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# Live Problem Solving via Computer in the Classroom to Avoid "Death by PowerPoint" 

## Introduction

Extensive use of the computer for primarily presentations in class, such as the review of PowerPoint ${ }^{\mathrm{TM}}$ notes for example, may have many undesired effects: 1) The attendance in the class session may drop as students have access to copies of the presentation in the course web site. 2) The class may become mind-numbing for students who have studied the material, and the pace may be too fast for students who did not. 3) The students may not appreciate the knowledge of the instructor as he/she only "repeats what is already written on the slides". Felder and Brent ${ }^{[3]}$ have described the undesired effects of the computer use in class as "Death by PowerPoint" and cautioned against the excessive use of pre-prepared PowerPoint visuals for teaching.

Fortunately, there are uses of the computer in teaching in addition to PowerPoint presentations that can be very beneficial in the classroom. A good example is the use of a personal computer for live demonstrations in the classroom for numerical problem solving. One successful scenario is to first discuss the principles and assumptions for a particular problem, and then to develop the mathematical model of the problem on the chalkboard (or a tablet PC). The model can then be entered into the computer in front of the class (or be preprogrammed), and the problem can then be immediately solved using a mathematical software package. Graphical and tabular presentation of the results can serve as the basis to critical analysis and discussion of these results. Questions can then be asked in class regarding the model and expected results when parameters are changed or the model further refined. The resulting model can then be solved in class with the results serving as a basis for further discussion.

In this paper three examples are presented. In these examples a pre-prepared definition of a practical problem is presented and explained. The algorithm and the equations required for the solution are developed in a live demonstration by on a chalkboard or a tablet PC. The problem is then solved using the software packages Polymath ${ }^{\ominus}$ (copyrighted by Polymath Software, http://www.polymath-software.com ), MATLAB ${ }^{\text {TM }}$ (trademark of MathWorks, Inc., http://www.mathworks.com) or Excel ${ }^{\text {TM }}$ (trademark of Microsoft Corporation, http://www.microsoft.com). During the live demonstration, the results are discussed and parametric studies are carried out.

## Example 1 - Solving a Two Point Boundary Value Problem with the Newton-Raphson Method (Shooting Method ${ }^{5}$ )

## Mathematical Model of the Problem and Explanation of the Need for Iterative Solution

This problem (Cutlip and Shacham ${ }^{[1]}$ ) involves the calculation of the concentration profiles and molar fluxes in simultaneous multi-component diffusion of gases. Gases A and B are diffusing through stagnant gas C . There is multicomponent molecular diffusion between two points where the compositions and distance apart are known. The model of the problem and the special numerical data are shown in Table 1. The problem is specified in a format that is also appropriate as Polymath input file for the solution. The Polymath input coding with the comments (marked by \#) provide a compete definition and clear documentation of the model.

Application of the Stefan Maxwell equations to this particular problem yields three differential equations representing the concentrations of components $\mathrm{A}, \mathrm{B}$ and C (lines 1 through 3 in Table 1). The parameters $N_{\mathrm{A}}$ and $N_{B}$ (the molar fluxes of components A and B respectively) are unknown. They can be calculated using the boundary conditions at point $2(z=0.001 \mathrm{~m})$ where $C_{A}=0$ and $C_{B}=0.002701$. Estimates of $N_{A}$ and $N_{B}$ can be obtained from application of the Fick's law assuming simple binary diffusion. An estimate for $N_{A}$ can be obtained, for example, from

$$
N_{A}=-D_{A C} \frac{\left(C_{A} \mathrm{I}_{2}-C_{A} \mathrm{I}_{1}\right)}{\left(z \mathrm{I}_{2}-z \mathrm{I}_{1}\right)}=-1.075 \times 10^{-4} \frac{\left(0-2.229 \times 10^{-4}\right)}{(0.001-0)}=2.396 \times 10^{-5}
$$

An estimate for $N_{B}$ can be similarly calculated, yielding $N_{B}=-3.363 \times 10^{-4}$. These estimates for $N_{A}$ and $N_{B}$ were introduced into the problem definition of Table 1. Integrating the system of differential equations using these parameter values yields the results shown in Table 2. Observe that the value of $C_{A}$ at the final point $(z=0.001)$ is $-1.692 \mathrm{E}-05$ rather than 0 and the value $C_{B}$ is 0.002284 rather than the specified value of 0.002701 . Thus, there is a need to develop a method for adjusting the values of $N_{A}$ and $N_{B}$ so as to obtain the correct boundary values of the variables.

