



Using group theoretic method to solve multi-dimensional diffusion equation

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Abstract

The nonlinear diffusion equation arises in many important areas of science and technology such as modeling of dopant diffusion in semiconductors. We give analytical solution to N -dimensional radially symmetric nonlinear diffusion equation of the form

$$\frac{\partial}{\partial r} \left[D(C) \frac{\partial C}{\partial r} \right] + \frac{N-1}{r} D(C) \frac{\partial C}{\partial r} = \frac{\partial C}{\partial t},$$

where $C(r, t)$ is the concentration and $D(C)$ is diffusion coefficient.

The transformation group theoretic approach is applied to present an analysis of the nonlinear diffusion equation. The one-parameter group transformation reduces the number of independent variables by one and the governing partial differential equation with the boundary conditions reduce to an ordinary differential equation with the appropriate boundary conditions. Effect of the time “ t ” and the number of dimension “ N ” on the concentration diffusion function $C(r, t)$ has been studied and the results are plotted. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

The problem of N -dimensional radially symmetric nonlinear diffusion equation was treated by King [11] in 1988. He introduced an approximate similarity solution to the porous-medium equation

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in one and two dimensions. He studied the case ($N = 1$) and assumed $D(C) = D_0 C^m$. The problems considered arise in the modeling of dopant diffusion in semiconductors.

He studied the cases $m = 1$ for arsenic and boron in silicon; $m = 2$ for phosphorus in silicon; $m = 2$ or 3 for zinc in gallium arsenide.

Also, Hill [9] in 1989 studied the case ($N = 1$) and assumed $D(C) = C^m$ but he introduced a new exact solution for the power-law diffusivity of index $m = -4/3$ using continuous one-parameter continuous group of transformations. Hill and Hill [10] in 1990 extended the results given in [9] for particular power-law diffusivities C^m (such as $m = -1/2, -1, -3/2$ and -2) using one-parameter continuous group of transformations.

King [12] in 1990 gave a new closed-form similarity solutions to N -dimensional radially symmetric nonlinear diffusion equation. He studied two cases. First $D(C) = C^m$ (power-law diffusivities) for both $m > 0$ (slow diffusion), and $m < 0$ (fast diffusion), second $D(C) = e^C$ (exponential diffusivities). The mathematical technique used in the present analysis is the one-parameter group transformation. The group methods, as a class of methods, which lead to reduction of the number of independent variables, were first introduced by Birkhoff [7] in 1948, where he made use of one-parameter transformation groups. In 1952, Morgan [13] presented a theory, which has led to improvements over earlier similarity methods.

The method has been applied intensively in [1–5,14,13]. In this work, we present a general procedure for applying a one-parameter group transformation to the multi-dimensional diffusion equation. Under the transformation, the partial differential equation with boundary conditions, is reduced to an ordinary differential equation with the appropriate corresponding conditions. The equation is then solved numerically using nonlinear finite difference method applied to the nonlinear second-order boundary value problem [8], see the appendix.

2. Formulation of the problem and the governing equation

Consider a multi-dimensional diffusion equation of the form

$$\frac{\partial}{\partial r} \left[D(C) \frac{\partial C}{\partial r} \right] + \frac{N - 1}{r} D(C) \frac{\partial C}{\partial r} = \frac{\partial C}{\partial t} \tag{2.1}$$

with the boundary conditions

$$(i) \ C(0, t) = F(t), \tag{2.2}$$

$$(ii) \ C(\infty, t) = 0 \tag{2.3}$$

and initial condition

$$C(r, 0) = 0, \tag{2.4}$$

where “ $C(r, t)$ ” is the concentration and “ $D(C)$ ” is diffusion coefficient. The functions “ $D(C)$ ” and “ $F(t)$ ” are unknown functions and their proper forms will be determined later on, and “ N ” is the number of dimensions.

Assume

$$D(C) = C^m \tag{2.5}$$

and

$$C(r, t) = F(t)q(r, t), \tag{2.6}$$

where “ $q(r, t)$ ” is unknown function and its proper form will be determined later on.

