Chemical Engineering Science 59 (2004) 781-788

Chemical Engineering Science

www.elsevier.com/locate/ces

Semianalytical method of lines for solving elliptic partial differential equations

Venkat R. Subramanian^{a,*}, Ralph E. White^b

Department of Chemical Engineering, Tennessee Technological University, Cookeville, TN 38505, USA
 Department of Chemical Engineering, University of South Carolina, Columbia, SC 29208, USA

Received 22 February 2002; received in revised form 6 March 2003; accepted 17 October 2003

Abstract

A semianalytical method of lines is presented for solving elliptic partial differential equations, which are often used to describe steady-state mass and energy transport in solids. The method provides a semianalytical solution for linear equations and can be used to obtain explicit symbolic series solutions in one of the independent variables for non-linear equations.

© 2003 Elsevier Ltd. All rights reserved.

Keywords: Method of lines; Exponential matrix

1. Introduction

Steady-state heat transfer in solids is governed by Laplace's equation and has been solved directly by various numerical methods such as the successive over-relaxation method and the implicit alternative direction method (see, e.g., Carnahan et al., 1969). Another method that has been used to solve Laplace's equation is the method of false transients (Schiesser, 1991, 1994). In this method, one adds a time derivative of the dependent variable to Laplace's equation, uses finite differences to approximate the spatial derivatives, and then solves the resulting system of equations by the method of lines (Davis, 1984; Schiesser, 1991, 1994; Rice and Do, 1995; Schiesser and Silebi, 1997; Cutlip and Shacham, 1998; Constantinides and Mostoufi, 1999; Taylor, 1999; Subramanian and White, 2000a). In this paper, we present a method for solving Laplace's equation using a semianalytical method of lines. This method consists of using a central difference approximation for the second-order derivative in one of the spatial directions followed by solving analytically the resulting system of second-order differential equations by an analytical method. That is, the system of second-order, two-point boundary value problems are solved analytically by casting them in first-order form and

solving the resulting set of first-order equations by using the matrix exponential. Subramanian and White (2000b) used this method previously to solve Laplace's equation to analyze current distribution problems in electrochemical systems. An important aspect of our technique is that the solution obtained is semianalytical (e.g., analytical in y, finite differences in x). A useful aspect of our technique is that the solution obtained is valid for both linear and non-linear boundary conditions at y=0 and 1. For non-linear elliptic PDEs, our semianalytical method combined with iteration for the non-linear term is used to obtain explicit symbolic series solutions in y.

2. Semianalytical method of lines for linear elliptic PDEs

Example 1. Consider heat transfer in a rectangle of length L and height H. The governing equation for the dimensionless temperature distribution can be written as (Carslaw and Jaeger, 1973, p. 166; Schiesser, 1991)

$$\varepsilon^2 \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0, \tag{1}$$

where $\varepsilon = H/L$ is the aspect ratio. For simplicity, the following boundary conditions are set:

$$u(0, y) = 0$$
 for $0 \le y \le 1$, (2)

^{*} Corresponding author.

E-mail address: vsubramanian@tntech.edu (V.R. Subramanian).

$$u(1, y) = 0 \quad \text{for } 0 \leqslant y \leqslant 1, \tag{3}$$

$$u(x,0) = 0 \quad \text{for } 0 \leqslant x \leqslant 1 \tag{4}$$

and

$$u(x, 1) = \sinh(\varepsilon \pi) \sin(\pi x)$$
 for $0 \le x \le 1$. (5)

Eq. (1) with the boundary conditions (2)–(5) has the analytical solution (Schiesser, 1991)

$$u = \sinh(\varepsilon \pi y) \sin(\pi x). \tag{6}$$

The first step in our solution process is to replace $\partial^2 u/\partial x^2$ in Eq. (1) by a finite difference approximation accurate to order h^2 to give

$$\frac{d^2 u_i}{d v^2} = -\varepsilon^2 \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}, \quad i = 1 \dots N,$$
 (7)

where N is the number of interior node points used in discretization of x and h = 1/(N+1) is the node spacing. The boundary conditions at x = 0 and 1 (Eqs. (2) and (3)) are transformed as follows:

$$u_0 = 0, (8)$$

$$u_{N+1} = 0.$$
 (9)