In this section the Polymath model of Table 1 is prepared in advance and used to explain the physical nature of the problem. The live demonstration includes the calculation of the initial estimates for $N_{A}$ and the integration of the model equations using Polymath.

## Description of the Application of the Newton-Raphson Method for the Solution of Two Point Boundary Value Problems

Let us define $\mathbf{x}$ as the vector of unknown parameters (in this particular case $\mathbf{x}=\left(N_{A} N_{B}\right)^{\mathrm{T}}$ ) and $\mathbf{f}$ as a vector of functions representing the difference between the desired and calculated concentration values as point 2 , thus

$$
\mathbf{f}=\left[\begin{array}{l}
C_{A} I_{2}-0  \tag{1}\\
C_{B} I_{2}-2.701 \times 10^{-3}
\end{array}\right]
$$

The Newton-Raphson (NR) method can be written

$$
\begin{equation*}
\mathbf{x}_{k+1}=\mathbf{x}_{k}-\frac{\partial \mathbf{f}^{-1}}{\partial \mathbf{x}} \mathbf{f}\left(\mathbf{x}_{k}\right) \quad k=0,1,2 \mathrm{~K} \tag{2}
\end{equation*}
$$

where $k$ is the iteration number, $\mathbf{x}_{0}$ is the initial estimate and $\boldsymbol{\partial} / \mathbf{\partial} \mathbf{x}$ is the matrix of partial derivatives at $\mathbf{x}=\mathbf{x}_{k}$. The matrix of partial derivatives can be calculated using forward differences, thus

$$
\begin{equation*}
\frac{\partial f_{i}}{\partial x_{j}}=\frac{f_{i}\left(\mathbf{x}_{k}+\boldsymbol{\delta}_{j}\right)-f_{i}\left(\mathbf{x}_{k}\right)}{\delta_{j}} \quad i=1,2 ; \quad j=1,2 \tag{3}
\end{equation*}
$$

where $\boldsymbol{\delta}_{j}$ is a vector containing the value of $\delta_{j}$ at the $j^{\text {th }}$ position and zeroes elsewhere. The iterations of the NR method are stopped when $\left\|f\left(\mathbf{x}_{k}\right)\right\| \leq \varepsilon_{d}$ and where $\varepsilon_{d}$ is the desired error tolerance.

The equations in this section are shown and explained in a live demonstration. In order to carry out the iterative solution process a programming language (such as MATLAB) should be used.

Translating the Model into a MATLAB Function and Implementing the NR Method to Find the Values of $N_{A}$ and $N_{B}$

An option within Polymath 6.1 can be used to automatically convert the model of the problem into a MATLAB function. The Polymath generated function is shown in Table 3. Note that Polymath reorders the equations and changes the syntax of the model according to the requirements of MATLAB. The "main program" that runs the Polymath generated function (shown in Table 4) is available as a template in the "Help" section of Polymath. Only the function name has to be added (see line 1) and the initial values of the variables had to be copied from the Polymath generated model (see lines 3 and 4). Execution of the complete MATLAB program as specified in Tables 4 and 3 does yield the same results obtained by Polymath (Table 2 ), thus verifying that the MATLAB representation of the model is correct.

The MATLAB implementation of the NR method using forward differences to calculate the matrix of partial derivatives is shown in Table 5. The modification of the programs shown in Tables 3 and 4 for iterative refinement of the $N_{A}$ and $N_{B}$ values involves replacement of lines 8 and 9 in Table 4 by the 24 lines of code shown in Table 5, addition of NA and NB to the function parameter list (line 1 in Table 3) and removing the specification of the values of the same variables (lines 5 and 6 in Table 3) from the function. The modified MATLAB program yields the sequence of $N_{A}, N_{B}, f_{1}$ and $f_{2}$ values shown in Table 6 . Note that five NR iterations are required for convergence with error tolerance of $\varepsilon_{d}=10^{-10}$. The converged solution values are $N_{A}$ $=2.1149 \mathrm{e}-5$ and $N_{B}=-4.1425 \mathrm{e}-4$. Using these solution values, the difference between the calculated and desired values of $C_{A}$ and $C_{B}$ at point 2 are $<10^{-10}$.

