

Using Group Theoretic Method to Solve Multi-Dimensional Diffusion Equation

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The nonlinear diffusion equation arises in many important areas of science and technology such as modelling of dopant diffusion in semiconductors. We give analytical solution to N -dimensional radially symmetric nonlinear diffusion equation. The transformation group theoretic approach is applied to analysis of this 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 on the concentration diffusion function $C(r, t)$ has been studied and the results are plotted.

1 Introduction

The problem of m -dimensional radially symmetric nonlinear diffusion equation, was treated by King [9] in 1988. He introduced an approximate similarity solution to the porous-medium equation in one and two dimensions. He studied the case ($m = 1$) and assumed $D(C) = D_0 C^n$. The problems considered arise in the modelling of dopant diffusion in semiconductors. He studied the cases $n = 1$ for arsenic and boron in silicon; $n = 2$ for phosphorus in silicon; $n = 2$ or 3 for zinc in gallium arsenide.

Also, Hill [10] in 1989 studied the case ($m = 1$) and assumed $D(C) = C^n$ but he introduced a new exact solution for the power law diffusivity of index $n = -4/3$ using one-parameter continuous group of transformations. D. Hill and J. Hill [11] in 1990 extended the results given in [10] for particular power law diffusivities C^n (such as $n = -1/2, -1, -3/2$ 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 $D(C) = C^n$ (power-law diffusivities) for both $n > 0$ (slow diffusion), and $n < 0$ (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 [13] in 1948, where he made use of one-parameter transformation groups. In 1952, Morgan [7] presented a theory, which has led to improvements over earlier similarity methods. The method has been applied intensively by Abd-el-Malek et al. [1, 2], Ames [3, 4, 5], Moran and Gaggioli [6] and A.J.A. Morgan [7]. 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 non-linear finite difference method applied to the non-linear second order boundary value problem [14], see appendix.

2 Formulation of the problem and the governing equation

Consider a multi-dimensional diffusion equation of the form:

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

with the boundary conditions

$$\begin{aligned} (i) \quad & C(0, t) = F(t), \\ (ii) \quad & C(\infty, t) = 0, \end{aligned}$$

and initial condition

$$C(r, 0) = 0,$$

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 m is an arbitrary constant.

Assume

$$C(r, t) = F(t)q(r, t), \quad (2)$$

and

$$D(C) = Z(r, t), \quad (3)$$

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

Substitution from (2) and (3) into (1) yields

$$\frac{\partial}{\partial r} \left(Z(r, t) \frac{\partial}{\partial r} [F(t)q(r, t)] \right) + \frac{m-1}{r} Z(r, t) \frac{\partial}{\partial r} [F(t)q(r, t)] = \frac{\partial}{\partial t} [F(t)q(r, t)]. \quad (4)$$

Equation (4) can be rewritten in the form:

$$F \left[\frac{\partial Z}{\partial r} \frac{\partial q}{\partial r} + Z \frac{\partial^2 q}{\partial r^2} \right] + FZ \frac{m-1}{r} \frac{\partial q}{\partial r} - F \frac{\partial q}{\partial t} - q \frac{dF}{dt} = 0 \quad (5)$$

with the boundary conditions

$$(i) \quad q(0, t) = 1, \quad (6)$$

$$(ii) \quad q(\infty, t) = 0, \quad (7)$$

and initial condition

$$q(r, 0) = 0. \quad (8)$$

3 Solution of the problem

Our method of solution depends on the application of a one-parameter group transformation to the partial differential equation (5). Under this transformation the two independent variables will be reduced by one and the differential equation (5) 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:

$$\begin{aligned}\bar{r} &= h^r(a)r + k^r, & \bar{t} &= h^t(a)t + k^t, & \bar{F} &= h^F(a)F + k^F, \\ \bar{q} &= h^q(a)q + k^q, & \bar{Z} &= h^Z(a)Z + k^Z,\end{aligned}\quad (9)$$

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 , q and Z are obtained from G via chain-rule operations:

$$\bar{S}_i = \left[\frac{h^S}{h^i} \right] S_i, \quad \bar{S}_{ij} = \left[\frac{h^S}{h^i h^j} \right] S_{ij}, \quad i, j = r, t, \quad (10)$$

where S stands for F , q and Z .