Substituting from (2.5) and (2.6) into (2.1) yields

$$\begin{aligned} & \frac{\partial}{\partial r} \left([F(t)q(r, t)]^m \frac{\partial}{\partial r} [F(t)q(r, t)] \right) + \frac{N-1}{r} [F(t)q(r, t)]^m \frac{\partial}{\partial r} [F(t)q(r, t)] \\ & = \frac{\partial}{\partial t} [F(t)q(r, t)]. \end{aligned} \tag{2.7}$$

Eq. (2.7) can be rewritten in the form

$$F^{m+1}q^m \frac{\partial^2 q}{\partial r^2} + mF^{m+1}q^{m-1} \left[\frac{\partial q}{\partial r} \right]^2 + \frac{N-1}{r} F^{m+1}q^m \frac{\partial q}{\partial r} - F \frac{\partial q}{\partial t} - q \frac{dF}{dt} = 0 \tag{2.8}$$

with the boundary conditions

$$(i) \quad q(0, t) = 1, \tag{2.9}$$

$$(ii) \quad q(\infty, t) = 0 \tag{2.10}$$

and initial condition

$$q(r, 0) = 0. \tag{2.11}$$

3. Solution of the problem

Our method of solution depends on the application of a one-parameter group transformation to the partial differential equation (2.8). Under this transformation the two independent variables will be reduced by one and the differential equation (2.8) transforms into an ordinary differential equation.

3.1. The group systematic formulation

The procedure is initiated with the group G , a class of transformation of one-parameter “ a ” of the form:

$$G: \begin{cases} \bar{r} = h^r(a)r + k^r, \\ \bar{t} = h^t(a)t + k^t, \\ \bar{F} = h^F(a)F + k^F, \\ \bar{q} = h^q(a)q + k^q, \end{cases} \tag{3.1}$$

where h 's and k 's are real-valued and at least differentiable in the real argument “ a ”.

3.2. The invariance analysis

To transform the differential equation, transformations of the derivatives of F and q are obtained from G via chain-rule operations

$$\bar{S}_i = \left[\frac{h^S}{h^i} \right] S_i, \quad \bar{S}_{ij} = \left[\frac{h^S}{h^i h^j} \right] S_{ij}, \quad i = r, t, \quad j = r, t, \tag{3.2}$$

where S stands for F and q .

Eq. (2.8) is said to be invariantly transformed, for some function $A(a)$ whenever:

$$\begin{aligned} & (\bar{F})^{m+1}(\bar{q})^m \bar{q}_{rr} + m(\bar{F})^{m+1}(\bar{q})^{m-1}(\bar{q}_r)^2 + \frac{N-1}{\bar{r}} (\bar{F})^{m+1}(\bar{q})^m \bar{q}_r - \bar{F} \bar{q}_t - \bar{q} \bar{F}_t \\ & = A(a) \left(F^{m+1} q^m q_{rr} + m F^{m+1} q^{m-1} (q_r)^2 + \frac{N-1}{r} F^{m+1} q^m q_r - F q_t - q F_t \right). \end{aligned} \tag{3.3}$$

Substituting from (3.1) and (3.2) into (3.3) yields

$$\begin{aligned} & (h^F F + k^F)^{m+1} (h^q q + k^q)^m \frac{h^q}{(h^r)^2} q_{rr} \\ & + m (h^F F + k^F)^{m+1} (h^q q + k^q)^{m-1} \left[\frac{h^q}{h^r} \right]^2 (q_r)^2 \\ & + \frac{N-1}{h^r r + k^r} (h^F F + k^F)^{m+1} (h^q q + k^q)^m \frac{h^q}{h^r} q_r - (h^F F + k^F) \frac{h^q}{h^t} q_t \\ & - (h^q q + k^q) \frac{h^F}{h^t} F_t \\ & = A(a) \left(F^{m+1} q^m q_{rr} + m F^{m+1} q^{m-1} (q_r)^2 + \frac{N-1}{r} F^{m+1} q^m q_r - F q_t - q F_t \right). \end{aligned} \tag{3.4}$$

The invariance of (3.4) implies

$$k^F = k^q = k^r = 0$$

and

$$\frac{(h^F)^{m+1} (h^q)^{m+1}}{(h^r)^2} = \frac{h^F h^q}{h^t} = A(a), \tag{3.5}$$

which yields

$$h^t = \frac{(h^r)^2}{(h^F)^m}. \tag{3.6}$$

The invariance of the auxiliary conditions (2.9)–(2.11) implies that

$$h^q = 1, \quad k^t = 0. \tag{3.7}$$

Finally, we get the one-parameter group G , which transforms invariantly the differential equation (2.8) and the auxiliary conditions (2.9)–(2.11).

