

Symbolic solutions for boundary value problems using Maple

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Abstract

A simple technique based on finite differences is presented for obtaining symbolic solutions for boundary value problems (BVPs). The governing equations for the node points are expressed in matrix form and the dependent variables (e.g. concentration) at both the boundaries (both at $x=0$ and $x=1$) are taken as unknown constants. The solution is obtained by finding the matrix inverse using Maple. The unique aspect of the technique presented here is that the solution obtained is valid for various boundary conditions (both linear and nonlinear) and geometries. Both linear ordinary differential equations (ODEs) and partial differential equations (PDEs) with linear and non-linear boundary conditions are treated in this paper. Solutions analytical in time are obtained for PDEs. © 2000 Elsevier Science Ltd. All rights reserved.

Keywords: Maple; Matrix inverse; Symbolic solution; Laplace transform technique

1. Introduction

We present here a symbolic inverse technique using Maple for solving systems of linear BVPs. We start by casting a given linear BVP into finite difference form accurate to the order h^2 . This discretization yields a set of linear algebraic equations that includes all the parameters of the system and the dependent variables (e.g. concentration) at the boundaries (both at $x=0$ and $x=1$) as unknown constants. These equations are expressed in a linear matrix form, from which an expression for the value of the dependent variable at each node point is obtained by finding the symbolic inverse using Maple.

First, the methodology is illustrated using a general ordinary differential equation with unknown values at both the boundaries. Once the solution is obtained, we explain how the same solution can be used to generate solutions for different boundary conditions and geometries. Next, we extend our symbolic inverse method to partial differential equations by applying the Laplace transform technique. The resulting BVP is solved in the Laplace domain symbolically by using our symbolic

inverse method. The solution obtained in the Laplace domain is then converted to the time domain by using Maple. Hence, a symbolic semi-analytical solution is obtained, which is similar to our previously presented semi-analytical method (De Vidts & White, 1992) and the method presented earlier by Villadsen and Michelsen (1978), pp. 166–176, for solving parabolic PDEs using orthogonal collocation. The method presented here is superior to these previous methods because the solutions obtained here are valid for various boundary conditions and geometries. The existing semi-analytical techniques (Villadsen & Michelsen, 1978; De Vidts & White, 1992; Subramanian & White, 2000) are valid for specific boundary conditions only. Our new technique (symbolic inverse) solves for the values at the boundaries as unknown constants and hence the solutions once obtained cover various boundary conditions and geometries.

2. Symbolic solution for ordinary differential equations (ODEs)

We demonstrate the technique for linear problems first by solving a general diffusion like equation. The governing differential equation in dimensionless form (e.g. diffusion with reaction, heat transfer, etc.) can be written as,

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$$\frac{d^2y}{dx^2} + \frac{p}{x} \frac{dy}{dx} = H^2y \tag{1}$$

where H is a dimensionless parameter and p is a geometry dependent parameter ($p = 0, 1, 2$ for rectangular, cylindrical, spherical coordinates, respectively). First, the boundary conditions are specified as arbitrary constants.

$$y(0) = c_0 \tag{2}$$

and

$$y(1) = c_L \tag{3}$$

Next, the x -axis is discretized into N (interior) node points. The step size in the x -axis is then given by,

$$h = \frac{1}{N+1} \tag{4}$$

Thus, for $N=2$ points, ($h = 1/3$), we seek expressions for the dependent variable at four node points (y_0, y_1, y_2 and y_3) in terms of H and p . The boundary condition at $x = 0$ (Eq. (2)) gives,

$$y_0 = c_0 \tag{5}$$

and the boundary condition at $x = 1$ (Eq. (3)) gives,

$$y_3 = c_L \tag{6}$$

The dependent variables at the interior node points (y_1 and y_2) satisfy the governing Eq. (1) with the second derivative in x expressed in three-point central difference form accurate to the order h^2 :

$$\frac{y_0 - 2y_1 + y_2}{h^2} + \frac{p}{h} \frac{y_2 - y_0}{2h} - H^2y_1 = 0 \tag{7}$$

at node 1 and,

$$\frac{y_1 - 2y_2 + y_3}{h^2} + \frac{p}{2h} \frac{y_3 - y_1}{2h} - H^2y_2 = 0 \tag{8}$$

at node 2.

The governing equations for y_1 and y_2 (Eqs. (7) and (8)) can be simplified using Eqs. (5) and (6) and expressed in matrix form as,

$$\mathbf{A}\mathbf{Y} = \mathbf{b} \tag{9}$$

where,

$$\mathbf{Y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \tag{10}$$

The coefficient matrix when $h = 1/3$ is,

$$\mathbf{A} = \begin{bmatrix} -H^2 - 18 & 9 + \frac{9}{2}p \\ 9 - \frac{9}{4}p & -H^2 - 18 \end{bmatrix} \tag{11}$$

and the forcing function is

$$\mathbf{b} = \begin{bmatrix} \frac{9}{2}c_0(p-2) \\ -\frac{9}{4}c_L(p+4) \end{bmatrix} \tag{12}$$

Eq. (9) can be solved by finding the inverse of \mathbf{A}

$$\mathbf{Y} = \mathbf{A}^{-1}\mathbf{b} \tag{13}$$

by using Maple:

$$\mathbf{Y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 9 \frac{144c_0 - 72pc_0 + 8c_0H^2 - 4c_0H^2p + 72c_L + 54pc_L + 9c_Lp^2}{1944 + 288H^2 + 8H^4 - 162p + 81p^2} \\ 9 \frac{144c_L - 54pc_0 + 8c_LH^2 + 2c_LH^2p + 72c_0 + 36pc_L + 9c_0p^2}{1944 + 288H^2 + 8H^4 - 162p + 81p^2} \end{bmatrix} \tag{14}$$

Note H, p, c_0 and c_L are parameters in Eq. (14). The complete solution can be written as:

$$\mathbf{Y} = \begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} c_0 \\ 9 \frac{144c_0 - 72pc_0 + 8c_0H^2 - 4c_0H^2p + 72c_L + 54pc_L + 9c_Lp^2}{1944 + 288H^2 + 8H^4 - 162p + 81p^2} \\ 9 \frac{144c_L - 54pc_0 + 8c_LH^2 + 2c_LH^2p + 72c_0 + 36pc_L + 9c_0p^2}{1944 + 288H^2 + 8H^4 - 162p + 81p^2} \\ c_L \end{bmatrix} \tag{15}$$

Thus, a symbolic solution is obtained for the given general linear differential equation. Eqs. (1)–(15) are easily modeled in Maple V as illustrated in the appendix. The solution once obtained can be extended for different boundary conditions as described below.

