APPLICATION OF THE QUASILINEARIZATION TECHNIQUE FOR PARAMETER ESTIMATION IN NONLINEAR DIFFERENTIAL EQUATIONS

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PART I

INTRODUCTION

The form of the differential equations used to describe a physical process can be specified from basic conservation principles. Very often the parameters associated with the differential equations are unknown. They are determined from a comparison of experimental measurements of the process and the solutions of the differential equations that describe the process. Parameter estimation is an integral part of the analysis of experimental data in terms of a model of known form with unknown coefficients.

There has been very little work done in the area of parameter estimation. The parameters or coefficients cannot be measured directly. The measurable variables are generally the dependent variables of the differential equations. Therefore it is not simple to identify the parameters.

The estimation of parameters in ordinary differential equations has received considerable interest in recent technical literature.

Rosenbrock and Storey [19] have presented a review of the techniques of generating and analyzing parameter estimates.

Bellman, Kagiwada and Sridhar [20] have shown how techniques from nonlinear filtering and estimation theory can be applied to the estimation of parameters in ordinary differential equations.

Lee [11] has presented the problem of parameter estimation using the quasilinearization method.

The objective of the present work is to estimate parameters in the differential equations resulting from tubular flow chemical reactors with axial diffusion. The physical process is assumed to be represented by a nonlinear ordinary differential equation. Linearization is carried through by considering the first two terms in the Taylor's series expansion of the original nonlinear equation. This technique is a generalized Newton-Raphson formula for functional equations. It is more commonly known as the quasilinearization method. The main advantage of this technique is that the procedure converges quadratically to the solution of the original equation, if it should converge.

Integration of the linearized equation is carried through by the fourth order Runge-Kutta-Gill method. An algorithm is devised based on the least squares method. Initial guesses are made for the parameters and also for the function value of concentration as a function of axial length. Initial values for the numerical integration are so chosen that the integration constants are identically equal to the unknown parameters. Parameters thus obtained are used recursively to obtain improved results.

Errors in the experimental data are considered small in magnitude. The mathematical model is devised to fit the data.

CHAPTER I

QUASILINEARIZATION TECHNIQUE

Solutions to initial value problems are well developed theoretically. They are also easily adaptable for solving on high speed digital and analog computers. Nonlinear differential equations having two or multipoint boundary values are common in engineering and physical sciences. There is no general proof for the existence and uniqueness of the solutions of such problems. Numerical difficulties in their solution are caused because not all the conditions are given at one point. A trial and error procedure is generally used to obtain the missing initial condition. This procedure has a relatively slow rate of convergence.

Quasilinearization is a useful technique for obtaining numerical solutions for these type of problems. In this method the nonlinear differential equation is solved recursively by a series of linear differential equations. The quasilinearization technique converges quadratically to the exact solution, if at all it should converge. Quadratic, convergences implies that the error in every succeeding iteration tends to be proportional to the square of the error in its immediately preceeding iteration.

Linearization of the original differential equation is carried through by considering the first two terms in the Taylor's series expansion. This is a generalized Newton-Raphson technique for functional equations. The Newton-Raphson technique is associated with two important properties. These are monotone convergence and quadratic convergence. The nature of the monotone convergence property depends on the function itself. The monotone convergence property exists for the Newton-Raphson formula only if the function is a monotone decreasing or monotone increasing function. The function should be strictly convex or strictly concave. In general the Newton-Raphson formula always has the quadratic convergence property provided that it converges [11].

The Newton-Raphson equation is always linear even if the original function is nonlinear. Linear boundary value problems can be solved fairly routinely on modern computers.

CHAPTER II

LINEARIZATION OF THE NONLINEAR ORDINARY DIFFERENTIAL EQUATION

The mathematical formulation for estimating the parameters in the differential equation for homogeneous tubular flow chemical reactor with axial mixing is presented in this chapter. The physical process is assumed to be represented by a nonlinear second-order ordinary differential equation.

$$\frac{1}{P}\frac{d^2x}{dt^2} - \frac{dx}{dt} - Rx^2 = 0 \qquad (1)$$

where,

P is the dimensionless Peclet group. Its magnitude is $\frac{Lv}{D}$,

R is the reaction rate group $\frac{kL}{v}$,

t is the dimensionless reactor length which varies between 0 and 1. It is obtained by dividing the actual position along the axial direction of the reactor by the total reactor length L,

x is the concentration of the reactant,

v is the flow velocity of the reaction mixture. It is assumed constant throughout the reactors,

D is the mean mass axial dispersion coefficient. It is assumed constant,

k is the specific chemical reaction rate. It is also assumed constant.

Boundary Conditions

$$x_e = x(0) - \frac{1}{P}\frac{dx}{dt}\Big|_{t=0} = c, \quad \text{say at } t = 0 \tag{2}$$

$$\frac{dx}{dt}\Big|_{t=t_f} = 0 \qquad\qquad \text{at } t = t_{final} \tag{3}$$

where,

x_e is the concentration of the reactant before it enters the reactor. It is a known quantity. $x(0)$ is the concentration just after entering the reactor. There is a discontinuity of the concentration x of the reactant at the entrance to the tubular reactor.

Equation (1) is a second order nonlinear differential equation of the boundary-value type with P and R as parameters. These parameters are unknown values that are to be determined.

The preliminary step involved for estimating the parameters is to linearize the original nonlinear equation (1) by the generalized Newton-Raphson method.

$$\frac{1}{P}\frac{d^2x}{dt^2} = \frac{dx}{dt} + Rx^2 \tag{4}$$

$$\frac{d^2x}{dt^2} = P\frac{dx}{dt} + PRx^2 \tag{5}$$

Equation (5) can be rewritten as,

$$x' = \frac{dx}{dt} = y \tag{6a}$$

$$y' = \frac{dy}{dt} = Py + PRx^2 \tag{6b}$$

The parameters P and R are considered as dependent variables parallel to x and as functions of the independent variable t. The parameters satisfy the following equations,

$$\frac{dR}{dt} = 0, \tag{6c}$$

and

$$\frac{dP}{dt} = 0. \tag{6d}$$

The generalized Newton-Raphson formula is applied to equation (6a) as follows.

$$x'_{n+1} = x'_n + \frac{\partial x'_n}{\partial y_n} \{y_{n+1} - y_n\} \tag{7a}$$

The subscripts n and n+1 denote the n^{th} and $(n+1)^{st}$ iteration respectively.

From equation (6a),

$$x' = y.$$

Thus,

$$x'_{n+1} = y_n + \frac{\partial y_n}{\partial y_n} \{y_{n+1} - y_n\} \tag{7b}$$

$$x'_{n+1} = y_n + 1 \cdot \{y_{n+1} - y_n\} \tag{7c}$$

$$x'_{n+1} = y_{n+1} \tag{8a}$$

Similarly equation (6b) is written as,

$$y' = Py + PRx^2 \tag{7d}$$

Thus,

$$y' = f(x,y,P,R) \tag{7e}$$

$$y'_{n+1} = y'_n + \frac{\partial y'_n}{\partial x_n}(x_{n+1} - x_n) + \frac{\partial y'_n}{\partial y_n}(y_{n+1} - y_n)$$

$$+ \frac{\partial y'_n}{\partial P_n}(P_{n+1} - P_n) + \frac{\partial y'_n}{\partial R_n}(R_{n+1} - R_n) \tag{7f}$$

Thus,

$$y'_{n+1} = (P_n y_n + P_n R_n x_n^2) + \frac{\partial}{\partial x_n}(P_n y_n + P_n R_n x_n^2)(x_{n+1} - x_n)$$

$$+ \frac{\partial}{\partial y_n}(P_n y_n + P_n R_n x_n^2)(y_{n+1} - y_n) + \frac{\partial}{\partial P_n}(P_n y_n + P_n R_n x_n^2)(P_{n+1} - P_n)$$

$$+ \frac{\partial}{\partial R_n}(P_n y_n + P_n R_n x_n^2)(R_{n+1} - R_n) \tag{7g}$$

$$y'_{n+1} = (P_n y_n + P_n R_n x_n^2) + (0 + 2P_n R_n x_n)(x_{n+1} - x_n)$$

$$+ (P_n \cdot 1 + 0)(y_{n+1} - y_n) + (1 \cdot y_n + 1 \cdot R_n x_n^2)(P_{n+1} - P_n)$$

$$+ (0 + P_n \cdot 1 \cdot x_n^2)(R_{n+1} - R_n) \tag{7h}$$

$$y'_{n+1} = (P_n y_n + P_n R_n x_n^2) + (2P_n R_n x_n)(x_{n+1} - x_n)$$

$$+ P_n(y_{n+1} - y_n) + (y_n + R_n x_n^2)(P_{n+1} - P_n)$$

$$+ P_n x_n^2(R_{n+1} - R_n) \tag{7i}$$

Rearranging the terms in equation (7i),

$$y'_{n+1} = P_n y_{n+1} + 2P_n R_n x_n x_{n+1} + P_n x_n^2 R_{n+1} + (y_n + R_n x_n^2) P_{n+1}$$

$$- (3P_n R_n x_n^2 + P_n y_n) \tag{8b}$$

Similarly equations (6c) and (6d) are written as,

$$R'_{n+1} = 0, \tag{8c}$$

$$P'_{n+1} = 0. \tag{8d}$$

The boundary conditions (2) and (3) are written below as

$$x_e = x(0) - \frac{1}{P} y(0) = c \quad \text{at } t = 0 \tag{9a}$$

$$y(t_f) = 0 \qquad \text{at } t = t_f \tag{9b}$$

$$x(t_1) = b_1 \qquad \text{at } t = t_1 \tag{9c}$$

$$x(t_2) = b_2 \qquad \text{at } t = t_2 \tag{9d}$$

where b_1 and b_2 are the true values of x at t_1 and t_2.

Applying the generalized Newton Raphson method to equations (9),

$$x_{n+1}(0) = c \tag{10a}$$

$$y_{n+1}(t_f) = 0 \tag{10b}$$

$$x_{n+1}(t_1) = b_1 \tag{10c}$$

$$x_{n+1}(t_2) = b_2 \tag{10d}$$

Equations (8) together with the boundary condititions (10) are solved by the use of the principle of superposition. Since one initial condition equation (2) is given, three sets of homogeneous solutions are needed for solving the equations (8). Initial values for solving equations (8) are so chosen that they satisfy the initial boundary condition and also set the integration constants equal to the unknown parameters.

The particular solution is obtained with the following initial values.

$$x_{p,n+1}(0) = c \tag{11a}$$

$$y_{p,n+1}(0) = 0 \tag{11b}$$

$$R_{p,n+1}(0) = 0 \tag{11c}$$

$$P_{p,n+1}(0) = 0 \tag{11d}$$

where, the subscript p denotes the particular value.

The homogeneous solutions are obtained by integrating the following equations.

$$x'_{n+1} = y_{n+1} \tag{12a}$$

$$y'_{n+1} = P_n y_{n+1} + 2P_n R_n x_n x_{n+1} + P_n x_n^2 R_{n+1} + (y_n + R_n x_n^2) P_{n+1} \tag{12b}$$

$$R'_{n+1} = 0 \tag{12c}$$

$$P'_{n+1} = 0 \tag{12d}$$

The three sets of initial values of obtaining the homogeneous solution are given below. Subscripts h_1, h_2, h_3 denote the three homogeneous values.

$$x_{h1,n+1}(0) = 0 \tag{13a}$$

$$y_{h1,n+1}(0) = 1 \tag{13b}$$

$$R_{h1,n+1}(0) = 0 \tag{13c}$$

$$P_{h1,n+1}(0) = 0 \tag{13d}$$

$$x_{h2,n+1}(0) = 0 \tag{14a}$$

$$y_{h2,n+1}(0) = 0 \tag{14b}$$

$$R_{h2,n+1}(0) = 1 \tag{14c}$$

$$P_{h2,n+1}(0) = 0 \tag{14d}$$

and,

$$x_{h3,n+1}(0) = 0 \tag{15a}$$

$$y_{h3,n+1}(0) = 0 \tag{15b}$$

$$R_{h3,n+1}(0) = 0 \tag{15c}$$

$$P_{h3,n+1}(0) = 1 \tag{15d}$$

The general solutions of the system of equations (8) are obtained by the principle of superposition.

$$x_{n+1}(t) = x_{p,n+1}(t) + \sum_{j=1}^{3} a_{j,n+1}\, x_{hj,n+1}(t) \tag{16a}$$

$$y_{n+1}(t) = y_{p,n+1}(t) + \sum_{j=1}^{3} a_{j,n+1}\, y_{hj,n+1}(t) \tag{16b}$$

$$R_{n+1}(t) + R_{p,n+1}(t) + \sum_{j=1}^{3} a_{j,n+1}\, R_{hj,n+1}(t) \tag{16c}$$

$$P_{n+1}(t) = P_{p,n+1}(t) + \sum_{j=1}^{3} a_{j,n+1}\, P_{hj,n+1}(t) \tag{16d}$$

It will be seen from equations (16c) and (16d) that,

$$R_{n+1}(0) = a_{2,n+1} \tag{17}$$

$$P_{n+1}(0) = a_{3,n+1} \tag{18}$$

It was initially assumed that both $R_{n+1}(t)$ and $P_{n+1}(t)$ are constant functions. Thus equations (17) and (18) are true for all values of t. Thus,

$$R_{n+1}(t) = a_{2,n+1} \tag{17a}$$

$$p_{n+1}(t) = a_{3,n+1} \tag{18a}$$

The integration constant $a_{1,n+1}$ can be expressed as a function of $a_{2,n+1}$ and $a_{3,n+1}$. The following equation is obtained from equation (16b) at $t = t_f$.

$$a_{1,n+1} = -\frac{(y_{p,n+1}(t_f) + a_{2,n+1}\, y_{h2,n+1}(t_f) + a_{3,n+1}\, y_{h3,n+1}(t_f))}{y_{h1,n+1}(t_f)} \tag{19}$$

CHAPTER III

NUMERICAL ANALYSIS

The fourth order Runge-Kutta Gill method has been used for carrying through the numerical integration. Integration over the interval (0,1) is carried through with a step size of 0.01.

Assuming that a solution exists, the linear differential equation is solved in two steps. First one set of particular and three sets of homogeneous solutions are obtained numerically. Initial values for obtaining these have been discussed in the preceeding chapter. Then the integration constants are obtained by the least square method.

The error between the general solution and the experimental values is minimized as follows

$$Q_{n+1} = \sum_{s=1}^{m_1} [x_{n+1}(t_s) - b_s]^2 \tag{1}$$

$$Q_{n+1} = \sum_{s=1}^{m_1} [x_{p,n+1}(t_s) + a_{1,n+1}\, x_{h1,n+1}(t_s) + a_{2,n+1}\, x_{h2,n+1}(t_s) + a_{3,n+1}\, x_{h3,n+1}(t_s) - b_s]^2 \tag{2}$$

From equation (19) of the preceeding chapter,

$$a_{1,n+1} = -\frac{(y_{p,n+1}(t_f) + a_{2,n+1}\, y_{h2,n+1}(t_f) + a_{3,n+1}\, y_{h3,n+1}(t_f))}{y_{h1,n+1}(t_f)} \tag{3}$$

Introducing equation (3) in equation (2),

$$Q_{n+1} = \sum_{s=1}^{m_1} [x_{p,n+1}(t_s) - \frac{x_{h1,n+1}(t_s)}{y_{h1,n+1}(t_f)} (y_{p,n+1}(t_f) + a_{2,n+1}\, y_{h2,n+1}(t_f)$$

$$+ a_{3,n+1}\, y_{h3,n+1}(t_f)) + a_{2,n+1}\, x_{h2,n+1}(t_s) + a_{3,n+1}\, x_{h3,n+1}(t_s) - b_s]^2 \quad (4)$$

Rearranging the terms and writing $A_{n+1} = \frac{x_{h1,n+1}(t_s)}{y_{h1,n+1}(t_f)}$

$$Q_{n+1} = \sum_{s=1}^{m_1} [x_{p,n+1}(t_s) - A_{n+1}\, y_{p,n+1}(t_f) + a_{2,n+1}(x_{h2,n+1}(t_s)$$

$$- A_{n+1}\, y_{h2,n+1}(t_f)) + a_{3,n+1}(x_{h3,n+1}(t_s) - A_{n+1} y_{h3,n+1}(t_f)) - b_s]^2 \quad (5)$$

Since all the particular and homogeneous solutions are known quantities equation (5) can be written as

$$Q_{n+1} = \sum_{s=1}^{m_1} [q_{1,n+1}(t_s) + a_{2,n+1} \cdot q_{2,n+1}(t_s) + a_{3,n+1} \cdot q_{3,n+1}(t_s) - b_s]^2 \quad (6)$$

Minimizing equation (6) wrt $a_{2,n+1}$ and $a_{3,n+1}$ the following two equations are obtained.

$$\sum_{s=1}^{m_1} q_{3,n+1}(t_s)[q_{1,n+1}(t_s) + a_{2,n+1} \cdot q_{2,n+1}(t_s) + a_{3,n+1} \cdot q_{3,n+1}(t_s)$$

$$- b_s] = 0 \quad (7a)$$

$$\sum_{s=1}^{m_1} q_{3,n+1}(t_s)[q_{1,n+1}(t_s) + a_{2,n+1} \cdot q_{2,n+1}(t_s) + a_{3,n+1} \cdot q_{3,n+1}(t_s) - b_s] = 0 \quad (7b)$$

The two simultaneous algebraic equations (7a) and (7b) are to be solved to obtain the integration constants, which are equal to the unknown parameters. The parameters are used recursively to obtain improved results.