Equation (5) is said to be invariantly transformed, for some function $A(a)$ whenever:

$$\begin{aligned}\bar{F} [\bar{Z}_r \bar{q}_r + \bar{Z} \bar{q}_{rr}] + \bar{F} \bar{Z} \frac{m-1}{\bar{r}} \bar{q}_r - \bar{F} \bar{q}_t - \bar{q} \bar{F}_t \\ = A(a) \left(F [Z_r q_r + Z q_{rr}] + F Z \frac{m-1}{r} q_r - F q_t - q F_t \right).\end{aligned}\quad (11)$$

Substitution from (9) and (10) into (11) yields

$$\begin{aligned}(h^F F + k^F) \left[\frac{h^Z h^q}{(h^r)^2} Z_r q_r + (h^Z Z + k^Z) \frac{h^q}{(h^r)^2} q_{rr} \right] \\ + (h^F F + k^F) (h^Z Z + k^Z) \frac{m-1}{h^r r + k^r} \frac{h^q}{h^r} q_r - (h^F F + k^F) \frac{h^q}{h^t} q_t - (h^q q + k^q) \frac{h^F}{h^t} F_t \\ = A(a) \left(F [Z_r q_r + Z q_{rr}] + F Z \frac{m-1}{r} q_r - F q_t - q F_t \right).\end{aligned}\quad (12)$$

The invariance of (12) implies

$$k^F = k^Z = k^q = k^r = 0, \quad \text{and} \quad \frac{h^F h^Z h^q}{(h^r)^2} = \frac{h^F h^q}{h^t} = A(a).$$

which yields

$$h^t = \frac{(h^r)^2}{h^Z}.$$

The invariance of the auxiliary conditions (6)–(8) implies that $h^q = 1$, $k^t = 0$.

Finally, we get the one-parameter group G , which transforms invariantly the differential equation (5) and the auxiliary conditions (6)–(8).

The group G is of the form:

$$\bar{r} = h^r r, \quad \bar{t} = \frac{(h^r)^2}{h^Z} t, \quad \bar{F} = h^F F, \quad \bar{q} = q, \quad \bar{Z} = h^Z Z. \quad (13)$$

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

$$g_j(r, t; F, q, Z) = \Psi_j [\eta(r, t)], \quad j = 1, 2, 3$$

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

$$\sum_{i=1}^5 (\alpha_i S_i + \beta_i) \frac{\partial g}{\partial S_i} = 0, \quad S_i \equiv r, t, F, q, Z, \quad (14)$$

where

$$\alpha_i = \frac{\partial h^{S_i}}{\partial a} (a^0) \quad \text{and} \quad \beta_i = \frac{\partial k^{S_i}}{\partial a} (a^0), \quad i = 1, 2, 3, 4, 5 \quad (15)$$

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 the condition (14) is used.

At first, we seek the absolute invariant of the independent variables. Owing to equation (14), $\eta(r, t)$ is an absolute invariant if it satisfies the following first-order linear differential equation,

$$(\alpha_1 r + \beta_1) \frac{\partial \eta}{\partial r} + (\alpha_2 t + \beta_2) \frac{\partial \eta}{\partial t} = 0. \quad (16)$$

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

Now, equation (16) may be rewritten in the form,

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

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

$$\eta = rt^{-B}, \quad \text{where} \quad B = \frac{\alpha_1}{\alpha_2}. \quad (17)$$

The second step is to obtain the absolute invariants of the dependent variables F , q and Z . By a similar analysis, using equations (13), (14) and (15), we get

$$F(t) = R(t)\phi(\eta), \quad (18)$$

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

$$F(t) = R(t), \quad (19)$$

and the second absolute invariant is

$$q(r, t) = \theta(\eta). \quad (20)$$

Also, the last absolute invariant is

$$Z(r, t) = \Gamma(t)W(\eta). \quad (21)$$

4 The reduction to an ordinary differential equation

By means of substitution from (17)–(21) into equation (5), we get

$$R\Gamma t^{-2B}W'\theta' + R\Gamma t^{-2B}W\theta'' + R(m-1)\Gamma W\theta' \frac{t^{-B}}{r} + \frac{RB\theta'}{t}\eta - \theta R' = 0.$$

Dividing by $R\Gamma t^{-2B}$

$$W'\theta' + W\theta'' + \frac{m-1}{\eta}W\theta' + \frac{\eta t^{2B-1}}{\Gamma}\theta' - \frac{R't^{2B}}{R\Gamma}\theta = 0. \quad (22)$$

For (22) 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

$$C_1 = \frac{Bt^{2B-1}}{\Gamma}, \quad C_2 = \frac{R't^{2B}}{R\Gamma}. \quad (23)$$

Using (23) we get,

$$\Gamma(t) = \frac{Bt^{2B-1}}{C_1}, \quad R(t) = t^{\frac{BC_2}{C_1}}.$$

Hence, equation (22) will be,

$$W\theta'' + W'\theta' + \frac{m-1}{\eta}W\theta' + C_1\eta\theta' - C_2\theta = 0. \quad (24)$$

Under the similarity variable η , the boundary conditions are

$$\theta(0) = 1, \quad \theta(\infty) = 0.$$

5 Numerical solution

Consider $W = \eta$.