The group G is of the form:

$$G: \begin{cases} \bar{r} = h^r r, \\ \bar{t} = \frac{(h^r)^2}{(h^F)^m} t, \\ \bar{F} = h^F F, \\ \bar{q} = q. \end{cases} \tag{3.8}$$

3.3. The complete set of absolute invariants

Our aim is to make use of group methods to represent the problem in the form of an ordinary differential equation. Then, we have to proceed in our analysis to obtain a complete set of absolute invariants. If $\eta \equiv \eta(r, t)$ is the absolute invariant of the independent variables, then

$$g_j(r, t; F, q) = \Psi_j[\eta(r, t)], \quad j = 1, 2 \tag{3.9}$$

are the two absolute invariants corresponding to F and q represented by g_j . The application of a basic theorem in group theory, see [6], states that: a function $g(r, t; F, q)$ is an absolute invariant of a one-parameter group if it satisfies the following first-order linear differential equation:

$$\sum_{i=1}^4 (\alpha_i S_i + \beta_i) \frac{\partial g}{\partial S_i} = 0, \quad S_i \equiv r, t, F, q, \tag{3.10}$$

where

$$\alpha_i = \frac{\partial h^{S_i}}{\partial a}(a^0) \quad \text{and} \quad \beta_i = \frac{\partial k^{S_i}}{\partial a}(a^0), \quad i = 1, 2, 3, 4 \tag{3.11}$$

and a^0 denotes the value of “ a ” which yields the identity element of the group G .

The group method applied to the given partial differential equation with the specific boundary conditions yields a unique solution as condition (3.10) is used.

At first, we seek the absolute invariant of the independent variables. Owing to equation (3.10), $\eta(r, t)$ is an absolute invariant if it satisfies the following first-order linear differential equation:

$$(\alpha_1 r + \beta_1) \frac{\partial \eta}{\partial r} + (\alpha_2 t + \beta_2) \frac{\partial \eta}{\partial t} = 0. \tag{3.12}$$

Since $k^r = k^t = 0$, and according to the definition of the β 's then $\beta_1 = \beta_2 = 0$.

Now Eq. (3.12) may be rewritten in the form:

$$\alpha_1 r \frac{\partial \eta}{\partial r} + \alpha_2 t \frac{\partial \eta}{\partial t} = 0. \tag{3.13}$$

Applying separation of variables method, one can obtain a solution in the form:

$$\eta = r t^{-B} \quad \text{where} \quad B = \frac{\alpha_1}{\alpha_2}. \tag{3.14}$$

The second step is to obtain the absolute invariants of the dependent variables F and q .

By a similar analysis, using Eqs. (3.8), (3.10) and (3.11), we get

$$F(t) = R(t)\phi(\eta). \tag{3.15}$$

Since $F(t)$ and $R(t)$ are independent of r , while η is a function of r and t , then $\phi(\eta)$ must be constant, say $\phi(\eta) = 1$, and from which

$$F(t) = R(t) \tag{3.16}$$

and the second absolute invariant is

$$q(r, t) = \theta(\eta). \tag{3.17}$$

4. The reduction to an ordinary differential equation

Substitution from (3.14)–(3.17) into Eq. (2.8), we get

$$\begin{aligned} &(R^{m+1}t^{-2B})\theta^m \frac{d^2\theta}{d\eta^2} + (mR^{m+1}t^{-2B})\theta^{m-1} \left[\frac{d\theta}{d\eta} \right]^2 \\ &+ \left(\frac{N-1}{r} R^{m+1}\theta^m t^{-B} + \frac{RB\eta}{t} \right) \frac{d\theta}{d\eta} - \frac{dR}{dt} \theta = 0. \end{aligned} \tag{4.1}$$