2.1. Heat transfer in a rectangular fin

Consider the conduction of heat in a rectangular cooling fin. The governing differential equation (Davis, 1984, pp. 72–75, Subramanian, Haran & White, 1999) in dimensionless form is,

$$\frac{d^2y}{dx^2} = H^2y \tag{16}$$

subject to the following boundary conditions,

$$y(0) = 1 \tag{17}$$

and

$$\frac{dy}{dx}(1) = 0 \tag{18}$$

The rectangular cooling fin has an analytical solution:

$$y = \frac{\cosh H(1 - x)}{\cosh H} \tag{19}$$

The general solution obtained earlier (Eq. (15)) is valid for this BVP where

$$p = 0 \text{ (rectangular geometry)} \tag{20}$$

$$c_0 = 1 \text{ (Eq. (17))} \tag{21}$$

$$\frac{y_1 - 4y_2 + 3c_L}{2h} = 0 \text{ (Eq. (18))} \tag{22}$$

Note that, three point backward difference expressions, accurate to the order h^2 are used for accurate dy/dx in Eq. (22). To obtain c_L , the expressions for y_1 and y_2 from Eq. (15) are substituted into Eq. (22):

$$c_L = -3 \frac{H^2 - 18}{54 + 24H^2 + H^4} \tag{23}$$

Hence the complete solution for a rectangular fin is

$$y = \begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 9 \frac{6 + H^2}{54 + 24H^2 + H^4} \\ 54 \frac{1}{54 + 24H^2 + H^4} \\ -3 \frac{18 - H^2}{54 + 24H^2 + H^4} \end{bmatrix} \tag{24}$$

The profiles obtained for $N = 10$ points are plotted in Fig. 1 with H as a parameter. The values of y at the node points with $N = 10$ agree with the analytical solution (Eq. (19)) to within three digits. The computer time required to produce Fig. 1 was less than 1 min.

2.2. Cylindrical catalyst pellet

Eq. (1) with $p = 1$ can be used to describe diffusion with reaction in a cylindrical catalyst pellet (Villadsen & Michelsen, 1978, pp. 72–75):

$$\begin{aligned} \frac{d^2y}{dx^2} + \frac{1}{x} \frac{dy}{dx} &= H^2y \\ \frac{dy}{dx}(0) &= 0 \\ y(1) &= 1 \end{aligned} \tag{25}$$

where H is the Thiele modulus. In this case,

$$\begin{aligned} p &= 1 \\ c_0 &= -\frac{15}{4} \frac{H^2 - 36}{135 + 30H^2 + H^4} \\ c_L &= 1 \end{aligned} \tag{26}$$

where a three point forward difference expression accurate to the order h^2 was used with y_1 and y_2 from Eq. (15) to obtain c_0 . The final solution at all the node points for this case is,

$$y = \begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} -\frac{15}{4} \frac{H^2 - 36}{135 + 30H^2 + H^4} \\ 135 \frac{1}{135 + 30H^2 + H^4} \\ 45 \frac{H^2 + 12}{12(135 + 30H^2 + H^4)} \\ 1 \end{bmatrix} \tag{27}$$

The results for $N = 10$ for various values of H are plotted in Fig. 2. These results agree to within three

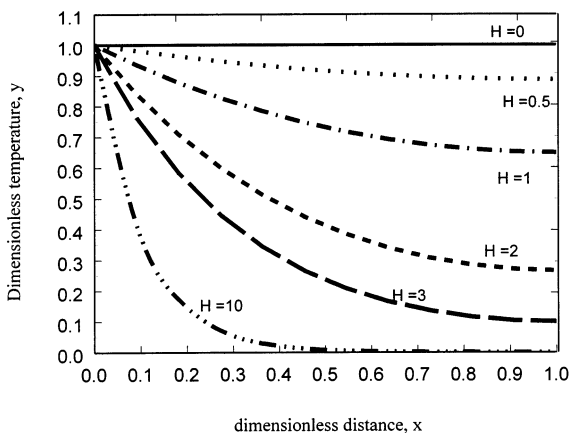


Fig. 1. Dimensionless temperature profiles in a rectangular fin as a function of dimensionless heat transfer coefficient, H-Symbolic solutions for linear ODEs.

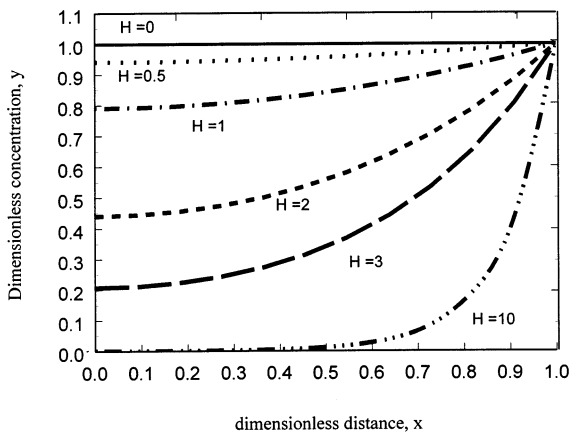


Fig. 2. Dimensionless concentration profiles in a cylindrical catalyst pellet as a function of the Thiele modulus, H-Symbolic solutions for cylindrical coordinate systems.

