all six sets of initially assumed functions. The convergence rates for the unknown parameters V_1, V_2, V_3, V_4 , and V_5 are shown in Table 3,4,5,6,7, and 8 respectively. Notice that large improvement obtained during the first iteration. It can be seen from Table 3,4,5,6,7, and 8 that a five-digit accuracy is obtained in only three or four iterations. It should be noted that the initially assumed functions as given by Eq. (3.117)

are very far removed from the correct solutions.

3.4.2 Estimation with Experimental Errors - Five Parameters

In practical situations, the data obtained always have measurement or experimental errors. To test the influence of the experimental errors on the rate of convergence of this approach, the data listed in Table 1 are corrupted with noise by the equations

$$x_{1Z}^{(exp)}(I) = x_{1S}(I) + R_1 \quad (3.118)$$

$$x_{2Z}^{(exp)}(I) = x_{2S}(I) + R_2 \quad (3.119)$$

$$\vdots \quad \quad \quad \vdots$$

$$x_{15Z}^{(exp)}(I) = x_{15S}(I) + R_{15} \quad (3.122)$$

where $I = 1, 11, 21, 31, 41, 51, 61, 71, 81, 91, 101$ with 11 data points for each variable. x_Z represents the noise data and x_S represents actual data. The noises $R_1, R_2, \dots, R_{15}$ represent normally distributed random numbers. These random numbers are generated by using IBM Scientific Subroutine GAUSS and RANDU. The means for these normally distributed random members are zeros and the standard deviations are 0.0015 for $R_1, R_2, \dots, R_{15}$. These standard deviations are approximately five percent of the data listed in Table 1. These noisy data are listed in Table 9. The noisy data with 10% variation about the actual data are also generated and listed in Table 10. Both 5% and 10% noisy data for x_5, x_6 , and x_{13} are plotted in Figure 9, 10, and 11 respectively.

The problem is solved with the other numerical values remaining the same as that used for the case without noise. When 11 data points

$(S = R = \dots = Q)$ were used, the convergence rate for the one of the six sets of initial functions listed in Eq. (3.117) are shown in Tables 11 and 12 for 5% and 10% noisy data respectively. It can be seen that the presence of experimental errors does not slow the convergence rates. However, due to the presence of noise, the values of V_1 , V_2 , V_3 , V_4 , and V_5 obtained are not the same as the original given values. The larger the noise, the less the accuracy, as can be seen from Table 11 and 12. It is expected that as the number of the noisy data increases, the estimated values of V_1 , V_2 , V_3 , V_4 , and V_5 should approach the original given values. This problem was also been solved with 101 data points ($S = R = \dots = Q = 101$) for $x_1, x_2, \dots, x_{15}$ and with all the other numerical values remaining the same. The convergence rates for this 101 data points problem are approximately the same as that shown in Tables 11 and 12. However, the estimated values of V_1 , V_2 , V_3 , V_4 , and V_5 are improved as can be seen from Tables 13 and 14. The values of V_1 , V_2 , V_3 , V_4 , and V_5 are now fairly close to the original given values.

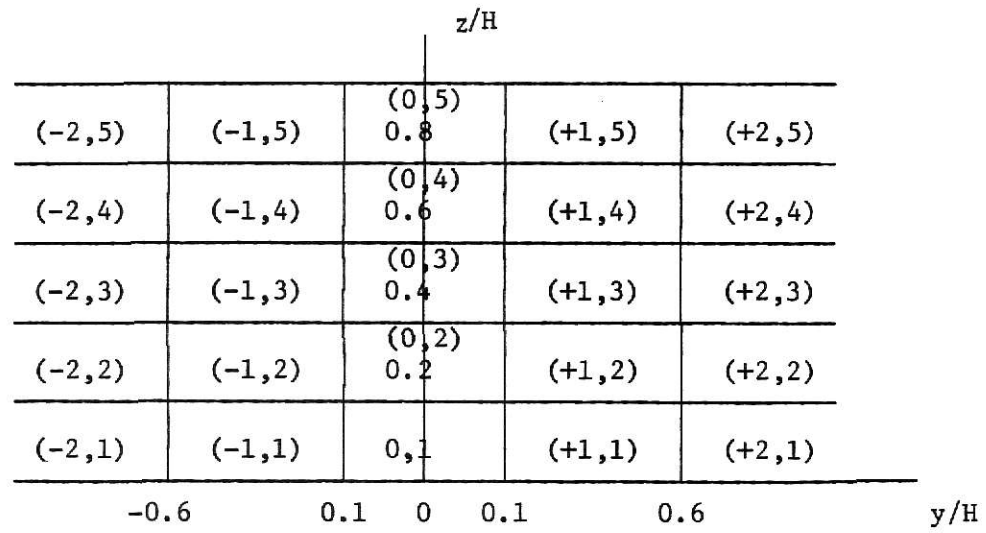


FIGURE 1.

Schematic representation of a 25-cell model [17]

Table 1. Experimental Data without noise

X	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	x11	x12	x13	x14	x15
0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
0.5	0.029582	0.10662	0.237953	0.106643	0.029626	0.006688	0.022023	0.045326	0.018904	0.004896	0.004595	0.018569	0.045216	0.021691	0.006389
1.0	0.037132	0.068230	0.095764	0.068328	0.037367	0.019507	0.032805	0.042562	0.028309	0.014530	0.013664	0.027703	0.042196	0.032216	0.018676
1.5	0.034806	0.047397	0.056159	0.047581	0.035268	0.028140	0.035137	0.038349	0.030309	0.021246	0.019975	0.029488	0.037820	0.034369	0.026980
2.0	0.032449	0.038301	0.042033	0.038568	0.033089	0.032525	0.035282	0.035537	0.030375	0.024785	0.023256	0.029372	0.034845	0.034388	0.031206
2.5	0.031082	0.034229	0.036169	0.034565	0.031864	0.03449	0.034925	0.033778	0.030020	0.026405	0.024597	0.028868	0.032956	0.033942	0.033058
3.0	0.030301	0.032247	0.033434	0.032637	0.031181	0.035135	0.034465	0.032649	0.029600	0.027024	0.025180	0.028327	0.031727	0.033420	0.033710
3.5	0.029763	0.031145	0.031991	0.031579	0.030717	0.035223	0.033996	0.031869	0.029189	0.027149	0.025198	0.027817	0.030869	0.032909	0.033783
4.0	0.029313	0.030423	0.031110	0.030892	0.030324	0.035026	0.033538	0.031276	0.028795	0.027033	0.024999	0.027305	0.030215	0.032421	0.033581
4.5	0.028893	0.029869	0.030483	0.030366	0.029948	0.034693	0.033089	0.030779	0.028415	0.026803	0.024699	0.026902	0.029673	0.031953	0.033249
5.0	0.029483	0.029393	0.029973	0.029912	0.029572	0.034295	0.032648	0.030334	0.028045	0.026517	0.024361	0.026483	0.029192	0.031499	0.032859

Table 2

Initial Values Used for Obtaining the
Particular and Homogeneous Solutions

Variable	Particular Solution	Homogeneous Solutions				
$x1_{k+1}(0)$	0	0	0	0	0	0
$x2_{k+1}(0)$	0	0	0	0	0	0
$x3_{k+1}(0)$	1	0	0	0	0	0
$x4_{k+1}(0)$	0	0	0	0	0	0
$x5_{k+1}(0)$	0	0	0	0	0	0
$x6_{k+1}(0)$	0	0	0	0	0	0
$x7_{k+1}(0)$	0	0	0	0	0	0
$x8_{k+1}(0)$	0	0	0	0	0	0
$x9_{k+1}(0)$	0	0	0	0	0	0
$x10_{k+1}(0)$	0	0	0	0	0	0
$x11_{k+1}(0)$	0	0	0	0	0	0
$x12_{k+1}(0)$	0	0	0	0	0	0
$x13_{k+1}(0)$	0	0	0	0	0	0
$x14_{k+1}(0)$	0	0	0	0	0	0
$x15_{k+1}(0)$	0	0	0	0	0	0
$v_{1,k+1}(0)$	0	1	0	0	0	0
$v_{2,k+1}(0)$	0	0	1	0	0	0
$v_{3,k+1}(0)$	0	0	0	1	0	0
$v_{4,k+1}(0)$	0	0	0	0	1	0
$v_{5,k+1}(0)$	0	0	0	0	0	1

Table 3. Convergence Rates for V_1 , V_2 , V_3 , V_4 ,
and V_5 with Data Set 1

Iteration	V_1	V_2	V_3	V_4	V_5
0	4	2	0	-1.5	-3
1	2.99951	1.35099	-0.00113	-1.10902	-1.99744
2	2.99998	1.35486	-0.00025	-1.11531	-1.99613
3	2.99996	1.35484	-0.00017	-1.11537	-1.99608
4	2.99996	1.35484	-0.00017	-1.11538	-1.99608
5	2.99996	1.35484	-0.00017	-1.11538	-1.99608

Table 4. Convergence Rates for V_1 , V_2 , V_3 , V_4 ,
and V_5 with Data Set 2

Iteration	V_1	V_2	V_3	V_4	V_5
0	6	4	0	-3	-5
1	3.00084	1.33788	-0.00290	-1.09169	-2.00125
2	3.00004	1.35491	-0.00040	-1.11519	-1.99623
3	2.99996	1.35484	-0.00018	-1.11537	-1.99608
4	2.99996	1.35484	-0.00017	-1.11538	-1.99608
5	2.99996	1.35484	-0.00017	-1.11538	-1.99608

Table 5. Convergence Rates for V_1 , V_2 , V_3 , V_4 ,
and V_5 with Data Set 3

Iteration	V_1	V_2	V_3	V_4	V_5
0	10	6	0	-5	-8
1	3.00950	1.30775	-0.00339	-1.05963	-2.01194
2	3.00017	1.35482	-0.00044	-1.11504	-1.99638
3	2.99996	1.35484	-0.00019	-1.11536	-1.99608
4	2.99996	1.35484	-0.00017	-1.11538	-1.99608
5	2.99996	1.35484	-0.00017	-1.11538	-1.99608

Table 6. Convergence Rates for V_1 , V_2 , V_3 , V_4 ,
and V_5 with Data Set 4

Iteration	V_1	V_2	V_3	V_4	V_5
0	15	10	0	-5	-10
1	3.03736	1.27961	-0.01666	-1.01652	-2.02538
2	3.00017	1.35509	-0.00148	-1.11445	-1.99661
3	2.99996	1.35487	-0.00026	-1.11533	-1.99609
4	2.99996	1.35484	-0.00019	-1.11537	-1.99608
5	2.99996	1.35484	-0.00017	-1.11538	-1.99608
6	2.99996	1.35484	-0.00017	-1.11538	-1.99608

Table 7. Convergence Rates for V_1 , V_2 , V_3 , V_4 ,
and V_5 with Data Set 5

Iteration	V_1	V_2	V_3	V_4	V_5
0	20.	15	0	-10	-15
1	3.09554	1.21599	-0.01113	-0.96123	-2.07374
2	3.00020	1.35461	-0.00103	-1.11438	-1.99671
3	2.99997	1.35485	-0.00023	-1.11534	-1.99609
4	2.99996	1.35484	-0.00017	-1.11537	-1.99608
5	2.99996	1.35484	-0.00017	-1.11538	-1.99608
6	2.99996	1.35484	-0.00017	-1.11538	-1.99608

Table 8. Convergence Rates for V_1 , V_2 , V_3 , V_4 ,
and V_5 with Data Set 6

Iteration	V_1	V_2	V_3	V_4	V_5
0	50	40	0	-30	-35
1	3.29695	1.09387	-0.00368	-0.863527	-2.25716
2	2.99873	1.35311	-0.00021	-1.11403	-1.99529
3	2.99999	1.35480	-0.00014	-1.11536	-1.99610
4	2.99996	1.35484	-0.00016	-1.11538	-1.99608
5	2.99996	1.35484	-0.00017	-1.11538	-1.99608
6	2.99996	1.35484	-0.00017	-1.11538	-1.99608

Table 9. Experimental Data with 5% noise

X	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	x11	x12	x13	x14	x15
0	0.000705	0.000449	1.000466	-0.002118	0.003484	-0.000322	0.001571	0.002321	0.002234	0.001079	0.000624	-0.000892	0.000093	-0.001924	0.000790
0.5	0.030793	0.107317	0.239287	0.110252	0.028787	0.008763	0.022861	0.046634	0.018824	0.000728	0.005461	0.017619	0.045026	0.021749	0.005700
1.0	0.034692	0.067550	0.096011	0.068316	0.037147	0.017516	0.032548	0.041403	0.026133	0.015207	0.014272	0.026145	0.043732	0.031907	0.017401
1.5	0.034662	0.044417	0.055784	0.046865	0.034696	0.029637	0.037276	0.035728	0.031044	0.021911	0.018594	0.029606	0.038414	0.034629	0.026001
2.0	0.032621	0.036662	0.042504	0.039959	0.030776	0.032042	0.034542	0.034678	0.028636	0.024223	0.023968	0.026759	0.036014	0.034588	0.030520
2.5	0.032201	0.036655	0.037526	0.033948	0.032860	0.033948	0.035258	0.035875	0.027524	0.028612	0.023395	0.028612	0.031586	0.034478	0.032151
3.0	0.031974	0.033734	0.035227	0.033916	0.028781	0.036105	0.033256	0.031992	0.030242	0.025509	0.025579	0.029450	0.028926	0.033269	0.030530
3.5	0.031725	0.030779	0.030011	0.030609	0.029748	0.034583	0.032319	0.030547	0.030958	0.029061	0.025463	0.026413	0.029327	0.032177	0.033370
4.0	0.027621	0.030785	0.030815	0.032619	0.031498	0.035984	0.033954	0.029387	0.032353	0.028148	0.024593	0.027335	0.028419	0.028929	0.033811
4.5	0.027541	0.029012	0.207517	0.029886	0.028336	0.035722	0.034944	0.031397	0.026092	0.027456	0.026337	0.024867	0.030315	0.032380	0.030100
5.0	0.029784	0.029849	0.031199	0.030675	0.029260	0.032879	0.029838	0.031692	0.027649	0.023751	0.022356	0.026993	0.029627	0.033116	0.033370

Table 10. Experimental Data with 10% noise

X	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	x11	x12	x13	x14	x15
0	0.001411	0.000898	1.000932	-0.004236	0.006969	-0.000644	0.003142	0.004642	0.004467	0.002157	0.001248	-0.001984	0.000186	-0.003848	0.001580
0.5	0.032005	0.108018	0.240621	0.113861	0.027948	0.010838	0.023699	0.048021	0.018745	-0.003441	0.006328	0.016671	0.044836	0.021806	0.005011
1.0	0.032252	0.066869	0.096259	0.068305	0.036926	0.015526	0.032290	0.040279	0.023956	0.015885	0.014883	0.024584	0.045269	0.031598	0.016133
1.5	0.032518	0.041438	0.055407	0.046149	0.034124	0.031135	0.039415	0.033106	0.031779	0.022577	0.017212	0.029724	0.039008	0.034889	0.025022
2.0	0.032798	0.035023	0.042975	0.041351	0.026461	0.031559	0.033801	0.033818	0.426879	0.023662	0.024280	0.024146	0.037182	0.034788	0.029845
2.5	0.033319	0.039080	0.038883	0.033332	0.033856	0.03346	0.035592	0.037972	0.025659	0.028644	0.022094	0.028355	0.030216	0.035014	0.031248
3.0	0.033647	0.035221	0.037019	0.035195	0.026381	0.037075	0.032847	0.031295	0.030883	0.023994	0.025979	0.030573	0.026125	0.033117	0.027349
3.5	0.033686	0.030412	0.028032	0.029639	0.028779	0.033943	0.030643	0.029225	0.032727	0.030973	0.025729	0.025008	0.027786	0.031444	0.032970
4.0	0.025928	0.031146	0.030520	0.034346	0.032672	0.036943	0.034371	0.027497	0.035912	0.029262	0.024188	0.027324	0.026623	0.025437	0.034055
4.5	0.025189	0.028155	0.024552	0.029406	0.026724	0.036752	0.036799	0.032015	0.023769	0.028109	0.027976	0.022832	0.030958	0.032808	0.026969
5.0	0.031085	0.030306	0.032425	0.031438	0.028948	0.031464	0.027027	0.033049	0.027254	0.020986	0.020351	0.027502	0.030062	0.034733	0.034636

Table 11. Convergence Rates for V_1 , V_2 , V_3 , V_4 ,
and V_5 with 11 Data Points and 5% Noise

Iteration	V_1	V_2	V_3	V_4	V_5
0	6	4	0	-3	-5
1	2.7228	1.6857	-0.0690	-1.1877	-1.5817
2	2.6613	1.9111	-0.0713	-1.3678	-1.5496
3	2.6569	1.9144	-0.0690	-1.3865	-1.5283
4	2.6569	1.9144	-0.0686	-1.3884	-1.5258
5	2.6569	1.9144	-0.0686	-1.3887	-1.5255
6	2.6569	1.9144	-0.0686	-1.3887	-1.5255

Table 12. Convergence Rates for V_1 , V_2 , V_3 , V_4 ,
and V_5 with 11 Data Points and 10% Noise

Iteration	V_1	V_2	V_3	V_4	V_5
0	6	4	0	-3.	-5.
1	2.353	2.325	-0.114	-1.577	-1.006
2	2.279	2.505	-0.135	-1.706	-0.973
3	2.278	2.507	-0.131	-1.742	-0.929
4	2.278	2.507	-0.130	-1.750	-0.918
5	2.278	2.507	-0.130	-1.751	-0.916
6	2.278	2.507	-0.130	-1.751	-0.916

Table 13. Convergence Rates for V_1 , V_2 , V_3 , V_4 ,
and V_5 with 101 Data Points and 5% Noise

Iteration	V_1	V_2	V_3	V_4	V_5
0	10	6	0	-5.	-8.
1	3.18333	1.23393	0.00414	-1.21487	-1.85879
2	3.18228	1.26013	0.00878	-1.24539	-1.82955
3	3.18257	1.25985	0.00924	-1.24602	-1.82933
4	3.18258	1.25983	0.00928	-1.24605	-1.82931
5	3.18258	1.25883	0.00929	-1.24605	-1.82931
6	3.18258	1.25983	0.00929	-1.24605	-1.82931

Table 14. Convergence Rates for V_1 , V_2 , V_3 , V_4 ,
and V_5 with 101 Data Points and 10% Noise

Iteration	V_1	V_2	V_3	V_4	V_5
0	10.	6	0.	-5	-8.
1	3.37820	1.14119	0.01449	-1.37101	-1.70586
2	3.37276	1.15871	0.01998	-1.38363	-1.65298
3	3.37436	1.15741	0.02054	-1.38356	-1.65375
4	3.37446	1.15730	0.02059	-1.38356	-1.65378
5	3.37447	1.15729	0.02060	-1.38356	-1.65378
6	3.37447	1.15729	0.02060	-1.38356	-1.65378