The flow chart figure (2), and the computer program for solving the problem appear in the Appendix.

CHAPTER IV

CONCLUSION

The quasilinearization method combined with the superposition method is unstable under certain conditions [11]. For example, during the process of iteration one or more values of the particular and homogeneous solutions can become unreasonable. The solutions will not converge to the exact values even if the exact values of the parameters are used as the initial approximations.

Extremely large or small values of the parameters are obtained at the end of the first few iterations. Since the original nonlinear equations are very sensitive to these values, extremely large positive or negative values are obtained for the dependent variable of the differential equation. Thus the final boundary condition cannot be fulfilled.

The linear differential equation is obtained by the generalized Newton-Raphson method. Therefore these unreasonable values of the parameters during the first few iterations should be expected.

In order to avoid these unreasonable values, the parameters should be changed to within reasonable ranges. When these restrictions are used, the convergence problems are reduced.

The method converged to the exact values in six iterations. Figure (1) shows the nature of convergence of the method.

PART II

INTRODUCTION

The estimation of parameters in nonlinear partial differential equations is much more difficult than in ordinary differential equations. If the model equations are linear an analytical solution is usually obtainable from which the parameters may be estimated. When the partial differential equation is nonlinear some sort of extremely time-consumming trial and error integration of the equations becomes necessary.

Parameter estimation for the humidity diffusion in concrete has been presented. The drying of concrete is one of the basic factors in creep, shrinkage and crack formation. In the construction of massive structures, knowledge of the rate and the amount of heat evolved during the process of hardening are desirable. The physical process is assumed to be represented by a nonlinear parabolic differential equation.

The phenomenological characteristics of the drying of concrete were studied experimentally by Pihlajavaara [1]. A mathematical equation for the moisture dependence of the diffusion coefficient was proposed. It was observed in the experiments that the diffusion coefficient underwent a significant change when the process of drying proceeded from 100 per cent to 70 per cent relative humidity of the pores. Definite conclusions have not been reached so far. This is partly due to the lack of experimental data for the drying of concrete.

Bazant and Najjar [2] performed numerical analysis with the diffusion coefficient proposed by [1]. Trial and error was used. Finite differencing of the space and the time derivatives was carried through based on the Crank Nicolson method. A more pertinent form of the diffusion coefficient was proposed. It contained three parameters.

The objective of the present work is to estimate the parameters in the diffusion equation by the quasilinearization technique. The diffusion coefficient suggested by [2] is used. Experimental data of Abrams and Orals [3] is also used.

Integration of the linearized equation is carried through by the finite difference method. Both the space and the time derivatives are discretized. The Crank-Nicolson method has been used in the finite differencing. An algorithm is devised based on the least squares method. Initial guesses are made for the parameters and also for the function value of humidity as a function of space and time. The initial values chosen for the purpose of integration comply with the initial boundary condition and set the integration constants equal to the unknown parameters. The parameters thus obtained are used recursively to obtain improved values.

The error in the experimental data of [3] is considered small in magnitude. The mathematical model is devised to fit the experimental data. The concrete medium is assumed isotropic macroscopically. It has been assumed that the process of drying takes place isothermally.

CHAPTER I

THE BASIC DIFFUSION EQUATION

Concrete is a capillary porous colloidal material. It has a wide range of pore sizes. The complicated physico-chemical microstructure allows different kinds of individual flow to occur simultaneously. Vapor diffusion, saturated and unsaturated capillary transfer are typical examples of these flows.

The process of diffusion is a result of random particle motions within the medium. Matter is transported from one part of the system to another as a result of the random particle motions. The flow due to diffusion is not caused by external forces but it is due to concentration gradients.

Inadequate knowledge of the actual mechanisms of heat and mass transfer during the drying process makes the formulation of a detailed kinetic-mathematical model difficult. Generally engineering problems that have a multiplicity of fundamental laws in operation are nonlinear mathematical models.

Concentration dependent diffusion in an isotropic medium is governed by the Ficks equation,

$$\frac{\partial Y_d}{\partial t} = \frac{\partial}{\partial x}\left[C(Y_d)\frac{\partial Y}{\partial x}\right] \tag{1}$$

or

$$\frac{\partial Y_d}{\partial t} = \nabla(C(Y_d)\ \nabla Y_d) \tag{2}$$

Equation (2) is expressed in vector notation. The diffusion coefficient undergoes a significant change when the drying process progresses from 100 per cent relative humidity of the pores to 70 per cent relative humidity of the pores.

Pihlajavaara [1] proposed the following mathematical equation for the diffusion coefficient:

$$C[Y_d] = C_1 \cdot (1 + \alpha\, Y_d^{\gamma}) \tag{3}$$

where,

α and γ are parameters,

C_1 is the diffusion coefficient at 100 per cent relative humidity of the pores,

Y_d is the relative humidity of the pores.

Bazant and Najjar [2] proposed the following equations:

$$C[Y_d] = C_1 \cdot \{1 + (1 - \alpha)(1 - Y_d)^{\gamma}\} \tag{4}$$

and

$$C[Y_d] = C_1 \cdot \left\{\alpha + \frac{1-\alpha}{1 + \left(\frac{1-Y_d}{1-h}\right)^{\gamma}}\right\} \tag{5}$$

where,

h is another parameter.

The diffusion coefficient characterizes the diffusion process and represents the rate of drying. Besides its dependence on the moisture, the diffusion coefficient also depends on the properties of the cement paste, history of hydration, moisture concentration and the ambient temperature.

Figure (3) illustrates the various phases of drying experienced by concrete. It shows a plot of the rate of drying against the average moisture content.

The medium is initially at saturation, constant temperature and constant external condition. AB denotes the constant rate period. The surface of the medium is sufficiently wet during this phase. It enables to simulate a free water surface. The surface remains wet during the period.

BC denotes the first-following rate period. The rate of evaporation from the saturated surface is higher than the rate of liquid diffusion. The surface begins to dry out. The effective area of the wetted surface decreases linearly with the moisture content [17]. In this period the rate of drying is approximately a linear function of the moisture content. The first falling-rate period ends when dryness is reached at the surface. The moisture content will be in equilibrium with the moisture in the environment.

CD denotes the falling rate period. It is characterized by sub-surface evaporation. The plane of evaporation receedes further into the body. The liquid evaporates from a relatively dry surface. The evaporation rate depends on liquid transfer from the interior of the mass. The liquid transfer will be from the surface into the environment.

The rate of hydration tends to retard over extended time intervals. This is because of the dependence of the diffusivity on the pore humidity.

CHAPTER II

LINEARIZATION OF THE NONLINEAR PARABOLIC DIFFERENTIAL EQUATION

The development of high speed digital and analog computing devices has spurred a substantial growth of the mathematical science of numerical analysis. There is no extant theory for solving nonlinear partial differential equations. Many of the methods used are suggested from procedures that can solve linear equations. Extension of these ideas to nonlinear partial differential equations is very difficult if a thorough analysis of stability, convergence and error is carried through.

The preliminary step involved in all numerical methods is to introduce nondimensional variables in place of dimensional variables.

$$\frac{\partial Y}{\partial t} = \frac{\partial}{\partial x} (C([Y] \frac{\partial Y}{\partial x}) \qquad (1)$$

The variables Y, t, x and C[Y] are dimensionless

where,

$$x = \frac{x_d}{L_d} ,$$

$$Y = \frac{Y_d - Y_{en}}{1 - Y_{en}} ,$$

$$t = \frac{(t_d - t_0) \cdot C_1}{L_d^2} ,$$

x_d, t_d, Y_d are dimensional variables of space, time and relative humidity of pores respectively. Y_{en}, t_0, L_d and C_1 are dimensional variables of relative humidity of the environment, curing time, half-length of slab and the diffusion coefficient at 100 per cent relative humidity of pores respectively.

The dimensionless diffusion coefficient C[Y] is given by,

$$C[Y] = \alpha + \frac{(1 - \alpha)}{1 + \beta^{\gamma} (1-Y)^{\gamma}} \tag{2}$$

where,

$$\beta = \frac{1 - Y_{en}}{1 - h}, \qquad \text{is a parameter.}$$

$$Y = \frac{Y_d - Y_{en}}{1 - Y_{en}}$$

Introducing equation (2) in the basic diffusion equation (1),

$$\frac{\partial Y}{\partial t} = \frac{\partial}{\partial x} \left(\left\{ \alpha + \frac{(1 - \alpha)}{1 + \beta^{\gamma}(1-Y)^{\gamma}} \right\} \frac{\partial Y}{\partial x} \right) \tag{3}$$

Thus,

$$\frac{\partial Y}{\partial t} = \frac{\partial}{\partial x} \left\{ \alpha + \frac{(1 - \alpha)}{1 + \beta^{\gamma}(1-Y)^{\gamma}} \right\} \frac{\partial Y}{\partial x} + \left\{ \alpha + \frac{(1 - \alpha)}{1 + \beta^{\gamma}(1-Y)^{\gamma}} \right\} \frac{\partial^2 Y}{\partial x^2} \tag{4}$$

For simplicity in the derivation, equation (4) is written as,

$$\frac{\partial Y}{\partial t} = \frac{\partial C}{\partial x}\frac{\partial Y}{\partial x} + C\,\frac{\partial^2 Y}{\partial x^2} \tag{5}$$

Thus,

$$Y' = f[Y, \frac{\partial Y}{\partial x}, \frac{\partial^2 Y}{\partial x^2}, \alpha, \beta, \gamma] \tag{6}$$

Equation (5) is nonlinear and it is linearized by the generalized Newton-Raphson method as below:

$$Y'_{n+1} = Y'_n + \frac{\partial Y'_n}{\partial Y_n}(Y_{n+1} - Y_n) + \frac{\partial Y'_n}{\partial \left.\frac{\partial Y}{\partial x}\right|_n}\left(\left.\frac{\partial Y}{\partial x}\right|_{n+1} - \left.\frac{\partial Y}{\partial x}\right|_n\right)$$

$$+ \frac{\partial Y'_n}{\partial \left.\frac{\partial^2 Y}{\partial x^2}\right|_n}\left(\left.\frac{\partial^2 Y}{\partial x^2}\right|_{n+1} - \left.\frac{\partial^2 Y}{\partial x^2}\right|_n\right) + \frac{\partial Y'_n}{\partial \alpha_n}(\alpha_{n+1} - \alpha_n)$$

$$+ \frac{\partial Y'_n}{\partial \beta_n}(\beta_{n+1} - \beta_n) + \frac{\partial Y'_n}{\partial \gamma_n}(\gamma_{n+1} - \gamma_n) \tag{7}$$

where the subscripts n+1 and n denote the $(n+1)^{st}$ iteration and the n^{th} iteration respectively.

Equation (5) may be written for the n^{th} iteration as,

$$Y'_n = \left.\frac{\partial C}{\partial x}\right|_n \left.\frac{\partial Y}{\partial x}\right|_n + C_n \left.\frac{\partial^2 Y}{\partial x^2}\right|_n \tag{8}$$

Introducing equation (8) in equation (7),

$$
\begin{aligned}
Y'_{n+1} = {} & \left(\frac{\partial C}{\partial x}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n + C_n \cdot \frac{\partial^2 Y}{\partial x^2}\bigg|_n\right) + \frac{\partial}{\partial Y_n}\left(\frac{\partial C}{\partial x}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n\right. \\
& \left. + C_n \cdot \frac{\partial^2 Y}{\partial x^2}\bigg|_n\right)(Y_{n+1} - Y_n) + \frac{\partial}{\partial \left.\frac{\partial Y}{\partial x}\right|_n}\left(\frac{\partial C}{\partial x}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n\right. \\
& \left. + C_n \cdot \frac{\partial^2 Y}{\partial x^2}\bigg|_n\right)\left(\frac{\partial Y}{\partial x}\bigg|_{n+1} - \frac{\partial Y}{\partial x}\bigg|_n\right) + \frac{\partial}{\partial \left.\frac{\partial^2 Y}{\partial x^2}\right|_n}\left(\frac{\partial C}{\partial x}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n\right. \\
& \left. + C_n \frac{\partial^2 Y}{\partial x^2}\bigg|_n\right)\left(\frac{\partial^2 Y}{\partial x^2}\bigg|_{n+1} - \frac{\partial^2 Y}{\partial x^2}\bigg|_n\right) + \frac{\partial}{\partial \alpha_n}\left(\frac{\partial C}{\partial x}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n\right. \\
& \left. + C_n \cdot \frac{\partial^2 Y}{\partial x^2}\bigg|_n\right)(\alpha_{n+1} - \alpha_n) + \frac{\partial}{\partial \beta_n}\left(\frac{\partial C}{\partial x}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n + C_n \cdot \frac{\partial^2 Y}{\partial x^2}\bigg|_n\right)(\beta_{n+1} - \beta_n) \\
& + \frac{\partial}{\partial \gamma_n}\left(\frac{\partial C}{\partial x}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n + C_n \cdot \frac{\partial^2 Y}{\partial x^2}\bigg|_n\right)\left(\gamma_{n+1} - \gamma_n\right)
\end{aligned}
\tag{9}
$$

$$
\begin{aligned}
Y'_{n+1} = {} & \left(\frac{\partial C}{\partial x}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n + C_n \cdot \frac{\partial^2 Y}{\partial x^2}\bigg|_n\right) \\
& + \left(\frac{\partial^2 C}{\partial x \partial Y}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n + \frac{\partial C}{\partial Y}\bigg|_n \cdot \frac{\partial^2 Y}{\partial x^2}\bigg|_n\right)(Y_{n+1} - Y_n) \\
& + \left(\frac{\partial C}{\partial x}\bigg|_n + 0\right)\left(\frac{\partial Y}{\partial x}\bigg|_{n+1} - \frac{\partial Y}{\partial x}\bigg|_n\right) + (0 + C_n)\left(\frac{\partial^2 Y}{\partial x^2}\bigg|_{n+1} - \frac{\partial^2 Y}{\partial x^2}\bigg|_n\right) \\
& + \left(\frac{\partial^2 C}{\partial x \partial \alpha}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n + \frac{\partial C}{\partial \alpha}\bigg|_n \cdot \frac{\partial^2 Y}{\partial x^2}\bigg|_n\right)(\alpha_{n+1} - \alpha_n)
\end{aligned}
$$

$$+ \left(\frac{\partial^2 C}{\partial x\ \partial\beta}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n + \frac{\partial C}{\partial\beta}\bigg|_n \cdot \frac{\partial^2 Y}{\partial x^2}\bigg|_n\right)(\beta_{n+1} - \beta_n)$$

$$+ \left(\frac{\partial^2 C}{\partial x\ \partial\gamma}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n + \frac{\partial C}{\partial\gamma}\bigg|_n\right)(\gamma_{n+1} - \gamma_n) \tag{10}$$

Since,

$$C = g(Y) \tag{11}$$

$$\frac{\partial C}{\partial x} = \frac{\partial C}{\partial Y}\frac{\partial Y}{\partial x} \tag{12}$$

Thus,

$$\frac{\partial C}{\partial x}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n \tag{13a}$$

Similarly,

$$\frac{\partial^2 C}{\partial x\ \partial\alpha}\bigg|_n = \frac{\partial^2 C}{\partial Y\ \partial\alpha}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n \tag{13b}$$

$$\frac{\partial^2 C}{\partial x\ \partial\beta}\bigg|_n = \frac{\partial^2 C}{\partial Y\ \partial\beta}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n \tag{13c}$$

$$\frac{\partial^2 C}{\partial x\ \partial\gamma}\bigg|_n = \frac{\partial^2 C}{\partial Y\ \partial\gamma}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n \tag{13d}$$

$$\frac{\partial^2 C}{\partial x\ \partial Y}\bigg|_n = \frac{\partial^2 C}{\partial Y^2}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n \tag{13e}$$