For (4.1) to be reduced to an ordinary differential equation in one variable η , it is necessary that the coefficients should be constants or functions of η only. Thus,

$$m + 1 = 2B, \tag{4.2}$$

$$R(t) = t. \tag{4.3}$$

Hence, Eq. (4.1) takes the form:

$$\theta^m \frac{d^2\theta}{d\eta^2} + m\theta^{m-1} \left[\frac{d\theta}{d\eta} \right]^2 + \left(\frac{N-1}{\eta} \theta^m + B\eta \right) \frac{d\theta}{d\eta} - \theta = 0. \tag{4.4}$$

Under the similarity variable η , the boundary conditions are

$$\theta(0) = 1, \tag{4.5}$$

$$\theta(\infty) = 0. \tag{4.6}$$

5. Numerical solution

5.1. Study the effect of “ t ”

Consider $m = -\frac{1}{2}$ and $N = 2$. From Eq. (4.2), $B = \frac{1}{4}$, which yields $\eta = r/\sqrt[3]{t}$.

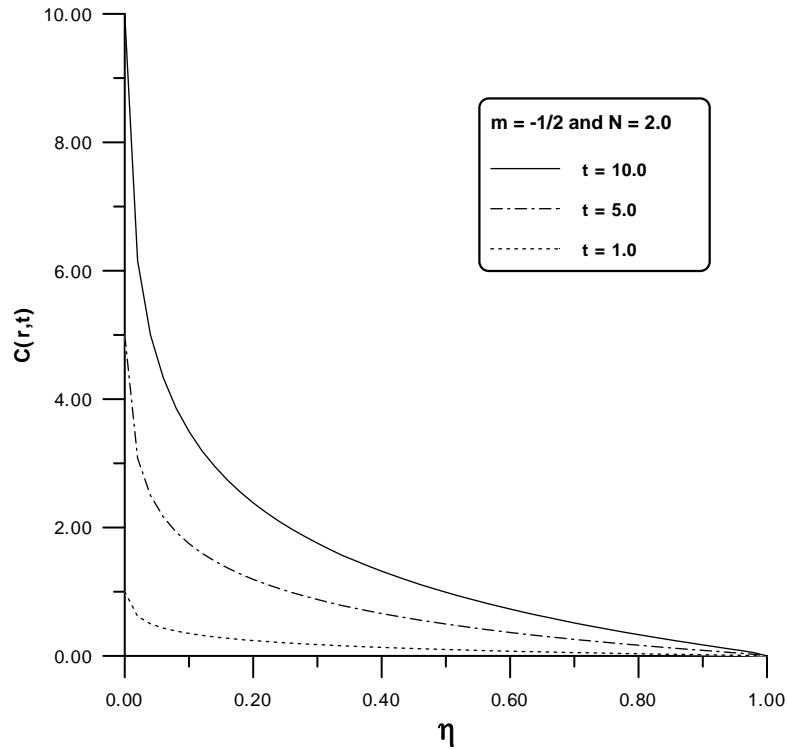


Fig. 1. Effect of time t on the concentration function $C(r,t)$ for $m = -\frac{1}{2}$ and $N = 2$.

Eq. (4.4) takes the form:

$$\frac{d^2\theta}{d\eta^2} - \frac{1}{2\theta} \left[\frac{d\theta}{d\eta} \right]^2 + \frac{1}{\eta} \frac{d\theta}{d\eta} + \frac{\eta\sqrt{\theta}}{4} \frac{d\theta}{d\eta} - \theta^{3/2} = 0. \tag{5.1}$$

To know the final value of η , using order of magnitude analysis [6]

$$\frac{d\theta}{d\eta} \cong \frac{\Delta\theta}{\eta_{\max}} \cong \frac{1}{\eta_{\max}},$$

$$\frac{d^2\theta}{d\eta^2} = \frac{d}{d\eta} \left[\frac{d\theta}{d\eta} \right] \cong \frac{1}{\eta_{\max}^2}.$$

The result for different values of time “ t ” is plotted in Fig. 1.

5.2. Study the effect of “ N ”

Consider $m = -\frac{1}{2}$ and $t = 1$. From Eq. (4.2), $B = \frac{1}{4}$, which yields $\eta = r/\sqrt[4]{t}$.