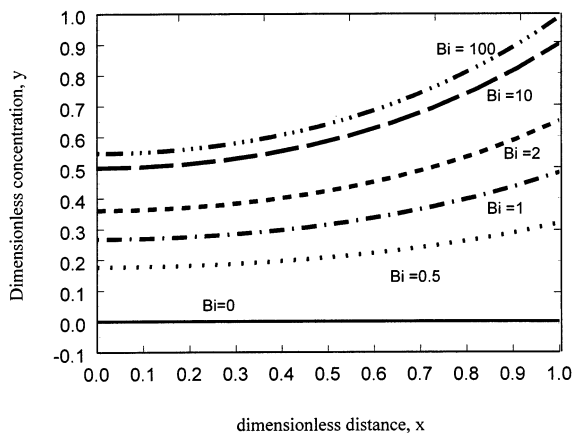


Fig. 3. Dimensionless concentration profiles in a spherical particle as a function of the Biot number, Bi-Symbolic solutions for spherical particles with a new parameter in the boundary condition.

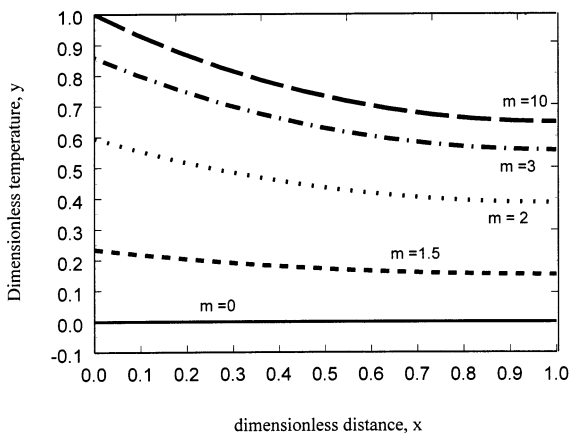


Fig. 4. Symbolic inverse method for nonlinear boundary conditions-dimensionless temperature distribution.

digits with those from Villadsen and Michelsen (1978), pp. 72–75.

2.3. Spherical domain

Eq. (1) written with $p = 2$ describes diffusion with reaction in a spherical catalyst pellet (Finlayson, 1980, pp. 168):

$$\frac{d^2y}{dx^2} + \frac{2}{x} \frac{dy}{dx} = H^2y$$

$$\frac{dy}{dx}(0) = 0$$

$$\frac{dy}{dx}(1) = Bi(1 - y(1))$$
(28)

where H is the Thiele modulus and Bi is the Biot number. Again, Eq. (15) with $p = 2$ can be used with three point forward and backward finite difference expressions for the derivatives at the boundaries to obtain:

$$c_0 = -9 \frac{H^2 - 54}{162H^2 + 9H^4 + 486Bi + 72BiH^2 + 2BiH^4}$$

$$c_L = 2 \frac{Bi(243 + 36H^2 + 9H^4)}{162H^2 + 9H^4 + 486Bi + 72BiH^2 + 2BiH^4}$$
(29)

The final solution for this case can be obtained by substituting c_0 and c_L from Eq. (29) into Eq. (15). For brevity, the final solution is not given here. Again for $N = 10$ node points, the concentration profiles inside the spherical catalyst pellet for different values of Biot numbers are plotted in Fig. 3 for the Thiele modulus $H = 2$.

2.4. Non-linear boundary conditions

One of the advantages of the technique presented here is that it obviates the need for iterations for nonlinear boundary conditions. For example, if one has to solve the BVP

$$\frac{d^2y}{dx^2} = y$$

$$y(0) = 1 - \exp(-m * \left| \frac{dy}{dx}(0) \right|)$$

$$\frac{dy}{dx}(1) = 0$$
(30)

where m is a constant. We see in Eq. (30) that as m approaches infinity, the BVP reduces to the fin problem (Section 2.1) with $H = 1$. Even now the solution obtained (Eq. (15)) is valid. For this case c_0 and c_L are solved in Maple using the fsolve command for specific values of m (see the Appendix A). The procedure consists of writing the equation for $y(0)$ in Eq. (30) in finite difference expression form followed by solving simultaneously the resulting equation together with Eq. (22) for c_0 and c_L (see the Appendix A). For example, when m is 2, c_0 is 0.57 and c_L is 0.37. Profiles for different values of m with $N = 10$ are presented in Fig. 4.

3. Symbolic solutions for partial differential equations (PDEs)

The methodology developed in the previous section for ODEs is extended to partial differential equations (PDEs) here. First, the given PDE is converted into an ODE by applying the Laplace transform technique in time (or time like independent variable). Then, the resulting ODE is solved symbolically in the Laplace

$$\begin{aligned}
 \left(\begin{array}{c} \text{solution in the} \\ \text{Laplace domain} \end{array} \right) &= \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \end{bmatrix} \\
 &= \left[\begin{array}{c} \frac{c_0}{s} \\ \left[\frac{1296c_0 + 648pc_0 - 216s - 72sc_0 + 36spc_0 - 8s^2 - 648c_L - 486pc_L - 81p^2c_L - 36ps}{s(1944 + 288s + 8s^2 - 162p + 81p^2)} \right] \\ \left[\frac{648c_0 - 486pc_0 + 216s + 72sc_L + 18spc_L + 8s^2 + 1296c_L + 324pc_L + 81p^2c_0 - 18ps}{s(1944 + 288s + 8s^2 - 162p + 81p^2)} \right] \\ \frac{c_L}{s} \end{array} \right] \tag{39}
 \end{aligned}$$

domain by using Maple. Once the solution is obtained in the Laplace domain, the final solution is obtained by finding the inverse Laplace transform again by using Maple. To illustrate our method, consider the diffusion equation:

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} + \frac{p}{x} \frac{\partial c}{\partial x} \tag{31}$$

with the initial condition:

$$c = 1 \quad @ \quad t = 0 \tag{32}$$

and boundary conditions:

$$c = c_0 \quad @ \quad x = 0 \tag{33}$$

$$c = c_L \quad @ \quad x = 1 \tag{34}$$

Applying the Laplace transform technique (by using Maple) for t in Eq. (31), we obtain:

$$sc(s) - c_{t=0} = \frac{d^2c(s)}{dx^2} + \frac{p}{x} \frac{dc(s)}{dx} \tag{35}$$

If we replace $c(s)$ by u for brevity and use the initial condition (Eq. (32)), Eq. (31) simplifies to:

$$\frac{d^2u}{dx^2} + \frac{p}{x} \frac{du}{dx} - su + 1 = 0 \tag{36}$$

The boundary conditions (Eqs. (33) and (34)) in the Laplace domain are:

$$u(0) = \frac{c_0}{s} \tag{37}$$

and

$$u(1) = \frac{c_L}{s} \tag{38}$$

Eqs. (36)–(38) are similar to Eqs. (1)–(3). The method applied in Section 2 is applied to solve Eq. (36) and the solution obtained for $N = 2$ is:

Hence a solution is obtained in the Laplace domain as a function of c_0 , c_L and p as parameters.