The boundary conditions at y = 0 and 1 are transformed as follows:

$$u_i(y=0) = 0, \quad i = 1...N,$$
 (10)

$$u_i(y=1) = \sinh(\varepsilon \pi) \sin(\pi i h), \quad i=1...N.$$
 (11)

For convenience, let $\zeta = y\varepsilon/h$. This converts the governing equation (Eq. (7)) and boundary conditions (Eqs. (8)–(11)) into the following system of equations:

$$\frac{d^2 u_i}{d\zeta^2} = -u_{i+1} + 2u_i - u_{i-1}, \quad i = 1...N,$$

 $u_0 = 0$,

 $u_{N+1} = 0$,

$$u_i(\zeta = 0) = 0, \quad i = 1...N,$$

$$u_i\left(\zeta = \frac{\varepsilon}{h}\right) = \sinh(\varepsilon\pi)\sin(\pi i h), \quad i = 1...N.$$
 (12)

In Eq. (12), there are N second-order equations. These are converted to 2N first-order equations as follows (Rice and Do, 1995; Subramanian and White, 2000b)

$$\frac{\mathrm{d}u_i}{\mathrm{d}\zeta}=u_{N+1+i}, \quad i=1\ldots N,$$

$$\frac{\mathrm{d}u_{N+1+i}}{\mathrm{d}\zeta} = -u_{i+1} + 2u_i - u_{i-1}, \quad i = 1...N$$
 (13)

with $u_0 = 0$ and $u_{N+1} = 0$. The conditions at $\zeta = 0$ for these 2N differential equations are

$$u_i(\zeta = 0) = 0, \quad i = 1...N$$
 (14)

and

$$u_{N+1+i}(\zeta=0)=c_i, \quad i=1...N.$$
 (15)

In Eq. (15), the unknown constants c_i , i = 1...N are found after integrating the equations in Eq. (13) and by using the boundary conditions at y = 1 ($\zeta = \varepsilon/h$):

$$u_i\left(\zeta = \frac{\varepsilon}{h}\right) = \sinh(\varepsilon\pi)\sin(\pi i h), \quad i = 1...N.$$
 (16)

Eq. (13) is a system of 2N linear first-order differential equations and can be written in matrix form as

$$\frac{\mathrm{d}\mathbf{Y}}{\mathrm{d}\zeta} = \mathbf{A}\mathbf{Y} + \mathbf{b}(\zeta),\tag{17}$$

where

$$\mathbf{Y} = [u_1, u_2, \dots, u_N, u_{N+2}, u_{N+3}, \dots, u_{2N+1}]^{\mathrm{T}}.$$
 (18)

(Note that Eq. (18) does not contain u_{N+1} because it is set equal to zero by the boundary condition at x = 1 (Eq. (12))). **A** is the $2N \times 2N$ coefficient matrix defined by

$$\mathbf{A} = \begin{bmatrix} \mathbf{0} & \mathbf{I} \\ \mathbf{a} & \mathbf{0} \end{bmatrix},\tag{19}$$

where $\mathbf{0}$ is the zero matrix of order $N \times N$, \mathbf{I} is the identity matrix of order $N \times N$ and \mathbf{a} is an $N \times N$ matrix given by

$$\mathbf{a} = \begin{bmatrix} 2 & -1 & 0 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & -1 & 2 & -1 & 0 \\ 0 & \cdots & 0 & 0 & -1 & 2 & -1 \\ 0 & \cdots & 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$
 (20)

and $\mathbf{b}(\zeta)$ is a column vector of order $2N \times 1$ which is a zero vector since $u_0 = u_{N+1} = 0$ in this case. Eq. (17) can be integrated analytically by using the exponential matrix (Amundson, 1966; Taylor and Krishna, 1993; Varma and Morbidelli, 1997; Subramanian and White, 2000a):

$$\mathbf{Y} = \exp(\mathbf{A}\zeta)\mathbf{Y}_0 + \int_0^\zeta \exp[\mathbf{A}(\zeta - \lambda)]\mathbf{b}(\lambda) \, d\lambda, \tag{21}$$

where λ is a dummy variable of integration. \mathbf{Y}_0 is the initial condition vector ($\mathbf{Y}_0 = \mathbf{Y}$ at $\zeta = 0$). For the example chosen, \mathbf{Y}_0 is given by Eqs. (14) and (15):

$$\mathbf{Y}_{0} = [u_{1}, u_{2}, ...u_{N}, u_{N+2}, u_{N+3}, ..., u_{2N+1}]_{\varsigma=0}^{\mathsf{T}}$$

$$= [0, 0, ..., 0, c_{1}, c_{2}, ..., c_{N}]^{\mathsf{T}}.$$
(22)