Case 1. $C_1=1$ and $C_2 = 1$. Equation (24) will be

$$\eta\theta'' + m\theta' + \eta\theta' - \theta = 0.$$

To know the final value of η , using order of Magnitude Analysis [8]

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

Subcase 1a. Take $B = \frac{1}{2}$, then

$$\eta = \frac{r}{\sqrt{t}}, \quad \Gamma(t) = \frac{1}{2}, \quad D(C) = \frac{r}{2\sqrt{t}} = \frac{\eta}{2}, \quad F(t) = \sqrt{t}, \quad C(r, t) = \sqrt{t}\theta(\eta).$$

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

Subcase 1b. Take $B = 1$, then

$$\eta = \frac{r}{t}, \quad \Gamma(t) = t, \quad D(C) = r, \quad F(t) = t, \quad C(r, t) = t\theta(\eta).$$

The result for different values of time t is plotted in Fig. 2.

Case 2. $C_1 = 1$ and $C_2 = 2$. Equation (24) will be

$$\eta\theta'' + m\theta' + \eta\theta' - 2\theta = 0.$$

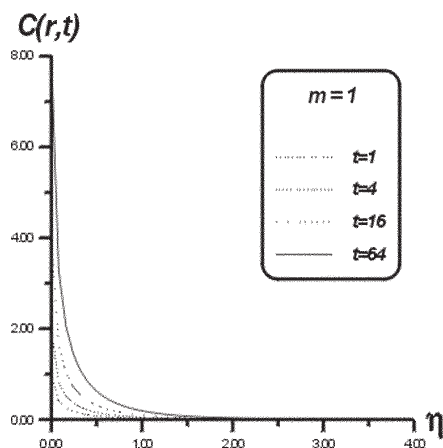


Figure 1. Effect of time t on the concentration function $C(r,t)$ for $C_1 = 1$, $C_2 = 1$ and $B = 1/2$ at $m = 1$.

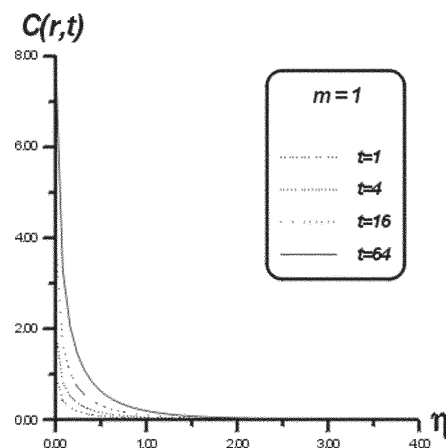


Figure 2. Effect of time t on the concentration function $C(r,t)$ for $C_1 = 1$, $C_2 = 1$ and $B = 1$ at $m = 1$.

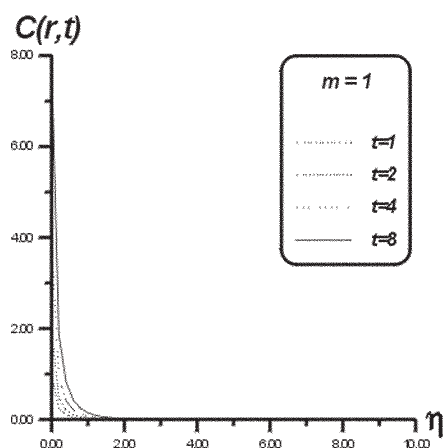


Figure 3. Effect of time t on the concentration function $C(r,t)$ for $C_1 = 1$, $C_2 = 2$ and $B = 1/2$ at $m = 1$.

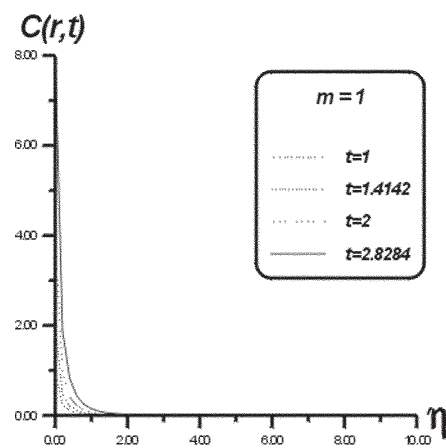


Figure 4. Effect of time t on the concentration function $C(r,t)$ for $C_1 = 1$, $C_2 = 2$ and $B = 1$ at $m = 1$.

Subcase 2a. Take $B = \frac{1}{2}$, then

$$\eta = \frac{r}{\sqrt{t}}, \quad \Gamma(t) = \frac{1}{2}, \quad D(C) = \frac{r}{2\sqrt{t}} = \frac{\eta}{2}, \quad F(t) = t, \quad C(r,t) = t\theta(\eta).$$

The result for different values of time t is plotted in Fig. 3.