3.1. Diffusion in a plane sheet

Eq. (39) can be used with $p = 0$ to solve for the diffusion in a plane sheet (Crank, 1994 pp.47–51). The governing equation is:

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} \tag{40}$$

with the initial condition $c(x, 0) = 1$ and boundary conditions,

$$\begin{aligned}
 c(0, t) &= 1 \\
 c(1, t) &= 0
 \end{aligned} \tag{41}$$

Maple is used to convert the boundary conditions to the Laplace domain as:

$$\begin{aligned}
 u(0) &= \frac{1}{s} \\
 u(1) &= 0
 \end{aligned} \tag{42}$$

These boundary conditions can be substituted into Eq. (39) to obtain:

$$\begin{aligned}
 \left(\text{Solution in the Laplace domain} \right) &= \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \end{bmatrix} \\
 &= \begin{bmatrix} \frac{1}{s} \\ \frac{1296 + 288s + 8s^2}{s(1944 + 288s + 8s^2)} \\ \frac{648 + 216s + 8s^2}{s(1944 + 288s + 8s^2)} \\ 0 \end{bmatrix}
 \end{aligned}
 \tag{43}$$

Once the solution is obtained in the Laplace domain, the solution in the time domain is obtained by finding the inverse Laplace transform using Maple:

$$\begin{aligned}
 \text{Solution} &= \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{bmatrix} \quad \text{Solution} = \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{bmatrix} \\
 &= \begin{bmatrix} 1 \\ \left[\frac{2}{3} + \frac{1}{2} \exp(-9t) - \frac{1}{6} \exp(-27t) \right] \\ \left[\frac{1}{3} + \frac{1}{2} \exp(-9t) + \frac{1}{6} \exp(-27t) \right] \\ 0 \end{bmatrix}
 \end{aligned}
 \tag{44}$$

Note that the expressions for the dependent variable obtained at the node points are analytical in time. The results obtained for this case with $N = 10$ are plotted with time t as a parameter in Fig. 5.

3.2. Other examples

Different BVPs can be solved by just recalculating c_0 and c_L . Some of the examples are solved here. For all the cases considered in this section the initial condition is $c(x, 0) = 1$. Consider diffusion with constant flux at the surface of a plane sheet (Crank, 1994, pp. 61–62). The BVP can be written as:

$$\begin{aligned}
 \frac{\partial c}{\partial t} &= \frac{\partial^2 c}{\partial x^2} \\
 \frac{\partial c}{\partial x}(0, t) &= 0 \\
 \frac{\partial c}{\partial x}(1, t) &= -1
 \end{aligned}
 \tag{45}$$

As before by using Eq. (39) ($p = 0$) and $N = 10$, the solution is plotted in Fig. 6 with t as a parameter. It should be noted that a completely different BVP is solved by just recalculating the constants c_0 and c_L in Eq. (39).

Next, consider diffusion in a cylinder with a time dependent concentration at the surface (Crank, 1994, pp.75–76)

$$\begin{aligned}
 \frac{\partial c}{\partial t} &= \frac{\partial^2 c}{\partial x^2} + \frac{1}{x} \frac{\partial c}{\partial x} \\
 \frac{\partial c}{\partial x}(0, t) &= 0 \\
 c(1, t) &= 2 - \exp(-t)
 \end{aligned}
 \tag{46}$$

The profiles obtained by using the procedure presented here with $N = 10$ are plotted in Fig. 7. Note that Maple

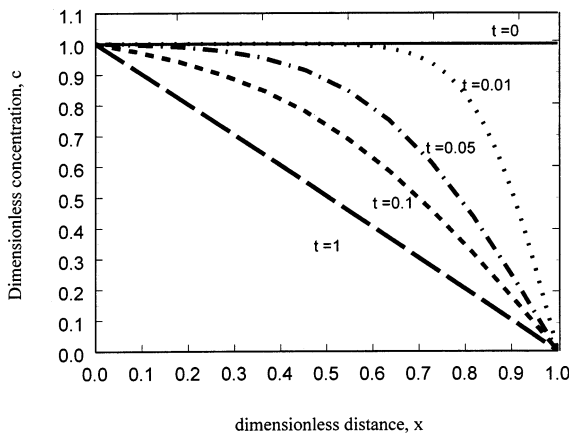


Fig. 5. Symbolic solutions for PDEs in rectangular coordinates-dimensionless concentration profiles with constant surface boundary conditions at both ends.

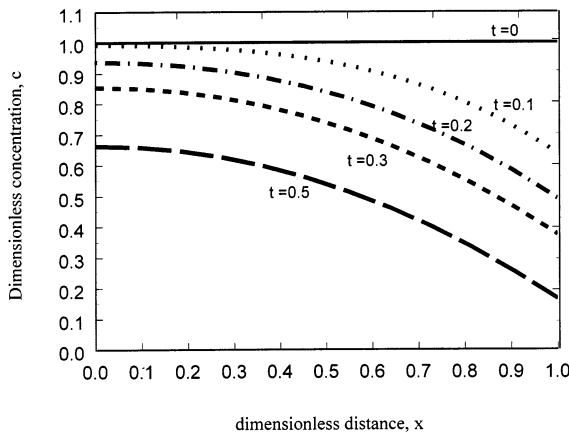


Fig. 6. Symbolic solutions for PDEs-dimensionless concentration profiles under a flux boundary condition at both the surfaces.