For the example chosen, when N=1 interior node point is used, the dependent variable at x=0 and 1 are given by the boundary conditions (Eq. (12)) as

$$u_0 = 0$$
 and $u_2 = 0$. (23)

The solution at the interior node point (i = 1) is given by Eq. (21). When N = 1 interior node point is used (with $\varepsilon = 1$), the solution at the interior node point is obtained using Eq. (21) as (note that $\mathbf{b}(\zeta)$ is zero for the example chosen)

$$\mathbf{Y} = \begin{bmatrix} u_1 \\ u_3 \end{bmatrix} = \begin{bmatrix} u_1 \\ \frac{du_1}{d\zeta} \end{bmatrix}$$

$$= \begin{bmatrix} \cosh(\sqrt{2}\zeta) & \frac{1}{\sqrt{2}}\sinh(\sqrt{2}\zeta) \\ \sqrt{2}\sinh(\sqrt{2}\zeta) & \cosh(\sqrt{2}\zeta) \end{bmatrix} \begin{bmatrix} 0 \\ c_1 \end{bmatrix}. \quad (24)$$

Eq. (24) can be simplified as

$$\mathbf{Y} = \begin{bmatrix} u_1 \\ u_3 \end{bmatrix} = \begin{bmatrix} u_1 \\ \frac{\mathrm{d}u_1}{\mathrm{d}\zeta} \end{bmatrix} = \begin{bmatrix} \frac{c_1}{\sqrt{2}} \sinh\left(\sqrt{2}\zeta\right) \\ c_1 \cosh\left(\sqrt{2}\zeta\right) \end{bmatrix}. \tag{25}$$

We call this a semianalytical solution (Eq. (25)), as the solution obtained is analytical in ζ (or y). In Eq. (25), c_1 is the unknown initial condition for $du_1/d\zeta$. The constant c_1 is obtained using the boundary condition at y=1 (Eq. (16) with $\varepsilon=1$) as

$$\mathbf{Y}_{y=1} = \begin{bmatrix} 1 \\ \frac{\mathrm{d}u_1}{\mathrm{d}\zeta_{\zeta=\frac{1}{h}}} \end{bmatrix} = \begin{bmatrix} \frac{c_1}{\sqrt{2}} \sinh\left(2\sqrt{2}\right) \\ c_1 \cosh\left(2\sqrt{2}\right) \end{bmatrix}. \tag{26}$$

Next, the first row of Eq. (26) is substituted in the boundary condition at y = 1 (Eq. (11)) to get

$$c_1 = \sqrt{2} \frac{\sinh(\pi)}{\sinh(2\sqrt{2})}. (27)$$

By substituting this value for c_1 in Eq. (25), analytical solutions for u_1 and $du_1/d\zeta$ are obtained. Note that since we have used only one interior node point (N=1), we only have one constant c_1 . If we use N interior node points, we will have N constants c_i , i=1...N that can be found using the boundary condition at y=1 ($\zeta=\varepsilon/h$).

2.1. Expediting the calculation of exponential matrix

We have used Maple® to calculate the exponential matrix in Eq. (24). When N increases, the time taken by Maple to calculate the exponential matrix increases drastically. For N=10, the matrix order is 20×20 . For this matrix, Maple takes around 10 min to calculate the exponential matrix in a 2.6 GHz processor with 2 GB RAM. For this particular problem, one can derive analytical expression for the exponential matrix by calculating the eigenvalues and eigenvectors analytically (Varma and Morbidelli, 1997). However, these expressions are valid for a particular problem only. If the governing equation or the boundary condition changes,

one has to redo all the steps. When the boundary condition at y = 0 or 1 changes the coefficient matrix **A** does not change. But, if the boundary condition at x = 0 or 1 changes, the first or last row of **a** matrix (Eq. (20)) changes according to the boundary condition. Hence obtaining analytical expressions for the eigenvalues and eigenvectors for every problem would involve tedious algebra. To avoid this, the coefficient matrix **A** can be converted to canonical form (Amundson, 1966; Varma and Morbidelli, 1997)