Introducing equations (13) in equation (10),

$$Y'_{n+1} = \left(\frac{\partial C}{\partial Y}\Big|_n \cdot \left(\frac{\partial Y}{\partial x}\right)^2\Big|_n + C_n \cdot \frac{\partial^2 Y}{\partial x^2}\Big|_n\right) +$$

$$\left(\frac{\partial^2 C}{\partial Y^2}\Big|_n \cdot \left(\frac{\partial Y}{\partial x}\right)^2\Big|_n + \frac{\partial C}{\partial Y}\Big|_n \cdot \frac{\partial^2 Y}{\partial x^2}\Big|_n\right) (Y_{n+1} - Y_n) +$$

$$\left(\frac{\partial C}{\partial Y}\Big|_n \cdot \frac{\partial Y}{\partial x}\Big|_n\right) \left(\frac{\partial Y}{\partial x}\Big|_{n+1} - \frac{\partial Y}{\partial x}\Big|_n\right) +$$

$$\left(\frac{\partial^2 C}{\partial Y \partial \alpha}\Big|_n \cdot \left(\frac{\partial Y}{\partial x}\right)^2\Big|_n + \frac{\partial C}{\partial \alpha}\Big|_n \cdot \frac{\partial^2 Y}{\partial x^2}\Big|_n\right) (\alpha_{n+1} - \alpha_n) +$$

$$\left(\frac{\partial^2 C}{\partial Y \partial \beta}\Big|_n \cdot \left(\frac{\partial Y}{\partial x}\right)^2\Big|_n + \frac{\partial C}{\partial \beta}\Big|_n \cdot \frac{\partial^2 Y}{\partial x^2}\Big|_n\right) (\beta_{n+1} - \beta_n) +$$

$$\left(\frac{\partial^2 C}{\partial Y \partial \gamma}\Big|_n \cdot \left(\frac{\partial Y}{\partial x}\right)^2\Big|_n + \frac{\partial C}{\partial \gamma}\Big|_n \cdot \frac{\partial^2 Y}{\partial x^2}\Big|_n\right) (\gamma_{n+1} - \gamma_n) \tag{14}$$

On cancellation of terms,

$$Y'_{n+1} = \frac{\partial C}{\partial Y}\Big|_n \cdot \frac{\partial Y}{\partial x}\Big|_n \cdot \frac{\partial Y}{\partial x}\Big|_{n+1} + C_n \frac{\partial^2 Y}{\partial x^2}\Big|_{n+1}$$

$$+ \left(\frac{\partial^2 C}{\partial Y \partial \alpha}\Big|_n \cdot \left(\frac{\partial Y}{\partial x}\right)^2\Big|_n + \frac{\partial C}{\partial \alpha}\Big|_n \cdot \frac{\partial^2 Y}{\partial x^2}\Big|_n\right) (\alpha_{n+1} - \alpha_n)$$

$$+ \left(\frac{\partial^2 C}{\partial Y \partial \beta}\Big|_n \cdot \left(\frac{\partial Y}{\partial x}\right)^2\Big|_n + \frac{\partial C}{\partial \beta}\Big|_n \cdot \frac{\partial^2 Y}{\partial x^2}\Big|_n\right) (\beta_{n+1} - \beta_n)$$

$$+ \left\{ \frac{\partial^2 C}{\partial Y \partial \gamma} \Big|_n \cdot \left(\frac{\partial Y}{\partial x}\right)^2 \Big|_n + \frac{\partial C}{\partial \gamma} \Big|_n \cdot \frac{\partial^2 Y}{\partial x^2} \Big|_n \right\} (\gamma_{n+1} - \gamma_n)$$

$$+ \left\{ \frac{\partial^2 C}{\partial Y^2} \Big|_n \cdot \left(\frac{\partial Y}{\partial x}\right)^2 \Big|_n + \frac{\partial C}{\partial Y} \Big|_n \cdot \frac{\partial^2 Y}{\partial x^2} \Big|_n \right\} (\Upsilon_{n+1} - \Upsilon_n) \qquad (15)$$

Equation (15) will determine the particular solution. To obtain the homogeneous solution, the equation is

$$Y'_{n+1} = \frac{\partial C}{\partial Y} \Big|_n \cdot \frac{\partial Y}{\partial x} \Big|_n \cdot \frac{\partial Y}{\partial x} \Big|_{n+1} + C_n \cdot \frac{\partial^2 Y}{\partial x^2} \Big|_{n+1}$$

$$+ \left\{ \frac{\partial^2 C}{\partial Y \partial \alpha} \Big|_n \cdot \left(\frac{\partial Y}{\partial x}\right)^2 \Big|_n + \frac{\partial C}{\partial \alpha} \Big|_n \cdot \frac{\partial^2 Y}{\partial x^2} \Big|_n \right\} \cdot \alpha_{n+1}$$

$$+ \left\{ \frac{\partial^2 C}{\partial Y \partial \beta} \Big|_n \cdot \left(\frac{\partial Y}{\partial x}\right)^2 \Big|_n + \frac{\partial C}{\partial \beta} \Big|_n \cdot \frac{\partial^2 Y}{\partial x^2} \Big|_n \right\} \cdot \beta_{n+1}$$

$$+ \left\{ \frac{\partial^2 C}{\partial Y \partial \gamma} \Big|_n \cdot \left(\frac{\partial Y}{\partial x}\right)^2 \Big|_n + \frac{\partial C}{\partial \gamma} \Big|_n \cdot \frac{\partial^2 Y}{\partial x^2} \Big|_n \right\} \cdot \gamma_{n+1}$$

$$+ \left\{ \frac{\partial^2 C}{\partial Y^2} \Big|_n \cdot \left(\frac{\partial Y}{\partial x}\right)^2 \Big|_n + \frac{\partial C}{\partial Y} \cdot \frac{\partial^2 Y}{\partial x^2} \Big|_n \right\} \cdot Y_{n+1} \qquad (16)$$

In equations (8) to (16) the equations for C, $\frac{\partial C}{\partial Y}$, $\frac{\partial^2 C}{\partial Y^2}$, $\frac{\partial^2 C}{\partial Y \partial \alpha}$, $\frac{\partial^2 C}{\partial Y, \partial \beta}$, $\frac{\partial^2 C}{\partial Y, \partial \gamma}$, etc are as follows:

$$C = \alpha + \frac{(1-\alpha)}{1 + \beta^{\gamma}(1-Y)^{\gamma}} \tag{17a}$$

$$\frac{\partial C}{\partial Y} = \frac{(1-\alpha)\gamma\beta^{\gamma}(1-Y)^{\gamma-1}}{\{1 + \beta^{\gamma}(1-Y)^{\gamma}\}^{2}} \tag{17b}$$

$$\frac{\partial C}{\partial \alpha} = 1 - \frac{1}{\{1 + \beta^{\gamma}(1-Y)^{\gamma}\}} \tag{17c}$$

$$\frac{\partial C}{\partial \beta} = -\frac{(1-\alpha)\gamma\beta^{\gamma-1}(1-Y)^{\gamma}}{\{1 + \beta^{\gamma}(1-Y)^{\gamma}\}^{2}} \tag{17d}$$

$$\frac{\partial C}{\partial \gamma} = -\frac{(1-\alpha)\beta^{\gamma}(1-Y)^{\gamma}\ln[\beta(1-Y)]}{\{1 + \beta^{\gamma}(1-Y)^{\gamma}\}^{2}} \tag{17c}$$

$$\frac{\partial^{2} C}{\partial Y^{2}} = \frac{(1-\alpha)\gamma\beta^{\gamma}(1-Y)^{\gamma-2}\{\beta^{\gamma}(1-Y)^{\gamma}(\gamma+1) - \gamma+1\}}{\{1 + \beta^{\gamma}(1-Y)^{\gamma}\}^{3}} \tag{17f}$$

$$\frac{\partial^{2} C}{\partial Y \partial \alpha} = \frac{\gamma\beta^{\gamma}(1-Y)^{\gamma-1}}{\{1 + \beta^{\gamma}(1-Y)^{\gamma}\}^{2}} \tag{17g}$$

$$\frac{\partial^{2} C}{\partial Y \partial \beta} = \frac{(1-\alpha)\gamma^{2}\beta^{\gamma-1}(1-Y)^{\gamma-1}\{1-\beta^{\gamma}(1-y)^{\gamma}\}}{\{1 + \beta^{\gamma}(1-Y)^{\gamma}\}^{3}} \tag{17h}$$

$$\frac{\partial^2 C}{\partial Y \partial \gamma} = \frac{(1-\alpha)\beta^{\gamma}(1-Y)^{\gamma-1}\{\beta^{\gamma}(1-Y)^{\gamma}[1-\gamma \ln\{\beta(1-Y)\}] + [1+\gamma \ln\{\beta(1-Y)\}]\}}{\{1 + \beta^{\gamma}(1-Y)^{\gamma}\}^3} \tag{17i}$$

Equations (15) and (16) are rewritten with the terms all rearranged as follows,

$$Y'_{n+1} = \frac{\partial C}{\partial Y}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_{n+1} + C_n \cdot \frac{\partial^2 Y}{\partial x^2}\bigg|_{n+1}$$

$$+ \left(\frac{\partial Y}{\partial x}\right)^2\bigg|_n \cdot \Bigg(\frac{\partial^2 C}{\partial Y \partial \alpha}\bigg|_n \cdot (\alpha_{n+1} - \alpha_n) + \frac{\partial^2 C}{\partial Y \partial \beta}\bigg|_n \cdot (\beta_{n+1} - \beta_n)$$

$$+ \frac{\partial^2 C}{\partial Y \partial \gamma}\bigg|_n \cdot (\gamma_{n+1} - \gamma_n) + \frac{\partial^2 C}{\partial Y^2}\bigg|_n \cdot (Y_{n+1} - Y_n)\Bigg)$$

$$+ \frac{\partial^2 Y}{\partial x^2}\bigg|_n \cdot \Bigg(\frac{\partial C}{\partial \alpha}\bigg|_n \cdot (\alpha_{n+1} - \alpha_n) + \frac{\partial C}{\partial \beta}\bigg|_n \cdot (\beta_{n+1} - \beta_n) +$$

$$\frac{\partial C}{\partial \gamma}\bigg|_n \cdot (\gamma_{n+1} - \gamma_n) + \frac{\partial C}{\partial Y}\bigg|_n \cdot (Y_{n+1} - Y_n)\Bigg) \tag{15a}$$

$$Y'_{n+1} = \frac{\partial C}{\partial Y}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_n \cdot \frac{\partial Y}{\partial x}\bigg|_{n+1} + C_n \cdot \frac{\partial^2 Y}{\partial x^2}\bigg|_{n+1}$$

$$+ \left(\frac{\partial Y}{\partial x}\right)^2\bigg|_n \cdot \Bigg(\frac{\partial^2 C}{\partial Y \partial \alpha}\bigg|_n \cdot \alpha_{n+1} + \frac{\partial^2 C}{\partial Y \partial \beta}\bigg|_n \cdot \beta_{n+1} + \frac{\partial^2 C}{\partial Y \partial \gamma}\bigg|_n \cdot \gamma_{n+1}$$

$$+ \frac{\partial^2 C}{\partial Y^2}\bigg|_n \cdot Y_{n+1}\Bigg)$$

$$+ \frac{\partial^2 Y}{\partial x^2}\bigg|_n \cdot \left\{\frac{\partial C}{\partial \alpha}\bigg|_n \cdot \alpha_{n+1} + \frac{\partial C}{\partial \beta}\bigg|_n \cdot \beta_{n+1} + \frac{\partial C}{\partial \gamma}\bigg|_n \cdot \gamma_{n+1} + \frac{\partial C}{\partial Y}\bigg|_n \cdot Y_{n+1}\right\}$$

(16a)

Boundary Conditions

At the exposed surface,

$$Y(t) = Y_{\text{environment}}(t) \,, \qquad \text{for all time } t. \qquad (18)$$

At the center of the slab,

$$\frac{\partial Y(t)}{\partial x} = 0, \qquad \text{for all time } t. \qquad (19)$$

(i) Initial boundary condition

$$Y(0) = 1, \qquad \text{at } t = 0 \text{ for all } x\text{, except at the exposed surface.} \qquad (20)$$

(ii) Final boundary condition

$$Y(t_f) = b \qquad \text{at } t = t_{\text{final}} \qquad (21)$$

where,

b is the experimental value at $t = t_{\text{final}}$.

Applying the generalized Newton-Raphson formula to equations (18) to (21),

$$Y_{n+1}(t) = Y_{\text{environment}}(t), \qquad (22)$$

$$\frac{\partial Y(t)}{\partial x}\bigg|_{n+1} = 0 \,, \qquad (23)$$

$$Y_{n+1}(0) = 1, \tag{24}$$

and,

$$Y_{n+1}(t_f) = b. \tag{25}$$

CHAPTER III

FINITE DIFFERENCE METHOD

The equations (15a) and (16a) of the preceeding chapter are solved by the finite difference method. Finite differences of both the space and the time derivatives are carried through. The increments in Y at each time step can be computed from either implict or explicit methods. The explicit method leads to a numerically unstable solution even if the diffusivity is considered constant.

Backward or central differences in time steps reduce the instability of the problem. For both the schemes, the numerical process at constant diffusivity is stable [2]. They also allow the time-step to be increased or decreased as desired. The dampening of error in subsequent steps is stronger when the backward differences are used. The central differences are usually more advantageous because of their accuracy.

The Crank-Nicolson method of averaging the approximations in the t^{th} and $(t+1)^{st}$ rows is considered more accurate and has therefore been used. The explicit and implicit methods lead to discretization errors of $O[\Delta t + (\Delta x)^2]$. The Crank-Nicolson method is stable for all values of the ratio $\Delta t/(\Delta x)^2$. It converges with a discretization error of $O[\Delta t^2 + (\Delta x)^2]$ [18]. Although this is a distinct improvement over the explicit and the implicit methods, the computation is more complicated than for the implicit method.

The following difference equations are obtained based on the Crank-Nicolson method,

$$Y'_{n+1} = \frac{Y_{n+1}(p,t+1) - Y_{n+1}(p,t)}{\Delta t} \tag{1}$$

$$\frac{\partial Y}{\partial x}\Big|_{n+1} = \frac{Y_{n+1}(p+1,t+1) - Y_{n+1}(p,t+1) + Y_{n+1}(p+1,t) - Y_{n+1}(p,t)}{2\Delta x} \tag{2}$$

$$\frac{\partial^2 Y}{\partial x^2}\Big|_{n+1} = \frac{Y_{n+1}(p+1,t+1)-2Y_{n+1}(p,t+1)+Y_{n+1}(p-1,t+1)+Y_{n+1}(p+1,t)-2Y_{n+1}(p,t)}{2(\Delta x)^2}$$

$$\frac{+Y_{n+1}(p-1,t)}{2(\Delta x)^2} \tag{3}$$

$$\frac{\partial Y}{\partial x}\Big|_{n} = \frac{Y_n(p+1,t+1) - Y_n(p,t+1) + Y_n(p+1,t) - Y_n(p,t)}{2\Delta x} \tag{4}$$

$$\frac{\partial^2 Y}{\partial x^2}\Big|_{n} = \frac{Y_n(p+1,t+1)-2Y_n(p,t+1)+Y_n(p-1,t+1)+Y_n(p+1,t)-2Y_n(p,t)+Y_n(p-1,t)}{2(\Delta x)^2}$$

$$Y_{n+1} = \frac{Y_{n+1}(p,t+1) + Y_{n+1}(p,t)}{2} \tag{6}$$

$$Y_n = \frac{Y_n(p,t+1) + Y_n(p,t)}{2} \tag{7}$$

Introducting equations (1) to (7) in equation (15a) of the preceeding chapter,

$$\frac{Y_{n+1}(p,t+1) - Y_{n+1}(p,t)}{\Delta t} =$$

$$\frac{\partial C}{\partial Y}\Big|_n \cdot \left(\frac{Y_n(p+1,t+1) - Y_n(p,t+1) + Y_n(p+1,t) - Y_n(p,t)}{2\Delta x}\right) \cdot$$

$$\left(\frac{Y_{n+1}(p+1,t+1) - Y_{n+1}(p,t+1) + Y_{n+1}(p+1,t) - Y_{n+1}(p,t)}{2\Delta x}\right)$$

$$+ C_n \cdot \left(\frac{Y_{n+1}(p+1,t+1)-2Y_{n+1}(p,t+1)+Y_{n+1}(p-1,t+1)+Y_{n+1}(p+1,t)-2Y_{n+1}(p,t)}{2(\Delta x)^2}\right.$$

$$\left. \cdot \frac{+ Y_{n+1}(p-1,t)}{2(\Delta x)^2}\right)$$

$$+ \left(\frac{Y_n(p+1,t+1) - Y_n(p,t+1) + Y_n(p+1,t) - Y_n(p,t)}{2\Delta x}\right)^2 \cdot$$

$$\left(\frac{\partial^2 C}{\partial Y \partial \alpha}\Big|_n \cdot (\alpha_{n+1}-\alpha_n) + \frac{\partial^2 C}{\partial Y \partial \beta}\Big|_n \cdot (\beta_{n+1}-\beta_n) + \frac{\partial^2 C}{\partial Y \partial \gamma}\Big|_n \cdot (\gamma_{n+1}-\gamma_n) + \frac{\partial^2 C}{\partial Y^2}\Big|_n \cdot\right.$$

$$\left.\left(\frac{Y_{n+1}(p,t+1)+Y_{n+1}(p,t)}{2} - \frac{Y_n(p,t+1)+Y_n(p,t)}{2}\right)\right)$$

$$+ \left(\frac{Y_n(p+1,t+1)-2Y_n(p,t+1)+Y_n(p-1,t+1)+Y_n(p+1,t)-2Y_n(p,t)+Y_n(p-1,t)}{2(\Delta x)^2}\right) \cdot$$

$$\left\{\frac{\partial C}{\partial \alpha}\bigg|_n \cdot (\alpha_{n+1}-\alpha_n) + \frac{\partial C}{\partial \beta}\bigg|_n \cdot (\beta_{n+1}-\beta_n) + \frac{\partial C}{\partial \gamma}\bigg|_n \cdot (\gamma_{n+1}-\gamma_n)+\frac{\partial C}{\partial Y}\bigg|_n \cdot\right.$$

$$\left.\left(\frac{Y_{n+1}(p,t+1)+Y_{n+1}(p,t)}{2} - \frac{Y_n(p,t+1)+Y_n(p,t)}{2}\right)\right\} \qquad (8)$$