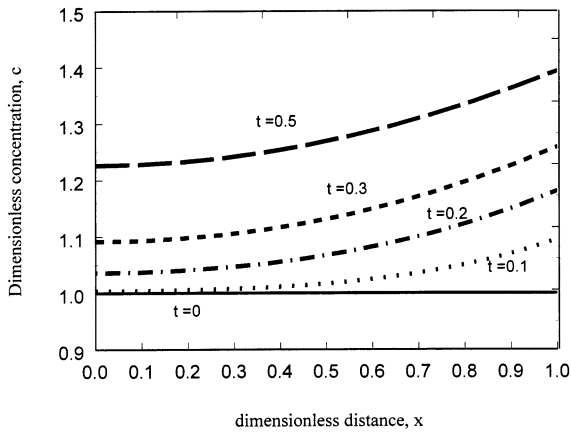


Fig. 7. Symbolic solutions for PDEs in cylindrical domain-dimensionless concentration profiles under time dependent boundary conditions.

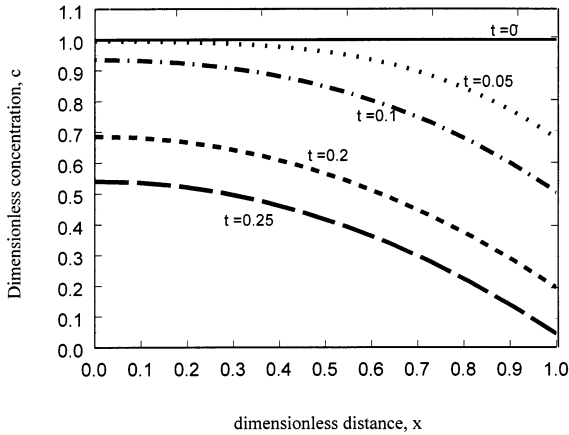


Fig. 8. Symbolic solutions for PDEs in spherical domain-dimensionless concentration profiles under flux boundary conditions at both the surfaces; electrochemical discharge of a spherical particle electrode.

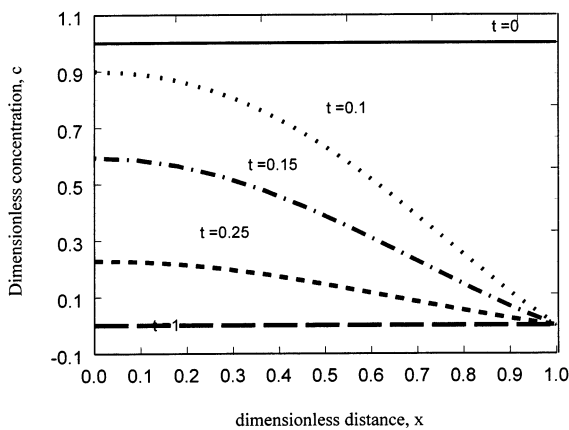


Fig. 9. Symbolic solutions for PDEs with nonlinear boundary conditions-dimensionless concentration profiles.

was used to convert the time dependent boundary condition to the Laplace domain. Spherical diffusion can also be treated. For example, consider electrochem-

ical discharge of a spherical electrode under galvanostatic discharge:

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} + \frac{2}{x} \frac{\partial c}{\partial x}$$

$$\frac{\partial c}{\partial x}(0, t) = 0$$

$$\frac{\partial c}{\partial x}(1, t) = -1$$
(47)

The concentration profiles are solved as before and plotted in Fig. 8 and agree with those presented in the literature (Subramanian & White, 1999a). Again, the solution is also valid for nonlinear boundary conditions, as was illustrated in Section 2. In this case, at a particular time, the nonlinear boundary condition is solved in Maple by using fsolve. For example, consider diffusion in a sphere with a nonlinear surface boundary condition:

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} + \frac{2}{x} \frac{\partial c}{\partial x}$$

$$\frac{\partial c}{\partial t}(0, t) = 0$$

$$c(1, t) = 100 \exp(c(1, t))$$
(48)

The values at the node points were solved using the fsolve command in Maple for a particular value of time. The profiles for this case with $N = 10$ are plotted in Fig. 9.

4. Discussion

A symbolic finite difference method is presented for ODEs. The advantage of the technique over that presented earlier (Subramanian & White, 1999b) is that the solution is independent of the boundary conditions (as illustrated in Section 2) and is valid for nonlinear boundary conditions also.

The method is then extended to PDEs by applying the Laplace transform technique for the time variable. A semi-analytical solution in time is obtained which is consistent with the existing literature (De Vidts & White, 1992; Subramanian & White, 2000). The advantage of the method presented here is that the solution is valid for various boundary conditions (both linear and nonlinear) as illustrated in Section 3.

The order of accuracy used in this paper is h^2 . We have used $N = 10$ interior node points for all the figures. Even though the symbolic solution looks complex for even $N = 2$ node points (Eq. (15)), Maple handles it very well. In the Appendix a simple Maple program is given to explain the technique and show how the same solution can be used for different boundary conditions. By using the same program by substituting $N = 10$ in the program and not changing anything else Figs. 1–4 can be produced. By just mod-

ifying the same program for just redefining A matrix all the results in Figs. 5–9 can be obtained. Total time taken on a 333 MHz Pentium processor for producing Figs. 1–4 starting from the first step (Eq. (1)) is less than 1 min. Total time taken for producing Figs. 5–9 is less than 2 min. An important difference between Eq. (39) and the matrix exponential method presented earlier (De Vidts & White, 1992) is that it is not necessary to find eigen-values of the coefficient matrix for using the method presented here.

Only diffusion like PDEs are solved in this paper. However the same method can be extended to the Laplace equation to solve current distribution problems (Subramanian & White, 2000). A computer with minimum RAM of 64 MB is recommended as Maple is a memory intensive software. The number of node points required depends upon the problem. We don't go beyond $N = 20$ node points. Instead of increasing N beyond 20 node points we increase the order of accuracy to h^4 or h^6 . Finite difference expressions for h^4 or higher order accuracy (look complicated) can be derived from Taylor's series (Maple program for obtaining finite difference expressions of any order is not reported here, but can be obtained from the authors upon request).