$$\mathbf{A} = \mathbf{P}\mathbf{D}\mathbf{P}^{-1},\tag{28}$$

Where **D** is the diagonal matrix of order $2N \times 2N$ with the 2N distinct eigenvalues (λ_k , k = 1...2N) as its diagonal elements. For elliptic partial differential equations, it can be shown that all the eigenvalues are distinct and real. **P** is the eigenvector matrix defined as

$$\mathbf{P} = [P_1, P_2, \dots, P_{2N}], \tag{29}$$

where P_k is an $2N \times 1$ eigenvector corresponding to the eigenvalue λ_k . One of the main advantages of Eq. (28) is that it simplifies the calculation of exponential matrix (Amundson, 1966; Varma and Morbidelli, 1997):

$$\exp(\mathbf{A}\zeta) = \mathbf{P}\exp(\mathbf{D}\zeta)\mathbf{P}^{-1}.$$
 (30)

Since **D** is a diagonal matrix, the exponential matrix of **D** is easily obtained as follows (Amundson, 1966; Varma and Morbidelli, 1997):

$$\exp(\mathbf{D}\zeta) = \begin{bmatrix} e^{\lambda_1 \zeta} & 0 & \cdots & 0 & 0 \\ 0 & e^{\lambda_2 \zeta} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & e^{\lambda_{2N-1} \zeta} & 0 \\ 0 & 0 & \cdots & 0 & e^{\lambda_{2N} \zeta} \end{bmatrix}.$$
(31)

Maple can be used to obtain the eigenvalues and the eigenvector matrix (**P**). Maple takes a few seconds to calculate the eigenvalues (e.g., it takes 5 s for a 20×20 matrix). However, Maple takes a long time to calculate the eigenvector matrix, **P**. To overcome this problem, we can obtain a particular eigenvector P_k using the equation (Varma and Morbidelli, 1997):

$$(\mathbf{A} - \lambda_k \mathbf{U}) P_k = \mathbf{0},\tag{32}$$

where **U** is the identity matrix of order $2N \times 2N$. We define P_k as

$$P_k = [\beta_1, \beta_2, \dots, \beta_{2N}]^{\mathrm{T}}.$$
(33)

On substituting Eq. (33) in Eq. (32), we obtain for $N \ge 3$

$$\begin{bmatrix}
-\lambda_{k}\beta_{1} + \beta_{N+1} \\
\vdots \\
-\lambda_{k}\beta_{N} + \beta_{2N} \\
2\beta_{1} - \beta_{2} - \lambda_{k}\beta_{N+1} \\
-\beta_{1} + 2\beta_{2} - \beta_{3} - \lambda_{k}\beta_{N+2} \\
\vdots \\
-\beta_{N-2} + 2\beta_{N-1} - \beta_{N} - \lambda_{k}\beta_{2N-1} \\
-\beta_{N-1} + 2\beta_{N} - \lambda_{k}\beta_{2N}
\end{bmatrix} = \mathbf{0}.$$
(34)

Next, Eq. (34) can be solved to obtain the following expressions for P_k

$$P_k = [\beta_1, \beta_2, \dots, \beta_{2N}]^{\mathrm{T}},$$

where

$$\beta_{1} = 1,
\beta_{2} = (2 - \lambda_{k}^{2})\beta_{1},
\beta_{i} = -\beta_{i-2} + (2 - \lambda_{k}^{2})\beta_{i-1}, \quad i = 3 ... N,
\beta_{N+i} = \lambda_{k}\beta_{i}, \quad i = 1 ... N.$$
(35)

Note that we have arbitrarily chosen $\beta_1 = 1$ in Eq. (35). The exponential matrix (Eq. (30)) once obtained is valid for any set of boundary conditions at y = 0 and/or y = 1. Note that Eq. (35) is valid for the Laplace's equation (Eq. (1)) for any boundary conditions at x = 1, y = 0 and 1. When the boundary condition at x = 0 changes, only the equation for β_2 will change (depending on the boundary condition) and all other expressions are still valid. In addition, it can be shown that the last expression in Eq. (35) $(\beta_{N+i} = \lambda_k \beta_i, i = 1...N)$ is valid for any elliptic PDE in rectangular and cylindrical coordinates. A simple procedure was written in Maple to simulate this example (worksheet available upon request). Maple's inbuilt command can be used to obtain the eigenvalues. Once the eigenvalues are obtained, eigenvectors can be obtained using Eq. (35). The total time taken for this program with N=18 node points (A is a 36 \times 36 matrix) to obtain the exponential matrix, semianalytical solution and 3D plots is less than 1 min (of which nearly 30 s are consumed by Maple for setting up the equations, and obtaining the 3D plot).