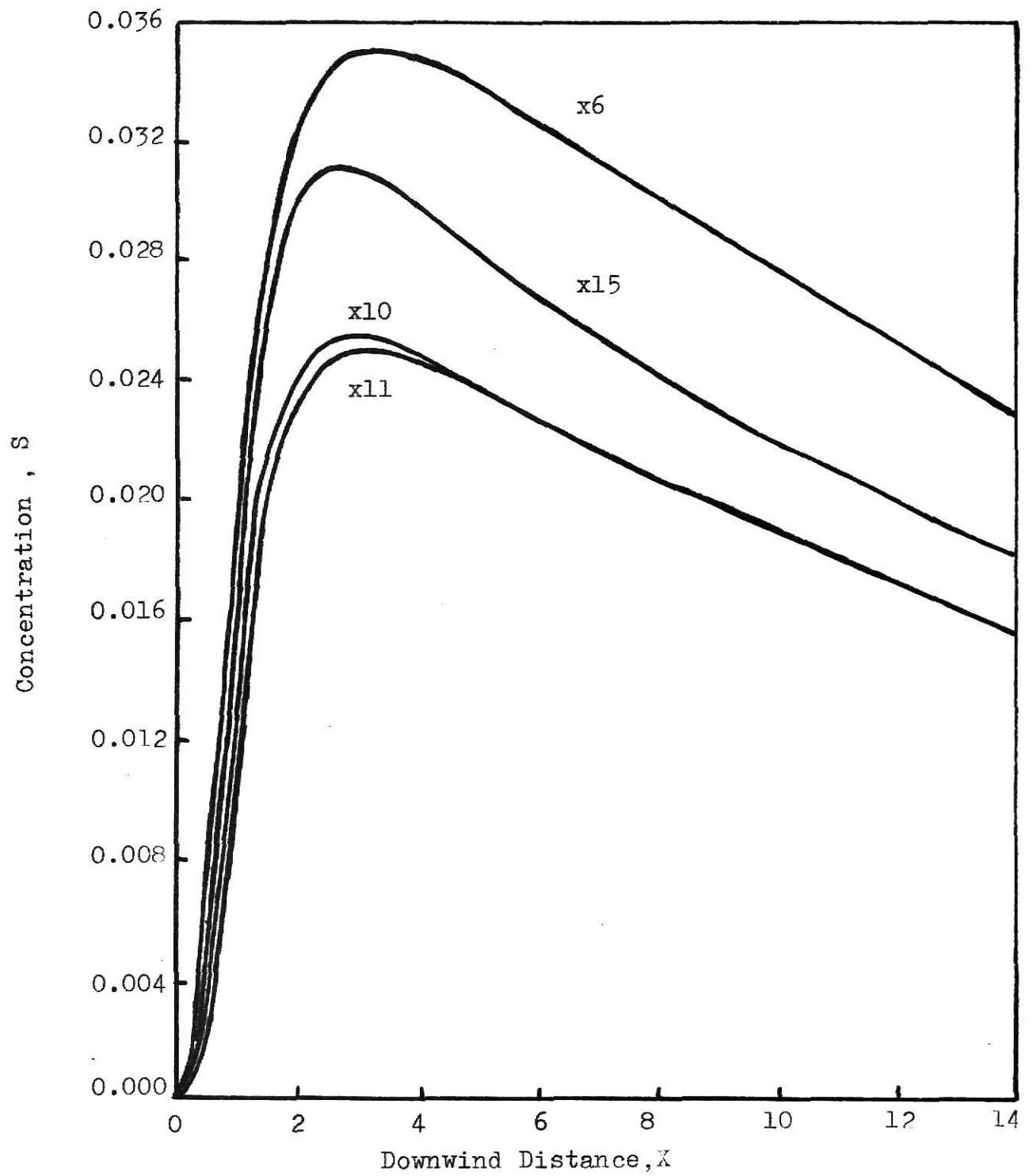


Figure 4. The Profiles of SO_2 Concentration in Regions x6, x10, x11, and x15

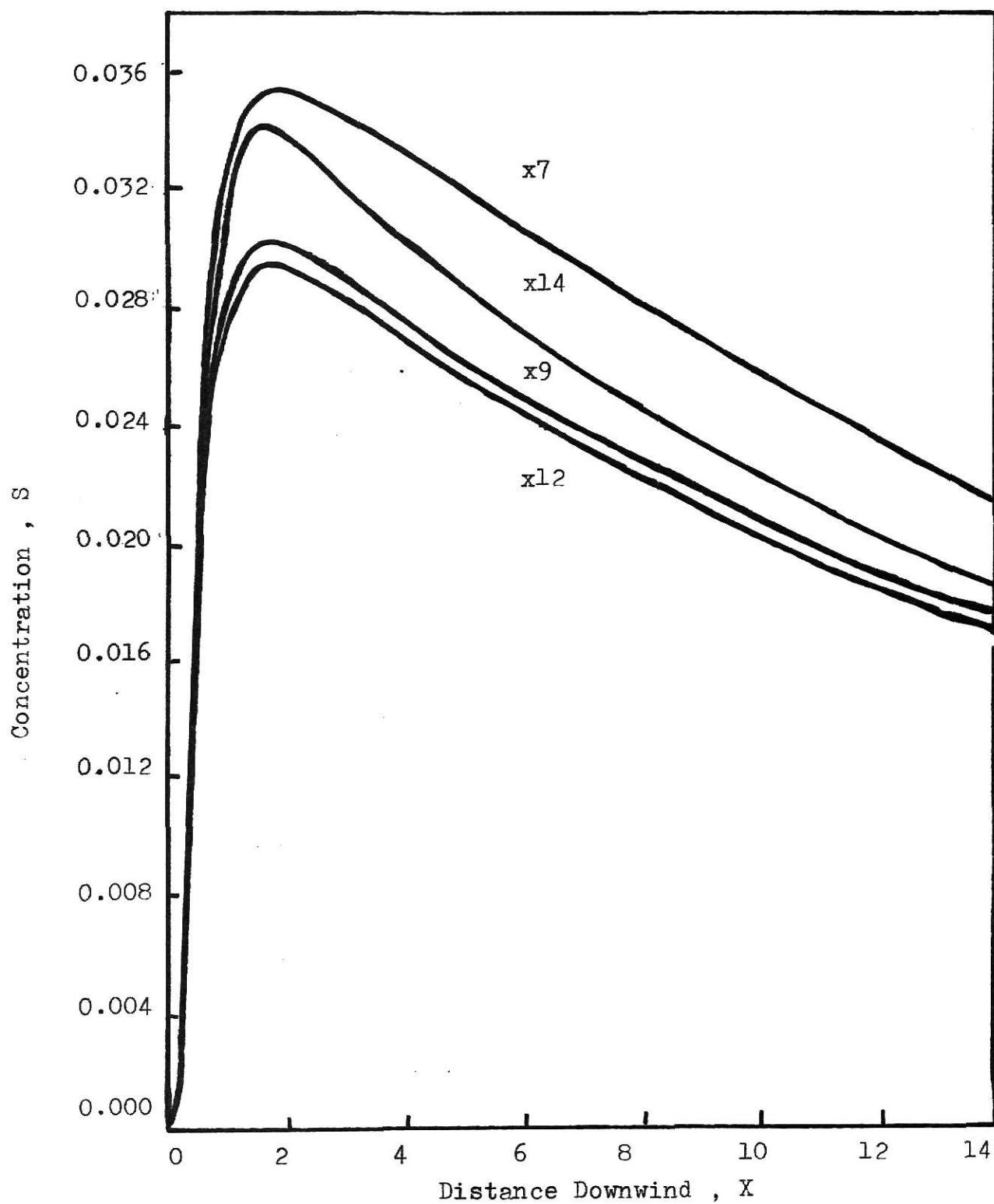


Figure 5. The profiles of SO₂ Concentration in Regions x7, x9, x12, and x14

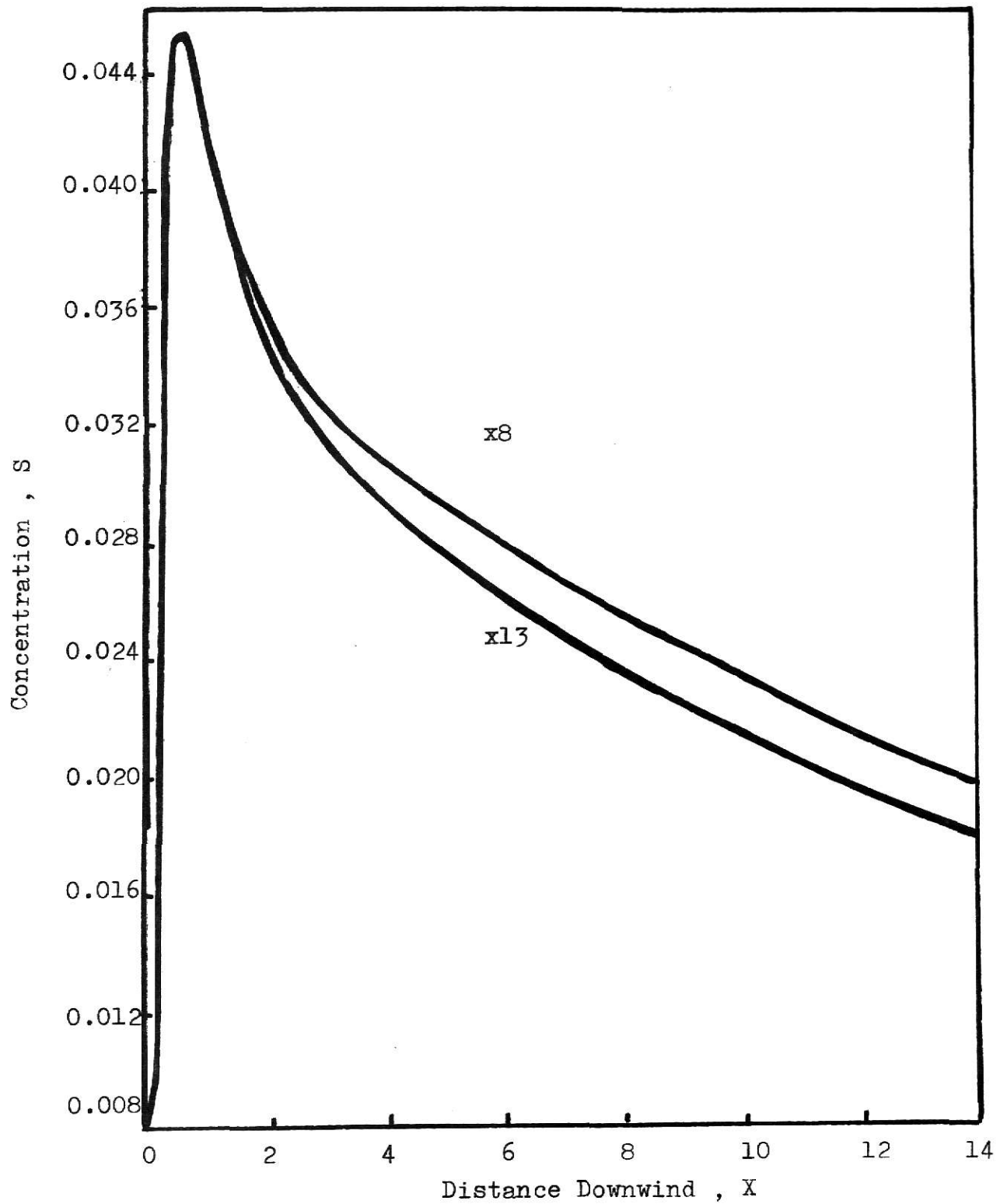


Figure 6. The Profiles of SO_2 Concentration in Regions x8 and x13

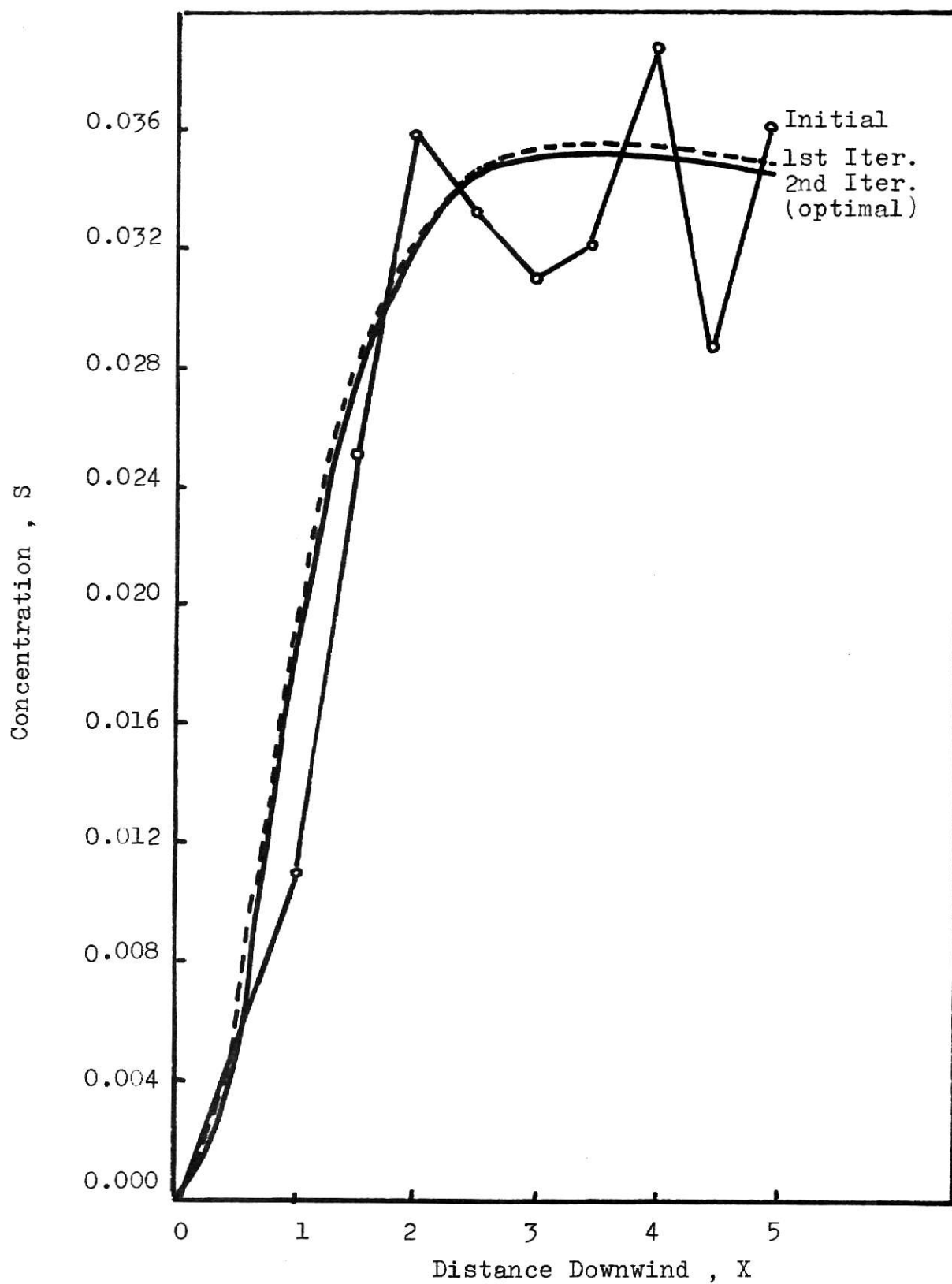


Figure 7. Convergence Rates of Region x_6

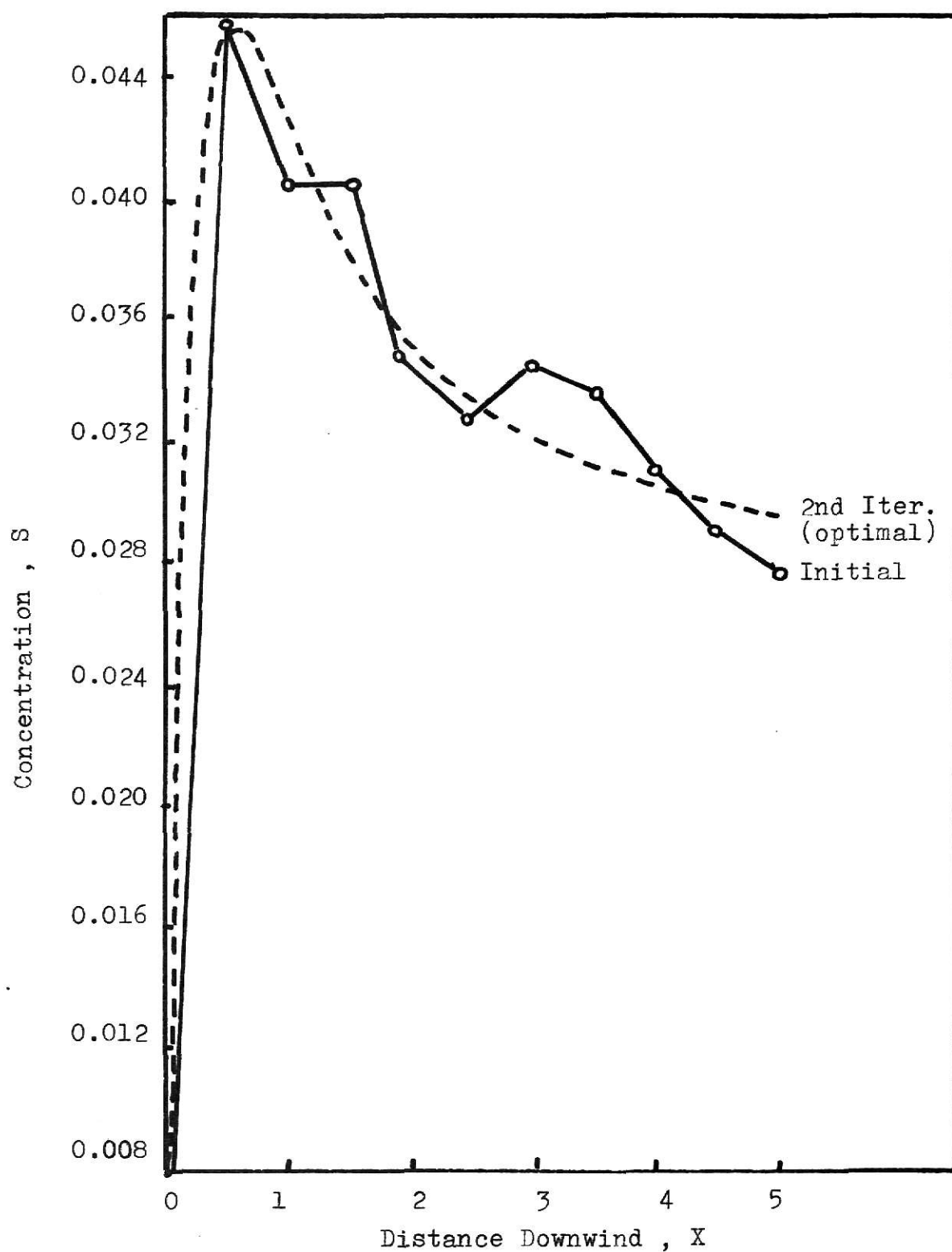


Figure 8. Convergence Rates of Region xl3

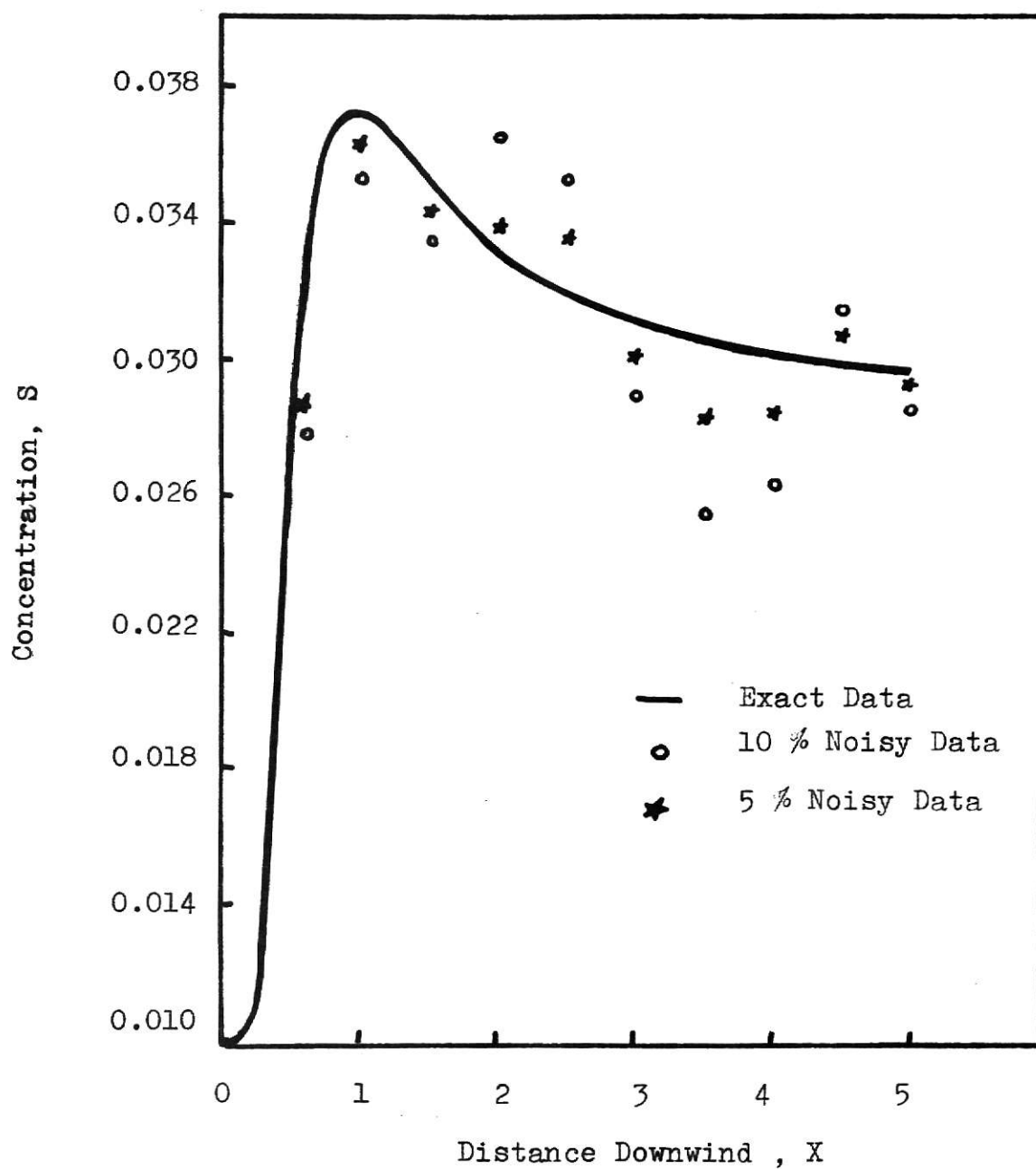


Figure 9. Actual and Noisy Measurements of SO_2 Concentration in Region x5

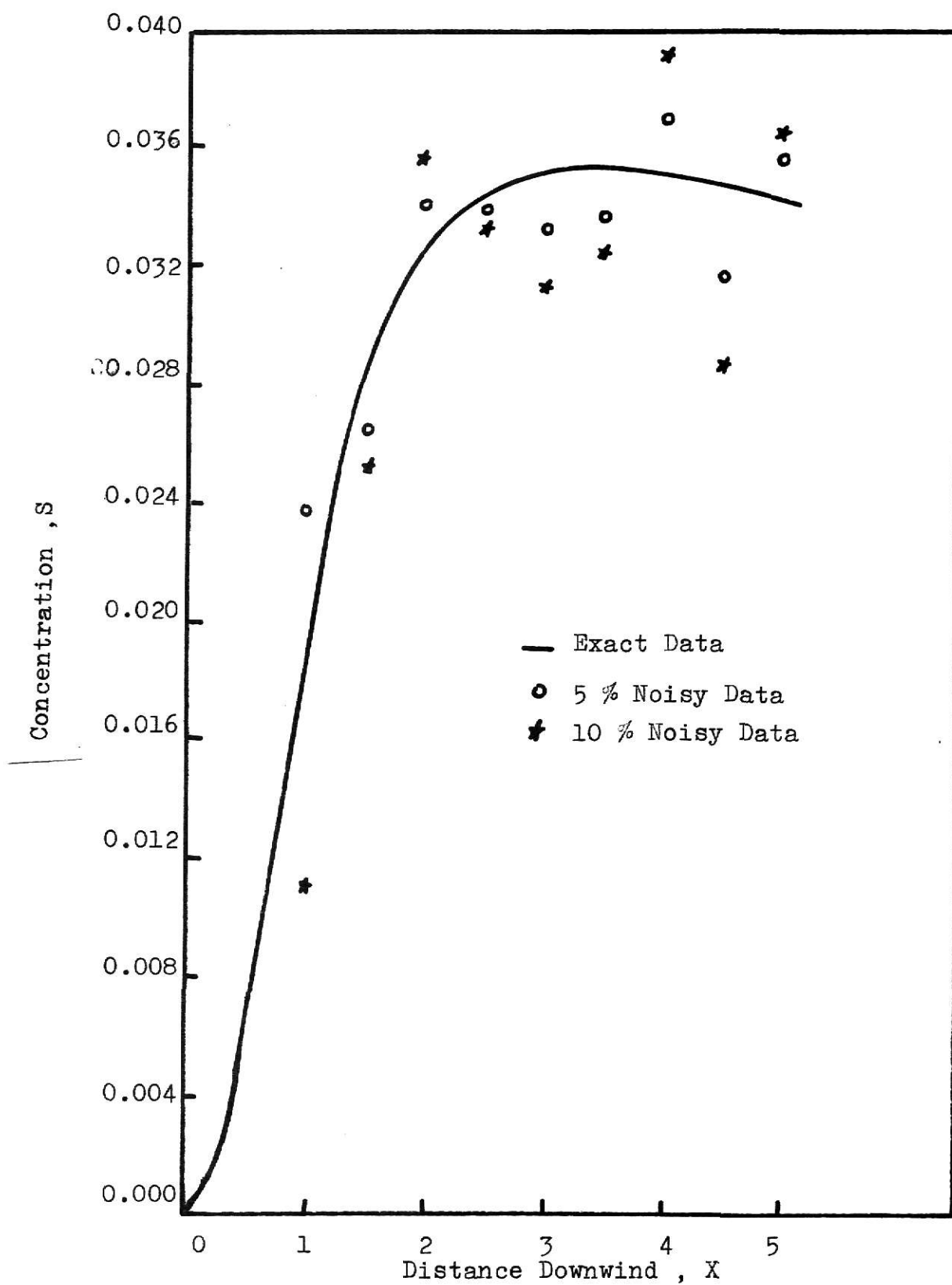


Figure 10. Actual and Noisy Measurements of SO_2 Concentration in Region X6

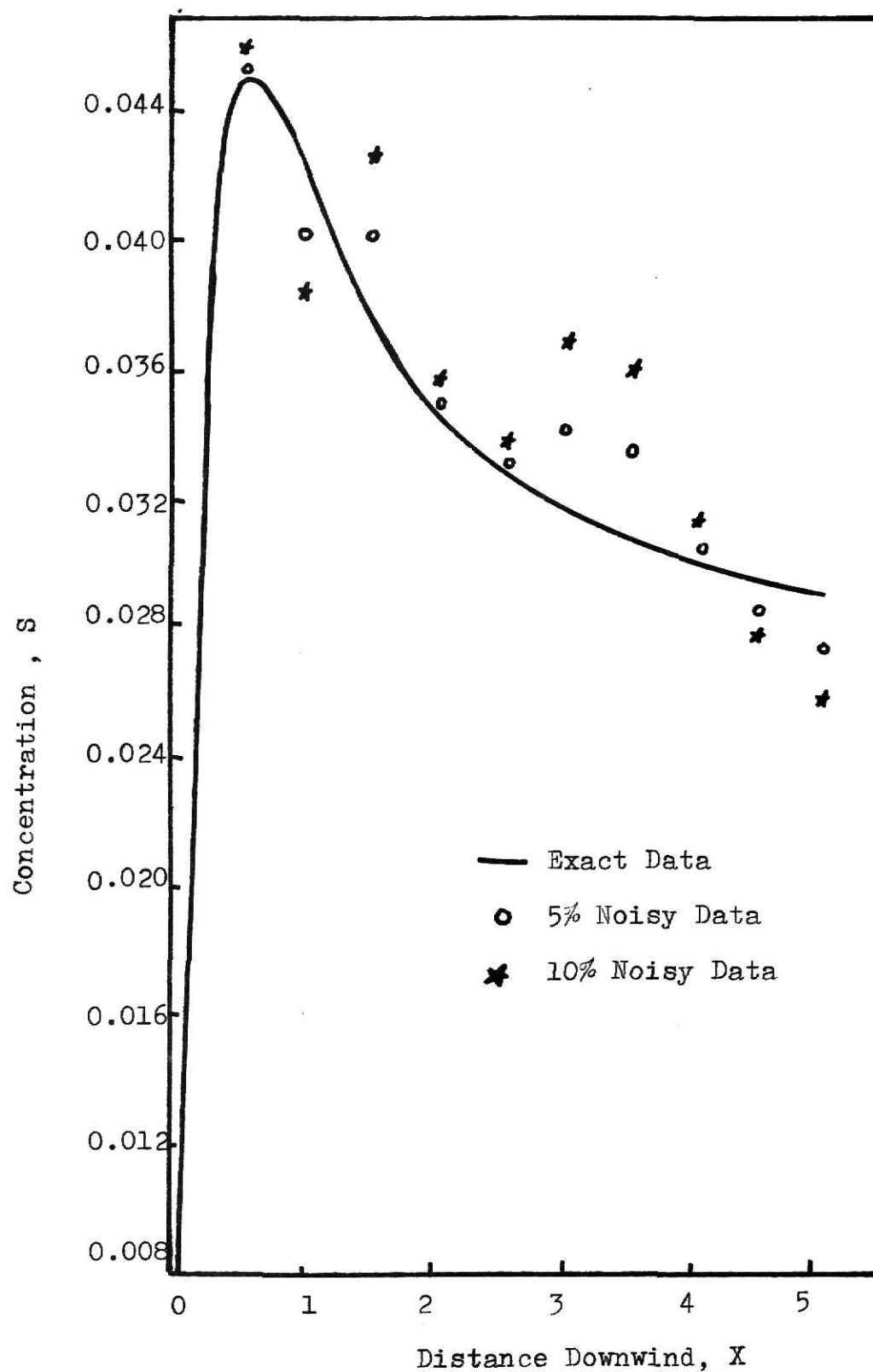


Figure 11. Actual and Noisy Measurements of SO_2 Concentration in Region X13

CHAPTER 4

Optimization of a revised dynamic decomposition model
by Linear Programming

4.1 INTRODUCTION

Generally speaking, there are two approaches to control air quality. One is the improvement or purification of the emission sources, and the other is to allocate in an optimal way the source distribution. The former approach consists of the desulfurization of fuel, improvement of internal combustion engine or the use of antiexhaust devices, and the development of nonpollution power sources such as nuclear energy. Due to technical and financial problems, the implementation of this approach cannot be carried out easily. The second approach is the system approach which gives the general policy of optimal pollutant emission distribution. By using this optimal distribution, the requirement on the purification of emission sources can be minimized. Thus, essentially, the second approach complements the first approach and reduces the losses of industrial and social activities due to air pollution control to a minimum.

For the purpose of using the system approach, a mathematical model representing the area of interest is required. Since the equations representing the flow, diffusion, and reaction of pollutants are fairly complicated and highly nonlinear, it cannot be used easily for optimization purposes. Furthermore, the meteorological factors such as wind direction, wind speed, atmospheric stability, temperature lapse rate, turbulent diffusivity, reaction rates, and even emission rates are

changing with time. In this work, a simplified model based on deviding the area of interest into regions is employed.

To consider the dynamic behavior of the pollutants, a day is devided into several time periods. The pollutants concentration are assumed uniform within each region and during each time period. By doing so, a complicated nonlinear dynamic system can be optimized by the linear dynamic decomposition programming approach [16].

In recent years, various pollution models have been proposed based on various simplifying assumptions [1,7,9-11,19]. However, none of these models can be used to optimize a large metropolitan area. Since the linear programming algorithm can solve fairly large problem with a large number of inequality constraints, this approach of linearly decomposing the nonlinear dynamic system appears to be a very powerful tool for optimizing the air pollution distribution in a large metropolitan area.

The approach discussed above has been found to be fairly practical and has been used in a large number of industrial situations to solve similarly complex problems [24,25,29,30]. Kohn [15] used linear programming technique to solve a static model which selects the fuels to be used to a least cost basis. The time period he uses is one year. However, this model does not include the dynamic nature of the problem because a time period of one year is used. To establish a model for effective online control, the dynamic aspects such as wind direction and speed must be included. The time period used must also be in fraction of a day in order to include the dynamic influences. Tillman and Lee [16] have proposed a dynamic decomposition model and they have solved this problem by linear

programming. This model does include the dynamic nature of the problem with a time period of one hour.

Concentrations of pollutants in each region transported into another region by wind within a time period are functions of background source, emission source, and the amount of pollutants transported into this region. However, since these concentrations are unknown until the problem is solved, some trial-and-error procedures are needed. In other words, the direct iteration method is used in order to employ linear programming. In this work, an equation which relating the amount of pollutants transported out of a region with background concentrations of the region, emission source of the region, and the amount of pollutants transported into this region is derived based on the theory of conservation of Mass. This equation can be established for each region. By substituting this equation into Tillman and Lee's model, the optimal solution can be obtained by using linear programming. Thus, no trial-and-error is needed. The computation work can be reduced.

4.2 THE MODEL

In order to establish the model, a metropolitan area is divided into n regions. In this work, the hypothetical metropolitan area is divided into 4 regions (see Figure 3). Three classes of pollution sources are considered: emission sources X , background sources W , and sources transported from and to other regions Y . Background sources are defined as those pollutants which are in the region at the beginning of the time period. Emission sources are pollutants emitted during the time period.

Note that emission sources include both stationary sources and mobile sources. Thus, exhaust from vehicles can be considered as emission sources.

A day is divided into several time periods. Each time period is represented by a mathematical model. In this work, the time period used is one hour.

Two emission sources are assumed in region 1, namely, a power plant and a municipal incinerator. A power plant and a refinery are located in region 2. One steam boiler and one power plant are located in region 3. Only one mobile source is assumed for region 5. The amounts of pollutants from each emission source can be reduced by either purifying the exhaust or by the use of a better grade of fuel.

The problem can be stated as given the costs and the heat values of the various grades of fuels and the purification costs of the various pollution sources, find the grades of fuels to be used and the amount of purifications needed at the various emission sources so that the overall cost is a minimum. At the same time, the energy required and a certain maximum allowable pollutants concentrations are not violated.