Writing $r = \frac{\Delta t}{(\Delta x)^2}$ and rearranging the terms in equation (8) above,

$$Y_{n+1}(p,t+1) \cdot r \cdot \left\{\frac{1}{r} + C_n + \frac{\partial C}{\partial Y}\bigg|_n \cdot \frac{1}{4} \cdot \{Y_n(p,t+1)-Y_n(p-1,t+1)+Y_n(p,t)\right.$$

$$- Y_n(p-1,t)\} - \frac{\partial^2 C}{\partial Y^2}\bigg|_n \cdot \frac{1}{8} \cdot \{Y_n(p+1,t+1) - Y_n(p,t+1) + Y_n(p+1,t)$$

$$\left. - Y_n(p,t)\}^2\right\} + Y_{n+1}(p+1,t+1) \cdot r \cdot (-1) \cdot \left\{C_n \cdot \frac{1}{2} + \frac{\partial C}{\partial Y}\bigg|_n \cdot \frac{1}{4} \cdot\right.$$

$$\left.\{Y_n(p+1,t+1) - Y_n(p,t+1) + Y_n(p+1,t) - Y_n(p,t)\}\right\}$$

$$+ Y_{n+1}(p-1,t+1) \cdot r \cdot (-1) \cdot C_n \cdot \frac{1}{2} = Y_{n+1}(p,t)$$

$$+ \frac{r}{2} \cdot [Y_n(p+1,t+1)-2Y_n(p,t+1)+Y_n(p-1,t+1)+Y_n(p+1,t)-2Y_n(p,t)+Y_n(p-1,t)].$$

$$\left\{\frac{\partial C}{\partial \alpha}\bigg|_n \cdot (\alpha_{n+1}-\alpha_n) + \frac{\partial C}{\partial \beta}\bigg|_n \cdot (\beta_{n+1}-\beta_n) + \frac{\partial C}{\partial \gamma}\bigg|_n (\gamma_{n+1}-\gamma_n) + \frac{\partial C}{\partial Y}\bigg|_n \cdot \frac{1}{2} \cdot\right.$$

$$\left.(Y_{n+1}(p,t)-Y_n(p,t+1)-Y_n(p,t))\right\} + \frac{r}{4} \cdot [Y_n(p+1,t+1)-Y_n(p,t+1)+Y_n(p+1,t)-Y_n(p,t)]^2.$$

$$\left[\frac{\partial^2 C}{\partial Y \partial \alpha}\bigg|_n \cdot (\alpha_{n+1}-\alpha_n) + \frac{\partial^2 C}{\partial Y \partial \beta}\bigg|_n \cdot (\beta_{n+1}-\beta_n) + \frac{\partial^2 C}{\partial Y \partial \gamma}\bigg|_n \cdot (\gamma_{n+1}-\gamma_n) + \frac{\partial^2 C}{\partial Y^2}\bigg|_n \cdot \frac{1}{2} \cdot\right.$$

$$\left.(Y_{n+1}(p,t)-Y_n(p,t+1)-Y_n(p,t))\right] + \frac{r}{4} \cdot \frac{\partial C}{\partial Y}\bigg|_n \cdot [Y_{n+1}(p+1,t+1)-Y_{n+1}(p,t+1)$$

$$+ Y_n(p+1,t) - Y_n(p,t)] \cdot [Y_{n+1}(p+1,t) - Y_{n+1}(p,t)] + \frac{r}{2} \cdot C_n \cdot$$

$$[Y_{n+1}(p+1,t) - 2Y_{n+1}(p,t) + Y_{n+1}(p-1,t)] . \tag{9}$$

Equation (9) is written explicitly below:

$$Y_{n+1}(p,t+1) \cdot r \cdot \left[\frac{1}{r} + \alpha_n + \frac{1-\alpha_n}{1+\beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1)+Y_n(p,t)}{2}\right)^{\gamma_n}} + \right.$$

$$\frac{1}{4} \cdot \frac{(1-\alpha_n)\gamma_n\beta_n^{\gamma_n}\left(1 - \frac{Y_n(p,t+1)+Y_n(p,t)}{2}\right)^{\gamma_n-1}}{\left\{1+\beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1)+Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^2} \cdot \{Y_n(p,t+1)-Y_n(p-1,t+1)+Y_n(p,t)$$

$$- Y_n(p-1,t)\} - \frac{1}{8} \cdot \frac{(1-\alpha_n)\gamma_n\beta_n^{\gamma_n}\left(1 - \frac{Y_n(p,t+1)+Y_n(p,t)}{2}\right)^{\gamma_n-2}}{\left\{1+\beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^3}$$

$$\frac{\left\{\beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n} \cdot (\gamma_n+1) - (\gamma_n-1)\right\}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}\right\}^3} \cdot$$

$$\left\{Y_n(p+1,t+1) - Y_n(p,t+1) + Y_n(p+1,t) - Y_n(p,t)\right\}^2\Big]$$

$$+ Y_{n+1}(p+1,t+1) \cdot r \cdot (-1) \cdot \left[\left\{\alpha_n + \frac{1-\alpha_n}{1 + \beta_n^{\gamma_n}\left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}}\right\} \cdot \frac{1}{2}\right.$$

$$+ \frac{1}{4} \cdot \frac{(1-\alpha_n)\beta_n^{\gamma}\left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n-1}}{\left\{1 + \beta_n^{\gamma_n}\left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}\right\}^2}$$

$$\left.\cdot \left\{Y_n(p+1,t+1) - Y_n(p,t+1) + Y_n(p+1,t) - Y_n(p,t)\right\}\right]$$

$$+ Y_{n+1}(p+1,t+1) \cdot r \cdot \left(-\frac{1}{2}\right) \cdot \left\{\alpha_n + \frac{1-\alpha_n}{1 + \beta_n^{\gamma_n}\left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}}\right\}$$

$$= Y_{n+1}(p,t) + \frac{r}{2} \cdot [Y_{n+1}(p+1,t+1) - 2Y_n(p,t+1) + Y_n(p-1,t+1) + Y_n(p+1,t)$$

$$- 2Y_n(p,t) + Y_n(p-1,t)]$$

$$\cdot \left[\left\{1 - \frac{1}{1 + \beta_n^{\gamma_n}\left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n}}\right\} \cdot (\alpha_{n+1} - \alpha_n)\right.$$

$$- \frac{(1-\alpha_n)\gamma_n\beta_n^{\gamma_n - 1}\left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n}}{\left\{1 + \beta_n^{\gamma_n}\left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n}\right\}^2} \cdot (\beta_{n+1} - \beta_n)$$

$$- \frac{(1-\alpha_n)\beta_n^{\gamma_n}\left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n} \cdot \ln\left[\beta_n \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}\right]}{\left\{1 + \beta_n^{\gamma_n} \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n}\right\}^2} \cdot$$

$$(\gamma_{n+1} - \gamma_n) +$$

$$\left.\frac{1}{2} \cdot \frac{(1-\alpha_n)\gamma_n\beta_n^{\gamma_n}\left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n}\right\}^2} \cdot \left\{Y_{n+1}(p,t) - Y_n(p,t+1) - Y_n(p,t)\right\}\right]$$

$$+ \frac{r}{4} \cdot [Y_n(p+1,t+1) - Y_n(p,t+1) + Y_n(p+1,t) - Y_n(p,t)]^2.$$

$$\left[\frac{-\gamma_n \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n} \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^2} \cdot (\alpha_{n+1} - \alpha_n) \right.$$

$$+ \frac{(1-\alpha_n)\gamma_n^2 \beta_n^{\gamma_n - 1} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^3} \cdot$$

$$\frac{\cdot \left\{1 - \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^3} \cdot (\beta_{n+1} - \beta_n) +$$

$$\frac{(1-\alpha_n)\beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)}{\left\{1 + \beta_n^{\gamma_n} \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}} \cdot$$

$$\left\{\beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n} \cdot \left\{1 - \gamma_n \cdot \ln \left[\beta_n \cdot \right.\right.\right.$$

$$\left.\left.\left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)\right]\right\} + \left\{1 + \gamma_n \cdot \ln \left[\beta_n \cdot \right.\right.$$

$$\left.\left.\left.\left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)\right]\right\}\right\} \cdot (\gamma_{n+1} - \gamma_n)$$

$$+ \frac{(1-\alpha_n)\gamma_n \cdot \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n - 2}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^3} \cdot$$

$$\frac{\left\{\beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n} \cdot (\gamma_n + 1) - (\gamma_n - 1)\right\}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^3} \cdot$$

$$\left.\frac{1}{2} \cdot \left\{Y_{n+1}(p,t) - Y_n(p,t+1) - Y_n(p,t)\right\}\right]$$

$$+ \frac{r}{4} \cdot \frac{(1-\alpha_n)\gamma_n\beta_n^{\gamma_n}\left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n}\left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^2} \cdot$$

$$[Y_n(p+1,t+1) - Y_n(p,t+1) + Y_n(p+1,t) - Y_n(p,t)]$$

$$\cdot\ [Y_{n+1}(p+1,t) - Y_{n+1}(p,t)]$$

$$+ \frac{r}{4} \cdot \left\{\alpha_n + \frac{1 - \alpha_n}{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}}\right\} \cdot$$

$$[Y_{n+1}(p+1,t) - 2Y_{n+1}(p,t) + Y_{n+1}(p-1,t)] \tag{10}$$

If the space domain is divided into $M-1$ equidistant spaces by M nodes, there will be M equations corresponding to equation (10). The first and the last of these equations satisfy the boundary conditions,

$$Y_{n+1}(1,t) = Y_{environment}(t) \, , \tag{11a}$$

and

$$\frac{\partial Y_{n+1}(M,t)}{\partial x} = 0 \, .$$

Thus,

$$\frac{Y_{n+1}(M+1,t) - Y_{n+1}(M-1,t)}{2\Delta x} = 0$$

and

$$Y_{n+1}(M+1,t) = Y_{n+1}(M-1,t) \tag{11b}$$

The system of M simultaneous algebraic equations is written in matrix form as,

$$[A]_{MxM} \cdot [Y]_{Mx1} = [K]_{Mx1} \tag{12}$$

where,

$[A]_{MxM}$ is a tridiagonal band matrix,

$[Y]_{Mx1}$ is the column matrix with relative humdiity predictions at the subsequent time step,

$[K]_{Mx1}$ is the column matrix with elements of known values.

Typical values that constitute the p^{th} row of the matrices [A] and [K] are written below

$$A[p,p-2] = 0, \qquad p = 1,M \tag{13a}$$

$$A[p,p-1] = r\,(-\tfrac{1}{2}) \cdot \left\{\alpha_n + \frac{1-\alpha_n}{1+\beta_n^{\gamma_n}\left\{1 - \frac{Y_n(p,t+1)+Y_n(p,t)}{2}\right\}^{\gamma_n}}\right\}, \quad p=1,M \tag{13b}$$

$$A[p,p] = r \cdot \left[\frac{1}{r} + \left\{ \alpha_n + \frac{1 - \alpha_n}{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}} \right\} + \right.$$

$$\frac{1}{4} \cdot \frac{(1-\alpha_n)\gamma_n\beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^2} \cdot$$

$$\{Y_n(p,t+1) - Y_n(p-1,t+1) + Y_n(p,t) - Y_n(p-1,t)\}$$

$$- \frac{1}{8} \cdot \frac{(1-\alpha_n)\gamma_n\beta_n^{\gamma_n} \cdot \left(1 - Y_n(p,t+1) + Y_n(p,t)\right)^{\gamma_n - 2}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^3} \cdot$$

$$\frac{\left\{\beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n} \cdot (\gamma_n + 1) - (\gamma_n - 1)\right\}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^3}$$

$$\left. \cdot \left\{Y_n(p+1,t+1) - Y_n(p,t+1) + Y_n(p+1,t) - Y_n(p,t)\right\}^2 \right] , \quad p = 1,M \qquad (13c)$$

$$A(p,p+1) = r \cdot (-1) \cdot \left[\left\{ \alpha_n + \frac{1 - \alpha_n}{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}} \right\} \cdot \frac{1}{2} \right.$$

$$+ \frac{(1-\alpha_n)\gamma_n\beta_n^{\gamma_n} \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n}\left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^2} \cdot$$

$$\left. \frac{1}{4} \cdot \{Y_n(p+1,t+1) - Y_n(p,t+1) + Y_n(p+1,t) - Y_n(p,t)\} \right] , \quad p = 1, M \tag{13d}$$

$$A(p,p+2) = 0, \qquad p = 1, M \tag{13e}$$

$$K[p] = Y_{n+1}(p,t) + \frac{r}{2} \cdot \left[Y_n(p+1,t+1) - 2Y_n(p,t+1) + Y_n(p-1,t+1) + Y_n(p+1,t) \right.$$

$$\left. - 2Y_n(p,t) + Y_n(p-1,t) \right]$$

$$\cdot \left[\left\{ 1 - \frac{1}{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}} \right\} \cdot (\alpha_{n+1} - \alpha_n) \right.$$

$$- \frac{(1-\alpha_n)\gamma_n\beta_n^{\gamma_n - 1} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^2} \cdot (\beta_{n+1} - \beta_n)$$

$$- \frac{(1-\alpha_n)\beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n} \cdot \ln\left[\beta_n \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]\right]}{\left\{1 + \beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}\right\}^2} \cdot$$

$$(\gamma_{n+1} - \gamma_n) + \frac{(1-\alpha_n)\gamma_n\beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}\right\}^2} \cdot$$

$$\left.\frac{1}{2} \cdot \{Y_{n+1}(p,t) - Y_n(p,t+1) - Y_n(p,t)\}\right] + \frac{r}{4} \cdot [Y_n(p+1,t+1) - Y_n(p,t+1)$$

$$+ Y_n(p+1,t) - Y_n(p,t)]^2$$

$$\cdot\left[\frac{-\gamma_n\beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}\right\}^2} \cdot (\alpha_{n+1} - \alpha_n)\right.$$

$$+ \frac{(1-\alpha_n)\gamma_n^2\beta_n^{\gamma_n - 1} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}\right\}^3} \cdot$$

$$\frac{\left\{1 - \beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}\right\}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}\right\}^3}$$

$$\cdot\ (\beta_{n+1} - \beta_n) + \frac{(1-\alpha_n)\beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}\right\}^3}\ \cdot$$

$$\left[\beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n} \cdot \left\{1 - \gamma_n \cdot \ln\left[\beta_n \cdot\ 1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]\right]\right\}$$

$$+ \left\{1 + \gamma_n \ln\left[\beta_n \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]\right]\right\} \cdot (\gamma_{n+1} - \gamma_n)$$

$$+ \frac{(1-\alpha_n) \cdot \gamma_n \beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n - 2}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}\right\}^3}\ \cdot$$

$$\frac{\left\{\beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n} \cdot (\gamma_n + 1) - (\gamma_n - 1)\right\}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}\right\}^3}$$

$$\cdot \frac{1}{2} \cdot \{Y_{n+1}(p,t) - Y_n(p,t+1) - Y_n(p,t)\}\Big\}\Big)$$

$$+ \frac{r}{4} \cdot \frac{(1-\alpha_n)\gamma_n \cdot \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^2 \cdot} \cdot$$

$$[Y_n(p+1,t+1) - Y_n(p,t+1) + Y_n(p+1,t) - Y_n(p,t)] \cdot [Y_{n+1}(p+1,t) - Y_{n+1}(p,t)]$$

$$+ \frac{r}{4} \cdot \left(\alpha_n + \frac{1 - \alpha_n}{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)}\right) \cdot$$

$$\cdot [Y_{n+1}(p+1,t) - 2Y_{n+1}(p,t) + Y_{n+1}(p-1,t)] \qquad (14)$$

Matrix $[Y]_{Mx1}$ is composed of,

$$\begin{bmatrix} Y_{n+1}(1,t+1) \\ Y_{n+1}(2,t+1) \\ \vdots \\ Y_{n+1}(p,t+1) \\ \vdots \\ Y_{n+1}(M-1,t+1) \\ Y_{n+1}(M,t+1) \end{bmatrix}_{M\times 1} \tag{15}$$