2.2. Error analysis

For the example chosen, the average flux at x = 0 can be calculated and used to estimate the error. The average flux

Table 1 Error estimation

Number of interior node points, N in the x direction	Error associated with the semianalytical method, Error _{Semianalytical} (%)	Error associated with the method of false transients, Error _{false transients} (%)
2	28.20	147.21
4	12.75	57.87
6	6.90	30.12
10	2.88	12.33
14	1.57	6.65
18	0.99	4.15

in the x direction at x = 0 (along y) can be obtained as

flux =
$$\int_{v=0}^{y=1} \left[\frac{\partial u}{\partial x} \right]_{x=0} dy.$$
 (36)

The exact value of this can be obtained from Eq. (6) (with $\varepsilon = 1$) as follows:

$$flux_{exact} = \int_{y=0}^{y=1} \left[\frac{\partial}{\partial x} \left(\sinh(\pi y) \sin(\pi x) \right) \right]_{x=0} dy$$
$$= \cosh(\pi) - 1. \tag{37}$$

The error associated with our semianalytical technique can be calculated as follows:

$$Error_{semianalytical}(\%) = \frac{|flux_{semianalytical} - flux_{exact}|}{flux_{exact}} 100.$$
(38)

The error calculated by Eq. (38) decreases with an increase in the number of interior node points N as shown in Table 1. N=18 node points are found to be sufficient to obtain less than 1% error for the average flux.

The error associated with the semianalytical method presented here is on the order of Δx^2 . However, the error associated with the method of false transients is on the order of $\Delta x^2 + \Delta y^2$. To illustrate the superiority of the semianalytical technique compared to the method of false transients, we solved Eq. (1) by adding the pseudo-time derivative (Schiesser, 1991) and applying finite differences in both x and y directions. We chose the same number of interior node points (N) in both x and y directions. The method of false transients was performed until the process reached steady state. The error associated with the method of false transients can be calculated as follows:

$$Error_{false\ transients}(\%) = \frac{|flux_{false\ transients} - flux_{exact}|}{flux_{exact}} 100$$
(39)

and are presented in Table 1. As shown in Table 1, semianalytical method is superior to the method of false transients when the same number of node points is used. For a fixed number of node points in the x-direction (N) (accurate to order h^2), to get higher accuracy with the method of false transients, either a higher number of node points or higher-order finite differences should be used in the y direction. This is

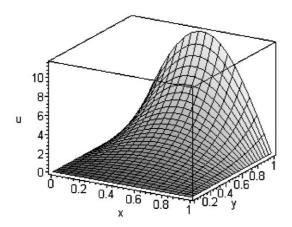


Fig. 1. Dimensionless temperature distribution inside a rectangle—analytical method of lines for linear elliptic partial differential equations. ($\varepsilon = H/L = 1, \ N = 18$).

true because our semianalytical method is analytical in the y direction and the method of false transients is numerical in the y direction.

The dimensionless temperature profile obtained for this example (for $\varepsilon = 1$) is plotted in Fig. 1 for N = 18 node points. Because of symmetry, we get $u_1 = u_2$, etc.

Note that **A** depends only on the governing equation and the boundary conditions at x = 0 and 1. It is convenient that once the exponential matrix $(\exp(\mathbf{A}\zeta))$ is found, the exponential matrix can be used for a different set of boundary conditions at y = 0 and 1. This is true because the solution obtained is analytical in the y direction and valid for any boundary conditions in y.