In this part of the solution the MATLAB implementation of the NR method is prepared in advance. The export of the model to MATLAB, the assembly of the complete program and the iterative solution can be carried out as live classroom demonstrations.

## Example 2 - Solving Systems of Linear Equations Arising from Finite Difference Approximation of PDEs Using Both the Jacoby and Gauss-Seidel Methods

## Description of the Jacoby and Gauss-Seidel Methods

Let us consider a linear system of equations $\mathbf{A x}=\mathbf{b}$ where $\mathbf{x}$ is the $n$-vector of unknowns, $\mathbf{A}$ is an $n \times n$ matrix of coefficients and $\mathbf{b}$ is an $n$ vector of constants. Assuming that $a_{i i} \neq 0 i=1,2, \ldots$, $n$, the system of equations can be written

$$
\begin{equation*}
x_{i}=\left(-\sum_{\substack{j=1 \\ j \neq i}}^{n} a_{i j} x_{j}+b_{i}\right) a_{i i}^{-1}, \mathrm{i}=1,2, \ldots, n \tag{4}
\end{equation*}
$$

Using this formulation of the system of equations, a sequence of approximate solutions $\mathbf{x}_{1}, \mathbf{x}_{2}, \ldots$ can be calculated using the Jacobi method (Dahlquist et al. ${ }^{[2]}$, p. 189)

$$
\begin{equation*}
x_{i, k}=\left(-\sum_{\substack{j=1 \\ j \neq i}}^{n} a_{i j} x_{j, k-1}+b_{i}\right) a_{i i}^{-1}, \mathrm{i}=1,2, \ldots, n ; k=1,2, \ldots \tag{5}
\end{equation*}
$$

where $k$ is the iteration number and $x_{0}$ is the initial estimate. The iterations are stopped when $\left\|\mathbf{x}_{k}-\mathbf{x}_{k-1}\right\| \leq \varepsilon_{d}$.

In the Gauss-Seidel method, new values of the unknowns are used as soon as they are computed. Thus

$$
\begin{equation*}
x_{i, k}=\left(-\sum_{j=1}^{i-1} a_{i j} x_{j, k-1}-\sum_{j=i+1}^{n} a_{i j} x_{j, k-1}+b_{i}\right) a_{i i}^{-1} \mathrm{i}=1,2, \ldots, n ; k=1,2, \ldots \tag{6}
\end{equation*}
$$

The equations of this section are presented and explained in a live demonstration.

## Finite Difference Representation of a Steady-State, Two-Dimensional Heat Transfer Problem

A two-dimensional problem is used to demonstrate the application of the Jacobi and GaussSeidel methods. Such a problem requires the solution of the Laplace equation.

$$
\begin{equation*}
\frac{\partial^{2} T}{\partial x^{2}}+\frac{\partial^{2} T}{\partial y^{2}}=0 \tag{7}
\end{equation*}
$$

Dividing the two dimensional space into squares with edge lengths of $\Delta x=\Delta y=1$ enables a finite difference representation of Eq. (7)

$$
\begin{equation*}
T_{i, j+1}+T_{i, j-1}+T_{i+1, j}+T_{i-1, j}-4 T_{i, j}=0 \tag{8}
\end{equation*}
$$

In this problem (Geankoplis ${ }^{[4]}$, p. 340), the steady state temperature profile in a hollow rectangular chamber (see Figure 1) has to be determined. The inside dimensions of the chamber $4 \times 2 \mathrm{~m}$ and the outside dimensions $8 \times 8 \mathrm{~m}$. The inside walls are held at 600 K and the outside at 300 K .