For illustration, only one time period (one hour) is considered. The revised dynamic decomposition model can be written in the form

Objective function

$$\begin{aligned}
 \text{Minimize } J = & C_1 x_{111} + C_2 x_{211} + C_3 z_{11} + C_4 x_{121} + C_5 z_{21} + \\
 & C_6 x_{112} + C_7 x_{212} + C_8 z_{12} + C_9 x_{122} + C_{10} z_{22} + \\
 & C_{11} x_{113} + C_{12} x_{213} + C_{13} z_{13} + C_{14} x_{123} + C_{15} z_{23} + \\
 & C_{16} x_{115} + C_{17} x_{215} + C_{18} z_{15}
 \end{aligned} \tag{4.10}$$

Subject to (constraints)

A. Balance Equations (4.11)

$$W_1 + a_{11}x_{111} + a_{12}x_{211} - P_{13}Z_{11} + a_{14}x_{121} - P_{17}Z_{21} + Q_{15}Y_{01} - Q_{16}Y_1 - C_d = S_1 \quad (\text{Region 1})$$

$$W_2 + a_{21}x_{112} + a_{22}x_{212} - P_{23}Z_{12} + a_{24}x_{122} - P_{25}Z_{25} + Q_{26}Y_{12} - Q_{27}Y_2 - C_d = S_2 \quad (\text{Region 2})$$

$$W_3 + a_{31}x_{113} + a_{32}x_{213} - P_{33}Z_{13} + a_{34}x_{123} - P_{35}Z_{23} + Q_{36}Y_{03} - Q_{37}Y_3 - C_d = S_3 \quad (\text{Region 3})$$

$$W_5 + a_{41}x_{115} + a_{42}x_{215} - P_{43}Z_{15} + a_{44}Y_{35} - a_{45}Y_5 - C_d = S_5 \quad (\text{Region 5})$$

B. Background Concentrations: (4.12)

$$W_1 = W_1^0 \quad (\text{Region 1})$$

$$W_2 = W_2^0 \quad (\text{Region 2})$$

$$W_3 = W_3^0 \quad (\text{Region 3})$$

$$W_5 = W_5^0 \quad (\text{Region 5})$$

C. Conservation of Mass equations (4.13)

Eq. (4.9) for Region 1

Eq. (4.9) for Region 2

Eq. (4.9) for Region 3

Eq. (4.9) for Region 5

D. Required Energy

(4.14)

$$d_1 x_{111} + d_2 x_{211} = R_3$$

$$x_{121} = R_4$$

$$d_5 x_{112} + d_6 x_{212} = R_7$$

$$x_{122} = R_8$$

$$d_9 x_{113} + d_{10} x_{213} = R_{11}$$

$$x_{123} = R_{12}$$

$$d_{13} x_{115} + d_{14} x_{215} = R_{15}$$

E. Purification Limits

(4.15)

$$d_1 x_{111} + d_2 x_{211} - Z_{11} \geq 0$$

$$x_{121} - Z_{21} \geq 0$$

$$d_5 x_{112} + d_6 x_{212} - Z_{12} \geq 0$$

$$x_{122} - Z_{22} \geq 0$$

$$d_9 x_{113} + d_{10} x_{213} - Z_{13} \geq 0$$

$$x_{123} - Z_{23} \geq 0$$

$$x_{113} - Z_{15} \geq 0$$

F. Air quality standard limitation

(4.16)

$$S_1 \leq L$$

$$S_2 \leq L$$

$$S_3 \leq L$$

$$S_5 \leq L$$

G. Relationships between pollutants in and out among regions (4.17)

$$Y_k = Y_{kj}$$

$$Y_j = Y_{jk}$$

where

X_{ijk} = total amount of fuel used per hour in tons for fuel grade i ,
emission source j , and region k .

Z_{jk} = total amount of fuel whose emission is cleaned for emission
source j and region k (in tons)

W_k = background pollutants concentration in region k (in p.p.m.)

Y_{jk} = average concentrations of pollutants in region j from where
the pollutants are transported into region k by wind. (in
p.p.m.)

Y_k = Average concentration of pollutants in region K (in p.p.m.)

S_k = Air quality of region k (in p.p.m.)

L = air quality standard (in p.p.m.)

C_d = upward dispersion pollutants concentration (in p.p.m.)

C_i 's = cost of various fuels

d_i 's = relative heat values among different fuels

R_i 's = amount of energy required. (in tons)

A_i 's = the total amount of pollutants emitted per ton of certain
fuel (in p.p.m.)

P_i 's = the total amount of pollutants cleaned per ton of certain
fuel (in p.p.m.)

Q_i 's = number of times the air of certain region are completely
replaced by the air of upwind region.

For the first time period, the value of W_i must be obtained by measuring the amount of pollutants in the region. For the second and later time periods, these values are calculated from the result of the previous time periods.

The values for Y_k are the most difficult to obtain. Since Y_k are dependent on X , Z , W , and Y_{jk} , it cannot be determined until X , Z , W , and Y_{jk} are determined. In this work, an equation relating Y_k with X , Z , W , and Y_{jk} is obtained by using the theory of Conservation of Mass. For illustration, let us consider a region k (see Figure 2.) with xyz cubic miles. The wind speed and direction are shown in Figure 2. Now, according to the theory of Conservation of Mass, we have

$$\frac{dM}{dt} = yzU_{in}\rho_{in} + M_p - yzU_{out}\rho_{out} - M_d \quad (4.1)$$

where

$\frac{dM}{dt}$ = the rate of change of mass of certain pollutant in the region (in lbs/min.)

M_p = mass of certain pollutant produced during a unit of time (min.)

M_d = mass of certain pollutant dispersed upward during a unit of time (min.)

U_{in} = wind speed in (in ft./min.)

U_{out} = wind speed out (in ft./min.)

ρ_{in} = density of certain pollutant transported into the region (in lbs/ft³)

ρ_{out} = density of certain pollutant transported out of the region
(in lbs/ft³)

$V = xyz$

$M = V \rho$

where

V = volume of the region (in ft³)

ρ = density of certain pollutants in the region (in p.p.m.)

Since we assume that the pollutants are uniform during the time period within the region, we have

$$\rho = \rho_{out} \quad (4.2)$$

Rewrite Eq. (4.1), we have

$$V \frac{d\rho}{dt} = U_{in} yz \rho_{in} + \rho_p \cdot V - yz U_{out} \rho - \rho_d V \quad (4.3)$$

where

ρ_p = density of certain pollutant produced per unit of time (in lbs/ft³)

ρ_d = density of certain pollutant dispersed upward per unit of time (in lbs/ft³)

Divide V for both sides, we have

$$\frac{d\rho}{dt} = \frac{U_{in}}{x} \cdot \rho_{in} + \rho_p - \frac{U_{out}}{x} \cdot \rho - \rho_d \quad (4.4)$$

Change the unit of ρ , ρ_{in} , ρ_p and ρ_d , we have

$$\frac{dc}{dt} = \frac{U_{in}}{x} \cdot c_{in} + c_p - \frac{U_{out}}{x} \cdot c - c_d \quad (4.5)$$

where

c , c_{in} , c_p , c_d correspond to ρ , ρ_{in} , ρ_p , ρ_d , in p.p.m

The initial condition for Eq. (4.5) is

$$C(0) = W \quad (4.6)$$

where

W = background concentration

Solve Eqs. (4.5) and (4.6), we obtain

$$C(t) = \frac{A}{k_2} + \left(W - \frac{A}{k_2}\right) e^{-k_2 t} \quad (4.7)$$

where

$$A = C_p - C_d + \frac{U_{in}}{a} \cdot y \cdot C_{in}$$

$$k_2 = \frac{U_{out}}{a} \cdot y$$

$a = xy$ = area of the region

Now, we can find the average pollutants concentration of the region k during the time period.

$$\bar{C} = Y_k = \frac{1}{60} \int_0^{60} C(t) dt \quad (4.8)$$

$$\begin{aligned} &= \frac{1}{60} \int_0^{60} \left(\frac{A}{k_2} + \left(W - \frac{A}{k_2}\right) e^{-k_2 t} \right) dt \\ &= \frac{A}{k_2} + \frac{W - \frac{A}{k_2}}{60 k_2} [1 - e^{-60 k_2}] \end{aligned} \quad (4.9)$$

Note that the value of C_{in} for the first region which faces the wind is assumed known. The value of C_{in} for the downwind area is the C_{out} of the upwind area.

For each region and each pollutant, relationship such as Eq. (4.9) can be found. Substituting these relationships into Eq. (4.15), the model can be optimized by linear programming.