Example 2. Consider the following boundary value problem

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \tag{40}$$

with the following boundary conditions:

$$u(0, y) = 0 \quad \text{for } 0 \leqslant y \leqslant 1, \tag{41}$$

$$u(1, y) = 0$$
 for $0 \le y \le 1$, (42)

$$u(x,0) = 1$$
 for $0 \le x \le 1$, (43)

$$\frac{\partial u}{\partial y}(x,1) = 1 - u(x,1)^4 \quad \text{for } 0 \leqslant x \leqslant 1.$$
 (44)

Eq. (44) is non-linear and consequently the solution of this example problem will require iteration. However, the exponential matrix obtained earlier in Example 1 is valid for this case also. We just need to change the boundary condition \mathbf{Y}_0 according to Eq. (43) and recalculate the constants c_1, c_2, \ldots, c_N by using Eq. (44). The average surface temperature at y=1 is used as a criterion for convergence. The profiles obtained for this example are plotted in Fig. 2. N=13 node points was found to be sufficient to obtain three digit accuracy for this example.

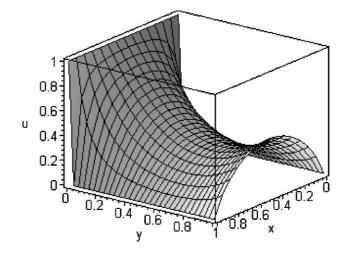


Fig. 2. Dimensionless temperature distribution inside a rectangle—analytical method of lines for linear elliptic partial differential equations with non-linear boundary conditions. ($\varepsilon = 1$, N = 13).

Example 3. The technique described in this paper can also be used for solving PDEs in cylindrical coordinates. For example, consider the Graetz problem (Schiesser and Silebi, 1997)

$$2Pe(1-r^2)\frac{\partial T}{\partial z} = \frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2}$$
 (45)

with the following boundary conditions:

$$\frac{\partial T}{\partial r}(0,z) = 0 \quad \text{for } 0 \leqslant z \leqslant z_L, \tag{46}$$

$$T(1,z) = 1 \quad \text{for } 0 \leqslant z \leqslant z_L, \tag{47}$$

$$T(r,0) = 0$$
 for $0 \le r < 1$ (48)

and

$$\frac{\partial T}{\partial z}(r, z_L) = 0 \quad \text{for } 0 \leqslant r \leqslant 1.$$
 (49)

The temperature distribution obtained by using our semianalytical method is plotted in Fig. 3 for Pe = 10 and $z_L = 2$. Note that values of Peclet number and z_L are chosen so that the effect of the axial conduction can be seen. For this example, the average temperature at $z = z_L$ was used as a criterion for convergence (i.e., the number of interior node points was increased until the temperature at $z = z_L$ converged). N = 10node points was found to be sufficient to obtain three digit accuracy.

3. Semianalytical method of lines for non-linear elliptic PDEs

Example 4. The semianalytical method presented above can be extended to treat certain non-linear PDEs. For example, consider a non-linear diffusion-reaction problem

$$\varepsilon^2 \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = u^2 \tag{50}$$

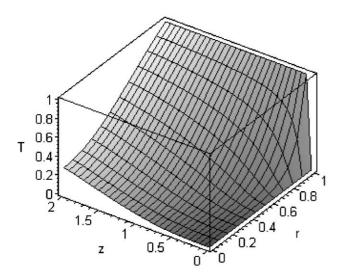


Fig. 3. Dimensionless temperature distribution inside a cylinder—analytical method of lines for linear elliptic partial differential equations in cylindrical coordinates Graetz problem. (Pe=10, $z_L=2$, N=10).

with the following boundary conditions:

$$u(0, y) = 1$$
 for $0 \le y \le 1$, (51)

$$\frac{\partial u}{\partial x}(1, y) = 0 \quad \text{for } 0 \le y \le 1, \tag{52}$$

$$\frac{\partial u}{\partial y}(x,0) = 0 \quad \text{for } 0 \le x \le 1$$
 (53)

and

$$u(x, 1) = 0$$
 for $0 < x \le 1$. (54)

Eq. (50) is non-linear only because of the term u^2 . The procedure for solving this problem using our semianalytical technique is as follows:

- 1. Replace the non-linear term in the equation (u^2) by g(x, y).
- 2. Next, finite differences are applied in the *x*-direction and the governing equation is converted to $\zeta = y\varepsilon/h$ coordinate as

$$\frac{\mathrm{d}u_i}{\mathrm{d}\zeta}=u_{N+1+i}, \quad i=1\ldots N,$$

$$\frac{\mathrm{d}u_{N+1+i}}{\mathrm{d}\zeta} = -u_{i+1} + 2u_i - u_{i-1}$$

$$+\frac{h^2}{\varepsilon^2}g_i(\zeta), \quad i=1...N.$$
 (55)