The initial values for obtaining the particular solution are,

$$\begin{bmatrix} Y_{p,n+1}(1,0) \\ Y_{p,n+1}(2,0) \\ Y_{p,n+1}(3,0) \\ \vdots \\ Y_{p,n+1}(j,t) \\ \vdots \\ Y_{p,n+1}(M-1,t) \\ Y_{p,n+1}(M,t) \\ \alpha_{p,n+1}(0) \\ \beta_{p,n+1}(0) \\ \gamma_{p,n+1}(0) \end{bmatrix} = \begin{bmatrix} Y^{(0)}_{environment} \\ 1 \\ 1 \\ \vdots \\ 1 \\ \vdots \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{16}$$

Equation (16a) of the preceeding chapter is used to determine the homogeneous solution. It is rewritten below

$$\gamma'_{n+1} = \frac{\partial C}{\partial \gamma}\Big|_n \cdot \frac{\partial Y}{\partial x}\Big|_n \cdot \frac{\partial Y}{\partial x}\Big|_{n+1} + C_n \cdot \frac{\partial^2 Y}{\partial x^2}\Big|_{n+1} + \left(\frac{\partial Y}{\partial x}\right)^2\Big|_n \cdot$$

$$\left\{\frac{\partial^2 C}{\partial Y \partial \alpha}\Big|_n \cdot \alpha_{n+1} + \frac{\partial^2 C}{\partial Y \partial \beta}\Big|_n \cdot \beta_{n+1} + \frac{\partial^2 C}{\partial Y \partial \gamma}\Big|_n \cdot \gamma_{n+1} + \frac{\partial^2 C}{\partial Y^2}\Big|_n \cdot Y_{n+1}\right\}$$

$$+ \frac{\partial^2 Y}{\partial x^2}\Big|_n \cdot \left\{\frac{\partial C}{\partial \alpha}\Big|_n \cdot \alpha_{n+1} + \frac{\partial C}{\partial \beta}\Big|_n \cdot \beta_{n+1} + \frac{\partial C}{\partial \gamma}\Big|_n \cdot \gamma_{n+1} + \frac{\partial C}{\partial Y}\Big|_n \cdot Y_{n+1}\right\} \tag{17}$$

Using the finite differences in equations (1) to (7) in equation (17) and proceeding in a similar manner as in equation (10), the final form obtained is,

$$Y_{n+1}(p,t+1) \cdot r \cdot \left[\frac{1}{r} + \left\{\alpha_n + \frac{1-\alpha_n}{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}}\right\}\right.$$

$$+ \frac{1}{4} \cdot \frac{(1-\alpha_n)\gamma_n \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^2} \cdot$$

$$[Y_n(p,t+1) - Y_n(p-1,t+1) + Y_n(p,t) - Y_n(p-1,t)]$$

$$- \frac{1}{8} \cdot \frac{(1-\alpha_n)\gamma_n\beta_n^{\gamma_n} \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n - 2}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n}\right\}^3} \cdot$$

$$\frac{\left\{\beta_n^{\gamma_n} \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n} \cdot (\gamma_n+1) - (\gamma_n-1)\right\}}{\left\{1 + \beta_n^{\gamma_n} \cdot \; 1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n}\Big\}^3}$$

$$\cdot \{Y_n(p+1,t+1) - Y_n(p,t+1) + Y_n(p+1,t) - Y_n(p,t)\}^2]$$

$$+ Y_{n+1}(p+1,t+1) \cdot r \cdot (-1) \cdot \left[\left\{\alpha_n + \frac{1 - \alpha_n}{1 + \beta_n^{\gamma_n} \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n}}\right\} \cdot \frac{1}{2}\right.$$

$$+ \frac{(1-\alpha_n)\gamma_n\beta_n^{\gamma_n} \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n}\right\}^2} \cdot$$

$$\left.\frac{1}{4} \cdot \{Y_n(p+1,t+1) - Y_n(p,t+1) + Y_n(p+1,t) - Y_n(p,t)\}\right]$$

$$+ Y_{n+1}(p-1,t+1) \cdot r \cdot (- \tfrac{1}{2}) \cdot \left\{\alpha_n + \frac{1 - \alpha_n}{1 + \beta_n^{\gamma_n} \cdot \; 1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\Big\}^{\gamma_n}}\right\}$$

$$= Y_{n+1}(p,t) + \frac{r}{2} \cdot \Big[Y_n(p+1,t+1) - 2Y_n(p,t+1) + Y_n(p-1,t+1) + Y_n(p+1,t)$$

$$- 2Y_n(p,t) + Y_n(p-1,t)] \cdot \left[\left\{1 - \frac{1}{1 + \beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}}\right\} \cdot \alpha_{n+1}\right.$$

$$- \frac{(1-\alpha_n)\gamma_n\beta_n^{\gamma_n-1} \cdot 1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}^{\gamma_n}}{\left\{1 + \beta_n^{\gamma_n}\left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}\right\}^2} \cdot \beta_{n+1}$$

$$- \frac{(1-\alpha_n)\beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n} \cdot \ln\left[\beta_n - \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]\right]}{\left\{1 + \beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}\right\}^2}$$

$$\left. \cdot \gamma_{n+1} + \frac{(1-\alpha_n)\gamma_n\beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n-1}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}\right\}^2} \cdot \frac{1}{2} \cdot Y_{n+1}(p,t) \right]$$

$$+ \frac{r}{4} \cdot [Y_n(p+1,t+1) - Y_n(p,t+1) + Y_n(p+1,t) - Y_n(p,t)]^2.$$

$$\left[- \frac{\gamma_n \beta_n^{\gamma_n} \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n}\right\}^2} \cdot \alpha_{n+1} + \right.$$

$$\frac{(1-\alpha_n)\gamma_n^2 \beta^{\gamma_n - 1} \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n}\right\}^3} \cdot$$

$$\frac{\left\{1 - \beta_n^{\gamma_n} \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n}\right\}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n}\right\}^3} \cdot \beta_{n+1}$$

$$+ \frac{(1-\alpha_n)\beta_n^{\gamma_n} \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n}\right\}^3} \cdot \left\{\beta_n^{\gamma_n} \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}^{\gamma_n} \cdot \right.$$

$$\left. [1 - \gamma_n \cdot \ln\left\{\beta_n \cdot \left\{1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right\}\right\}\right\}]$$

$$+ \left\{1 + \gamma_n \ln \left\{\beta_n \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]\right\}\right\}\}$$

$$\cdot\ \gamma_{n+1} + \frac{(1-\alpha_n)\gamma_n \beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n - 2}}{\left\{1 + \beta_n^{\gamma_n} \cdot\ 1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}\Big\}^3} \cdot$$

$$\left\{\beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n} \cdot (\gamma_n + 1) - (\gamma_n - 1)\right\} \cdot \frac{1}{2} \cdot Y_{n+1}(p,t)\Big]$$

$$+ \frac{r}{4} \cdot \frac{(1-\alpha_n) \cdot \gamma_n \beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}\right\}^2} \cdot$$

$$[Y_n(p+1,t+1) - Y_n(p,t+1) + Y_n(p+1,t) - Y_n(p,t)] \cdot [Y_{n+1}(p+1,t) - Y_{n+1}(p,t)]$$

$$+ \frac{r}{4} \cdot \left\{\alpha_n + \frac{1 - \alpha_n}{1 + \beta_n^{\gamma_n} \cdot \left[1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right]^{\gamma_n}}\right\} \cdot$$

$$[Y_{n+1}(p+1,t) = 2Y_{n+1}(p,t) + Y_{n+1}(p-1,t)] \qquad (18)$$

Equation (18) also consists of a system of M simultaneous equations. In matrix form the simultaneous equations are written as,

$$[A]_{MxM} \cdot [Y]_{Mx1} = [K']_{Mx1} \tag{19}$$

The elements in the p^{th} row of [A] and [Y] are identical to those in equation [12]. However the elements in the p^{th} row of [K'] are different.

$$K'[p] = Y_{n+1}(p,t) + \frac{r}{2} \cdot [Y_n(p+1,t+1) - 2Y_n(p,t+1) + Y_n(p-1,t+1) + Y_n(p+1,t)$$

$$-2Y_n(p,t) + Y_n(p-1,t)] \cdot \left\{\left\{1 - \frac{1}{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}}\right\} \alpha_{n+1}\right.$$

$$- \frac{(1-\alpha_n)\gamma_n\beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^2} \cdot \beta_{n+1}$$

$$- \frac{(1-\alpha_n)\beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n} \cdot \ln\left(\beta_n\left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)\right)}{\left\{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^2} \cdot \gamma_{n+1}$$

$$+ \frac{(1-\alpha_n) \cdot \gamma_n \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t+1)}{2}\right)^{\gamma_n}\right\}^2} \cdot \frac{1}{2} \cdot Y_{n+1}(p,t) \Bigg]$$

$$+ \frac{r}{4} \cdot [Y_n(p+1,t+1) - Y_n(p,t+1) + Y_n(p+1,t) - Y_n(p,t)]^2 \ .$$

$$\left(- \frac{\gamma_n \beta_n^{\gamma_n} \cdot \ 1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\Big)^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^2} \cdot \alpha_{n+1} \ + \right.$$

$$\frac{(1-\alpha_n)\gamma_n^2 \beta^{\gamma_n - 1} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n - 1}}{\left\{1 + \beta_n^{\gamma_n} \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^3} \ \cdot$$

$$\frac{\left\{1 - \beta_n^{\gamma_n} \cdot \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}}{\left\{1 + \beta_n^{\gamma_n} \left(1 - \frac{Y_n(p,t+1) + Y_n(p,t)}{2}\right)^{\gamma_n}\right\}^3} \cdot \beta_{n+1}$$

$$+\frac{(1-\alpha_n)\beta^{\gamma_n}\cdot\left\{1-\frac{Y_n(p,t+1)+Y_n(p,t)}{2}\right\}^{\gamma_n-1}}{\left\{1+\beta_n^{\gamma_n}\cdot\left\{1-\frac{Y_n(p,t+1)+Y_n(p,t)}{2}\right\}^{\gamma_n}\right\}^3}\cdot$$

$$\left\{\beta_n^{\gamma_n},\left\{1-\frac{Y_n(p,t+1)+Y_n(p,t)}{2}\right\}^{\gamma_n}\cdot\left\{1-\gamma_n\ell n\left\{\beta_n\cdot\left\{1-\frac{Y_n(p,t+1)+Y_n(p,t)}{2}\right\}\right\}\right\}\right.$$

$$\left.+\left\{1+\gamma_n\cdot\ell n\left\{\beta_n\cdot\left\{1-\frac{Y_n(p,t+1)+Y_n(p,t)}{2}\right\}\right\}\right\}\right\}\cdot\gamma_{n+1}$$

$$+\frac{(1-\alpha_n)\cdot\gamma_n\cdot\beta_n^{\gamma_n}\left\{1-\frac{Y_n(p,t+1)+Y_n(p,t)}{2}\right\}^{\gamma_n-2}}{\left\{1+\beta_n^{\gamma_n}\, n\left\{1-\frac{Y_n(p,t+1)+Y_n(p,t)}{2}\right\}^{\gamma_n}\right\}^3}\cdot$$

$$\left.\frac{\left\{\beta_n^{\gamma_n}\left\{1-\frac{Y_n(p,t+1)+Y_n(p,t)}{2}\right\}^{\gamma_n}\cdot(\gamma_n+1)-(\gamma_n-1)\right\}}{\left\{1+\beta_n^{\gamma_n}\cdot\left\{1-\frac{Y_n(p,t+1)+Y_n(p,t)}{2}\right\}^{\gamma_n}\right\}^3}\cdot\frac{1}{2}\cdot Y_{n+1}(p,t)\right\} \quad (20)$$

There are three sets of homogeneous solutions. The initial values for obtaining these are given below,

$$\begin{bmatrix}
Y_{h1,n+1}(1,0) & Y_{h2,n+1}(1,0) & Y_{h3,n+1}(1,0) \\
Y_{h1,n+1}(2,0) & Y_{h2,n+1}(2,0) & Y_{h3,n+1}(2,0) \\
Y_{h1,n+1}(3,0) & Y_{h2,n+1}(3,0) & Y_{h3,n+1}(3,0) \\
\vdots & \vdots & \vdots \\
Y_{h1,n+1}(p,0) & Y_{n2,n+1}(p,0) & Y_{h3,n+1}(p,0) \\
\vdots & \vdots & \vdots \\
Y_{h1,n+1}(M-1,0) & Y_{h2,n+1}(M-1,0) & Y_{h3,n+1}(M-1,0) \\
Y_{h1,n+1}(M,0) & Y_{h2,n+1}(M-0) & Y_{h3,n+1}(M,0) \\
\alpha_{h1,n+1}(0) & \alpha_{h2,n+1}(0) & \alpha_{h3,n+1}(0) \\
\beta_{h1,n+1}(0) & \beta_{h2,n+1}(0) & \beta_{h3,n+1}(0) \\
\gamma_{h1,n+1}(0) & \gamma_{h2,n+1}(0) & \gamma_{h3,n+1}(0)
\end{bmatrix}
=
\begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
\vdots & \vdots & \vdots \\
0 & 0 & 0 \\
\vdots & \vdots & \vdots \\
0 & 0 & 0 \\
0 & 0 & 0 \\
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix} \tag{21}$$

The general solution of the system of equations is obtained by the principle of superposition

$$Y_{n+1}(j,t) = Y_{p,n+1}(j,t) + \sum_{k=1}^{3} a_{k,n+1} \cdot Y_{hk,n+1}(j,t), \quad j = 1,M \tag{22a}$$

$$\alpha_{n+1}(j,t) = \alpha_{p,n+1}(t) + \sum_{k=1}^{3} a_{k,n+1} \cdot \alpha_{hk,n+1}(t) \tag{22b}$$

$$\beta_{n+1}(j,t) = \beta_{p,n+1}(t) + \sum_{k=1}^{3} a_{k,n+1} \cdot \beta_{hk,n+1}(t) \tag{22c}$$

$$\gamma_{n+1}(j,t) = \gamma_{p,n+1}(t) + \sum_{k=1}^{3} a_{k,n+1} \cdot \gamma_{hk,n+1}(t) \tag{22d}$$

The subscripts p, h1, h2 and h3 denote the particular and three sets of homogeneous solutions. The initial values for obtaining these four sets have been selected to satisfy the initial boundary condition and also to set the integration constants equal to the parameters.

It may be seen from equations (22b), (22c) and (22d) that,

$$\alpha_{n+1}(0) = a_{1,n+1} \tag{23a}$$

$$\beta_{n+1}(0) = a_{2,n+1} \tag{23b}$$

and

$$\gamma_{n+1}(0) = a_{3,n+1} \tag{23c}$$

Since the parameters are assumed constant functions, therefore,

$$\alpha_{n+1}(t) = a_{1,n+1} \tag{24a}$$

$$\beta_{n+1}(t) = a_{2,n+1} \tag{24b}$$

$$\gamma_{n+1}(t) = a_{3,n+1} \tag{24c}$$

CHAPTER IV

NUMERICAL ANALYSIS

The linear differential equation is solved in two steps, assuming that a solution exists for the problem. First one set of particular and three sets of homogeneous solutions are obtained numerically. Initial values for obtaining each of these sets have been stated in the preceeding chapter. The tridiagonal band matrix is inverted at every time increment by using the Thomas' algorithm. This algorithm expedites the numerical work involved at each time-step.