Subcase 2b. Take $B = 1$, then

$$\eta = \frac{r}{t}, \quad \Gamma(t) = t, \quad D(C) = r, \quad F(t) = t^2, \quad C(r,t) = t^2\theta(\eta).$$

The result for different values of time t is plotted in Fig. 4.

Case 3. $C_1 = 3$ and $C_2 = 2$. Equation (24) will be

$$\eta\theta'' + m\theta' + 3\eta\theta' - 2\theta = 0.$$

Subcase 3a. Take $B = \frac{1}{2}$, then

$$\eta = \frac{r}{\sqrt{t}}, \quad \Gamma(t) = \frac{1}{6}, \quad D(C) = \frac{r}{6\sqrt{t}} = \frac{\eta}{6}, \quad F(t) = t^{\frac{1}{3}}, \quad C(r,t) = t^{\frac{1}{3}}\theta(\eta).$$

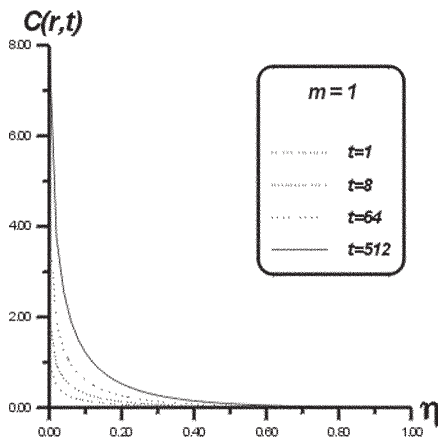


Figure 5. Effect of time t on the concentration function $C(r, t)$ for $C_1 = 3$, $C_2 = 2$ and $B = 1/2$ at $m = 1$.

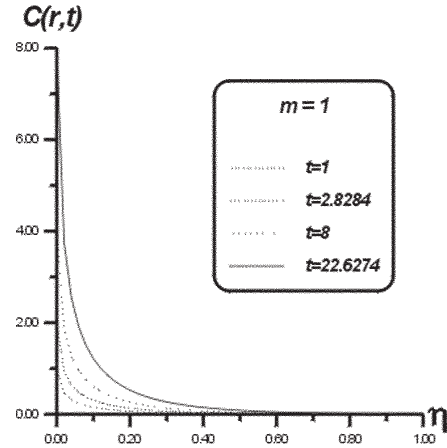


Figure 6. Effect of time t on the concentration function $C(r, t)$ for $C_1 = 3$, $C_2 = 2$ and $B = 1$ at $m = 1$.

The result for different values of time t is plotted in Fig. 5.

Subcase 3b. Take $B = 1$, then

$$\eta = \frac{r}{t}, \quad \Gamma(t) = \frac{t}{3}, \quad D(C) = \frac{r}{3}, \quad F(t) = t^{\frac{2}{3}}, \quad C(r, t) = t^{\frac{2}{3}}\theta(\eta).$$

The result for different values of time t is plotted in Fig. 6.

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 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 equation (1) is solved without made any assumption for the function $D(C)$ and the constant m . It is found that no numerical results could be obtained for equation (24) if we take $W = \eta^2$, $W = e^\eta$, $W = e^{-\eta}$, $W = \frac{1}{\eta}$ and $W = \frac{1}{\eta^2+1}$. The only value of W , to obtain results that $W = \eta$. Studying different cases for values of C_1 and C_2 show that, for constant value of m ($m = 1$), $C(r, t)$ is exponential increasing as t increases.

7 Appendix

Assume $\theta'' = f(\eta, \theta, \theta')$, $\theta(0) = \alpha$ and $\theta(\infty) = \beta$. 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

$$\frac{W_{i-1} - 2W_i + W_{i+1}}{h^2} = f\left(\eta_i, W_i, \frac{W_{i+1} - W_{i-1}}{2h}\right), \quad (25)$$

where h is the step size in η .

Equation (25) can be written in the form

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

which can be rewritten as,

$$F(W_{i-1}, W_i, W_{i+1}) = 0. \quad (26)$$

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,

$$J^{(K)} \left[\overline{W}^{(K+1)} - \overline{W}^{(K)} \right] = -\overline{F}^{(K)}.$$

where $J^{(K)}$ denotes the Jacobian of the system evaluate at the iterative step K . $\overline{W}^{(K)}$ and $\overline{W}^{(K+1)}$ represent the unknown vector at step K and $K + 1$, respectively. $\overline{F}^{(K)}$ is the vector representing the expression in (26) above evaluated at the iterative step K . The Jacobian matrix J is obtained which is three-diagonal matrix. The resulting system is solved using the Lower-Upper decomposition.

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