4.3 COMPUTATIONAL PROCEDURE

- (1) Divide the area of interest into several reasonable regions (usually according to the number of monitoring stations).
- (2) Calculate the area in each region.
- (3) Obtain the following data
 - A. the number of emission sources in each region and the alternative fuels available in each source.
 - B. the emission rates, relative heat value, and cost of each fuel.
 - C. the total amount of fuels needed for each source.
 - D. the efficiency and cost of each control method.
- (4) obtain the following meteorological data from monitoring stations in each region
 - A. Wind speed and direction for each time period
 - B. Background concentrations for each region and each time period.
- (5) Construct the revised dynamic decomposition model
 - A. Set the objective function [Eq. (4.10)]
 - B. Set all the constraints [Eqs. (4.11) - (4.17)]
- (6) Solve the model established in step (5) by IBM special program for linear programming.

4.4 NUMERICAL RESULTS

A hypothetical metropolitan area is divided into four regions (see Figure 3). The area of region 1 is 31.645 square miles. The area of region 2 is 21.09375 square miles. The area of region 3 is 35.1563 square miles. The area of region 5 is 21.09375 square miles. To illustrate, the time period chosen is from 12:01 Dec. 28, 1970 to 13:00 Dec. 28, 1970. For simplicity, only SO_2 is considered. The meteorological data of each region were obtained from the monitoring stations of each region. The numerical data are given as follows

Region 1

$$W_1 = 0.09 \text{ p.p.m.}$$

$$U_{\text{in}} = U_{\text{out}} = 3.325 \text{ M.P.H.}$$

$$\text{Wind direction} = 98^\circ$$

Region 2

$$W_2 = 0.06 \text{ p.p.m.}$$

$$U_{\text{in}} = U_{\text{out}} = 3.325 \text{ M.P.H.}$$

$$\text{Wind direction} = 98^\circ$$

Region 3

$$W_3 = 0.11 \text{ p.p.m.}$$

$$U_{\text{in}} = U_{\text{out}} = 3.325 \text{ M.P.H.}$$

$$\text{Wind direction} = 98^\circ$$

Region 5

$$W_5 = 0$$

$$U_{in} = U_{out} = 3.325 \text{ MPH}$$

$$\text{Wind direction} = 98^{\circ}$$

The data required for step 3 are

Region 1

Source 1

$$\begin{aligned} \text{Emission rate of fuel 1} &= a_{11} = 1 \text{ lb/Ton} \\ &= 0.00000656 \text{ p.p.m./TON (fuel)} \end{aligned}$$

$$\begin{aligned} \text{Emission rate of fuel 2} &= a_{12} = 0.5 \text{ lb/Ton} \\ &= 0.00000328 \text{ p.p.m./TON (fuel)} \end{aligned}$$

relative heat value of fuel 1 and fuel 2 is 1: 0.95

$$\text{The cost of fuel 1} = C_1 = \$7/\text{TON}$$

$$\text{The cost of fuel 2} = C_2 = \$20/\text{TON}$$

Total fuel required

$$x_{111} + 0.95 x_{211} = 10000 \text{ (Tons)}$$

The purification rate is

$$P_{13} = 0.000003 \text{ p.p.m./Ton (fuel)}$$

$$\text{The cost of purification} = C_3 = \$4/\text{Ton}$$

Source 2

$$\text{Emission rate} = a_{14} = 0.0656 \text{ p.p.m./Ton}$$

$$\text{cost of fuel} = C_4 = \$7/\text{TON}$$

$$\text{purification rate} = p_{17} = 0.000004 \text{ p.p.m./TON}$$

$$\text{The cost of purification} = C_5 = \$10/\text{TON}$$

Total fuel required

$$x_{121} = 9734.4 \text{ Tons}$$

Region 2:

Source 1:

Emission rate of fuel 1 = a_{21} = 0.00000 474 p.p.m./TON

Emission rate of fuel 2 = a_{22} = 0.00000948 p.p.m./TON

purification rate = p_{23} = 0.000003 p.p.m./TON

Relative heat value = 1.1 : 1

Cost of fuel 1 = C_6 = \$20/TON

Cost of fuel 2 = C_7 = \$10/TON

Cost of purification = C_8 = \$12/TON

Total fuel required

$$1.1 x_{112} = x_{212} = 248 \text{ (TONS)}$$

Source 2:

Emission rate = a_{24} = 0.00000948 p.p.m./TON

Purification rate = p_{25} = 0.000005 p.p.m./TON

cost of fuel = C_9 = \$10/TON

cost of purification = C_{10} = \$20/TON

Total fuel required

$$x_{122} = 200 \text{ (TONS)}$$

Region 3

Source 1

Emission rate of fuel 1 = a_{31} = 0.00000569 p.p.m./TON

Emission rate of fuel 2 = a_{32} = 0.00000285 p.p.m./TON

Purification Rate = p_{33} = 0.000002 p.p.m./TON

relative heat value = 1 : 0.95

cost of fuel 1 = C_{11} = \$7/TON

cost of fuel 2 = C_{12} = \$20/TON

cost of purification = C_{13} = \$4/TON

Total fuel required

$$x_{113} + 0.95 x_{213} = 340.1 \text{ (Tons)}$$

Source 2

Emission rate = a_{34} = 0.00000569 p.p.m./TON

purification rate = p_{35} = 0.000004 p.p.m./TON

cost of fuel = C_{14} = \$7/TON

cost of purification = C_{15} = \$10/TON

Total fuel required = x_{123} = 100 (TONS)

Region 5

Emission rate of fuel 1 = a_{41} = 0.00000984 p.p.m./TON

Emission rate of fuel 2 = a_{42} = 0.00000492 p.p.m./TON

Purification rate = p_{43} = 0.000004 p.p.m./TON

Relative heat value = 1 : 0.8

Cost of fuel 1 = C_{16} = \$5/TON

Cost of fuel 2 = C_{17} = \$20/TON

Cost of purification = C_{18} = \$16/TON

According to the data given above, three different cases are considered: (1) Assuming there is not upward dispersion ($M_d = 0$), and the allowable air quality is $L = 0.1$ p.p.m.; (2) Assuming there is upward dispersion ($M_d = 1/3 M_p$), and $L = 0.08$ p.p.m., (3) Same as (2), except the background concentration changed, and $L = 0.05$ p.p.m.

4.4.1 Case 1

$$M_d = 0$$

$$S_1 \leq 0.1 \text{ ppm}$$

$$S_2 \leq 0.1 \text{ ppm}$$

$$S_3 \leq 0.1 \text{ ppm}$$

$$S_5 \leq 0.1 \text{ ppm}$$

By using the numerical data given and following the procedures cited in Section 4.3, a revised dynamic decomposition model can be established which is shown in Table 17. By using IBM special program for linear programming this model can be optimized. The optimal, solution is presented in Table 24.

4.4.2 Case 2:

$$M_d = 1/3 M_p,$$

$$S_1 \leq 0.08 \text{ p.p.m.}$$

$$S_2 \leq 0.08 \text{ p.p.m.}$$

$$S_3 \leq 0.08 \text{ p.p.m.}$$

$$S_5 \leq 0.08 \text{ p.p.m.}$$

By using the new set of data and following the same procedure as case 1, a new optimal solution can be obtained. Table 15 is the optimal solution.

4.4.3. Case 3:

$$M_d = 1/3 M_p$$

$$S_1 \leq 0.05 \text{ p.p.m.} \quad W_1 = 0.045 \text{ p.p.m.}$$

$$S_2 \leq 0.05 \text{ p.p.m.} \quad W_2 = 0.06 \text{ p.p.m.}$$

$$S_3 \leq 0.05 \text{ p.p.m.} \quad W_3 = 0.055 \text{ p.p.m.}$$

$$S_5 \leq 0.05 \text{ p.p.m.} \quad W_5 = 0. \quad \text{p.p.m.}$$

The optimal solution for this case is shown in Table 11.

4.5 DISCUSSION

From the above results, we can see that air quality control can be simulated by a linear programming model. The model could also be extended to include many more pollution sources and to cover a larger metropolitan area composed of many more regions. In addition, the model can be extended to cover a sequence of time periods where the output of one time period became the input of the next time period for the same region. By using this model, a desired air quality level can be established with a minimal cost.

It should be emphasized that the pollutants concentrations are assumed uniform within each region and within a specific time period. Thus, the region must be reasonably small.

The values of Y_k depend on X , Z , W , and Y_{jk} . The equality constraints which representing the relationships among Y_k , X , Z , W , and Y_{jk} are needed in each time period for each pollutant in each region. Since Y_{jk} and Y_k are also dependent on meteorological data, such as wind direction, wind speed and upward dispersion rate, the values of Y_{jk} and Y_k are changing with time. In order to use this model more efficiently, an online computer which can update the values of Y_{jk} and Y_k is needed. By doing so, the online air pollution control system for the entire region can be established.

The application of this method will enable the industry and community to improve their planning and design of their environments considering the air pollution problems. By the use of this method, any desired air quality level can be established with a minimal cost requirement.

Table 24. Optimal Solution - Case 1

WD = 98° W1 = 0.09 W3 = 0.11 L = 0.1
 WS = 3.325 MPH W2 = 0.06 W5 = 0 M_d = 0

Total Minimum Cost = 261618.52359

Region 1	Region 2	Region 3	Region 5
X ₁₁₁ = 1000.	X ₁₁₂ = 0	X ₁₁₃ = 340	X ₁₁₅ = 281.792
X ₂₁₁ = 0	X ₂₁₂ = 248	X ₂₁₃ = 0	X ₂₁₅ = 0
Z ₁₁ = 10000	Z ₁₂ = 0	Z ₁₃ = 0	Z ₁₅ = 0
X ₁₂₁ = 9734.4	X ₁₂₂ = 200	X ₁₂₃ = 100	W ₅ = 0
Z ₂₁ = 7450.80636	Z ₂₂ = 0	Z ₂₃ = 0	Y ₀₅ = 0
W ₁ = 0.09	W ₂ = 0.06	W ₃ = 0.11	Y ₁₅ = 0.09485
Y ₀₁ = 0	Y ₀₂ = 0	Y ₁₃ = 0.09485	Y ₂₅ = 0.04467
Y ₂₁ = 0.04467	Y ₂ = 0.04467	Y ₅₃ = 0.03268	Y ₅ = 0.03268
Y ₁ = 0.09485	S ₂ = 0.03259	Y ₃ = 0.08606	S ₅ = 0.02862
S ₁ = 0.1		S ₃ = 0.06782	

Table 15. Optimal Solution - Case 2

WD = 98° W1 = 0.09 ppm W5 = 0
W5 = 3.325 MPH W2 = 0.06 ppm L = 0.09 ppm
Md = 1/3 Mp

Minimum total cost = \$277093.16848

Region 1	Region 2	Region 3	Region 5
X ₁₁₁ = 10000	X ₁₁₂ = 0	X ₁₁₃ = 340	X ₁₁₅ = 281.792
X ₂₁₁ = 0	X ₂₁₂ = 248	X ₂₁₃ = 0	X ₂₁₅ = 0
Z ₁₁ = 10000	Z ₁₂ = 0	Z ₁₃ = 0	Z ₁₅ = 0
X ₁₂₁ = 9734.4	X ₁₂₂ = 200	X ₁₂₃ = 100	W ₅ = 0
Z ₂₁ = 8998.27085	Z ₂₂ = 0	Z ₂₃ = 0	Y ₀₅ = 0
W ₁ = 0.09	W ₂ = 0.06	W ₃ = 0.11	Y ₁₅ = 0.08379
Y ₀₁ = 0	Y ₀₂ = 0	Y ₁₃ = 0.08379	Y ₂₅ = 0.04425
Y ₂₁ = 0.04425	Y ₂ = 0.04425	Y ₀₃ = 0	Y ₅ = 0.02874
Y ₁ = 0.08379	S ₂ = 0.03147	Y ₅₃ = 0.02874	S ₅ = 0.02475
S ₁ = 0.08		Y ₃ = 0.08568	
		S ₃ = 0.06615	

Table 16. Optimal Solution - Case 3

WD = 98° W1 = 0.045 W3 = 0.055 L = 0.05
 WS = 3.325 MPH W2 = 0.06 W5 = 0 M_d = 1/3 M_p

Total Minimum Cost = \$335,504.62051

Region 1	Region 2	Region 3	Region 5
X ₁₁₁ = 6367.21704	X ₁₁₂ = 0	X ₁₁₃ = 340	X ₁₁₅ = 281.792
X ₂₁₁ = 3823.98206	X ₂₁₂ = 248	X ₂₁₃ = 0	X ₂₁₅ = 0
Z ₁₁ = 10,000	Z ₁₂ = 0	Z ₁₃ = 0	Z ₁₅ = 0
X ₁₂₁ = 9734.4	X ₁₂₂ = 200	X ₁₂₃ = 100	W ₅ = 0
Z ₂₁ = 9734.4	Z ₂₂ = 0	Z ₂₃ = 0	Y ₀₅ = 0
W ₁ = 0.045	W ₂ = 0.06	W ₃ = 0.055	Y ₁₅ = 0.04712
Y ₀₁ = 0	Y ₀₂ = 0	Y ₁₃ = 0.04712	Y ₂₅ = 0.04425
Y ₂₁ = 0.04425	Y ₂ = 0.04425	Y ₀₃ = 0	Y ₅ = 0.01675
Y ₁ = 0.04712	S ₂ = 0.03147	Y ₅₃ = 0.01675	S ₅ = 0.00493
S ₁ = 0.05		Y ₃ = 0.04337	
		S ₃ = 0.03411	

Table 17. Formulation of the Revised Dynamic Decomposition Model - Case 1

Descriptions:		REGION 1											REGION 2									
		Col 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19		
Constraints:		Row	X_{111}	X_{112}	Z_{11}	X_{121}	Z_{21}	W_1	Y_{01}	Y_{21}	Y_1	S_1	X_{112}	X_{212}	Z_{12}	X_{122}	Z_{22}	W_2	Y_{02}	Y_2	S_2	
A Balance Equations:		1	0.0656	0.0328	-0.03	0.0656	-0.04	10000	1938	822.6	-6677	-10000	0.0474	0.0948	-0.03	0.0948	-0.05	10000	1500	-7086	-10000	
B Give Background Concentration:		2																				
		3																				
		4																				
		5																				
		6																				
		7																				
		8																				
C Conservation of Mass Eqs.:		9	0.0656	0.0328	-0.03	0.0656	-0.04	18018.66135.68	548.34	-24700			0.0474	0.0948	-0.03	0.0948	-0.05	17831	7069.11	-24900		
		10																				
		11																				
D Energy Required:		12	1	0.95		1							1.1	1		1						
		13																				
		14																				
		15																				
		16																				
		17																				
		18																				
		19																				
E Purification Limit:		20	1	0.95	-1	1	-1						1.1	1	-1	1	-1					
		21																				
		22																				
		23																				
		24																				
		25																				
		26																				
F Air Quality Standard:		27																				
		28																				
		29																				
		30																				
G Relationship of Pollutants in and out:		31								1												
		32									-1									-1		
		33																				
		34																				
		35																				
		36																				
		37																				
		38																				
		39																				
Objective function		7	20	4	7	10							20	10	12	10	20					

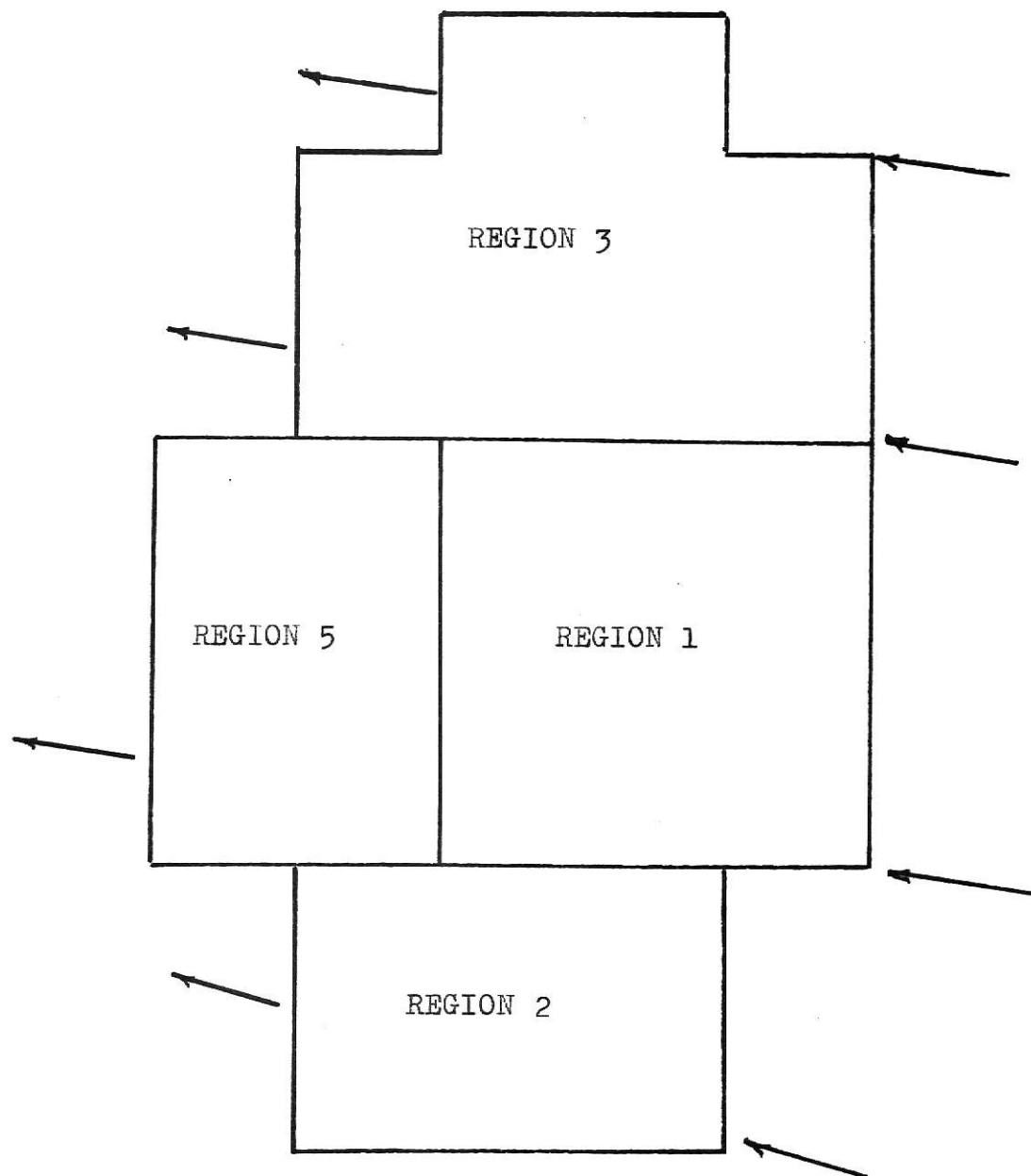


Figure 3. The Metropolitan Air Pollution Control Regions

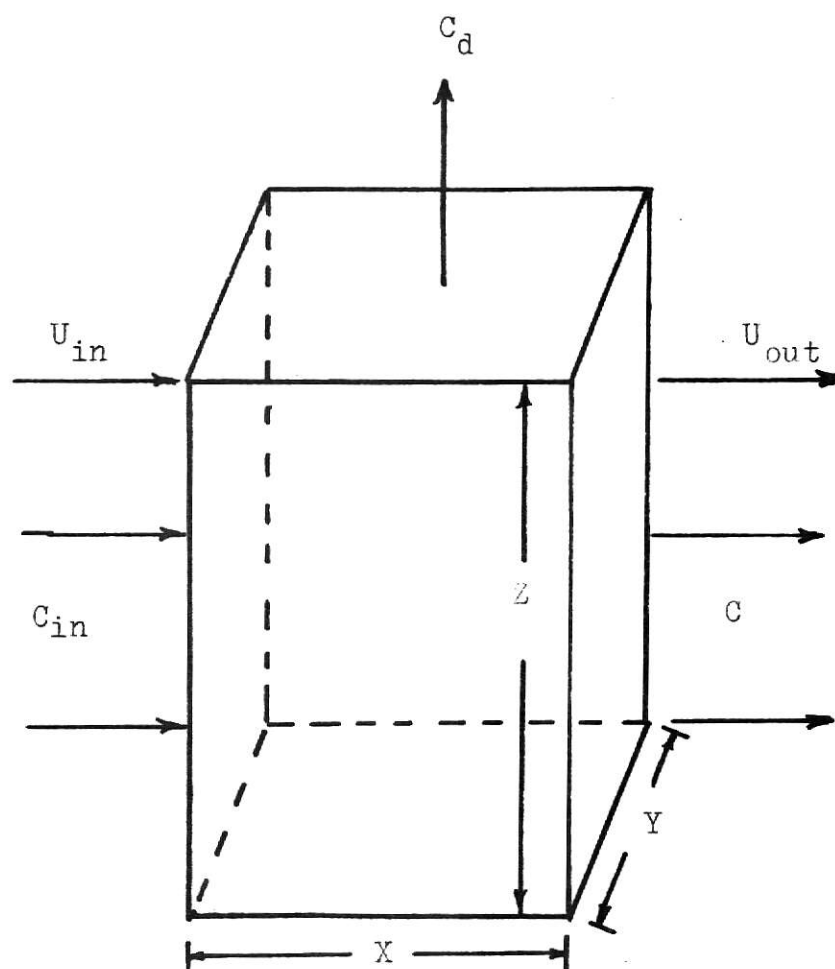


Figure 2. Schematic Representation of Pollutant Transportation

CHAPTER 5

IDENTIFICATION OF THE KINETICS OF GLUCOSE AND INSULIN IN PLASMA
BY QUASILINEARIZATION

5.1 INTRODUCTION

The purpose of this chapter is to introduce an effective technique for estimating parameters or coefficients in differential equations arising in glucose-insulin kinetics modeling. The parameter estimation problem is treated as a two-point or multipoint boundary-value problem by the quasilinearization technique [8, 20]. This technique for estimating parameters has been applied successfully in other fields [20, 21, 28]. It is shown that this technique is also a fairly useful approach for glucose-insulin kinetics modeling.