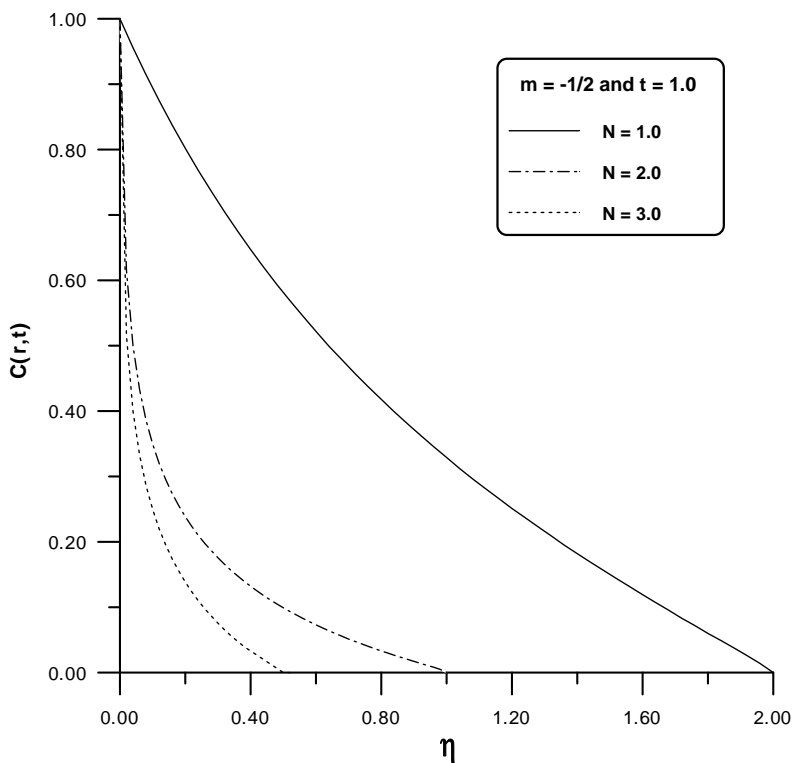


Fig. 2. Effect of N on the concentration function $C(r,t)$ for $m = -\frac{1}{2}$ and $t = 1$.

Eq. (4.4) takes the form:

$$\frac{d^2\theta}{d\eta^2} - \frac{1}{2\theta} \left[\frac{d\theta}{d\eta} \right]^2 + \frac{N-1}{\eta} \frac{d\theta}{d\eta} + \frac{\eta\sqrt{\theta}}{4} \frac{d\theta}{d\eta} - \theta^{3/2} = 0. \tag{5.2}$$

The result for different values of “ N ” is plotted in Fig. 2.

5.3. Study the effect of “ m ”

Consider $N = 2$ and $t = 1$.

Eq. (4.4) takes the form:

$$\theta^m \frac{d^2\theta}{d\eta^2} + m\theta^{m-1} \left[\frac{d\theta}{d\eta} \right]^2 + \frac{1}{\eta} \theta^m \frac{d\theta}{d\eta} + B\eta \frac{d\theta}{d\eta} - \theta = 0. \tag{5.3}$$

The result for different values of “ m ” is plotted in Fig. 3.

6. Results and discussion

The methods for obtaining similarity transformation were classified into (a) direct methods and (b) group-theoretic methods. The direct methods such as separation of variables do not invoke group