The next step involves the determination of the three integration constants. The least squares method is used. The error between the experimental data and the model prediction is minimized.

$$Q_{n+1} = \sum_{s=1}^{m_1} \sum_{j=1}^{M} [Y_{n+1}(j,t_s) - Y_{data}(j,t_s)]^2 \tag{1}$$

$$Q_{n+1} = \sum_{s=1}^{m_1} \sum_{j=1}^{M} [Y_{p,n+1}(j,t_s) + a_{1,n+1} \cdot Y_{h1,n+1}(j,t_s)$$

$$+ a_{2,n+1} \cdot Y_{h2,n+1}(j,t_s) + a_{3,n+1} \cdot Y_{h3,n+1}(j,t_s) - Y_{data}(j,t_s)]^2 \tag{2}$$

Since all the particular and homogeneous solutions are known, equation (2) is written as,

$$Q_{n+1} = \sum_{s=1}^{m_1} \sum_{j=1}^{M} [q_{1,n+1}(j,t_s) + a_{1,n+1} \cdot q_{2,n+1}(j,t_s)$$

$$+ a_{2,n+1} \cdot q_{3,n+1}(j,t_s) + a_{3,n+1} \cdot q_{4,n+1}(j,t_s)]^2 \tag{3}$$

Minimizing equation (3) wrt $a_{1,n+1}$, $a_{2,n+1}$ and $a_{3,n+1}$ the following three equations are obtained,

$$\sum_{s=1}^{m_1} \sum_{j=1}^{M} q_{2,n+1}(j,t_s) \cdot [q_{1,n+1}(j,t_s) + a_{1,n+1} \cdot q_{2,n+1}(j,t_s)$$

$$+ a_{2,n+1}(j,t_s)q_{3,n+1}(j,t_s) + a_{3,n+1} \cdot q_{4,n+1}(j,t_s)] = 0 \tag{4a}$$

$$\sum_{s=1}^{m_1} \sum_{j=1}^{M} q_{3,n+1}(j,t_s) \cdot [q_{1,n+1}(j,t_s) + a_{1,n+1} \cdot q_{2,n+1}(j,t_s)$$

$$+ a_{2,n+1} \cdot q_{3,n+1}(j,t_s) + a_{3,n+1} \cdot q_{4,n+1}(j,t_s)] = 0 \tag{4b}$$

$$\sum_{s=1}^{m_1} \sum_{j=1}^{M} q_{4,n+1}(j,t_s) \cdot [q_{1,n+1}(j,t_s) + a_{1,n+1} \cdot q_{2,n+1}(j,t_s)$$

$$+ a_{2,n+1} \cdot q_{3,n+1}(j,t_s) + a_{3,n+1} \cdot q_{4,n+1}(j,t_s)] = 0 \tag{4c}$$

The three simultaneous algebraic equations (4) are solved to obtain integration constants. They are equal to the unknown parameters. The parameters are used recursively to obtain improved results.

The flow chart figure (4) that was used in the numerical solution appears in the Appendix.

CHAPTER V

CONCLUSION

In the solution of the problem convergence was not obtained. The following factors may be attributed to this behavior.

Actual experience has shown that the generalized Newton-Raphson method is very sensitive to the error of the unknown or guessed initial condition, and is unstable. The guessed values of the unknown parameters as well as the functional equation of humidity for the first iteration have to be very close to the correct values for the problem to converge.

The lack of convergence encountered in solving the problem may also have been due to insufficient spacial nodes. Numerical analysis with upto thirty-four nodal points in the spacial coordinate and one hundred in the time coordinate was carried through.

The Newton-Raphson method can converge quadratically only if the method should at all converge [11].

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APPENDIX A

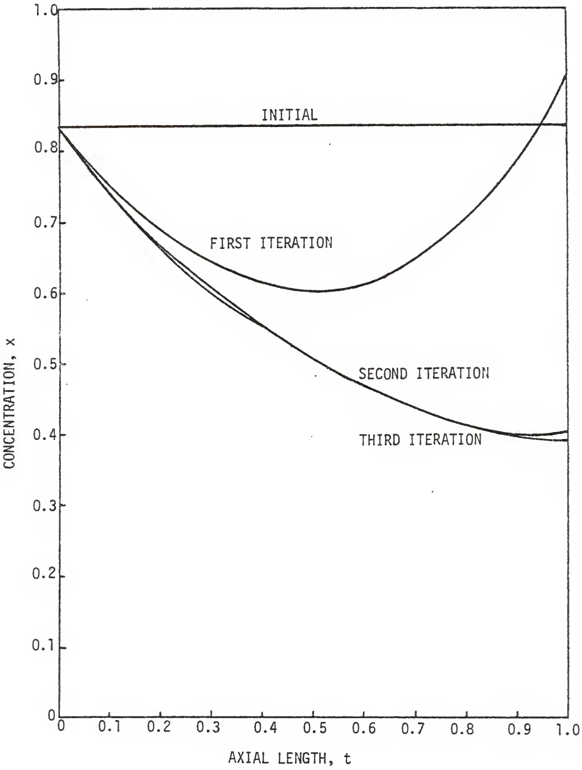

FIGURE 1. CONCENTRATION PROFILES WITH AXIAL DIFFUSION, SHOWING THE NATURE OF CONVERGENCE OF THE METHOD.

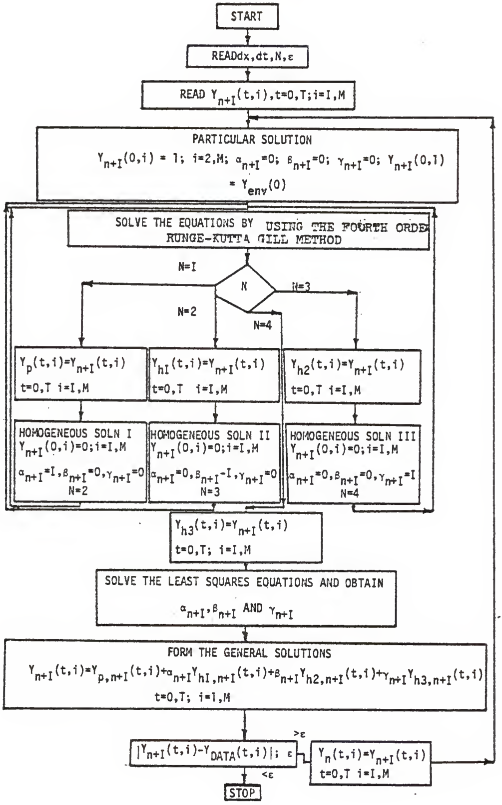

FIGURE 2. FLOW CHART FOR SOLVING THE NONLINEAR ORDINARY DIFFERENTIAL EQUATION.

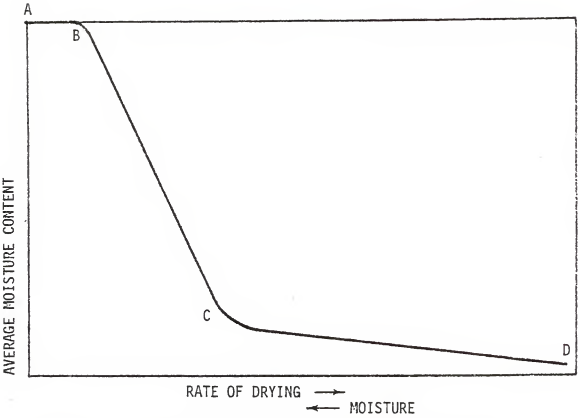

FIGURE 3: PLOT OF THE RATE OF DRYING AGAINST THE AVERAGE MOISTURE CONTENT.

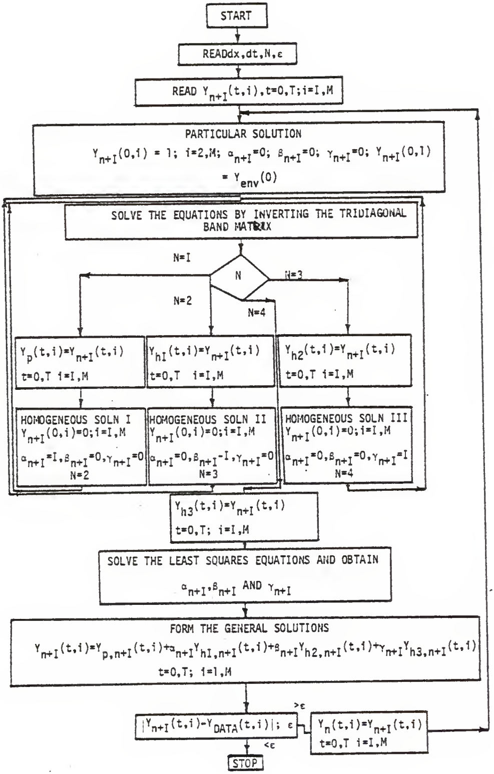

FIGURE 4. FLOW CHART FOR SOLVING THE NONLINEAR PARABOLIC DIFFERENTIAL EQUATION.

APPENDIX B

```
C
C     THIS PROGRAM ESTIMATES PARAMETERS IN A NONLINEAR ORDINARY
C     DIFFERENTIAL EQUATION. THE GENERALISED NEWTON-RAPHSON METHOD
C     IS USED TO LINEARISE THE EQUATION. USE OF THE RUNGE-KUTTA GILL
C     METHOD IS MADE FOR NUMERICAL INTEGRATION.
C
      DIMENSION X0(101),Y0(101),R0(1),P0(1),X1(101),Y1(101),R1(1),P1(1),
     *XP(101),YP(101),XH1(101),XH2(101),XH3(101),YH1(101),YH2(101),YH3(1
     *01),BS(10),W(4),F(28),DW(4),A(3)
      COMMON/FORMER/X0,Y0,R0,P0
      COMMON/ICONTR/INT,ICHECK
    1 FORMAT(F5.2,2X,F5.1,2X,I4,2X,I2,2X,I3,2X,F10.6,2X,F8.5)
    2 FORMAT(F8.5)
    3 FORMAT(///)
    4 FORMAT(9X,'R0', 5X,F3.1,/,9X,'P0', 5X,F3.1,//,T12,'N',T23,'R',T32,
     *'P',T43,'GENERAL SOLUTIONS AT CORRESPONDING DATA POINTS',/)
    5 FORMAT(1H1)
   13 FORMAT(2F10.6)
   63 FORMAT('0',8X,I3,5X,2F9.5,5X,10F5.2)
      WRITE(6,5)
      READ(5,1) DT,TF,M,N,NDATA,XE,EPS
      M1=M+1
      DO 10 I=1,NDATA
      READ(5,2) BS(I)
   10 CONTINUE
      KK=1
   97 CONTINUE
      READ(5,13) RINT,PINT
      KA=1
   94 CONTINUE
      READ(5,13) A2,A3
      WRITE(6,4) RINT,PINT
      DO 12 I=1,M1
      X0(I)=0.83129
      Y0(I)=-0.5
   12 CONTINUE
      R0(1)=RINT
      P0(1)=PINT
      NN=1
   90 CONTINUE
      X1(1)=XE
      Y1(1)=0.
      R1(1)=0.
      P1(1)=0.
      IDUMMY=1
      ICHECK=1
   20 CONTINUE
      W(1)=X1(1)
      W(2)=Y1(1)
      W(3)=R1(1)
      W(4)=P1(1)
C
C     INTEGRATE THE DIFFERENTIAL EQUATION FROM TIME=0 TO TIME=TFINAL
C
      DO 600 INT=1,M1
      CALL RKG(INT,DT,N,W,F,LX,MX,JX)
```

```
      X1(INT)=W(1)
      Y1(INT)=W(2)
      R1(1)=W(3)
      P1(1)=W(4)
  600 CONTINUE
      IF(IDUMMY.EQ.1) GO TO 100
      IF(IDUMMY.EQ.2) GO TO 200
      IF(IDUMMY.EQ.3) GO TO 300
      IF(IDUMMY.EQ.4) GO TO 400
  100 CONTINUE
      DO 31 I=1,M1
      XP(I)=X1(I)
      YP(I)=Y1(I)
   31 CONTINUE
C
C     SET THE INITIAL VALUES OF HOMOGENEOUS SOLUTION (1)
C
      X1(1)=0.
      Y1(1)=1.
      R1(1)=0.
      P1(1)=0.
      IDUMMY=2
      ICHECK=2
      GO TO 20
  200 CONTINUE
C
C     HOMOGENEOUS SOLUTION (1)
C
      DO 32 I=1,M1
      XH1(I)=X1(I)
      YH1(I)=Y1(I)
   32 CONTINUE
C
C     SET INITIAL VALUES OF HOMOGENEOUS SOLUTION (2)
C
      X1(1)=0.
      Y1(1)=0.
      R1(1)=1.
      P1(1)=0.
      IDUMMY=3
      ICHECK=2
      GO TO 20
  300 CONTINUE
C
C     HOMOGENEOUS SOLUTION (2)
C
      DO 33 I=1,M1
      XH2(I)=X1(I)
      YH2(I)=Y1(I)
   33 CONTINUE
C
C     INITIAL VALUES OF HOMOGENEOUS SOLUTION (3)
C
      X1(1)=0.
      Y1(1)=0.
      R1(1)=0.
      P1(1)=1.
      IDUMMY=4
```

```
      ICHECK=2
      GO TO 20
  400 CONTINUE
C
C     HOMOGENEOUS SOLUTION (3)
C
      DO 34 I=1,M1
      XH3(I)=X1(I)
      YH3(I)=Y1(I)
   34 CONTINUE
C
C     CALL THE SUBROUTINE TO EVALUATE THE INTEGRATION CONSTANTS
C
      CALL FUNC(XP,YP,XH1,XH2,XH3,YH1,YH2,YH3,BS,A)
C
C     FORM THE GENERAL SOLUTION
C
      IF(A(2).LE.0.) A(2)=1.
      IF(A(2).GE.10.) A(2)=10.
      IF(A(3).LE.0.) A(3)=1.
      IF(A(3).GE.10.) A(3)=10.
      DO 60 I=1,M1
      X1(I)=XP(I)+A(1)*XH1(I)+A(2)*XH2(I)+A(3)*XH3(I)
      Y1(I)=YP(I)+A(1)*YH1(I)+A(2)*YH2(I)+A(3)*YH3(I)
   60 CONTINUE
      WRITE(6,63) NN, A(2),A(3) ,X1(11),X1(21),X1(31),X1(41),X1(51),
     *X1(61),X1(71),X1(81),X1(91),X1(101)
      IF(NN.EQ.1) GO TO 61
      DR=R1(1)-R0(1)
      DP=P1(1)-P0(1)
      IF((ABS(DR).LE.EPS).AND.(ABS(DP).LE.EPS)) GO TO 68
   61 CONTINUE
      DO 73 I=1,M1
      X0(I)=X1(I)
      Y0(I)=Y1(I)
   73 CONTINUE
      R0(1)=A(2)
      P0(1)=A(3)
      NN=NN+1
      IF(NN-15) 90,90,68
   68 CONTINUE
      WRITE(6,3)
      KA=KA+1
      IF(KA-1) 94,94,95
   95 CONTINUE
      KK=KK+1
      IF(KK-1) 97,97,92
   92 CONTINUE
      WRITE(6,5)
      STOP
      END
```

```
C
C     FOURTH ORDER RUNGE-KUTTA GILL METHOD
C
      SUBROUTINE RKG(INT,DT,N,Y,F,L,M,J)
      DIMENSION DY(4),Y(4),F(28)
      T=(INT-1)*DT
      IF(INT.GT.1) GO TO 450
  410 L=3
      M=0
  450 CONTINUE
      GO TO (100,110,300),L
  100 GO TO (101,110),IG
  101 J=1
      L=2
      DO 106 K=1,N
      K1=K+3*N
      K2=K1+N
      K3=K+N
      F(K1)=Y(K)
      F(K3)=F(K1)
  106 F(K2)=DY(K)
      GO TO 406
  110 DO 140 K=1,N
      K1=K
      K2=K+5*N
      K3=K2+N
      K4=K+N
      GO TO (111,112,113,114),J
  111 F(K1)=DY(K)*DT
      Y(K)=F(K4)+0.5*F(K1)
      GO TO 140
  112 F(K2)=DY(K)*DT
      GO TO 124
  113 F(K3)=DY(K)*DT
      GO TO 134
  114 Y(K)=F(K4)+(F(K1)+2.*(F(K2)+F(K3))+DY(K)*DT)/6.
      GO TO 140
  124 Y(K)=0.5*F(K2)
      Y(K)=Y(K)+F(K4)
      GO TO 140
  134 Y(K)=F(K4)+F(K3)
  140 CONTINUE
      GO TO (170,180,170,180),J
  170 T=T+0.5*DT
  180 J=J+1
      IF(J-4) 404,404,299
  299 M=1
      GO TO 406
  300 IG=1
      GO TO 405
  404 IG=2
  405 L=1
  406 CONTINUE
      IF(M-1) 475,410,475
  475 GO TO (500,600,600),L
  500 CALL DFY(Y,DY)
```

```
      GO TO 450
  600 RETURN
      END
```