5.2 THE MODEL

To illustrate the approach, consider the following simple model of glucose and insulin in plasma (one compartment) proposed by Ackerman et al [33, 34]

$$\frac{dH}{dt} = -I_1 H + I_3 G + I_2 \quad (5.1)$$

$$\frac{dG}{dt} = -I_4 G - I_6 H + I_5 \quad (5.2)$$

where

$G \equiv$ plasma glucose concentration

$H \equiv$ plasma IRI concentration

I_i , $i = 1, 2, 3, 4, 5$ and 6 are constants; I_1 , I_3 , I_4 , I_5 , and I_6 must be positive if the equations (5.1) and (5.2) are to remain "physiological".

In actual experimental situations, the constants I_1 , I_2 , ..., I_6 cannot be measured directly. Only H and G can be measured at various values of t . The constants must be estimated from these experimental values. Eqs. (5.1) and (5.2) can be solved in closed form, so the estimation of these constants is not very difficult. However, if the closed form solutions for the equations representing the process cannot be obtained, the estimation of constants from experimental data is very difficult to obtain. Even if closed-form solutions for the process model could be obtained, as in Eqs. (5.1) and (5.2), the present approach of estimating the parameters directly from the differential equations, not from the closed form solution, still has distinct advantages. Note that the parameters or constants appear nonlinearly in the resulting analytical solution of Eqs. (1) and (2). The estimation of parameters for nonlinear algebraic equations is not easy. The quasilinearization approach seems to be much more powerful than the commonly used nonlinear regression, or nonlinear least square estimation techniques.

The problem can be stated as follows: estimate the constants I_1 , I_3 , I_4 , and I_6 for Eqs. (5.1) and (5.2) with the following measured or experimental data

$$I_2 = -1.56 \qquad I_5 = 6.94$$

$$H^{(\text{exp})}(t_s) = h_s, \quad s = 1, 2, \dots, m_1 \quad (5.3)$$

$$G^{(\text{exp})}(t_r) = g_r, \quad r = 1, 2, \dots, m_2 \quad (5.4)$$

with $m_1 + m_2 \geq 0$, $0 \leq t_s \leq t_f$, and

$0 \leq t_r \leq t_f$. The initial conditions for (1) and (2) are

$$H(0) = H^0 \quad G(0) = G^0 \quad (5.5)$$

The quantities h_s and g_r are known values and are obtained by measuring H and G experimentally at various values of t . The number of the experimental values must be larger than or equal to the number of the unknown constant parameters. The superscript (exp) denotes that the values are experimental values. Note that t_s and t_r are not necessarily the same. The data of H and G from reference [35] will be used as experimental data which is shown in Table 19. The technique to be discussed can be used in the same way if experimental data exist for only one of the variables.

For practical situations, the experimental data are not exact and have experimental errors. Thus, it is desirable to obtain a fairly large amount of data instead of just 6. For $m_1 + m_2 > 6$, the classical least squares criterion can be used. The object is to determine the parameters so that the sum of the deviations is minimized.

5.3 SIX EXPERIMENTAL DATA

First, the case in which $m_1 + m_2 = 6$ (including the initial conditions for H and G) is considered. Assume that only the following six data points are available for estimating the four constants, I_1 , I_3 , I_4 , and I_6 and two unknown initial conditions

$$\begin{aligned}
H^{(\text{exp})}(0) &= H^0 & G^{(\text{exp})}(0) &= G^0 \\
H^{(\text{exp})}(t_1) &= h_1 & G^{(\text{exp})}(t_1) &= g_1 \\
H^{(\text{exp})}(t_2) &= h_2 & G^{(\text{exp})}(t_2) &= g_2
\end{aligned} \tag{5.6}$$

It is assumed that the experimental errors resulting from obtaining the experimental data are very small, and thus these experimental data can be considered as the true values of H and G at the given values of t . To estimate the constants, it is convenient to consider the unknown parameters, I_1, I_3, I_4, I_6 as dependent variables parallel to H and G as functions of the independent variable t . Because these functions do not change with t , one can write

$$\frac{dI_1}{dt} = 0 \tag{5.7}$$

$$\frac{dI_3}{dt} = 0 \tag{5.8}$$

$$\frac{dI_4}{dt} = 0 \tag{5.9}$$

$$\frac{dI_6}{dt} = 0 \tag{5.10}$$

Now, the six simultaneous differential equations, Eqs. (5.1), (5.2), and (5.7) - (5.10), can be solved by the use of the following six boundary conditions

$$H(0) = H^0 \tag{5.11a}$$

$$G(0) = G^0 \tag{5.11b}$$

$$H(t_1) = h_1 \quad (5.11c)$$

$$H(t_2) = h_2 \quad (5.11d)$$

$$G(t_1) = g_1 \quad (5.11e)$$

$$G(t_2) = g_2 \quad (5.11f)$$

Note that the experimental data have been used as boundary conditions. Because these boundary conditions are not all given at one point, they form a multipoint boundary-value problem. The quantities t_1 and t_2 are two discrete values of t within the interval $0 \leq t \leq t_f$.

5.4 PROBLEM WITH MORE THAN SIX EXPERIMENTAL DATA

For nearly all practical situations, the experimental data are not exact and have experimental errors. Thus, it is desirable to obtain a fairly large amount of data instead of just six data points. For $m_1 + m_2 > 6$, the classical least squares criterion can be used. The object is to determine the parameters so that the sum of the squares of the deviations is minimized. Instead of boundary conditions (5.11a) through (5.11f), one can obtain these six conditions by minimizing the following least squares expression

$$Q = \sum_{s=1}^{m_1} [H(t_s) - h_s]^2 + \sum_{r=1}^{m_2} [G(t_r) - g_r]^2 \quad (5.12)$$

where the minimization is over the parameters, I_1 , I_3 , I_4 , and I_6 . $H(t_s)$ and $G(t_r)$ are obtained by solving Eqs. (5.1) and (5.2).

5.5 COMPUTATIONAL CONSIDERATION

Since both the parameters I_1 , I_3 , I_4 , and I_6 , and the original variables H and G are considered unknown functions, Eqs. (5.1) and (5.2)

are nonlinear equations. Thus, the system represented by Eqs. (5.1), (5.2), and (5.7) - (5.10) are nonlinear systems with multipoint boundary conditions. In general, nonlinear equations cannot be solved analytically. Furthermore, numerical solution cannot be obtained easily because of the fact that the boundary conditions are given at several different points. To overcome this computational difficulty, the quasilinearization technique, also known as the generalized Newton-Raphson method, can be used. In this method, the solution of the nonlinear equation is obtained by solving a sequence of linear equations. The solution of this sequence of linear equations converge rapidly to the solution of the original nonlinear equation provided that the process converges. This quadratic convergence property is the main advantage of the quasilinearization approach. Quadratic convergence means that the error in the current iteration tends to be proportional to the square of the error in the previous iteration.

5.6 COMPUTATIONAL PROCEDURE

The estimation problem for the model of the Kinetics of glucose and insulin in plasma can now be approached by the quasilinearization technique. The system represented by Eqs. (5.1), (5.2), and (5.7) - (5.10) can be linearized by using Eq. (2.3) with $M = 6$. The linearized equations are

$$\begin{aligned} \frac{dH_{n+1}}{dt} = & - I_{1,n} H_{n+1} + I_{3,n} G_{n+1} + I_2 + I_{3,n+1} G_n \\ & - I_{1,n+1} H_n + I_{1,n} H_n - I_{3,n} G_n \end{aligned} \quad (5.17)$$

$$\begin{aligned} \frac{dG_{n+1}}{dt} = & -I_{6,n}H_{n+1} - I_{4,n}G_{n+1} + I_5 + I_{4,n}G_n \\ & + I_{6,n}H_n - I_{4,n+1}G_n - I_{6,n+1}H_n \end{aligned} \quad (5.18)$$

$$\frac{dI_{1,n+1}}{dt} = 0 \quad (5.19)$$

$$\frac{dI_{3,n+1}}{dt} = 0 \quad (5.20)$$

$$\frac{dI_{4,n+1}}{dt} = 0 \quad (5.21)$$

$$\frac{dI_{6,n+1}}{dt} = 0 \quad (5.22)$$

The two assumed boundary conditions are

$$H_{n+1}(0) = H^0 = H^{(exp)}(t_0) \quad (5.23)$$

$$G_{n+1}(0) = G^0 = G^{(exp)}(t_0) \quad (5.24)$$

The six boundary conditions can be obtained either by using Eqs. (5.11a) through (5.11f) or by minimizing Eq. (5.12). Because the use of least squares is a more practical problem, this approach will use the minimization of Eq. (5.12).

Eqs. (5.17) through (5.22) are linear equations with variable coefficients. In general, they cannot be solved in closed form. However, since they are linear equations, the superposition principle can be used. It is known that for six simultaneous linear equations, the general solution can be represented by six sets of homogeneous solutions and one

set of particular solution. Thus, the general solutions of Eqs. (5.17) through (5.22) are

$$\begin{aligned}
 H_{n+1}(t) &= H_{p,n+1} + \sum_{j=1}^q A_{j,n+1} H_{hj,n+1}(t) \\
 G_{n+1}(t) &= G_{p,n+1} + \sum_{j=1}^q A_{j,n+1} G_{hj,n+1}(t) \\
 I_{1,n+1}(t) &= I_{1p,n+1}(t) + \sum_{j=1}^q A_{j,n+1} I_{1hj,n+1}(t) \\
 I_{3,n+1}(t) &= I_{3p,n+1}(t) + \sum_{j=1}^q A_{j,n+1} I_{3hj,n+1}(t) \\
 I_{4,n+1}(t) &= I_{4p,n+1}(t) + \sum_{j=1}^q A_{j,n+1} I_{4hj,n+1}(t) \\
 I_{6,n+1}(t) &= I_{6p,n+1}(t) + \sum_{j=1}^q A_{j,n+1} I_{6hj,n+1}(t)
 \end{aligned} \tag{5.25}$$

with $q = 6$. The subscript p is used to indicate particular solution, and subscripts $h1, h2, \dots, h6$ denote the first, second, ..., and sixth set of homogeneous solutions respectively. The A 's are integration constants to be determined from the boundary conditions.

The six sets of homogeneous solutions and one set of particular solutions must be obtained numerically. However, because they can be any solutions of Eqs. (5.17) through (5.22) as long as the homogeneous solutions are nontrivial and distinct, any set of initial conditions

can be used to obtain the particular solutions, and any six sets of initial conditions, as long as they are nontrivial and distinct, can be used to obtain the six sets of homogeneous solutions. In actual calculations, the following set of initial conditions is used for the particular solutions

$$H_{p,n+1}(0) = H^0 = H^{(\text{exp})}(t_0)$$

$$G_{p,n+1}(0) = G^0 = G^{(\text{exp})}(t_0)$$

$$I1_{p,n+1}(0) = 0$$

$$I3_{p,n+1}(0) = 0 \tag{5.26}$$

$$I4_{p,n+1}(0) = 0$$

$$I6_{p,n+1}(0) = 0.$$

The homogeneous forms of Eqs. (5.17) through (5.22) are

$$\frac{dH_{n+1}}{dt} = -I_{1,n}H_{n+1} + I_{3,n}G_{n+1} + I_{3,n+1}G_n - I_{1,n+1}H_n \tag{5.27}$$

$$\frac{dG_{n+1}}{dt} = -I_{6,n}H_{n+1} - I_{4,n}G_{n+1} - I_{4,n+1}G_n - I_{6,n+1}H_n \tag{5.28}$$

$$\frac{dI_{1,n+1}}{dt} = 0 \tag{5.29}$$

$$\frac{dI_{3,n+1}}{dt} = 0 \tag{5.30}$$

$$\frac{dI_{4,n+1}}{dt} = 0 \quad (5.31)$$

$$\frac{dI_{6,n+1}}{dt} = 0 \quad (5.32)$$

The initial conditions used to obtain the homogeneous solutions are listed in Table 18. The six integration constants, $A_{1,n+1}$, $A_{2,n+1}$, $A_{3,n+1}$, $A_{4,n+1}$, $A_{5,n+1}$, and $A_{6,n+1}$ can be obtained from the six boundary conditions. For the case $m_1 + m_2 > 6$, these six conditions can be obtained by minimizing Eq. (5.12) at various positions of t_s and t_r , $s = 1, 2, \dots, m_1$ and $r = 1, 2, \dots, m_2$. The following $m_1 + m_2$ equations can be obtained from the first two equations of Eq. (5.25) with $q = 6$

$$H_{n+1}(t_s) = H_{p,n+1}(t_s) + \sum_{j=1}^6 A_{j,n+1} H_{hj,n+1}(t_s) \quad (5.33)$$

$$G_{n+1}(t_r) = G_{p,n+1}(t_r) + \sum_{j=1}^6 A_{j,n+1} G_{hj,n+1}(t_r) \quad (5.34)$$

Substituting Eqs. (5.33) and (5.34) into Eq. (5.12), we have

$$Q = \sum_{s=1}^{m_1} [H_{p,n+1}(t_s) + \sum_{j=1}^6 A_{j,n+1} H_{hj,n+1}(t_s) - h_s]^2 + \sum_{r=1}^{m_2} [G_{p,n+1}(t_r) + \sum_{j=1}^6 A_{j,n+1} G_{hj,n+1}(t_r) - g_r]^2 \quad (5.35)$$

The particular and homogeneous solutions at the various positions of t are obtained numerically by using the initial values listed in Eq. (5.26) and Table 18. h_s and g_r are obtained from actual experimental

data. The only unknown values in the right-hand side of Eq. (5.35) are the six integration constants, $A_{1,n+1}$, $A_{2,n+1}$, $A_{3,n+1}$, $A_{4,n+1}$, $A_{5,n+1}$, and $A_{6,n+1}$. So, the problem is to find the values of these constants such that the value of Q is minimized. There are several techniques could handle the minimization problem. For this work, the extreme values will be obtained by partial differentiation. By differentiating Eq. (5.35) with respect to $A_{1,n+1}$, $A_{2,n+1}$, $A_{3,n+1}$, $A_{4,n+1}$, $A_{5,n+1}$, and $A_{6,n+1}$, and setting the results equal to zero, the following six equations can be obtained

$$\begin{aligned} \frac{\partial Q}{\partial A_{i,n+1}} = & 2 \sum_{s=1}^{m_1} H_{hi,n+1}(t_s) [H_{p,n+1}(t_s) + \sum_{j=1}^6 A_{j,n+1} \cdot \\ & H_{hj,n+1}(t_s) - h_s] + \sum_{r=1}^{m_2} 2 G_{hi,n+1}(t_r) \cdot \\ & [G_{p,n+1}(t_r) + \sum_{j=1}^6 A_{j,n+1} G_{hj,n+1}(t_r) - G_r] \\ = & 0 \quad i = 1, 2, 3, 4, 5, \text{ and } 6 \end{aligned} \quad (3.36)$$

These six equations form the six boundary conditions. The unknowns of these six algebraic equations are $A_{j,n+1}$, $j = 1, 2, 3, 4, 5, 6$. They can be obtained by solving these six equations. The Gauss Elimination method is used in this work. Thus, the computational procedure can be summarized as follows

1. Assume a set of reasonable initial functions for $H(t)$, $G(t)$, $I_1(t)$, $I_3(t)$, $I_4(t)$, and $I_6(t)$. Let these initial functions be $H_{n=0}(t)$,

$G_{n=0}(t)$, $I_{1,n=0}(t)$, $I_{3,n=0}(t)$, $I_{4,n=0}(t)$, and $I_{6,n=0}(t)$.

2. Integrate Eqs. (5.17) through (5.22) numerically using Eq. (5.26) as the initial values and with $n = 0$.
3. Integrate the homogeneous Eqs. (5.27) through (5.32) six times using Table 18 as the initial values and with $n = 0$.
4. Solve Eq. (5.36) for $A_{j,n+1=1}$, $j = 1, 2, 3, 4, 5, 6$, using the newly obtained particular and homogeneous solutions from step 2 and 3 and using the given experimental data h_s and G_r .
5. Calculate $H_{n+1}(t)$, $G_{n+1}(t)$, $I_{1,n+1}(t)$, $I_{3,n+1}(t)$, $I_{4,n+1}(t)$, and $I_{6,n+1}(t)$ by using Eq. (5.25) with $q = 6$.
6. Repeat steps 2 through 5 with $n = 1, 2, \dots$, until no further improvement on the values of $H(t)$, $G(t)$, I_1 , I_3 , I_4 , and I_6 can be obtained.

It should be noted that the best available initial functions should be used for step 1.

5.7 NUMERICAL RESULTS

To test the effectiveness of this approach, the parameters, I_1 , I_3 , I_4 , and I_6 in Eqs. (5.1) and (5.2) are estimated by using the following numerical data

$$I_2 = -1.56, \quad I_5 = 6.94, \quad t_f = 180 \text{ (minutes)}$$

$$\Delta t = 0.2 \text{ (minute)}, \quad H^0 = 177, \quad G^0 = 581$$

Experimental data for H and G are shown in Table 19.

By using the above numerical data and the procedures cited earlier, this four parameters estimation problem is solved. Four sets of solutions are obtained by using four different sets of initial functions

which is given as follows

$$1. \quad I_{1,n=0}(t) = 0.0457$$

$$I_{3,n=0}(t) = 0.0248$$

$$I_{4,n=0}(t) = 0.063$$

$$I_{6,n=0}(t) = 0.003$$

$$H^0 = H^{(\text{exp})}(t_0) = 177$$

$$G^0 = G^{(\text{exp})}(t_0) = 581$$

$$H_{n=0}(t) = H(t)^*$$

$$G_{n=0}(t) = G(t)^*$$

$$2. \quad I_{1,n=0}(t) = 0,01 \quad H^0 = 177 \quad G^0 = 581$$

$$I_{3,n=0}(t) = 0,01 \quad H_{n=0}(t) = H(t)^*$$

$$I_{4,n=0}(t) = 0,01$$

$$I_{6,n=0}(t) = 0.01 \quad G_{n=0}(t) = G(t)^*$$

$$3. \quad I_{1,n=0}(t) = 0.1 \quad H_0 = 177 \quad G_0 = 581$$

$$I_{3,n=0}(t) = 0.1 \quad H_{n=0}(t) = H(t)^*$$

$$I_{4,n=0}(t) = 0.1 \quad G_{n=0}(t) = G(t)^*$$

$$I_{6,n=0}(t) = 0.1$$

(5.37)

$$\begin{aligned}
4. \quad I_{1,n=0}(t) &= 0. & H_0 &= 177 & G_0 &= 581 \\
I_{3,n=0}(t) &= 0. & H_{n=0}(t) &= H(t)^* \\
I_{4,n=0}(t) &= 0. & G_{n=0}(t) &= G(t)^* \\
I_{6,n=0}(t) &= 0.
\end{aligned}$$

Where $H(t)^*$, $G(t)^*$ are solutions obtained by using assumed parameter values and assumed initial conditions of H and G to integrate Eqs. (5.1) and (5.2). The Runge-Kutta integration scheme with $\Delta t = 0.2$ was used. The convergence rates with the four different sets of initial functions are shown in tables 20_a , 20_b , 20_c , and 20_d respectively. The convergence rates of H and G with the set 1 data are shown in Figure 12 and 13 respectively.