3. Eq. (55) is cast into matrix form (see Eq. (17)). Note that the **A** matrix is independent of g and $g_i(\zeta)$ occurs only in the **b** matrix given as follows:

$$\mathbf{b} = \left[0, 0, \dots, 0, \frac{h^2}{\varepsilon^2} g_1(\zeta), \frac{h^2}{\varepsilon^2} g_2(\zeta), \dots, \frac{h^2}{\varepsilon^2} g_N(\zeta)\right]^{\mathrm{T}}.$$
 (56)

4. Since the **A** matrix is independent of g, the exponential matrix is found by finding eigenvalues and eigenvectors as in Example 1.

5. For the first iteration, the values for $g_i(\zeta)$ in Eq. (56) are taken as

$$g_i(\zeta) = 0.5, \quad i = 1...N.$$
 (57)

- 6. The semianalytical solution is then found using Eq. (21). Once the semianalytical solution is obtained, the unknown boundary condition constants at y=0 (c_i , i=1...N) are found using the boundary condition at y=1 (Eq. (54)).
- 7. After the first iteration, the values of g_i 's are updated using the semianalytical solution obtained as follows:

$$g_i(\zeta) = [(u_i(\zeta))_{\text{previous iteration}}]^2, \quad i = 1...N.$$
 (58)

- 8. Once new values for the g_i 's are obtained, step 6 is repeated until three digit accuracy is obtained for the constants $(c_i, i = 1...N)$.
- 9. To facilitate the integration involved in step 6, the g_i 's are converted to a series in ζ . For this example, 10 terms were found to be sufficient (these series are not reported here because of the space constraint).
- 10. This process yields series solutions for $u_i(y)$, i = 1...N. For this example, three iterations were found to be sufficient for convergence. When N = 2, the series solution obtained for the interior node points are $(\varepsilon = 0.5)$

$$u_1(y) = 0.43096 - 0.32384y^2 - 0.09129y^4$$

- 0.01461 $y^6 + \cdots$ (59)

and

$$u_2(y) = 0.17041 - 0.19178y^2 + 0.01515y^4 + 0.00567y^6 + \cdots$$
 (60)

A procedure was written in Maple to solve this non-linear example. This procedure gives series solutions in y as the output. The total time taken for this example with N=10 node points was about 2 min using a 2.6 GHz processor with 2 GB RAM. The average dimensionless concentration at y=0 is used as a measure for convergence. N=10 node points were found to be sufficient for this non-linear problem (to obtain three digit accuracy). The series solutions obtained (for N=10 node points) are not reported because of the space constraint. The dimensionless concentration distribution is plotted in Fig. 4.

4. Discussion

The main features of our semianalytical technique can be summarized as follows:

- 1. A semianalytical solution is obtained for linear elliptic partial differential equations, i.e., the solution obtained is analytical in the *y* direction and numerical in the *x* direction.
- 2. A closed-form semianalytical solution is obtained for linear and non-linear boundary conditions at y = 0 and 1.
- 3. The solution once obtained can be used to do different boundary condition case studies because the solution obtained is valid for arbitrary boundary conditions at v = 0

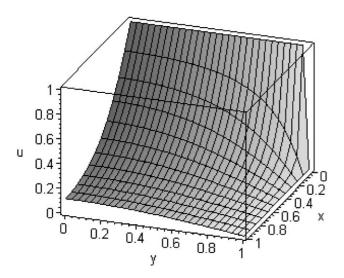


Fig. 4. Dimensionless concentration distribution inside a rectangle—analytical method of lines for non-linear elliptic partial differential equations. ($\varepsilon = 0.5$, N = 10).

and 1 and requires only recalculation of the unknown conditions (constants $c_1, c_2, ..., c_N$) for different sets of boundary conditions at y = 0 and 1.