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```
C
      SUBROUTINE DFY(Z,F)
      DIMENSION Z(4),F(4),XO(101),YO(101),RO(1),PO(1)
      COMMON/ICCNTR/I,METHOD
      COMMON/FORMER/XO,YO,RO,PO
      F(1)=Z(2)
      F(3)=0.
      F(4)=0.
      IF(METHOD.EQ.1) GO TO 10
      IF(METHOD.EQ.2) GO TO 20
C
C     PARTICULAR SOLUTION
C
   10 F(2)=PO(1)*Z(2)+2.*PO(1)*RO(1)*XO(I)*Z(1)+PO(1)*XO(I)**2*Z(3)+
     *(YO(I)+RO(1)*XO(I)**2)*Z(4)-(3.*PO(1)*RO(1)*XO(I)**2+PO(1)*YO(I))
      GO TO 30
C
C     HOMOGENEOUS SOLUTION
C
   20 F(2)=PO(1)*Z(2)+2.*PO(1)*RO(1)*XO(I)*Z(1)+PO(1)*XO(I)**2*Z(3)+
     *(YO(I)+RO(1)*XO(I)**2)*Z(4)
   30 CONTINUE
      RETURN
      END
```

```
C
C     SOLVE THE EQUATIONS TO OBTAIN THE INTEGRATION CONSTANTS
C
      SUBROUTINE FUNC(XP,YP,XH1,XH2,XH3,YH1,YH2,YH3,BS,AA)
      DIMENSION XP(101),XH1(101),XH2(101),XH3(101),BS(10),A(2,2),AA(3),
     *B(2),YH1(101),YH2(101),YH3(101),YP(101),Q1(10),Q2(10),Q3(10)
      SUM1=0.
      SUM2=0.
      SUM3=0.
      SUM4=0.
      SUM5=0.
      SUM6=0.
      DO 100 I=1,10
      AX=XH1(I*10+1)/YH1(101)
      Q1(I)=XP(I*10+1)-AX*YP(101)
      Q2(I)=XH2(I*10+1)-AX*YH2(101)
      Q3(I)=XH3(I*10+1)-AX*YH3(101)
  100 CONTINUE
      DO 105 I=1,10
      SUM1=SUM1+Q2(I)*Q2(I)
      SUM2=SUM2+Q3(I)*Q2(I)
      SUM3=SUM3-Q2(I)*(Q1(I)-BS(I))
      SUM4=SUM4+Q3(I)*Q2(I)
      SUM5=SUM5+Q3(I)*Q3(I)
      SUM6=SUM6-Q3(I)*(Q1(I)-BS(I))
  105 CONTINUE
      A(1,1)=SUM1
      A(1,2)=SUM2
      B(1)=SUM3
      A(2,1)=SUM4
      A(2,2)=SUM5
      B(2)=SUM6
C
C     SOLVE THE TWO SIMULTANEOUS EQUATIONS
C
      AA(2)=(A(2,2)*B(1)-A(1,2)*B(2))/(A(1,1)*A(2,2)-A(1,2)*A(2,1))
      AA(3)=(B(1)-A(1,1)*AA(2))/A(1,2)
      AA(1)=-(YP(101)+AA(2)*YH2(101)+AA(3)*YH3(101))/YH1(101)
      RETURN
      END
```

RO 1.0
PO 1.0

N	R	P	GENERAL SOLUTIONS AT CORRESPONDING DATA POINTS
1	1.00000	10.00000	0.75 0.69 0.64 0.61 0.60 0.61 0.64 0.70 0.78 0.90
2	1.73550	8.83985	0.74 0.67 0.60 0.55 0.51 0.47 0.44 0.41 0.40 0.40
3	1.87826	7.64583	0.74 0.67 0.60 0.55 0.51 0.47 0.44 0.41 0.39 0.39
4	1.97978	5.88460	0.74 0.67 0.60 0.55 0.51 0.47 0.44 0.41 0.40 0.39
5	2.00302	5.96851	0.74 0.67 0.60 0.55 0.51 0.47 0.44 0.41 0.39 0.39
6	1.99816	6.02124	0.74 0.67 0.60 0.55 0.51 0.47 0.44 0.41 0.39 0.39
7	1.99789	6.02708	0.74 0.67 0.60 0.55 0.51 0.47 0.44 0.41 0.39 0.39
8	1.99647	6.04628	0.74 0.67 0.60 0.55 0.51 0.47 0.44 0.41 0.39 0.39
9	1.99659	6.04449	0.74 0.67 0.60 0.55 0.51 0.47 0.44 0.41 0.39 0.39
10	1.99842	6.01924	0.74 0.67 0.60 0.55 0.51 0.47 0.44 0.41 0.39 0.39
11	1.99549	6.05949	0.74 0.67 0.60 0.55 0.51 0.47 0.44 0.41 0.39 0.39
12	1.99937	6.00918	0.74 0.67 0.60 0.55 0.51 0.47 0.44 0.41 0.39 0.39
13	1.99558	6.05777	0.74 0.67 0.60 0.55 0.51 0.47 0.44 0.41 0.39 0.39
14	1.99649	6.04573	0.74 0.67 0.60 0.55 0.51 0.47 0.44 0.41 0.39 0.39
15	1.99431	6.07467	0.74 0.67 0.60 0.55 0.51 0.47 0.44 0.41 0.39 0.39

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```
C
C     THE PARAMETERS IN THE NONLINEAR DIFFUSION EQUATION FOR DRYING
C     OF CONCRETE ARE DETERMINED BY THE GENERALISED NEWTON-RAPHSON
C     METHOD (OR THE QUASILINEARIZATION METHOD). THE CRANK-NICOLSON
C     TECHNIQUE HAS BEEN USED FOR NUMERICAL INTEGRATION. USE OF THE
C            THOMAS ALGORITHM HAS ALSO BEEN MADE.
C
      REAL L
      DIMENSION Y0(101,10),Y1(101,10),YH1(101,10),YH2(101,10),YH3(101,10
     *),YP(101,10),A10(1),A20(1),A30(1),A11(1),A21(1),A31(1),
     *A(3),W(10),L(10),D(10),U(10),B(10),BS(9),QP(9),Q1(9),Q2(9),Q3(9)
      COMMON/FORMER/Y0,A10,A20,A30,M0,M2,M3,M
      COMMON/ICONTR/INT,ICHECK
    1 FORMAT(4F10.8,6I5)
    2 FORMAT(10X,9F10.4)
    4 FORMAT(10X,3F8.4)
    6 FORMAT(5I5)
    7 FORMAT(F10.5)
    9 FORMAT(3I5)
   13 FORMAT(3F10.6)
   63 FORMAT(5X,I4,6X,3F12.4)
      READ(5,1) DX,TF,EPS,XE,M,M1,M0,M2,M3,NDATA
      READ(5,6) IX,IY,IZ,IX1,IY1
      READ(5,6) IA,IB,IC,ID,IE
      DO 11 I=1,NDATA
      READ(5,7) BS(I)
   11 CONTINUE
      READ(5,9) INN,IX2,IY2
      READ(5,13) DT1,DT2,DT3
      READ(5,13) DT10,DT20,DT30
      READ(5,13) A1INT,A2INT,A3INT
      WRITE(6,4) A1INT,A2INT,A3INT
      WRITE(6,2) (BS(I),I=1,NDATA)
      T=0.
      DO 12 I=1,M
      S=T+1.
      DO 120 J=1,M2
      Y0(I,J)=(1./S)**(0.002942*(ALOG(S))**2.26)*(DX*(J-1))**(0.12882-
     *0.03179*(1.-DX*(J-1))**2)
      Y0(I,M3)=Y0(I,M0)
  120 CONTINUE
      IF(I.GE.1.AND.I.LE.IX1) DT=DT10
      IF(I.GE.IX2.AND.I.LE.IY1) DT=DT20
      IF(I.GE.IY2.AND.I.LE.M1) DT=DT30
      T=T+DT
   12 CONTINUE
      WRITE(6,2) Y0(IX,IA),Y0(IX,IB),Y0(IX,IC),Y0(IX,ID),Y0(IY,IA),Y0(IY
     *,IB),Y0(IY,IC),Y0(IY,ID),Y0(IZ,IA)
      A10(1)=A1INT
      A20(1)=A2INT
      A30(1)=A3INT
      NN=1
   90 CONTINUE
C
C     SET INITIAL VALUES OF PARTICULAR SOLUTION
C
```

```
      DO 121 I=2,M3
      Y1(1,I)=XE
  121 CONTINUE
      Y1(1,1)=0.
      A11(1)=0.
      A21(1)=0.
      A31(1)=0.
      IDUMMY=1
      ICHECK=1
   20 CONTINUE
      DO 122 I=1,M3
      W(I)=Y1(1,I)
  122 CONTINUE
      T=0.
C
C     INTEGRATE THE DIFFERENTIAL EQUATION FROM TIME=0 TO TIME=TFINAL BY
C     THE CRANK NICOLSON METHOD, TAKING FINITE DIFFERENCES FOR BOTH
C                        SPACE AND TIME DERIVATIVES
C
      DO 600 INT=1,M1
      IF(INT.GE.1.AND.INT.LE.IX) DT=DT1
      IF(INT.GE.IX1.AND.INT.LE.IY) DT=DT2
      IF(INT.GE.IY1.AND.INT.LE.M1) DT=DT3
      R=DT/DX**2
      CALL MATRIX(R,W,L,D,U,B,A11,A21,A31)
      DO 123 J=1,M3
      Y1(INT,J)=W(J)
  123 CONTINUE
  600 CONTINUE
      IF(IDUMMY.EQ.1) GO TO 100
      IF(IDUMMY.EQ.2) GO TO 200
      IF(IDUMMY.EQ.3) GO TO 300
      IF(IDUMMY.EQ.4) GO TO 400
C
C     PARTICULAR SOLUTION
C
  100 CONTINUE
      DO 31 I=1,M1
      DO 124 J=1,M3
      YP(I,J)=Y1(I,J)
  124 CONTINUE
   31 CONTINUE
      QP(1)=YP(IX,IA)
      QP(2)=YP(IX,IB)
      QP(3)=YP(IX,IC)
      QP(4)=YP(IX,ID)
      QP(5)=YP(IY,IA)
      QP(6)=YP(IY,IB)
      QP(7)=YP(IY,IC)
      QP(8)=YP(IY,ID)
      QP(9)=YP(IZ,IA)
      WRITE(6,2) (QP(I),I=1,NDATA)
C
C     SET INITIAL VALUES OF HOMOGENEOUS SOLUTION (1)
C
      DO 125 I=1,M3
      Y1(1,I)=0.
  125 CONTINUE
```

```
      A11(1)=1.
      A21(1)=0.
      A31(1)=0.
      IDUMMY=2
      ICHECK=2
      GO TC 20
C
C     HOMOGENEOUS SOLUTION (1)
C
  200 CONTINUE
      DC 32 I=1,M1
      DO I26 J=1,M3
      YH1(I,J)=Y1(I,J)
  126 CCNTINUE
   32 CONTINUE
      Q1(1)=YH1(IX,IA)
      C1(2)=YH1(IX,IB)
      C1(3)=YH1(IX,IC)
      Q1(4)=YH1(1X,ID)
      Q1(5)=YH1(IY,IA)
      Q1(6)=YH1(IY,IB)
      C1(7)=YHI(IY,IC)
      Q1(8)=YH1(IY,ID)
      Q1(9)=YH1(IZ,IA)
      WRITE(6,2) (C1(I),I=1,NDATA)
C
C     SET INITIAL VALUES OF HOMOGENEOUS SOLUTICN (2)
C
      DO 127 J=1,M3
      Y1(1,J)=0.
  127 CCNTINUE
      A11(1)=0.
      A21(I)=1.
      A31(1)=0
      IDUMMY=3
      1CHECK=2
      GO TC 20
C
C     HOMCGENEOUS SOLUTION (2)
C
  300 CONTINUE
      DO 33 I=I,M1
      DO 128 J=1,M3
      YH2(I,J)=Y1(I,J)
  128 CONTINUE
   33 CCNTINUE
      Q2(I)=YH2(IX,IA)
      C2(2)=YH2(IX,IB)
      Q2(3)=YH2(1X,IC)
      Q2(4)=YH2(IX,ID)
      Q2(5)=YH2(IY,IA)
      C2(6)=YH2(IY,IB)
      Q2(7)=YH2(IY,IC)
      C2(8)=YH2(IY,ID)
      C2(9)=YH2(IZ,1A)
      WRITE(6,2) (Q2(I),I=1,NDATA)
C
C     INITIAL VALUES OF HOMCGENECUS SOLUTION (3)
```

```
C
      DO 129 J=1,M3
      Y1(1,J)=0
  129 CONTINUE
      A11(1)=0.
      A21(1)=0.
      A31(1)=1.
      IDUMMY=4
      ICHECK=2
      GO TO 20
C
C     HOMOGENEOUS SOLUTION (3)
C
  400 CONTINUE
      DO 34 I=1,MI
      DO 130 J=1,M3
      YH3(I,J)=Y1(I,J)
  130 CONTINUE
   34 CONTINUE
      Q3(1)=YH3(IX,IA)
      Q3(2)=YH3(IX,IB)
      Q3(3)=YH3(IX,IC)
      Q3(4)=YH3(IX,ID)
      Q3(5)=YH3(IY,IA)
      Q3(6)=YH3(IY,IB)
      Q3(7)=YH3(IY,IC)
      Q3(8)=YH3(IY,ID)
      Q3(9)=YH3(IZ,IA)
      WRITE(6,2) (Q3(I),I=1,NDATA)
C
C     CALL SUBROUTINE TO FIND INTEGRATION CONSTANTS
C
      CALL FUNC(CP,C1,C2,Q3,BS,A)
      WRITE(6,63) NN,A(1),A(2),A(3)
C
C     GENERAL SOLUTIONS FOR Y1(TIME,SPACE)
C
      DO 60 I=1,M1
      DO 131 J=2,M2
      Y1(I,J)=YP(I,J)+A(1)*YH1(I,J)+A(2)*YH2(I,J)+A(3)*YH3(I,J)
  131 CONTINUE
   60 CONTINUE
      WRITE(6,2) Y1(IX,IA),Y1(IX,IB),Y1(IX,IC),Y1(IX,ID),Y1(IY,IA),Y1(IY
     *,IB),Y1(IY,IC),Y1(IY,ID),Y1(IZ,IA)
      DA1= A(1)-A10(1)
      DA2= A(2)-A20(1)
      DA3= A(3)-A30(1)
      IF((ABS(DA1).LE.EPS).AND.(ABS(DA2).LE.EPS).AND.(ABS(DA3).LE.EPS))
     * GO TO 68
      DO 73 I=1,M1
      DO 132 J=1,M3
      Y0(I,J)=Y1(I,J)
  132 CONTINUE
   73 CONTINUE
      A10(1)=A(1)
      A20(1)=A(2)
      A30(1)=A(3)
      NN=NN+1
```

```
      IF(NN-INN) 90,90,68
   68 CONTINUE
      STOP
      END
```

```
      SUBROUTINE MATRIX(R,Z,L,C,U,B,A1N,A2N,A3N)
      REAL L
      DIMENSION Z(10),YO(101,10),A1N(1),A2N(1),A3N(1),L(10),U(10),D(10),
     * B(10),A1(1),A2(1),A3(1)
      COMMON/FORMER/YO,A1,A2,A3,M0,M2,M3,M
      COMMON/ICONTR/I,METHOD
      Z(1)=0.
      Z(M3)=Z(M0)
      DO 111 J=2,M2
      L(J) = -R*C(A1(1),A2(1),A3(1),YO(I,J),YO(I+1,J))/2.
      D(J) = R*(1./R+C(A1(1),A2(1),A3(1),YO(I,J),YO(I+1,J))+
     * CY(A1(1),A2(1),A3(1),YO(I,J),YO(I+1,J))/4.*(YO(I+1,J)-YO(I+1,J-1)
     *+YO(I,J)-YO(I,J-1))-CYY(A1(1),A2(1),A3(1),YO(I,J), YO(I+1,J))/8.*
     * (YO(I+1,J+1)-YO(I+1,J)+YO(I,J+1)-YO(I,J))**2)
      U(J) = -R*(C(A1(1),A2(1),A3(1),YO(I,J),YO(I+1,J))/2.+
     * CY(A1(1),A2(1),A3(1),YO(I,J),YO(I+1,J))/4.*(YO(I+1,J+1)-YO(I+1,J)
     * +YO(I,J+1)-YO(I,J)))
  111 CONTINUE
      L(2)=0
      L(M2)=U(M2)+L(M2)
      U(M2)=0
      IF(METHOD.EQ.1) GO TO 10
      IF(METHOD.EQ.2) GO TO 20
C
C     PARTICULAR SOLUTIONS
C
   10 CONTINUE
      DO 101 J=2,M2
      B(J) =  Z(J)  +R/2.*(YO(I+1,J+1)-2.*YO(I+1,J)+YO(I+1,J-1)+YO(I,J+1
     *  )-2.*YO(I,J)+YO(I,J-1))*(C1(A1(1),A2(1),A3(1),YO(I,J),YO(I+1,J))
     * *(A1N(1)-A1(1))+C2(A1(1),A2(1),A3(1),YO(I,J),YO(I+1,J))*(A2N(1)-A
     *2(1))+C3(A1(1),A2(1),A3(1),YO(I,J),YO(I+1,J))*(A3N(1)-A3(1))+CY(A1
     * (1),A2(1),A3(1),YO(I,J),YO(I+1,J))/2.*(Z(J)-YO(I+1,J)-YO(I,J)))+
     *R/4.*(YO(I+1,J+1)-YO(I+1,J)+YO(I,J+1)-YO(I,J))**2*(CY1(A1(1),A2(1)
     *,A3(1),YO(I,J),YO(I+1,J))*(A1N(1)-A1(1))+CY2(A1(1),A2(1),A3(1),
     *YO(I,J),YO(I+1,J))*(A2N(1)-A2(1))+CY3(A1(1),A2(1),A3(1),YO(I,J),
     *YO(I+1,J))*(A3N(1)-A3(1))+ CYY(A1(1),A2(1),A3(1),YO(I,J),YO(I+1,J)
     *)/2.*(Z(J)-YO(I+1,J)-YO(I,J)))+R/4.*CY(A1(1),A2(1),A3(1),YO(I,J),
     *YO(I+1,J))*(YO(I+1,J+1)-YO(I+1,J)+YO(I,J+1)-YO(I,J))*(Z(J+1)-Z(J))
     * +R/2.*C(A1(1),A2(1),A3(1),YO(I,J),YO(I+1,J))*(Z(J+1)-2.*Z(J)+Z(J-
     *1))
  101 CONTINUE
      GO TO 30
C
C     HOMOGENEOUS SOLUTIONS
C
   20 CONTINUE
      DO 102 J=2,M2
      B(J) =  Z(J)  +R/2.*(YO(I+1,J+1)-2.*YO(I+1,J)+YO(I+1,J-1)+YO(I,J+1
     *  )-2.*YO(I,J)+YO(I,J-1))*(C1(A1(1),A2(1),A3(1),YO(I,J),YO(I+1,J))
     * *(A1N(1))       +C2(A1(1),A2(1),A3(1),YO(I,J),YO(I+1,J))*(A2N(1))
     *      +C3(A1(1),A2(1),A3(1),YO(I,J),YO(I+1,J))*(A3N(1))       +CY(A1
     * (1),A2(1),A3(1),YO(I,J),YO(I+1,J))/2.*(Z(J)))+
     *R/4.*(YO(I+1,J+1)-YO(I+1,J)+YO(I,J+1)-YO(I,J))**2*(CY1(A1(1),A2(1)
     *,A3(1),YO(I,J),YO(I+1,J))*(A1N(1))       +CY2(A1(1),A2(1),A3(1),
     *YO(I,J),YO(I+1,J))*(A2N(1))       +CY3(A1(1),A2(1),A3(1),YO(I,J),
```

```
   *YO(I+1,J))*(A3N(1))        + CYY(A1(1),A2(1),A3(1),YC(I,J),YO(I+1,J)
   *)/2.*(Z(J)))                      +R/4.*CY(A1(1),A2(1),A3(1),YO(I,J),
   *YO(I+1,J))*(YO(I+1,J+1)-YO(I+1,J)+YO(I,J+1)-YC(I,J))*(Z(J+1)-Z(J))
   *  +R/2.*C(A1(1),A2(1),A3(1),YO(I,J),YO(I+1,J))*(Z(J+1)-2.*Z(J)+Z(J-
   *1))
102 CCNTINUE
 30 CONTINUE
    CALL TRIDAG(2,M2,L,D,U,B,Z)
    RETURN
    END

    FUNCTION CY3(A1,A2,A3,Y1,Y2)
    CY3= (1.-A1)*A2**A3*(1.-(0.5*(Y1+Y2))*(A3-1.)+(A3-1.)*(A3-2.)/2.*
   *().5*(Y1+Y2))**2-(A3-1.)*(A3-2.)*(A3-3.)/6.*(0.5*(Y1+Y2))**3)*(
   *(1.+A3*(ALOG(A2)-(0.5*(Y1+Y2))- (0.5*(Y1+Y2))**2 /2.- (C.5*(Y1+Y2)
   *)**3 /3.- (0.5*(Y1+Y2))**4 /4.- (0.5*(Y1+Y2))**5 /5.- ().5*(Y1+Y2
   *))**6 /6.))+
   *(1.-A3*(ALCG(A2)-(0.5*(Y1+Y2))- (0.5*(Y1+Y2))**2 /2.- (C.5*(Y1+Y2)
   *)**3 /3.- (0.5*(Y1+Y2))**4 /4.- (0.5*(Y1+Y2))**5 /5.- (0.5*(Y1+Y2
   *))**6 /6.)) *A2**A3*
   *(1.-A3*(0.5*(Y1+Y2))+A3*(A3-1.)/2.*(0.5*(Y1+Y2))**2-A3*(A3-1.)*
   *(A3-2.)/6.*(0.5*(Y1+Y2))**3))/
   * (1.+A2**A3*(1.-A3*(0.5*(Y1+Y2))+A3*(A3-1.)/2.*(C.5*(Y1+Y2))**2-
   *A3*(A3-1.)*(A3-2.)/6.*(0.5*(Y1+Y2))**3))**3
    RETURN
    END

    FUNCTICN CY2(A1,A2,A3,Y1,Y2)
    CY2= (1.-A1)*A3**2*A2*(A3-1.)*
   * (1.-(A3-1.)*(C.5*(Y1+Y2))+(A3-1.)*(A3-2.)/2.*(0.5*(Y1+Y2))**2-
   * (A3-1.)*(A3-2.)*(A3-3.)/6.*(0.5*(Y1+Y2))**3)*(1.-A2**A3*
   * (1.-A3*(0.5*(Y1+Y2))+A3*(A3-1.)/2.*(0.5*(Y1+Y2))**2-A3*(A3-1.)*
   * (A3-2.)/6.*(0.5*(Y1+Y2))**3))/
   * (1.+A2**A3*(1.-A3*(0.5*(Y1+Y2))+A3*(A3-1.)/2.*(0.5*(Y1+Y2))**2-
   *A3*(A3-1.)*(A3-2.)/6.*(0.5*(Y1+Y2))**3))**3
    RETURN
    END
```

```
 FUNCTION C(A1,A2,A3,Y1,Y2)
 C = A1+(1.-A1)/
* (1.+A2**A3*(1.-A3*(0.5*(Y1+Y2))+A3*(A3-1.)/2.*(0.5*(Y1+Y2))**2-
*A3*(A3-1.)*(A3-2.)/6.*(0.5*(Y1+Y2))**3))
 RETURN
 END

 FUNCTION CY(A1,A2,A3,Y1,Y2)
 CY = A3*(1.-A1)*A2**A3*
* (1.-(A3-1.)*(0.5*(Y1+Y2))+(A3-1.)*(A3-2.)/2.*(0.5*(Y1+Y2))**2-
* (A3-1.)*(A3-2.)*(A3-3.)/6.*(0.5*(Y1+Y2))**3)/
* (1.+A2**A3*(1.-A3*(0.5*(Y1+Y2))+A3*(A3-1.)/2.*(0.5*(Y1+Y2))**2-
*A3*(A3-1.)*(A3-2.)/6.*(0.5*(Y1+Y2))**3))**2
 RETURN
 END
 FUNCTION CYY(A1,A2,A3,Y1,Y2)
 CYY= A2**A3*A3*(1.-A1)*(1.-(A3-2.)*(0.5*(Y1+Y2))+(A3-2.)*(A3-3.)
*/2.*(0.5*(Y1+Y2))**2-(A3-2.)*(A3-3.)*(A3-4.)/6.*(0.5*(Y1+Y2))**3)
**(A2**A3*(A3+1.)*(1.-A3*(0.5*(Y1+Y2))+A3*(A3-1.)/2.*(0.5*(Y1+Y2))*
**2-A3*(A3-1.)*(A3-2.)/6.*(0.5*(Y1+Y2))**3)-(A3-1.))/
* (1.+A2**A3*(1.-A3*(0.5*(Y1+Y2))+A3*(A3-1.)/2.*(0.5*(Y1+Y2))**2-
*A3*(A3-1.)*(A3-2.)/6.*(0.5*(Y1+Y2))**3))**3
 RETURN
 END
 FUNCTION C1(A1,A2,A3,Y1,Y2)
 C1 = 1.-1./
* (1.+A2**A3*(1.-A3*(0.5*(Y1+Y2))+A3*(A3-1.)/2.*(0.5*(Y1+Y2))**2-
*A3*(A3-1.)*(A3-2.)/6.*(0.5*(Y1+Y2))**3))
 RETURN
 END
 FUNCTION C2(A1,A2,A3,Y1,Y2)
 C2 = -(1.-A1)*A3*A2**(A3-1.)*
* (1.-A3*(0.5*(Y1+Y2))+A3*(A3-1.)/2.*(0.5*(Y1+Y2))**2-A3*(A3-1.)*
* (A3-2.)/6.*(0.5*(Y1+Y2))**3)/
* (1.+A2**A3*(1.-A3*(0.5*(Y1+Y2))+A3*(A3-1.)/2.*(0.5*(Y1+Y2))**2-
*A3*(A3-1.)*(A3-2.)/6.*(0.5*(Y1+Y2))**3))**2
 RETURN
 END
 FUNCTION C3(A1,A2,A3,Y1,Y2)
 C3 = -(1.-A1)*(ALOG(A2)-(0.5*(Y1+Y2))-((0.5*(Y1+Y2))**2)/2.-
*((0.5*(Y1+Y2))**3)/3.-((0.5*(Y1+Y2))**4)/4.-((0.5*(Y1+Y2))**5)/5.
*-((0.5*(Y1+Y2))**6)/6.)*A2**A3*
* (1.-A3*(0.5*(Y1+Y2))+A3*(A3-1.)/2.*(0.5*(Y1+Y2))**2-A3*(A3-1.)*
* (A3-2.)/6.*(0.5*(Y1+Y2))**3)/
* (1.+A2**A3*(1.-A3*(0.5*(Y1+Y2))+A3*(A3-1.)/2.*(0.5*(Y1+Y2))**2-
*A3*(A3-1.)*(A3-2.)/6.*(0.5*(Y1+Y2))**3))**2
 RETURN
 END
 FUNCTION CY1(A1,A2,A3,Y1,Y2)
 CY1= -A3*A2**A3*
* (1.-(A3-1.)*(0.5*(Y1+Y2))+(A3-1.)*(A3-2.)/2.*(0.5*(Y1+Y2))**2-
* (A3-1.)*(A3-2.)*(A3-3.)/6.*(0.5*(Y1+Y2))**3)/
* (1.+A2**A3*(1.-A3*(0.5*(Y1+Y2))+A3*(A3-1.)/2.*(0.5*(Y1+Y2))**2-
*A3*(A3-1.)*(A3-2.)/6.*(0.5*(Y1+Y2))**3))**2
 RETURN
 END
```