5. Summary

A symbolic solution technique has been presented for solving linear ODEs and PDEs with linear and nonlinear boundary conditions. The method presented is simple and gives a general solution, which is valid for various boundary conditions and geometries. The general solution once obtained practically solves a large system of BVPs (not reported here). Several linear PDE examples in the current literature (Carslaw & Jaeger, 1973; Crank, 1994) were solved using our technique in less than 1 min.

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Appendix A. Symbolic solutions for boundary value problems (ODEs)

> **restart:**
Section 2 of paper

Enter the number of digits here

> **Digits:=5;**

Digits := 5

Enter the governing equation (Eq. (1)) here.

> **ge:=diff(y(x), x\$2)+p/x*diff(y(x), x)-H^2*y(x);**

$$ge := \left(\frac{\partial^2}{\partial x^2} y(x) \right) + \frac{p \left(\frac{\partial}{\partial x} y(x) \right)}{x} - H^2 y(x)$$

Enter the number of internal node points here.

> **N:=2;**

N := 2

Enter the boundary condition at $x = 0$ and 1 (Eqs. (2) and (3))

> **bc0:=y[0]=c0; bcL:=y[N+1]=cL;**

bc0 := $y_0 = c0$

bcL := $y_3 = cL$

Use these boundary conditions to solve for $y[0]$ and $y[3]$ (Eqs. (5) and (6))

> **y[0]:=solve(bc0, y[0]); y[N+1]:=solve(bcL, y[N+1]);**

y0 := $c0$

y3 := cL

User has to specify with (linalg) for linear algebra operations in Maple

> **with(linalg):**

Warning, new definition for norm

Warning, new definition for trace

Three point Finite difference expressions are substituted in the governing equation (accurate to the order h^2) given as

> **ge:=subs(diff(y(x), x\$2)=(y[i+1]-2*y[i]+y[i-1])/h^2, diff(y(x), x)=y[i+1]-y[i-1])/(2*h), y(x)=y[i], x=i*h, ge);**

$$ge := \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + \frac{1}{2} \frac{p(y_{i+1} - y_{i-1})}{ih^2} - H^2 y_i$$

The governing equations at the node points are given by (Eqs. (7) and (8))

> **for a from 1 to N do eq[a]:=subs(i=a, ge); od;**

$$eq_1 := \frac{y_2 - 2y_1 + y_0}{h^2} + \frac{1}{2} \frac{p(y_2 - y_0)}{h^2} - H^2 y_1$$

$$eq_2 := \frac{y_3 - 2y_2 + y_1}{h^2} + \frac{1}{4} \frac{p(y_3 - y_1)}{h^2} - H^2 y_2$$

3 point forward and backward differences are stored in fd and bd


```
> fd:=( -y[i+2]+4*y[i+1]-3*y[i])/2/h;
```

$$fd: = \frac{1}{2} \frac{-y_{i+2} + 4y_{i+1} - 3y_i}{h}$$

```
> bd:=(y[i-2]-4*y[i-1]+3*y[i])/2/h;
```

$$bd: = \frac{1}{2} \frac{y_{i-2} - 4y_{i-1} + 3y_i}{h}$$

Dimensions of A and b matrix are defined here

```
> A:=matrix(N, N); b:=matrix(N, 1);
```

```
A:=array(1..2, 1..2, [])
```

```
b:=array(1..2, 1..1, [])
```

First A matrix is initialized to 0

```
> for i from 1 to N do of j from 1 to N do A[i, j]:=0; od: od:
```

A matrix is formed now

```
> for i from 1 to N do for j from 1 to N do
A[i, j]:=coeff(eq[i], y[j]); od; od;
```

b matrix is formed here

```
> for i from 1 to N do
b[i, 1]:=-simplify(eq[i]-sum('A[i, j]*y[j]', 'j'=1..N)); od:
```

values of x are substituted in A and b matrix here

```
> for i from 1 to N do for j from 1 to N do
A[i, j]:=subs(x=i*h, A[i, j]); od; od;
> for i from 1 to N do b[i, 1]:=subs(x=i*h, b[i, 1]); od
```

step size is defined as (Eq. (4))

```
> h:=eval(1/(N+1));
```

$$h: = \frac{1}{3}$$

A and b matrix are evaluated here (Eqs. (11) and (12))

```
> for i from 1 to N do for j from 1 to N do
A[i, j]:=eval(A[i, j]); od: od: for i
from 1 to N do
```

```
B[i, 1]:=eval(b[i, 1]); od: evalm(A);
evalm(b);
```

$$\begin{bmatrix} -18 - H^2 & 9 + \frac{9}{2}p \\ 9 - \frac{9}{4}p & -18 - H^2 \end{bmatrix}$$

$$\begin{bmatrix} \frac{9}{2}c_0(-2+p) \\ -\frac{9}{4}cL(4+p) \end{bmatrix}$$

Eqs. (13)–(15) are done in Maple here

```
> sol:=evalm(inverse(A)*b):
```

```
> sol:=map(simplify, sol):
```

```
> soldf:=matrix(N+2, 1):
```

```
> for i from 1 to N do y[i]:=sol[i, 1];
```

```
od:=
```

```
> soldf[1, 1]:=y[0]: for i from 2 to N+1
do soldf[i, 1]:=simplify(y[i-1]): od:
soldf[N+2, 1]:=simplify(y[N+1]): evalm
(soldf);
```

$$\begin{bmatrix} 9 \frac{144 c_0 - 72 p c_0^2 + 8 c_0 H^2 - 4 c_0 H^2 p + 72 cL + 54 p cL + 9 cL p^2}{1944 + 288 H^2 + 8 H^4 - 162 p + 81 p^2} \\ 9 \frac{72 c_0 - 54 p c_0 + 9 c_0 p^2 + 144 cL + 36 p cL + 8 cL H^2 + 2 cL H^2 p}{1944 + 288 H^2 + 8 H^4 - 162 p + 81 p^2} \end{bmatrix}$$

Now the values at the node points are stored in $y[i]$.

```
> for i from 0 to N+1 do y[i]:=soldf[i+1, 1]; od:
```