- 4. A semianalytical solution can be obtained for cylindrical coordinates (Example 3), composite domains (Subramanian and White, 2000b) and arbitrary geometries (Subramanian and White, 2000b) in the *y* direction and for semi-infinite domains in the *y* direction.
- 5. A semianalytical solution can be obtained for certain non-linear elliptic PDEs as shown in Example 4. For non-linear problems, the number of iterations required will vary with the problem. In addition, one has to note that the coefficient of second derivative (both x and y) in Eq. (50) has to be independent of the dependent variable. Our semi-analytical method can be applied only if the right-hand side of the equation alone has non-linear terms.
- 6. In our paper, eigenvalues are obtained from Maple and a procedure was written to obtain the eigenvectors. Alternatively, one could use series approximations for the exponential matrix after scaling the matrix as described by Moler and van Loan (1978).
- 7. In this paper, we have used finite differences accurate to the order of Δx^2 . Using finite difference expressions accurate to the order of Δx^4 makes the coefficient matrix (**A**) in Eq. (17) dense and finding the exponential matrix difficult.
- 8. Even though the technique has been developed for a single elliptic PDE, the same concept could be extended to coupled linear and non-linear elliptic PDEs.
- 9. It should be straightforward to extend our methodology to 3D elliptic PDEs. One could apply finite differences in x and y directions and integrate analytically in z.

In this paper, finite differences were used to replace the derivatives in the x-direction. Alternatively, one could use orthogonal collocation or other discretization techniques and derive semianalytical solutions in y.

5. Conclusions

For linear elliptic PDEs, a semianalytical solution based on the matrix exponential method has been developed. For non-linear elliptic PDEs, series solutions are developed by using the semianalytical solution and iteration.

Notation

A coefficient matrix

 c_i dimensionless unknown constants

h step size in the x direction (dimensionless)

H height of the rectangle, cm

L length of the rectangle, cm

N total number of node points

Pe Peclet number

u dimensionless temperature

Y dependent variable in vector form

 z_L dimensionless length of the cylinder

Greek letters

 ε aspect ratio, H/L

 ζ dimensionless y ordinate $=\varepsilon y/h$

 λ dummy variable

Subscript and superscript

i index of the node point

Acknowledgements

The authors are grateful for the financial support of the project by National Reconnaissance Organization (NRO) under contract # NRO 000-03-C-0122.

References

Amundson, N.R., 1966. Mathematical Methods in Chemical Engineering. In: Matrices and Their Application, Vol. 1. Englewood Cliffs, New Jersey.

Carnahan, B., Luther, H.A., Wilkes, J.O., 1969. Applied Numerical Methods. Wiley, New York.

Carslaw, H.S., Jaeger, J.C., 1973. Conduction of Heat in Solids. Oxford University Press, London.

Constantinides, A., Mostoufi, N., 1999. Numerical Methods for Chemical Engineers with Matlab Applications. Prentice-Hall, New Jersey.

Cutlip, M.B., Shacham, M., 1998. The numerical method of lines for partial differential equations. CACHE News 47, 18–21.

Davis, M.E., 1984. Numerical Methods and Modeling for Chemical Engineers. Wiley, New York.

Moler, C., van Loan, C., 1978. Nineteen dubious ways to compute the exponential of a matrix. SIAM Review 20 (5), 801–836.

Rice, R.G., Do, D.D., 1995. Applied mathematics and modelling for chemical Engineers. John Wiley & Sons Inc., New York.

Schiesser, W.E., 1991. The Numerical Method of Lines. Academic Press, New York.

- Schiesser, W.E., 1994. Computational mathematics in Engineering and Applied Science: ODEs, DAEs and PDEs. CRC Press, Boca Raton.
- Schiesser, W.E., Silebi, C.A., 1997. Computational Transport Phenomena. Cambridge University Press, New York.
- Subramanian, V.R., White, R.E., 2000a. Solving differential equations with maple. Chemical Engineering Education 34, 328–336.
- Subramanian, V.R., White, R.E., 2000b. A semianalytical method for predicting primary and secondary current density distributions: linear
- and non-linear boundary conditions. Journal of Electrochemical Society 147 (5), 1636–1644.
- Taylor, R., 1999. Engineering computing with maple: solution of PDEs via method of lines. CACHE News 49, 5–8.
- Taylor, R., Krishna, R., 1993. Multi Component Mass Transfer. Wiley, New York.
- Varma, A., Morbidelli, M., 1997. Mathematical Methods in Chemical Engineering. Oxford University Press, New York, www.maplesoft.com.