5.8 DISCUSSION AND CONCLUSION

In practical situations, the parameters I_2 and I_5 cannot be measured directly for most cases. Thus, a practically important problem is to estimate I_1 , I_2 , I_3 , I_4 , I_5 , and I_6 . This problem can be solved in essentially the same way as before except for the presence of six unknown parameters. The system can be represented by Eqs. (5.1), (5.2), (5.7) - (5.10), and

$$\frac{dI_2}{dt} = 0 \tag{5.38}$$

$$\frac{dI_5}{dt} = 0 \tag{5.39}$$

This system can be solved in the same way as before. Since the original model which represented by Eqs. (5.1) and (5.2) can be simplified to [35]

$$\frac{dh}{dt} = -I_1 h + I_3 g \quad (5.40)$$

$$\frac{dg}{dt} = -I_4 g + I_6 h \quad (5.41)$$

where

$$h \equiv H - H_F$$

$$g \equiv G - G_F$$

$H_F \equiv$ fasting or steady state plasma **IRI** concentration

$G_F \equiv$ fasting or steady state plasma glucose concentration

Once we know the values of H_F and G_F , the original model can be transformed into a new model represented by Eqs. (5.40) and (5.41). So, essentially only I_1 , I_3 , I_4 and I_6 need to be estimated. The initial conditions for H and G are unknown in this problem. We use the experimental data at $t = 0$ as the assumed initial conditions for H and G . Even the initial conditions assumed are not exact, we still could find optimal initial conditions by using quasilinearization technique (See Tables 20_a, 20_b, 20_c, and 20_d). This is the advantage of this approach. Another important advantage is the quadratic convergence nature. The convergence rates for the four constant parameters are listed in Tables 20_a, 20_b, 20_c, and 20_d. It can be seen that only five iterations are needed to obtain a four-digit accuracy. Note that the initially assumed functions as given by Eq. (5.37) are very approximate. As long as the initial approximation are within the convergence interval, the convergence rate will remain the same as shown in Tables 20_a, 20_b, 20_c, and 20_d.

TABLE 18. Initial Conditions used for obtaining the Homogeneous Solutions

Variables	j					
	1	2	3	4	5	6
$H_{hj,n+1}^{(0)}$	1	0	0	1	1	0
$G_{hj,n+1}^{(0)}$	0	1	1	0	0	1
$I_{1hj,n+1}^{(0)}$	0.08	0	1	0.05	0	0
$I_{3hj,n+1}^{(0)}$	0	0.5	0	1	0	0.08
$I_{4hj,n+1}^{(0)}$	0	0.05	0.5	0	1	0
$I_{6hj,n+1}^{(0)}$	0.05	0	0	0	0.05	1

TABLE 19. Numerical Values used as Experimental Data

t_s	S	$H^{(exp)}(t_s) = R_s$	t_R	R	$G^{(exp)}(t_r) = g_r$
0.00	1	177	0.00	1	581
30.00	2	155	30.00	2	182
60.00	3	40	60.00	3	95
90.00	4	26	90.00	4	87
120.00	5	20	120.00	5	97
150.00	6	24	150.00	6	106
180.00	7	28	180.00	7	110

Table 20a. Convergence Rates with Data Set 1

Iteration	I_1	I_3	I_4	I_6	$H(0)$	$g(0)$
0	0.0457	0.0248	0.063	0.003	177.	581.
1	0.03763	0.014189	0.00644	0.06	177.42	579.89
2	0.045142	0.020978	0.025505	0.045667	177.49	580.1
3	0.046147	0.022111	0.028566	0.043367	177.29	580.32
4	0.046411	0.022281	0.028579	0.043292	177.24	580.38
5	0.046410	0.022287	0.028564	0.043512	177.23	580.39
6	0.046423	0.022293	0.028555	0.043523	177.23	580.39
7	0.046422	0.022292	0.028555	0.043523		
8	0.046422	0.022293	0.028555	0.043524		
9	0.046422	0.022293	0.028555	0.043524		

Table 20b. Convergence Rates with Data Set 2

Iteration	I_1	I_3	I_4	I_6	$H(0)$	$g(0)$
0	0.01	0.01	0.01	0.001	177.	581.
1	0.049825	0.025094	0.043074	0.029009	179.78	578.03
2	0.042125	0.019767	0.026236	0.04593	177.21	580.38
3	0.046305	0.022117	0.028411	0.043670	177.42	580.19
4	0.046243	0.022209	0.028638	0.043310	177.23	580.39
5	0.046435	0.022295	0.028559	0.043527	177.24	580.38
6	0.046411	0.022288	0.028561	0.043514	177.23	580.39
7	0.046424	0.022293	0.028554	0.043525	177.23	580.39
8	0.046422	0.022292	0.028555	0.043523		
9	0.046422	0.022293	0.028555	0.043524		
10	0.046422	0.022293	0.028555	0.043506		

Table 20c. Convergence Rates with Data Set 3

Iteration	I_1	I_3	I_4	I_6	H(0)	G(0)
0	0.1	0.1	0.1	0.1	177	581
1	0.057981	0.043455	-0.091183	0.11594	176.04	579.81
2	0.029460	0.010724	0.02330	0.0033317	176.08	581.31
3	0.044468	0.022018	0.041126	0.024042	178.79	578.89
4	0.044671	0.021177	0.027924	0.044250	177.44	580.17
5	0.046365	0.022202	0.028493	0.043597	177.33	580.28
6	0.046355	0.022261	0.028609	0.043443	177.23	580.39
7	0.046426	0.022293	0.028557	0.043524	177.23	580.39
8	0.046418	0.022291	0.028557	0.043520		
9	0.046423	0.022293	0.028555	0.043524		
10	0.046422	0.022293	0.028555	0.043524		
11	0.046422	0.022293	0.028555	0.043504		

Table 20d. Convergence Rates with Data Set 4

Iteration	I_1	I_2	I_4	I_6	$H(0)$	$G(0)$
0	0.	0.	0.	0.	177.	581.
1	0.051076	0.025872	0.048513	0.22224	181.31	576.58
2	0.038405	0.017182	0.020605	0.052089	177.16	580.37
3	0.045445	0.021543	0.028009	0.043957	177.56	580.06
4	0.046151	0.022149	0.028790	0.043174	177.27	580.35
5	0.046411	0.022281	0.028581	0.043500	177.24	580.38
6	0.046408	0.022286	0.028565	0.043510	177.23	580.39
7	0.046423	0.022293	0.028555	0.043523	177.23	580.39
8	0.046421	0.022292	0.028555	0.043523		
9	0.046422	0.022293	0.028555	0.043524		
10	0.046422	0.022293	0.028555	0.043524		

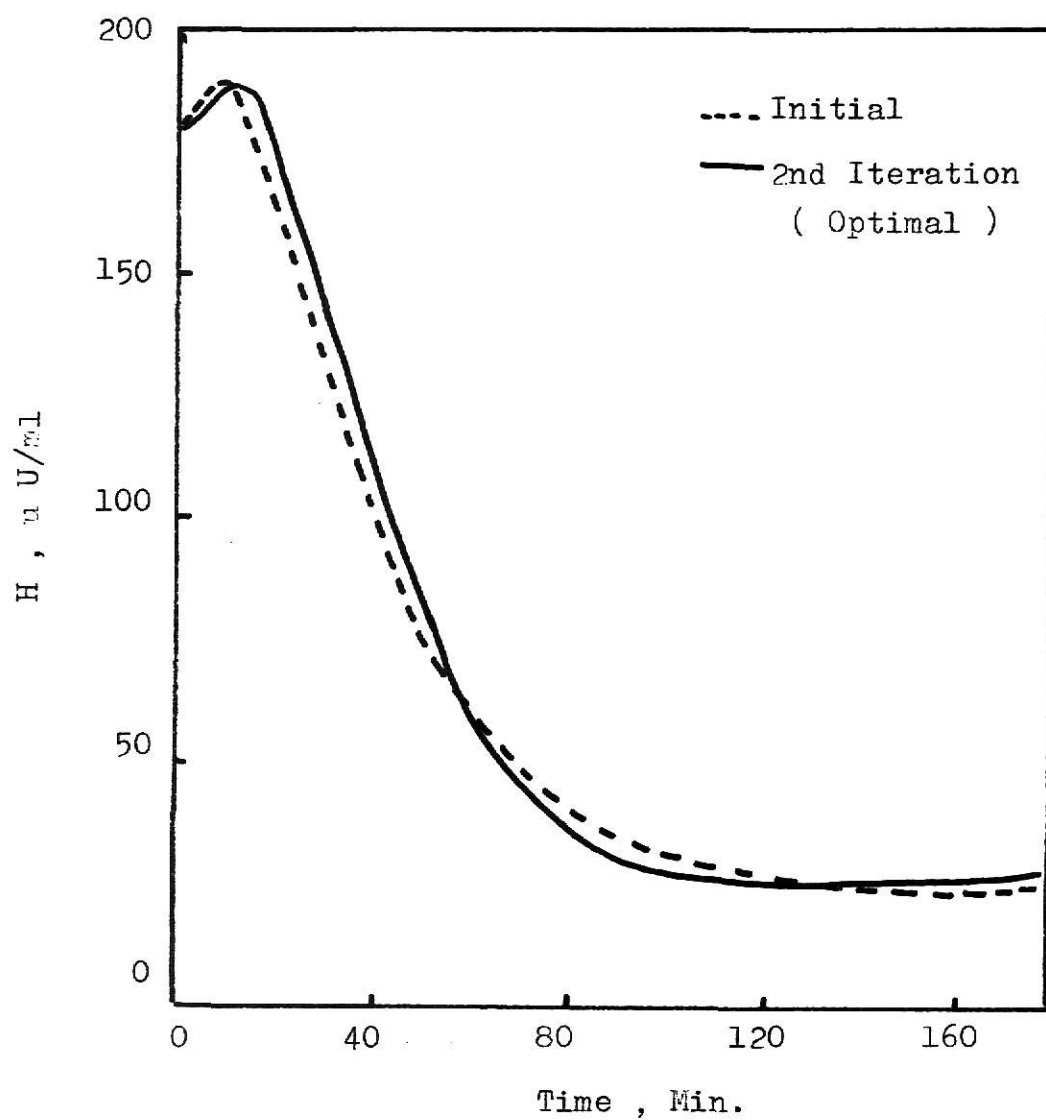


Figure 12. Convergence Rates of H

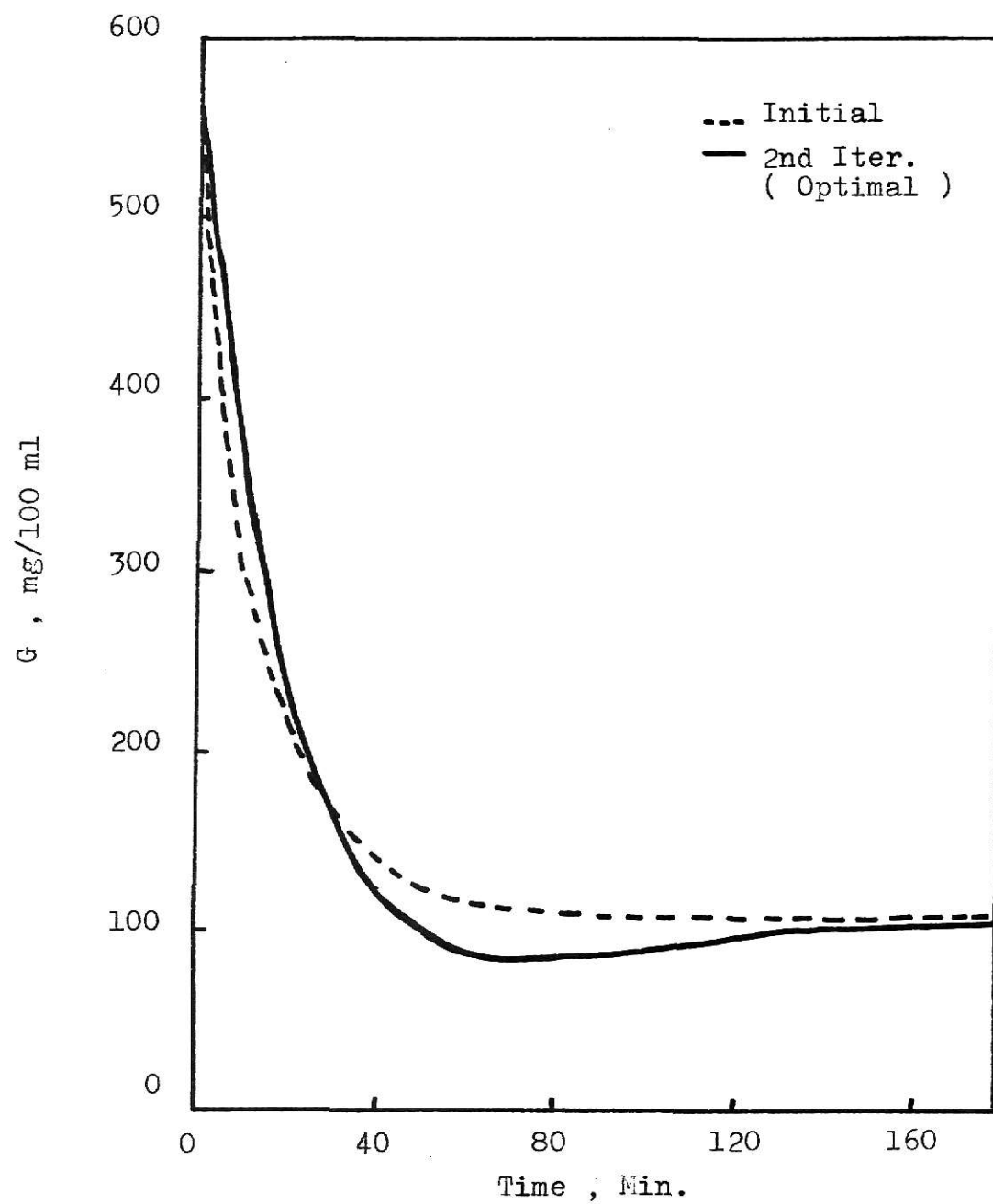


Figure 13. Convergence Rates of G

CHAPTER 6

Identification the model of cardiovascular
indicator-dilution curve by quasilinearization

6.1 INTRODUCTION

The purpose of this chapter is to introduce an effective technique for estimating parameters or coefficients in differential equations arising in cardiovascular indicator-dilution modeling. The parameter estimation problem is treated as a two-point or multipoint boundary-value problem by the quasilinearization technique [8, 20]. This technique for estimating parameters has been applied successfully in other fields [20, 21, 28]. It is shown that this technique is also a fairly useful approach for cardiovascular indicator-dilution curves modeling.

6.2 The model

To illustrate the approach, consider the following simple model of cardiovascular indication-dilution model [36].

$$\frac{dC_1}{dt} = -\frac{F}{V} C_1 + \frac{F_s}{V} C_4 \quad (6.1)$$

$$\frac{dC_2}{dt} = \frac{F}{V} (C_1 - C_2) \quad (6.2)$$

$$\frac{dC_3}{dt} = \frac{F}{V} (C_2 - C_3) \quad (6.3)$$

$$\frac{dC_4}{dt} = \frac{F}{V} (C_3 - C_4) \quad (6.4)$$

with boundary conditions

$$C_1(0) = \frac{M}{V} \quad (6.5)$$

$$C_2(0) = 0 \quad (6.6)$$

$$C_3(0) = 0 \quad (6.7)$$

$$C_4(0) = 0 \quad (6.8)$$

where

V = the volume of the well-mixed cells

F = volumetric flow rate

F_s = recycle volumetric flow rate

M = the mass of injection

Let

$$\begin{aligned} B_1 &= \frac{F}{V} \\ B_2 &= \frac{F_s}{V} \\ B_3 &= \frac{M}{V} \end{aligned} \quad (6.9)$$

The model represented by Eqs. (6.1) - (6.4) can be written as

$$\frac{dC_1}{dt} = -B_1 C_1 + B_2 C_4 \quad (6.10)$$

$$\frac{dC_2}{dt} = B_1 (C_1 - C_2) \quad (6.11)$$

$$\frac{dC_3}{dt} = B_1 (C_2 - C_3) \quad (6.12)$$

$$\frac{dC_4}{dt} = B_1(C_3 - C_4) \quad (6.13)$$

with boundary conditions

$$C_1(0) = B_3 \quad (6.14)$$

$$C_2(0) = 0 \quad (6.15)$$

$$C_3(0) = 0 \quad (6.16)$$

$$C_4(0) = 0 \quad (6.17)$$

where

C_1 = concentration of cell 1

C_2 = concentration of cell 2

C_3 = concentration of cell 3

C_4 = concentration of cell 4

B_1 = constant parameter

B_2 = constant parameter

B_3 = initial condition for C_1

In actual experimental situations, the constant parameters B_1 and B_2 cannot be measured directly. Only C_1 , C_2 , C_3 , and C_4 can be measured at various values of t . The constants must be estimated from these experimental values. Eqs. (6.1) - (6.4) can be solved in closed form, so the estimation of these constants is not very difficult. However,

if the closed form solutions for the equations representing the process cannot be obtained, the estimation of constants from experimental data is very difficult to obtain. Even if closed form solution for the process model could be obtained, as in Eqs. (6.1) - (6.4), the present approach of estimating the parameters directly from the differential equations, not from the closed form solution, still has distinct advantages. Note that the parameters or constants appear nonlinearly in the resulting analytical solution of Eqs. (6.1) - (6.4). The estimation of parameters for nonlinear algebraic equations is not easy. The quasi-linearization approach seems to be much more powerful than the commonly used nonlinear regression, or nonlinear least square estimation techniques.

The problem can be stated: Estimate the constants B_1 and B_2 for Eqs. (6.1) - (6.4) with the following measured or experimental data

$$C_1^{(\text{exp})}(t_s) = C_{1s}, \quad s = 1, 2, \dots, m_1 \quad (6.18)$$

$$C_2^{(\text{exp})}(t_R) = C_{2R}, \quad R = 1, 2, \dots, m_2 \quad (6.19)$$

$$C_3^{(\text{exp})}(t_P) = C_{3P}, \quad P = 1, 2, \dots, m_3 \quad (6.20)$$

$$C_4^{(\text{exp})}(t_Q) = C_{4Q}, \quad Q = 1, 2, \dots, m_4 \quad (6.21)$$

where $m_1 + m_2 + m_3 + m_4 \geq 3$, $0 \leq t_s \leq t_f$,

$$0 \leq t_R \leq t_f \quad 0 \leq t_P \leq t_f \quad 0 \leq t_Q \leq t_f$$

The initial conditions for (6.1) - (6.4) are

$$C_1(0) = B_3 \quad (6.22)$$

$$C_2(0) = 0 \quad (6.23)$$

$$C_3(0) = 0 \quad (6.24)$$

$$C_4(0) = 0 \quad (6.25)$$

The quantities, C_{1S} , C_{2R} , C_{3P} , and C_{4Q} are known values and are obtained by measuring C_1 , C_2 , C_3 , and C_4 experimentally at various values of t . The number of the experimental values must be larger or equal to the number of the unknown constant parameters. The superscript (exp) denotes that the values are experimental values. Note that t_S , t_R , t_P , and t_Q are not necessarily the same. The technique to be discussed can be used in the same way if experimental data exist for only one of the variables.

For practical situations, the experimental data are not exact and have experimental errors. Thus, it is desirable to obtain a fairly large amount of data instead of just three. For $m_1 + m_2 + m_3 + m_4 \geq 3$, the classical least squares criterion can be used. The object is to determine the parameters so that the sum of squares of the deviations is minimized.

6.3 THREE EXPERIMENTAL DATA

First the case in which $m_1 + m_2 + m_3 + m_4 = 3$ is considered. Assume that only the following three data points are available for estimating the two constant parameters, B_1 and B_2

$$c_1^{(\text{exp})}(t_0) = c_1(0)$$

$$c_2^{(\text{exp})}(t_1) = c_{21} \quad (6.23)$$

$$c_3^{(\text{exp})}(t_2) = c_{32}$$

It is assumed that the experimental errors resulting from obtaining the experimental data are very small. Thus, these experimental data can be considered as the true values of C_1 , C_2 , and C_3 at the given values of t . To estimate the constants, it is convenient to consider the unknown parameters, B_1 and B_2 , as dependent variables parallel to C_1 , C_2 , C_3 , and C_4 as functions of the independent variable t . Because these functions do not change with t , one can write

$$\frac{dB_1}{dt} = 0 \quad (6.24)$$

$$\frac{dB_2}{dt} = 0 \quad (6.25)$$

Now, the six simultaneous differential equations, (6.1) - (6.4) and (6.24) - (6.25), can be solved by using the following six boundary conditions

$$c_1(0) = B_3 = c_1^{(\text{exp})}(t_0) \quad (6.24a)$$

$$c_2(0) = 0 \quad (6.24b)$$

$$c_3(0) = 0 \quad (6.24c)$$

$$c_4(0) = 0 \quad (6.24d)$$

$$c_2(t_1) = c_{21} = c_2^{(\text{exp})}(t_1) \quad (6.24e)$$

$$c_3(t_2) = c_{32} = c_3^{(\text{exp})}(t_2) \quad (6.24f)$$

Note that the experimental data have been used as boundary conditions. Because these boundary conditions are not all given at one point, they form a multipoint boundary-value problem. The quantities, t_1 and t_2 , are two discrete values of t within the interval of $0 \leq t \leq t_f$.