Section 2.1 of paper — Heat transfer in fin

Enter the boundary conditions (Eqs. (16) and (17))

```
BC0:=Y(x)=1
```

```
> BCL:=diff(Y(x), x)=0;
```

$$BCL: = \frac{\partial}{\partial x} Y(x) = 0$$

```
> i='i':
```

Now equations Eqs. (20)–(22) in the paper are given as,

```
> p1=0;
```

```
p1:=0
```

```
> Eq0:=subs(diff(Y(x), x)=subs(i=0, fd), Y(x)=y[0], x=0, BC0);
```

```
Eq0:=c0=1
```

```
> EqN:=subs(diff(Y(x), x)=subs(i=0, bd), Y(x)=y[N+1], x=L, BCL);
```

$$EqN: = \frac{3}{2}y_1 - 6y_2 + \frac{9}{2}y_3 = 0$$

note that fd is used $Eq0$ (at $x=0$) and bd is used in EqN (at $x=L$). Now c_0 and cL are solved as (Eq. (26))

```
> soln:=solve({subs(p=p1, Eq0), subs(p=p1, EqN)}, {c0, cL});
```

$$soln: = \left\{ c_0 = 1, cL = -3 \frac{-18 + H^2}{54 + 24 H^2 + H^4} \right\}$$

The solution obtained should be assigned

```
> assign(soln);
```

Now the final solution can be obtained by evaluating $soldf$, the general solution to get Eq. (24) (transpose is printed for brevity)

```
> Yfinal:=simplify(map(eval, subs(p=p1, evalm(soldf)))):transpose(Yfinal);
```

$$\begin{bmatrix} 1 & 9 \frac{H^2 + 6}{54 + 24 H^2 + H^4} \\ 54 \frac{1}{54 + 24 H^2 + H^4} - 3 \frac{-18 + H^2}{54 + 24 H^2 + H^4} \end{bmatrix}$$

This general solution can be plotted for specific values of H as

```
> par:=[0, 0.5, 1, 2, 3, 10];
```

```
par:=[0, .5, 1, 2, 3, 10]
```

```
> for k from 0 to 5 do
  p2 [k]:=plot ([seq ([ (i) *h, Re (evalf
    (subs (H=par [k+1], Yfinal [i+1, 1])))]
    ,i=0..N+1) ], style=line): od:
> with (plots):
```

Fig. 10 can be obtained as

```
> display ( {seq (p2 [i], i=0..5) }, axes=
boxed, thickness=3);
```

Section 2.2 of paper — Cylindrical catalyst pellet

The constraints $c0$ and cL should be first unassigned

```
> unassign ('c0'): unassign ('cL');
```

The boundary conditions are given as (Eq. (25))

```
> BC0: =diff (Y (x), x)=0; BCL:=Y (x)=1;
```

$$BC0: = \frac{\partial}{\partial x} Y(x) = 0$$

$$BCL: = Y(X) = 1$$

```
> i:='i':
```

As before the boundary conditions are used to solve for $c0$ and cL (Eq. (26))

```
> p1:=1;
```

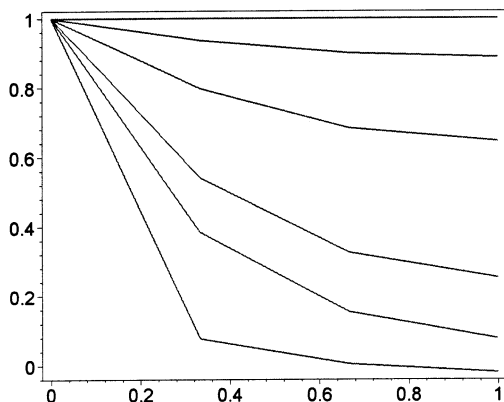


Fig. 10.

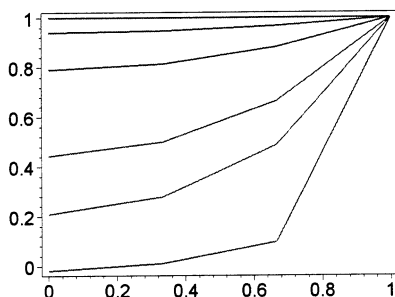


Fig. 11.

```
p1:=1
```

```
> Eq0:=subs (diff (Y(x), x)=subs (i=N+1,
f64), Y (x)=y [N+1], x=0, BCL);
```

$$Eq0: = -\frac{3}{2}y_2 + 6y_1 - \frac{9}{2}y_0 = 0$$

```
> EqN:=subs (diff (Y (x) , x)=subs (i=N+1,
bd), Y (x)=y [N+1], x=L, BCL);
```

```
EqN:=cL=1
```

```
> soln:=solve ( {subs (p=p1, Eq0), subs
(p=p1, EqN) }, {c0, cL});
```

$$soln: = \left\{ c0 = -\frac{15}{4} \frac{-36 + H^2}{135 + 30H^2 + H^4}, cL = 1 \right\}$$

```
> assign (soln);
```

As before the final solution can be obtained as

```
> Yfinal:=simplify (evalm (subs (p=p1, map
(eval, soldf)))):transpose (Yfinal);
```

$$\left[\begin{array}{c} -\frac{15}{4} \frac{-36 + H^2}{135 + 30H^2 + H^4} \\ 135 \frac{1}{135 + 30H^2 + H^4} \frac{45}{4} \frac{H^2 + 12}{135 + 30H^2 + H^4} 1 \end{array} \right]$$

```
> par:=[0, 0.5, 1, 2, 3, 10];
```

```
par:=[0, .5, 1, 2, 3, 10]
```

```
> for k from 0 to 5 do
```

```
  p2 [k]:=plot ([seq ([ (i)*h, Re (evalf
    (subs (H=par [k+1], Yfinal [i+1, 1] )))]
    ,i=0..N+1)], style=line) :od:
```

```
> with (plots):
```

Fig. 11 is obtained as

```
> display ( {seq (p2 [i], i=0..5) }, axes=
boxed, thickness=3);
```