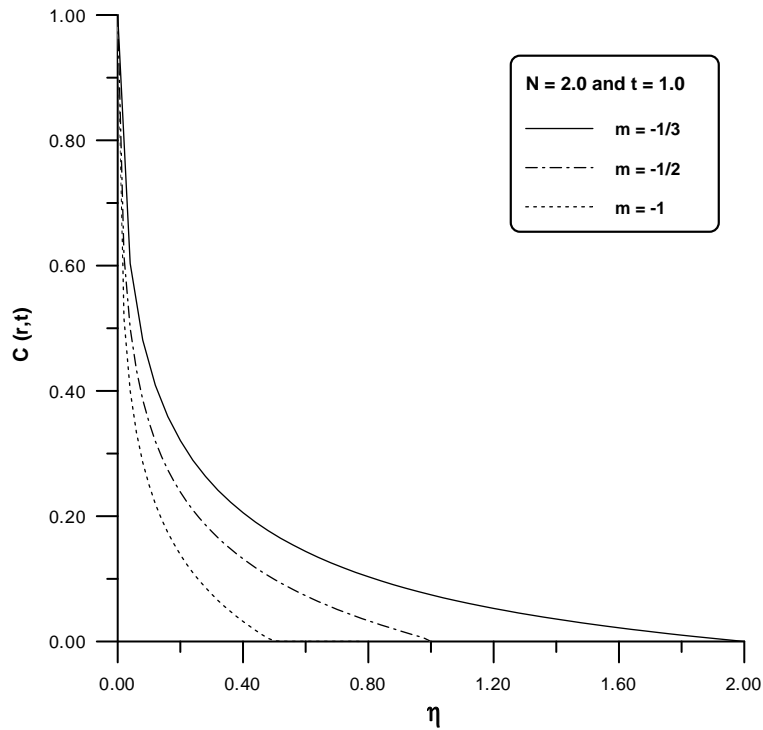


Fig. 3. Effect of m on the concentration function $C(r, t)$ for $N = 2$ and $t = 1$.

invariance. It is fairly straightforward and simple to apply. Group-theoretic methods on the other hand are mathematically more elegant and the important concept of invariance under a group of transformations is always invoked. In some group-theoretic procedures such as the Birkhoff–Morgan method and the Hellums–Churchill method, the specific form of the group is assumed a priori.

On the other hand, procedure such as the finite group method of Moran–Gaggioli is deductive. In this procedure, a general group of transformations is defined and similarity solutions are systematically deduced.

The N -dimensional radially symmetric nonlinear diffusion equation, which is given by Eq. (2.1) is solved with the assumption that, the function $D(C) = C^m$. Studying effect of the time on the concentration $C(r, t)$ show that, for constant value of m ($m = -\frac{1}{2}$), $C(r, t)$ is increasing as “ t ” increases, see Fig. 1. Studying effect of “ N ” on the concentration $C(r, t)$ show that, for constant value of m ($m = -\frac{1}{2}$), $C(r, t)$ is increasing as “ N ” decreases, see Fig. 2. Studying effect of “ m ” on the concentration $C(r, t)$ show that, for $N = 2$, $C(r, t)$ is increasing as “ m ” decreases, see Fig. 3.

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Appendix.

Assume

$$\theta'' = f(\eta, \theta, \theta'), \quad \theta(0) = \alpha \text{ and } \theta(\infty) = \beta. \tag{A.1}$$

Let W_i be the numerical solution for $\theta(\eta_i)$. Substituting for the derivatives θ', θ'' with their approximations in finite difference; we get

$$\frac{W_{i-1} - 2W_i + W_{i+1}}{h^2} = f\left(\eta_i, W_i, \frac{W_{i+1} - W_{i-1}}{2h}\right), \tag{A.2}$$

where “ h ” is the step size in η .

Eq. (A.2) can be written in the form:

$$W_{i-1} - 2W_i + W_{i+1} = h^2 f\left(\eta_i, W_i, \frac{W_{i+1} - W_{i-1}}{2h}\right), \tag{A.3}$$

which can be rewritten as

$$F(W_{i-1}, W_i, W_{i+1}) = 0. \tag{A.4}$$

Writing this equation for $i = 1, 2, 3, \dots, n$.

Taking into consideration that the space domain $\eta \in [0, \infty)$ is subdivided into the computational mesh $\eta_0 < \eta_1 < \eta_2 < \dots < \eta_n < \eta_{n+1}$ where η_{n+1} will be at a far away distance from the initial point η_0 to represent our artificial boundary at ∞ .

The result is a system of nonlinear equation in the unknowns W_1, W_2, \dots, W_n .

The system is solved iteratively using the Newton method for such problem, which leads to

$$J^{(K)}[\bar{W}^{(K+1)} - \bar{W}^{(K)}] = -\bar{F}^{(K)}, \tag{A.5}$$

where $J^{(K)}$ denotes the Jacobian of the system evaluate at the iterative step “ K ”.

$\bar{W}^{(K)}$ and $\bar{W}^{(K+1)}$ represent the unknown vector at step “ K ” and “ $K + 1$ ”, respectively.

$\bar{F}^{(K)}$ is the vector representing the expression in (7.4) above evaluated at the iterative step “ K ”.

The Jacobian matrix “ J ” is obtained which is tri-diagonal matrix.

The resulting system is solved using the Lower–Upper decomposition.

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