6.4 PROBLEM WITH MORE THAN THREE EXPERIMENTAL DATA

For nearly all practical situations, the experimental data are not exact and have experimental errors. Thus, it is desirable to obtain a fairly large amount of data instead of just three data points. For $m_1 + m_2 + m_3 + m_4 \geq 3$, the classical least squares criterion can be used. The object is to determine the parameters so that the sum of the squares of the deviations is minimized. Instead of boundary conditions, (6.24a), (6.24e), and (6.24f), one can obtain these three conditions by minimizing the following least squares expression

$$Q = \sum_{s=0}^{m_1} [c_1(t_s) - c_{1s}]^2 + \sum_{R=0}^{m_2} [c_2(t_R) - c_{2R}]^2 + \sum_{P=0}^{m_3} [c_3(t_P) - c_{3P}]^2 + \sum_{Q=0}^{m_4} [c_4(t_Q) - c_{4Q}]^2 \quad (6.25)$$

where the minimization is over the parameters, B_1 and B_2 . $c_1(t_s)$, $c_2(t_R)$, $c_3(t_P)$, and $c_4(t_Q)$ are obtained by solving Eqs. (6.1) - (6.4).

6.5 COMPUTATIONAL CONSIDERATIONS

Since both the parameters B_1 , B_2 , and the original variables C_1 , C_2 , C_3 and C_4 are considered unknown functions, Eqs. (6.1) - (6.4) are nonlinear equations. Thus, the system represented by Eqs. (6.1) - (6.24) and Eq. (25) are nonlinear systems with multipoint boundary conditions. Generally speaking, nonlinear equations can not be solved analytically. Furthermore, even numerical solutions cannot be obtained easily because of the fact that the boundary conditions are given at several different points. Quasilinearization technique, also known as the generalized Newton-Raphson method, can be used to overcome this computational difficulty. In this method, the solution of the nonlinear equation is obtained by solving a sequence of linear equations.

The solution of this sequence of linear equations converge rapidly to the solution of the original nonlinear equation provided that the process converges. This quadratic convergence property is the main advantage of the quasilinearization approach. Quadratic convergence means that the error in the current iteration tends to be proportional to the square of the error in the previous iteration.

6.6 COMPUTATIONAL PROCEDURE

The estimation problem for the simple cardiovascular indicator-dilution model can now be approached by the quasilinearization technique. The system of Equations (6.1) - (6.4) and (6.24) - (6.25) can be linearized by using Eq. (2.3) with $M = 6$. The linearized equations are

$$\frac{dC_{1,n+1}}{dt} = -B_{1,n} C_{1,n+1} + B_{2,n} C_{4,n+1} + B_{2,n+1} C_{4,n} \quad (6.30)$$

$$-B_{1,n+1} C_{1,n} + C_{1,n} B_{1,n} - C_{4,n} B_{2,n}$$

$$\frac{dC_{2,n+1}}{dt} = B_{1,n} C_{1,n+1} - B_{1,n} C_{2,n+1} + (C_{1,n} - C_{2,n}) B_{1,n+1} \quad (6.31)$$

$$- (C_{1,n} - C_{2,n}) B_{1,n}$$

$$\frac{dC_{3,n+1}}{dt} = B_{1,n} C_{2,n+1} - B_{1,n} C_{3,n+1} + (C_{2,n} - C_{3,n}) B_{1,n+1} \quad (6.32)$$

$$- (C_{2,n} - C_{3,n}) B_{1,n}$$

$$\frac{dC_{4,n+1}}{dt} = B_{1,n} C_{3,n+1} - B_{1,n} C_{4,n+1} + (C_{3,n} - C_{4,n}) B_{1,n+1} \quad (6.33)$$

$$- (C_{3,n} - C_{4,n}) B_{1,n}$$

$$\frac{dB_{1,n+1}}{dt} = 0 \quad (6.34)$$

$$\frac{dB_{2,n+1}}{dt} = 0 \quad (6.35)$$

The four boundary conditions are

$$C_1(0) = B_3 \quad (6.36)$$

$$C_2(0) = 0 \quad (6.37)$$

$$C_3(0) = 0 \quad (6.38)$$

$$C_4(0) = 0 \quad (6.39)$$

Since B_3 is unknown, so there are still three other boundary conditions need to find. These three boundary conditions can be obtained either by using Eqs. (6.24a), (6.24e) and (6.24f) or by minimizing Eq. (6.25). Because the use of least squares is a more practical problem, this work will use minimization of Eq. (6.25).

Equations (6.30) through (6.35) are linear equations with variable coefficients. In general, they cannot be solved in closed form. However, because they are linear equations, the superposition principle can be applied [20]. It is well known that for six simultaneous linear equations, the general solution can be represented by six set of homogeneous solutions and one set of particular solution [20]. Thus, the general solutions of Eqs. (6.30) through (6.35) are

$$\begin{aligned} C_{1,n+1}(t) &= C_{1p,n+1}(t) + \sum_{j=1}^q a_{j,n+1} C_{1hj,n+1}(t) \\ C_{2,n+1}(t) &= C_{2p,n+1}(t) + \sum_{j=1}^q a_{j,n+1} C_{2hj,n+1}(t) \\ C_{3,n+1}(t) &= C_{3p,n+1}(t) + \sum_{j=1}^q a_{j,n+1} C_{3hj,n+1}(t) \\ C_{4,n+1}(t) &= C_{4p,n+1}(t) + \sum_{j=1}^q a_{j,n+1} C_{4hj,n+1}(t) \end{aligned} \quad (6.40)$$

$$B_{1,n+1}(t) = B_{1p,n+1}(t) + \sum_{j=1}^q a_{j,n+1} B_{1hj,n+1}(t)$$

$$B_{2,n+1}(t) = B_{2p,n+1}(t) + \sum_{j=1}^q a_{j,n+1} B_{2hj,n+1}(t)$$

with $q = 6$. The subscript p is used to indicate particular solutions, and subscript $h1, h2, h3, h4, h5$, and $h6$ denote the first, second, ..., and sixth sets of homogeneous solutions, respectively. The a 's are integration constants to be determined from the boundary conditions.

The six sets of homogeneous solutions must be obtained numerically. However, because they can be any solutions of Equations (6.30) through (6.35) as long as the homogeneous solutions are nontrivial and distinct, any set of initial conditions can be used to obtain the particular solutions, and any six sets of initial conditions, as long as they are nontrivial and distinct, can be used to obtain the six sets of homogeneous solutions. Furthermore, if these seven sets of initial conditions are chosen in such a way that they satisfy the three given initial conditions, Eqs. (6.37) - (6.39), only three sets of homogeneous solutions are needed with three integration constants, $a_{j,n+1}$, $j = 1, 2, 3$. In actual calculations, the following set of initial conditions is used for the particular solutions

$$C_{1p,n+1}(0) = 0.5, \quad C_{2p,n+1}(0) = 0, \quad C_{3p,n+1}(0) = 0 \quad (6.41)$$

$$C_{4p,n+1}(0) = 0, \quad B_{1p,n+1}(0) = 0, \quad B_{2p,n+1}(0) = 0$$

The homogeneous forms of Eqs. (6.30) through (6.35) are

$$\frac{dC_{1,n+1}}{dt} = -B_{1,n} C_{1,n+1} + B_{2,n} C_{4,n+1} + B_{2,n+1} C_{4,n} - B_{1,n+1} C_{1,n} \quad (6.42)$$

$$\frac{dC_{2,n+1}}{dt} = B_{1,n} C_{1,n+1} - B_{1,n} C_{2,n+1} + (C_{1,n} - C_{2,n}) B_{1,n+1} \quad (6.44)$$

$$\frac{dC_{3,n+1}}{dt} = B_{1,n} C_{2,n+1} - B_{1,n} C_{3,n+1} + (C_{2,n} - C_{3,n}) B_{1,n+1} \quad (6.44)$$

$$\frac{dC_{4,n+1}}{dt} = B_{1,n} C_{3,n+1} - B_{1,n} C_{4,n+1} + (C_{3,n} - C_{4,n}) B_{1,n+1} \quad (6.45)$$

$$\frac{dB_{1,n+1}}{dt} = 0 \quad (6.46)$$

$$\frac{dB_{2,n+1}}{dt} = 0 \quad (6.47)$$

The initial conditions used to obtain the homogeneous solutions are listed in Table 21. Note that the initial values listed in Eq. (6.41) and Table 21 are chosen in such a way that at $t = 0$, they satisfy the given initial conditions, Eqs. (6.37) - (6.39). Because these chosen initial values satisfy the three given initial conditions, the fourth, fifth, and sixth homogeneous solutions are not needed. Thus, only three sets of initial conditions are needed for the homogeneous solutions and the value of q in Eq. (6.40) is now reduced to three.

The three given boundary conditions, Eqs. (6.37) - (6.39), have already been used in choosing the initial conditions for obtaining the particular and homogeneous solutions. The remaining three integration

constants, $a_{1,n+1}$, $a_{2,n+1}$, and $a_{3,n+1}$, can be obtained from the remaining three boundary conditions. For the case $m_1 + m_2 + m_3 + m_4 > 3$, these three conditions can be obtained by minimizing Eq. (6.25). At various positions of t_S , t_R , t_P , and t_Q ; $S = 1, 2, \dots, m_1$; $R = 1, 2, \dots, m_2$; $P = 1, 2, \dots, m_3$; $Q = 1, 2, \dots, m_4$ the following $m_1 + m_2 + m_3 + m_4$ equations can be obtained from the first four equations of Eq. (40)

with $q = 3$

$$C_{1,n+1}(t_s) = C_{1p,n+1}(t_s) + \sum_{j=1}^3 a_{j,n+1} C_{1hj,n+1}(t_s) \quad (6.48)$$

$$C_{2,n+1}(t_R) = C_{2p,n+1}(t_R) + \sum_{j=1}^3 a_{j,n+1} C_{2hj,n+1}(t_R) \quad (6.49)$$

$$C_{3,n+1}(t_P) = C_{3p,n+1}(t_P) + \sum_{j=1}^3 a_{j,n+1} C_{3hj,n+1}(t_P) \quad (6.50)$$

$$C_{4,n+1}(t_Q) = C_{4p,n+1}(t_Q) + \sum_{j=1}^3 a_{j,n+1} C_{4hj,n+1}(t_Q) \quad (6.51)$$

Substituting the above four equations into Eq. (25), gives

$$\begin{aligned} Q = & \sum_{s=1}^{m_1} [C_{1p,n+1}(t_s) + \sum_{j=1}^3 a_{j,n+1} C_{1hj,n+1}(t_s) - C_{1s}]^2 \\ & + \sum_{R=1}^{m_2} [C_{2p,n+1}(t_R) + \sum_{j=1}^3 a_{j,n+1} C_{2hj,n+1}(t_R) - C_{2R}]^2 \\ & + \sum_{p=1}^{m_3} [C_{3p,n+1}(t_P) + \sum_{j=1}^3 a_{j,n+1} C_{3hj,n+1}(t_P) - C_{3p}]^2 \end{aligned}$$

$$+ \sum_{Q=1}^{m_4} [C_{4p,n+1}(t_Q) + \sum_{j=1}^3 a_{j,n+1} C_{4hj,n+1}(t_Q) - C_{4Q}]^2 \quad (6.52)$$

Because the particular and homogeneous solutions at the various positions of t are known and are obtained numerically by using the initial values listed in Equation (6.41) and Table 21, the only unknown values in the right-hand side of Eq. (6.52) are the three integration constants, $a_{1,n+1}$, $a_{2,n+1}$, and $a_{3,n+1}$. Thus, the problem is to find the values of these constants such that the value of Q is minimized. There are many techniques that can be used to minimize Eq. (6.52). For this work, the extreme values will be obtained by partial Differentiation. By differentiating Eq. (6.52) with respect to $a_{1,n+1}$, $a_{2,n+1}$, and $a_{3,n+1}$, and setting the results equal to zero, the following three equations can be obtained

$$\begin{aligned} \frac{\partial Q}{\partial a_{i,n+1}} &= 2 \sum_{s=1}^{m_1} C_{1hi,n+1}(t_s) [C_{1p,n+1}(t_s) + \sum_{j=1}^3 a_{j,n+1} C_{1hj,n+1}(t_s) - C_{1s}]^2 \\ &+ 2 \sum_{R=1}^{m_2} C_{2hi,n+1}(t_R) [C_{2p,n+1}(t_R) + \sum_{j=1}^3 a_{j,n+1} C_{2hj,n+1}(t_R) - C_{2R}]^2 \\ &+ 2 \sum_{p=1}^{m_3} C_{3hi,n+1}(t_p) [C_{3p,n+1}(t_p) + \sum_{j=1}^3 a_{j,n+1} C_{3hj,n+1}(t_p) - C_{3p}]^2 \\ &+ 2 \sum_{Q=1}^{m_4} C_{4hi,n+1}(t_Q) [C_{4p,n+1}(t_Q) + \sum_{j=1}^3 a_{j,n+1} C_{4hj,n+1}(t_Q) - C_{4Q}]^2 \\ &= 0, \quad i = 1, 2, 3 \end{aligned} \quad (6.53)$$

These three equations form the remaining three boundary conditions.

Because the variables $C_1(t_s)$, $C_2(t_R)$, $C_3(t_p)$, $C_4(t_Q)$, t_s , t_R , t_p and t_Q are all known values, the three constants $a_{j,n+1}$, $j = 1,2,3$, can now be obtained by solving the above three algebraic equations. Once the integration constants are obtained, the general solutions for $C_{1,n+1}(t)$, $C_{2,n+1}(t)$, $C_{3,n+1}(t)$, $C_{4,n+1}(t)$, $B_{1,n+1}(t)$, $B_{2,n+1}(t)$, and $B_{3,n+1} = C_{1,n+1}(0)$ can be obtained by using Eq. (6.40) with $q = 3$ and the newly obtained particular and homogeneous solutions. The computational procedure can be summarized as follows

1. Assume a set of reasonable initial functions for $C_1(t)$, $C_2(t)$, $C_3(t)$, $C_4(t)$, $B_1(t)$ and $B_2(t)$. Let these initial functions be $C_{1,n=0}(t)$, $C_{2,n=0}(t)$, $C_{3,n=0}(t)$, $C_{4,n=0}(t)$, $B_{1,n=0}(t)$ and $B_{2,n=0}(t)$
2. Integrate Equations (6.30) through (6.35) numerically using Eq. (6.41) as initial value and with $n = 0$.
3. Integrate the homogeneous Equations (6.42) through (6.47) three times using Table 21 as the initial values and with $n = 0$.
4. Solve Eq. (6.53) for $a_{j,n+1}$, $j = 1,2,3$, using the newly obtained particular and homogeneous solutions from step 2 and 3 and using the given experimental data C_{1s} , C_{2R} , C_{3p} , and C_{4Q} .
5. Calculate $C_{1,n+1=1}(t)$, $C_{2,n+1=1}(t)$, $C_{3,n+1=1}(t)$, $C_{4,n+1=1}(t)$, $B_{1,n+1=1}(t)$, $B_{2,n+1=1}(t)$, and $B_{3,n+1=1} = C_{1,n+1=1}(0)$, using Eq. (6.40) with $q = 3$.
6. Repeat step 2 through 5 with $n = 1,2,\dots$, until no further improvement on the value of $C_1(t)$, $C_2(t)$, $C_3(t)$, B_1 , B_2 and B_3 can be obtained.

It should note that the best available initial functions should be used for step 1.

6.7 NUMERICAL RESULTS

To test the effectiveness of this approach, the parameters, B_1 and B_2 , in Eqs. (6.1) - (6.4) are estimated from a given set of data. These given data are obtained numerically by solving Eqs. (6.1) - (6.4). In other words, we use the following numerical values

$$\begin{aligned}
 C_1(0) &= 0.9997 & B_1 &= 0.8017 \\
 C_2(0) &= 0 & B_2 &= 0.4018 \\
 C_3(0) &= 0 & t_f &= 20 \\
 C_4(0) &= 0
 \end{aligned} \tag{6.54}$$

(6.55)

Eq. (6.1) - (6.4) were integrated numerically with the Runge-Kutta integration scheme [6]. The step size used in this integration is $\Delta t = 0.2$. Some of the results from this integration are listed in Table 22 and will be used as the experimental data. Note that $m_1 = m_2 = m_3 = m_4 = 11$ and $t_s = t_R = t_p = t_Q$ used for this particular problem.

Parameters B_1 and B_2 are estimated using the value listed in Table 22 as the experimental data. In other words, B_1 and B_2 are considered as the unknown parameters that must be estimated from the data given in Table 22, the given model represented by Eqs. (6.1) - (6.4), and the given values represented by Eqs. (6.54) and (6.55).

The system of equations for this problem is represented by Eqs. (6.1) - (6.4), (6.24), and (6.25). These six equations can be linearized in the same way as before.

The following initial conditions are used to obtain the one set of

particular and three sets of homogeneous solutions

$$C_{1p,n+1}(0) = 0.5$$

$$C_{2p,n+1}(0) = 0 \quad B_{1p,n+1}(0) = 0$$

$$C_{3p,n+1}(0) = 0 \quad B_{2p,n+1}(0) = 0$$

$$C_{4p,n+1}(0) = 0$$

$$C_{1h1,n+1}(0) = 1 \quad C_{1h2,n+1}(0) = 0 \quad C_{1h3,n+1}(0) = 0$$

$$C_{2h1,n+1}(0) = 0 \quad C_{2h2,n+1}(0) = 0 \quad C_{2h3,n+1}(0) = 0$$

$$C_{3h1,n+1}(0) = 0 \quad C_{3h2,n+1}(0) = 0 \quad C_{3h3,n+1}(0) = 0$$

$$C_{4h1,n+1}(0) = 0 \quad C_{4h2,n+1}(0) = 0 \quad C_{4h3,n+1}(0) = 0 \quad (6.56)$$

$$B_{1h1,n+1}(0) = 0 \quad B_{1h2,n+1}(0) = 1 \quad B_{1h3,n+1}(0) = 0$$

$$B_{2h1,n+1}(0) = 0 \quad B_{2h2,n+1}(0) = 0 \quad B_{2h3,n+1}(0) = 1$$

Note that the initial conditions for the particular and homogeneous solutions are chosen in such a way that they satisfy the given initial conditions. Thus, only three sets of homogeneous solutions are needed.

This problem was solved by using the computational procedure discussed earlier, and by using the initial conditions for the particular and homogeneous solutions given by Eq. (6.56). The Runge-Kutta numerical integration scheme was used with the step size $\Delta t = 0.2$. To test the influence of the initial functions used in step 1, the following four sets of initial functions were used for the unknown parameters and $C_1(0)$

$$\begin{array}{cccc}
B_{1,n=0}(t) = 0.1 & B_{1,n=0}(t) = 0.6 & B_{1,n=0}(t) = 1 & B_{1,n=0}(t) = 2 \\
B_{2,n=0}(t) = 0.01 & B_{2,n=0}(t) = 0.2 & B_{2,n=0}(t) = 0.6 & B_{2,n=0}(t) = 1.5 \\
B_{3,n=0}=C_{1,n=0}(0) & B_{3,n=0}=C_{1,n=0}(0) & B_{3,n=0}=C_{1,n=0}(0) & B_{3,n=0}=C_{1,n=0}(0) \\
= 0.1 & = 0.8 & = 1.2 & = 3
\end{array}$$

(6.57)

for $0 \leq t \leq t_f = 20$. The initial functions of C_1 , C_2 , C_3 , and C_4 are obtained by using the given initial conditions Eqs. (6.37) - (6.39), and the assumed values listed in Eq. (6.57) to integrate Eqs. (6.1) - (6.4). It should be noted that in order to increase the convergence rate, either the experimental data or the actual solutions of Eqs. (6.1) - (6.4) should be used as the initially assumed functions.

The problem converges rapidly to the correct solution for all four sets of initially assumed functions. The convergence rates for the unknown parameters are shown in Tables 23a, 23b, 23c, and 23d for first, second, third and fourth set of data, respectively. It can be seen that a four-digit accuracy is obtained in only four or less than eight iterations. Note that a unknown initial condition $C_1(0)$ can also be obtained by this approach. Noted also that though the assumed initial function for unknown parameters and original variables are far removed from the correct solution, we still can find the convergent value for these unknown parameters. The convergent rates of C_1 , C_2 , C_3 , and C_4 with $B_{1,n=0}(t) = 2$, $B_{2,n=0}(t) = 1.5$, and $C_{1,n=0}(0) = 3$ are shown in Figures 14, 15, 16 and 17 respectively. Notice that the large amount of improvement have been obtained in the first iteration.