LEVEL 21.7 (JAN 73)   OS/360 FORTRAN H   DATE 78.116/22.09.17

```
C
C     USE THE THOMAS ALGORITHM FOR THE TRIDIAGONAL BAND MATRIX
C
      SUBROUTINE TRIDAG(IF,L,A,B,C,D,V)
      DIMENSION A(1),B(1),C(1),D(1),V(1),BETA(101),GAMMA(101)
C
C     COMPUTE INTERMEDIATE ARRAYS BETA,GAMMA
C
      BETA(IF)=B(IF)
      GAMMA(IF)=D(IF)/BETA(IF)
      IFP1=IF+1
      DO 1 I=IFP1,L
      BETA(I)=B(I)-A(I)*C(I-1)/BETA(I-1)
    1 GAMMA(I)=(D(I)-A(I)*GAMMA(I-1)) /BETA(I)
C
C     COMPUTE FINAL SOLUTION VECTOR V
C
      V(L)=GAMMA(L)
      LAST=L-IF
      DO 2 K=1,LAST
      I=L-K
    2 V(I)=GAMMA(I)-C(I)*V(I+1)/BETA(I)
      RETURN
      END
```

```
C
C     SOLVE THE EQUATIONS TO OBTAIN THE INTEGRATION CONSTANTS
C
      SUBROUTINE FUNC(QP,C1,Q2,Q3,BS,AA)
      DIMENSION QP(9),Q1(9),C2(9),Q3(9),BS(9),A(3,3),B(3),AA(3)
      SUM1=0.
      SUM2=0.
      SUM3=0.
      SUM4=0.
      SUM5=0.
      SUM6=0.
      SUM7=0.
      SUM8=0.
      SUM9=0.
      DO 100 I=1,9
      SUM1=SUM1+C1(I)*Q1(I)
      SUM2=SUM2+Q1(I)*Q2(I)
      SUM3=SUM3+Q1(I)*Q3(I)
      SUM4=SUM4+C2(I)*C2(I)
      SUM5=SUM5+C2(I)*Q3(I)
      SUM6=SUM6+C3(I)*Q3(I)
      SUM7=SUM7-C1(I)*(QP(I)-BS(I))
      SUM8=SUM8-C2(I)*(QP(I)-BS(I))
      SUM9=SUM9-C3(I)*(QP(I)-BS(I))
  100 CONTINUE
      A(1,1)=SUM1
      A(1,2)=SUM2
      A(1,3)=SUM3
      A(2,1)=SUM2
      A(2,2)=SUM4
      A(2,3)=SUM5
      A(3,1)=SUM3
      A(3,2)=SUM5
      A(3,3)=SUM6
      B(1)=SUM7
      B(2)=SUM8
      B(3)=SUM9
C
C     SOLVE THE THREE SIMULTANEOUS EQUATIONS
C
      AA(3) =((B(1)*A(2,1)-B(2)*A(1,1))*(A(2,2)*A(3,1)-A(3,2)*A(2,1))-
     * (B(2)*A(3,1)-B(3)*A(2,1))*(A(1,2)*A(2,1)-A(2,2)*A(1,1)))/
     * ((A(1,3)*A(2,1)-A(2,3)*A(1,1))*(A(2,2)*A(3,1)-A(3,2)*A(2,1))-
     * (A(2,3)*A(3,1)-A(3,3)* A(2,1))*(A(1,2)*A(2,1)-A(2,2)*A(1,1)))
      AA(2) = (B(2)*A(3,1)-B(3)*A(2,1)-AA(3)*(A(2,3)*A(3,1)-A(3,3)*A(2,1
     * )))/(A(2,2)*A(3,1)-A(3,2)*A(2,1))
      AA(1) = (B(1)-AA(3)*A(1,3)-AA(2)*A(1,2))/A(1,1)
      RETURN
      END
```

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APPLICATION OF THE QUASILINEARIZATION TECHNIQUE
FOR PARAMETER ESTIMATION IN NONLINEAR
DIFFERENTIAL EQUATIONS

by

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ABSTRACT

Application of the quasilinearization technique for parameter estimation in nonlinear differential equations is investigated.

Parameter estimation of the nonlinear differential equation for a homogeneous tubular flow chemical reactor with axial mixing is presented in Part I. It is assumed that the physical process can be represented by a nonlinear ordinary differential equation of known form but containing unknown parameters. Linearization of the problem is carried through by the quasilinearization technique. The fourth order Runge Kutta Gill method is used for numerical integration.

An algorithm is devised based on the least squares method. It minimizes the error between the experimental data and the model predictions. Numerical data from Lee [11] has been treated as the experimental data.

Extension of the application of the quasilinearization technique to nonlinear parabolic differential equations is investigated in Part II. The mathematical model of moisture diffusion in concrete medium is presented. The Crank Nicolson method is used for numerical integration. Experimental data of Abrams and Orals [3] is used.

The method converges quadratically in the solution of the problem in Part I. Convergence was not attained in the solution of the problem in Part II.