Section 2.3 of paper — Spherical domain

For this section only final result is printed for brevity

```
> unassign ('c0'):unassign ('cL');
```

```
> BC0:=diff (Y (x), x)=0;
```

$$BC0: = \frac{\partial}{\partial x} Y(x) = 0$$

```
> BCL:=diff (Y (x), x)-Bi* (1-Y (x));
```

$$BCL: = \left(\frac{\partial}{\partial x} Y(x) \right) - Bi(1 - Y(x))$$

```
> i:='i':
```

```
> p1:=2;
```

```
p1:=2
```

```
> Eq0:=subs (diff (Y (x), x)=subs (i=0,
fd), Y (x)=y [0], x=0, BC0);
```

$$Eq0: = -\frac{3}{2}y_2 + 6y_1 - \frac{9}{2}y_0 = 0$$

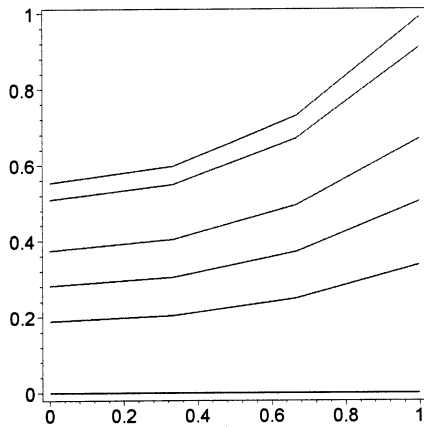


Fig. 12.

```
> EqN:=subs (diff (Y (x), x)=subs (i=N+1,
bd), Y (x)=y [N+1], x=L, BCL);
```

$$EqN: = \frac{3}{2}y_1 - 6y_2 + \frac{9}{2}y_3 - Bi(1 - cL)$$

```
> soln:=solve ({subs (p=p1, Eq0), subs
(p=p1, EqN)}, {c0, cL});
> assign (soln);
> Yfinal:=simplify (evalm (subs (p=p1, map
(eval, soldf))));
```

Yfinal:=

$$\begin{bmatrix} -9 \frac{(H^2 - 54)Bi}{162 H^2 + 9 H^4 + 486 Bi + 72 Bi H^2 + 2 Bi H^4} \\ 486 \frac{Bi}{162 H^2 + 9 H^4 + 486 Bi + 72 Bi H^2 + 2 Bi H^4} \\ 27 \frac{(18 + H^2) Bi}{162 H^2 + 9 H^4 + 486 Bi + 72 Bi H^2 + 2 Bi H^4} \\ 2 \frac{Bi (243 + 36 H^2 + H^4)}{162 H^2 + 9 H^4 + 486 Bi + 72 Bi H^2 + 2 Bi H^4} \end{bmatrix}$$

```
> par:=[0, 0.5, 1, 2, 10, 100];
```

```
par:=[0, .5, 1, 2, 10, 100]
```

```
> for k from 0 to 5 do
p2 [k]:=plot ([seq ([i]*h, Re (evalf
(subs (H=2, Bi=par [k+1], Yfinal [i+1,
1])))], i=0..N+1)], style=line) :od:
```

```
> with (plots):
```

Fig. 12 is obtained as

```
> display ({seq (p2 [i], i=0..5)}, axes=
boxed, thickness=3);
```

Section 2.4 of paper — Non-linear boundary conditions

```
> unassign ('c0'):unassign ('cL');
```

```
> BC0:=Y (x)=1-exp (-m*abs (diff (Y (x),
x)));
```

$$BC0: = Y(x) = 1 - e\left(-m\left|\frac{\partial}{\partial x}Y(x)\right|\right)$$

```
> BCL:=diff (Y (x), x);
```

$$BCL: = \frac{\partial}{\partial x}Y(x)$$

```
> i:='i':
```

```
> p1:=0;
```

```
p1:=0
```

```
> Eq0:=subs (diff (Y (x), x)=subs (i=0,
fd), Y (x)=y [0], x=0, BC0);
```

$$Eq0: = c0 = 1 - e^{(-m|-3/2y_2 + 6y_1 - 9/2y_0)}$$

```
> EqN:=subs (diff (Y (x), x)=subs (i=N+1,
bd), Y (x)=y [N+1], x=L, BCL);
```

$$EqN: = \frac{3}{2}y_1 - 6y_2 + \frac{9}{2}y_3$$

We demonstrate below how to solve for a nonlinear boundary condition

```
> m1:=2;
```

```
m1:=2
```

```
> soln:=fsolve ({subs (p=p1, m=m1, H=1,
Eq0), subs (p=p1, m=m1, H=1, EqN)}, {c0,
cL});
```

```
soln:={c0=.57017, cL=.36809}
```

```
> assign (soln);
```

```
> Yfinal:=simplify (evalm (subs (p=p1, H=
1, m=m1, map (eval, soldf)))):transpose
(Yfinal);
```

```
[.57017 .45470 .38975 .36809]
```

For a different value of m one can solve as

```
> unassign ('c0'):unassign ('cL');
```

```
> m1:=10;
```

```
m1:=10
```

```
> soln:=fsolve ({subs (p=p1, m=m1, H=1,
Eq0), subs (p=p1, m=m1, H=1, EqN)}, {c0,
cL});
```

```
soln:={c0=.99939, cL=.64519}
```

```
> assign (soln);
```

```
> Yfinal:=simplify (evalm (subs (p=p1, H=
1, m=m1, map (eval, soldf)))):transpose
(Yfinal);
```

```
[.99939 .79699 .68312 .64519]
```

The user can just change $N = 10$ at the beginning of this program and run the program to produce Figs. 1–4 in less than 2 min.

Total time taken for $N = 2$ node points is around 8 s.

Appendix B. Nomenclature

- A** coefficient matrix
- b** forcing function
- c dimensionless concentration
- c_i dimensionless concentration at the i^{th} node point
- c_0 dimensionless concentration at $x = 0$
- c_L dimensionless concentration at $x = 1$
- c_I constants (initial derivatives, only in Section 4)
- h step size in x direction
- H dimensionless heat transfer coefficient, Thiele modulus
- L length (cm)
- N number of interior node points used
- s laplace transform variable
- t time (s)
- u dependent variable in the Laplace domain
- x independent variable
- y dependent variable (dimensionless)
- y_i dependent variable at the i^{th} node point (dimensionless)
- Y** dependent variable vector
- y independent variable (only in Section 4)

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