TABLE 21. Initial Conditions used for Obtaining the Homogeneous Solutions

Variables	j		
	1	2	3
$C_{1hj,n+1}^{(0)}$	1	0	0
$C_{2hj,n+1}^{(0)}$	0	0	0
$C_{3hj,n+1}^{(0)}$	0	0	0
$C_{4hj,n+1}^{(0)}$	0	0	0
$B_{1,n+1}^{(0)}$	0	1	0
$B_{2,n+1}^{(0)}$	0	0	1

TABLE 22. Numerical Values used as Experimental Data

t_s	S	$C_{1(\text{exp})}(t_s) = C_{1s}$	$C_{2(\text{exp})}(t_s) = C_{2s}$	$C_{3(\text{exp})}(t_s) = C_{3s}$	$C_{4(\text{exp})}(t_s) = C_{4s}$
0.0	1	0.9997	0.0	0.0	0.0
2.0	2	0.2289	0.3314	0.2609	0.1387
4.0	3	0.1327	0.1887	0.2391	0.2366
6.0	4	0.1141	0.1347	0.1682	0.2009
8.0	5	0.0909	0.1066	0.1269	0.1528
10.0	6	0.0702	0.0834	0.0988	0.1175
12.0	7	0.0543	0.0646	0.0768	0.0912
14.0	8	0.0421	0.0501	0.0595	0.0707
16.0	9	0.0327	0.0388	0.0462	0.0549
18.0	10	0.0253	0.0301	0.0358	0.0425
20.0	11	0.0196	0.0234	0.0278	0.0329

TABLE 23a. CONVERGENCE RATES WITH DATA SET 1

ITERATION	B1	B2	B3(c1(0))
0	0.1	0.01	0.1
1	0.4379	0.0725	0.4969
2	0.4896	0.1772	0.8993
3	0.6522	0.2679	0.9658
4	0.7616	0.3635	0.9952
5	0.7974	0.3979	0.9993
6	0.8014	0.4015	0.9997
7	0.8017	0.4018	0.9997
8	0.8017	0.4018	0.9997

TABLE 23b. CONVERGENCE RATES WITH DATA SET 2

ITERATION	B1	B2	B3[c1(0)]
0	0.6	0.2	0.8
1	0.7663	0.3755	0.9903
2	0.7966	0.3970	0.9992
3	0.8013	0.4015	0.9996
4	0.8017	0.4018	0.9997
5	0.8017	0.4018	0.9997

TABLE 23c. CONVERGENCE RATES WITH DATA SET 3

ITERATION	B1	B2	B3[c1(0)]
0	1.	0.6	1.2
1	0.8123	0.4123	0.9991
2	0.8025	0.4025	0.9997
3	0.8017	0.4018	0.9997
4	0.8017	0.4018	0.9997
5	0.8017	0.4018	0.9997

TABLE 23d. CONVERGENCE RATES WITH DATA SET 4

ITERATION	B1	B2	B3[c1(0)]
0	2.	1.5	3
1	1.7167	1.2619	1.0049
2	0.6846	0.2886	0.9983
3	0.8014	0.4021	0.9992
4	0.8017	0.4018	0.9997
5	0.8017	0.4018	0.9997

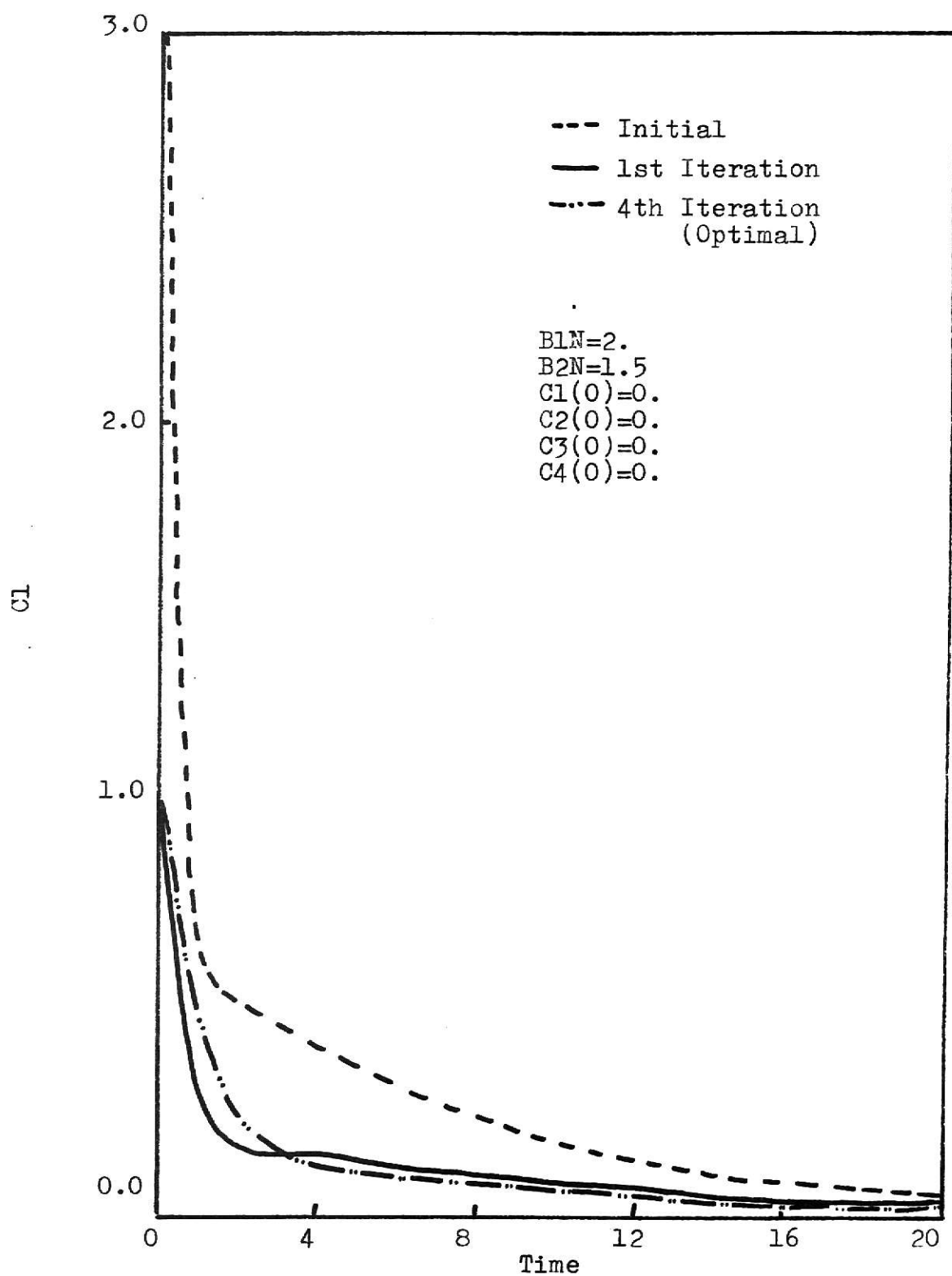


Figure 14. Convergence Rates of C1

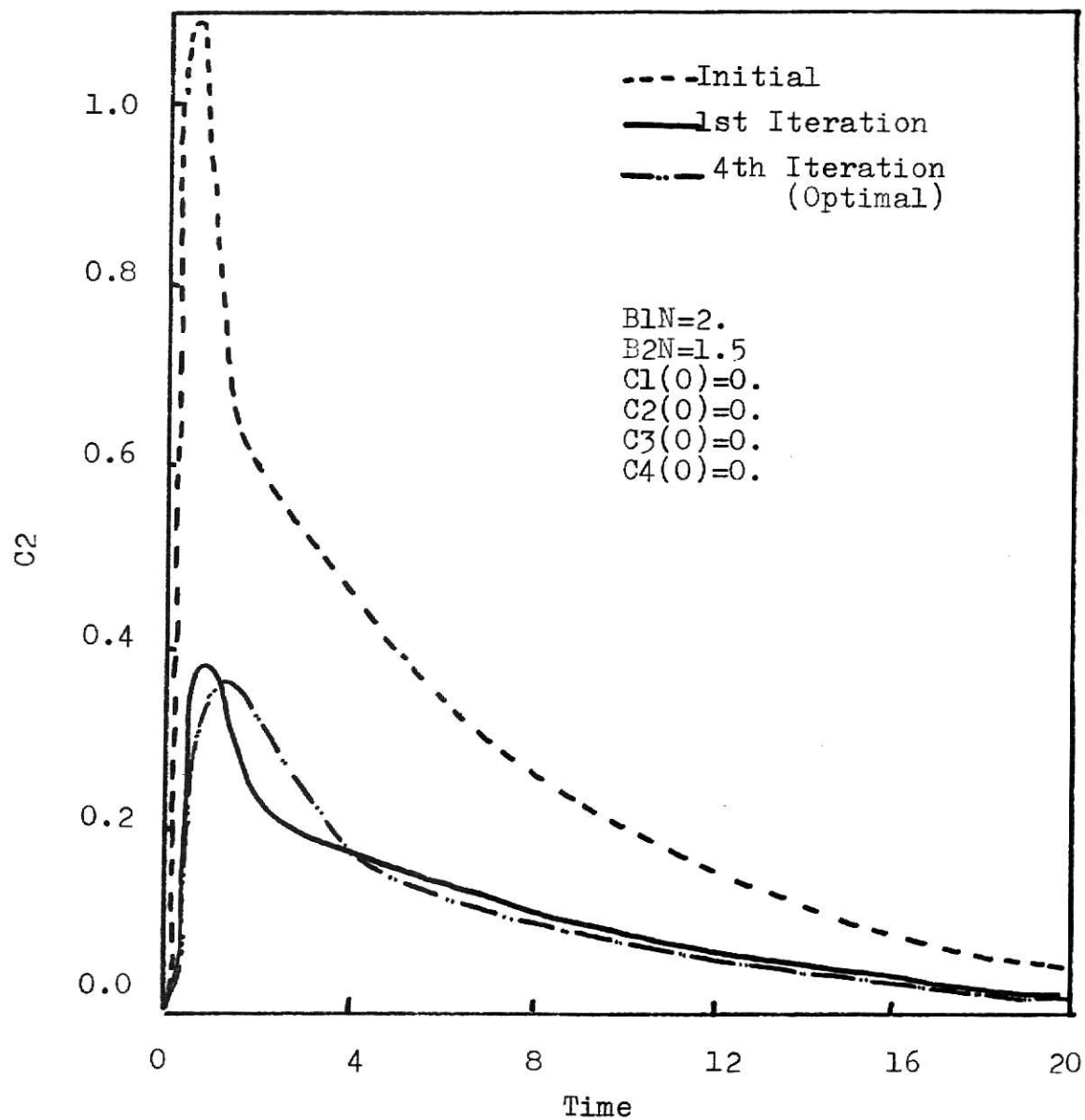
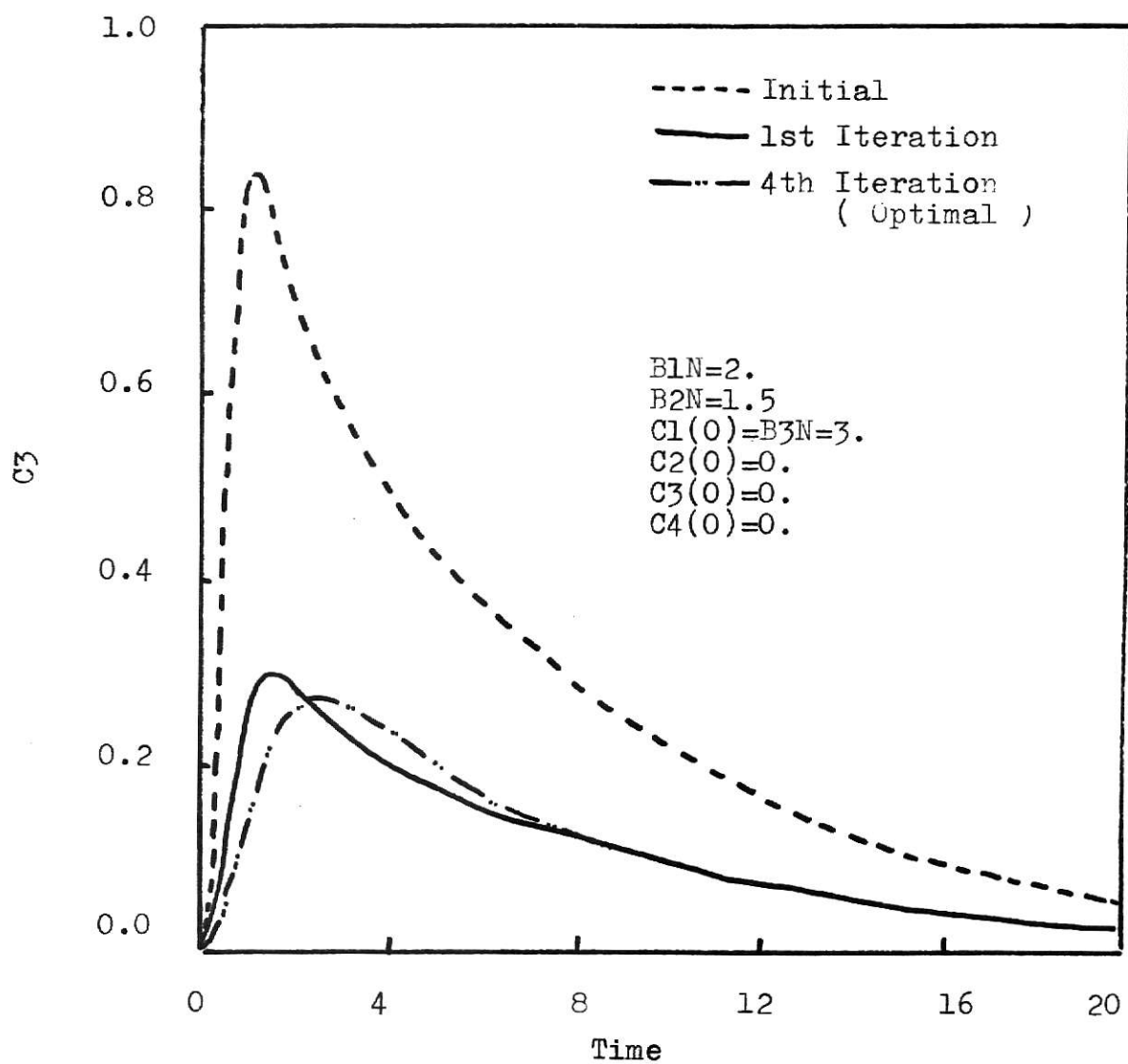


Figure 15. Convergence Rates of C2

Figure 16. Convergence Rates of $C3$

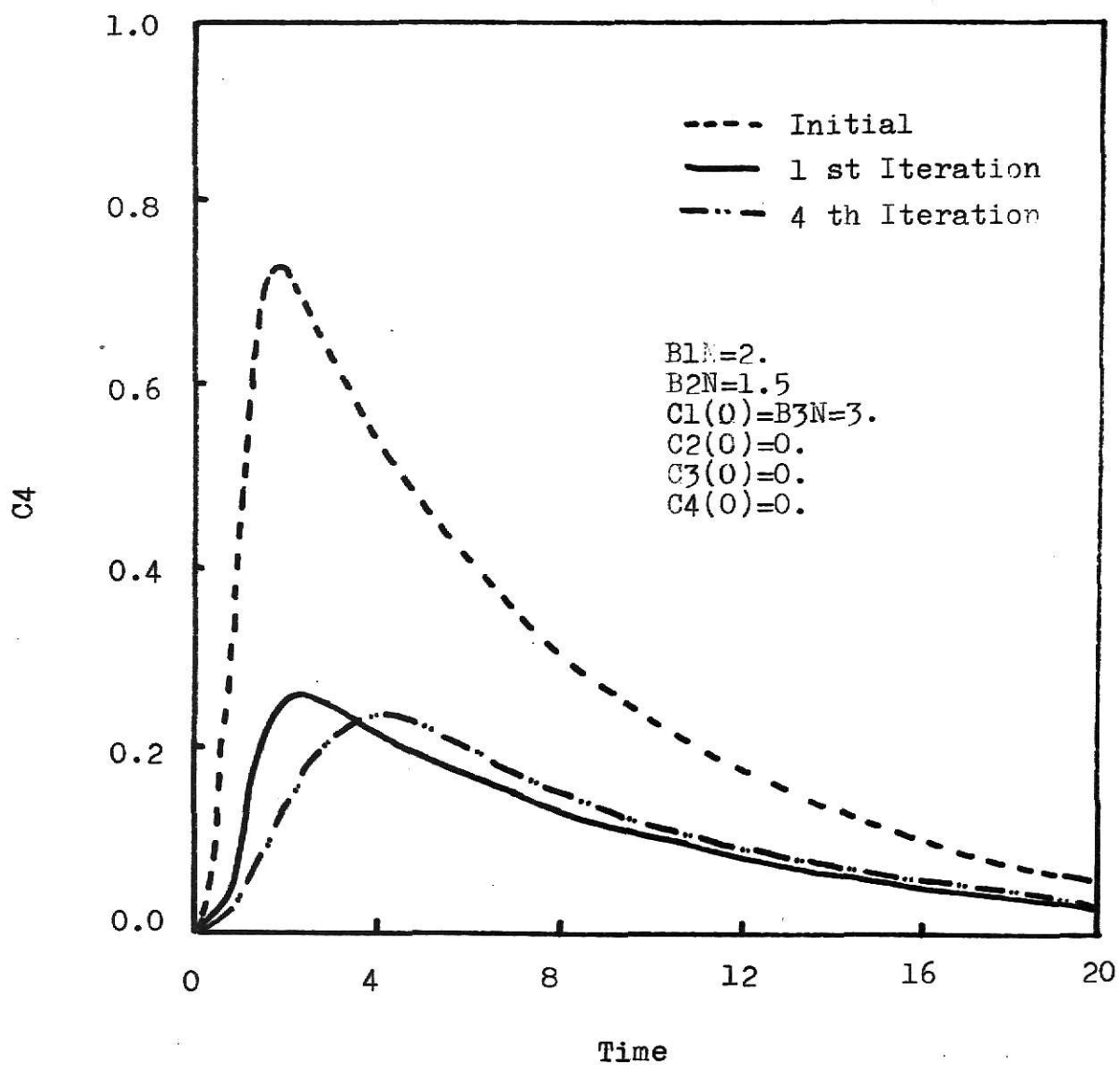


Figure 17. Convergence Rates of C4

CHAPTER 7

CONCLUSION

The difficulties in estimating nonlinear system represent one of the obstacles to the sythesis and analysis of dynamic nonlinear systmes such as air pollution and bioengineering systems. The reasons are

- 1) absence of explicit analytical solutions to the nonlinear models which represent the systems; and
- 2) difficulties of obtaining numerical solutions from the nonlinear models of the boundary-value type on digital computers. Quasi-linearization technique represents a powerful computational tools for overcoming these difficulties.

From the numerical examples presented in this work, we can see that the parameter estimation problems are effectively solved by the quasi-linearization technique. This proves that quasilinearization technique is a promising technique for the dynamic modeling and adaptive forecasting of air quality and bioengineering systems.

The most attractive feature of the quasilinearization technique lies in its general applicability to a large class of complicated nonlinear models and its rapid convergence property. Solutions to the examples in this current work reveal

- 1) Accurate initial conditions are not required and only reasonable approximations are needed.
- 2) The convergence rate of state variables and parameters are fairly rapid. Generally, four digits accuracy are obtained within six iterations.

- 3) The presence of noises or experimental errors do not slow down the convergence rates noticeably.

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APPLYING QUASILINEARIZATION TECHNIQUE TO
AIR POLLUTION AND BIOENGINEERING SYSTEMS MODELING

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The air pollution modeling and optimization and the modeling of certain bioengineering systems are studied in this work. The recently developed modeling techniques such as the quasilinearization technique and linear programming are used for modeling and optimization purposes.

Quasilinearization technique is a useful technique for obtaining the numerical solutions of nonlinear boundary-value problems. Furthermore, this technique has been proved to be a powerful tool for solving various estimation problems. Combined with estimation criteria such as the least square criteria, the parameters to be estimated converges quadratically to the desired accuracy. Another property of this approach is that the parameters can be estimated directly from the set of differential equations representing the model and from the experimental data. The parameters of one air pollution model and two bioengineering models are identified by using quasilinearization technique to show the effectiveness of this approach.

A diffusion model with continuous point source which located between an inversion layer and the ground is identified under the assumption that the wind speed and eddy diffusivity are constant over the diffusion region and the wind direction shear presents in the diffusion layers. The rate constants in the one compartment model of the kinetics of glucose and insulin in plasma also have been estimated. Also, the model of cardiovascular indicator-dilution curves is identified by quasilinearization. It is shown that with very approximate initial guesses for the unknown parameters, only three to six iterations are needed to obtain a four to five-digit accuracy.

The dynamic decomposition model of Tillman and Lee is revised by using the principle of conservation of mass. This model is optimized for the control of the dynamic movement of air pollution. The optimal amounts of different grades of fuel for each source in each region and the optimal purification levels for each source are obtained by linear programming. By using these optimal amounts of different grades of fuel and optimal purification levels, the total cost to maintain a certain air quality standard and maintain a desired energy level is minimized. The principle advantages of this approach are

- 1) The dynamic aspects of air pollution are considered so that on-line control of air quality can be considered.
- 2) Because of the flexibility of the model and also because linear programming can be used to solve very large practical problems, the proposed approach appears to be a feasible one for the optimal on-line control of air pollution of a large metropolitan area.