Since the chamber is symmetrical, equations in the form of Eq. 8 have to be written only for one fourth of the chamber. The equations, as arranged in the form appropriate for the use of the Jacobi method, are shown in lines 1 through 10 of the $2^{\text {nd }}$ column in Table 7. Note that variable names have been replaced by temperature values at the boundaries and relationships based on symmetry allow replacement of three of the unknown temperatures ( $T_{0,2}=T_{2,2} ; T_{3,6}=T_{3,4}$ and $T_{4,6}=T_{4,4}$ ). Variable names ending with the letter "i" indicate initial estimates for the temperature and the initial estimates suggested by Geankoplis are introduced in lines 11 through 20. In lines 21 through 30, the elements needed to calculate the norm of the error in the first iteration are computed. Solving this set of equations with Polymath yields the results of the first iteration of the Jacobi method.

Polymath 6.1 can be used to export the problem definition to Excel with a single key-press. A slight modification of the Polymath exported problem enables carrying out additional iterations just by copying the column which contains the formulas for calculating $T_{i, j}$ and $\operatorname{err}_{i, j}$ and pasting them into additional columns as shown in Table 8. Note that every column represents one iteration.

Solution of the problem using the Gauss-Seidel method the equations is shown in the third column of Table 7. Observe that the only difference between the Jacobi and the Gauss-Seidel methods is that the newly calculated unknown values are immediately being used in the former method. For example, the calculation of T22 (in line 2) the Jacobi method uses T12i while the Gauss-Seidel method uses T12 which was calculated in the previous line. The equations of the Gauss-Seidel method can be exported to Excel similarly to what was done for the equations of the Jacobi method. The iterations can be carried out and the results compared in one worksheet.

In this case, the equations shown in Table 7 are prepared in advance. The export to Excel, rearrangement and extension of the worksheet along with the iterative solution are carried out as a live demonstration.

## Example 3 - Ill-Conditioning in Multiple Linear Regression - Detection and Harmful Effects

## Regression Model for Heat of Cement Hardening

Woods et al. ${ }^{[7]}$ investigated the integral heat of hardening of cement as a function of composition. Some of the reported results are shown in Table 9. The independent variables represent weight percent of the clinker compounds: $x_{1}$ - tricalcium aluminate ( $3 \mathrm{CaO} \cdot \mathrm{Al}_{2} \mathrm{O}_{3}$ ), $x_{2}$ tricalcium silicate $\left(3 \mathrm{CaO} \cdot \mathrm{SiO}_{2}\right)$, $x_{3}$ - tetracalcium alumino-ferrite $\left(4 \mathrm{CaO} \cdot \mathrm{Al}_{2} \mathrm{O}_{3} \cdot \mathrm{Fe}_{2} \mathrm{O}_{3}\right)$, and $x_{4}$ -$\beta$-dicalcium silicate ( $3 \mathrm{CaO} \cdot \mathrm{SiO}_{2}$ ). The dependent variable $y$ is the total heat evolved (in calories per gram cement) in a 180-day period. Two multiple linear regression models, one with zero y intercept (no free parameter) and one with non-zero intercept, are to be compared.

The regression model for this problem is

$$
\begin{equation*}
\mathbf{y}=\hat{\beta}_{0} \mathbf{x}_{0}+\hat{\beta}_{1} \mathbf{x}_{1}+\hat{\beta}_{2} \mathbf{x}_{2}+\hat{\beta}_{3} \mathbf{x}_{3}+\hat{\beta}_{4} \mathbf{x}_{4} \tag{9}
\end{equation*}
$$

where $\hat{\beta}_{0}, \hat{\beta}_{1}, \hat{\beta}_{2}, \hat{\beta}_{3}$ and $\hat{\beta}_{4}$ are the model parameter estimates and $\mathbf{x}_{0}$ is a vector whose components are unity (included in the model only in case of non-zero y intercept).

The model parameter estimates can be calculated using the least squares method by solving the "normal" equation

$$
\begin{equation*}
\left(\mathbf{X}^{T} \mathbf{X}\right) \hat{\boldsymbol{\beta}}=\mathbf{X}^{T} \mathbf{y} \tag{10}
\end{equation*}
$$

where $\mathbf{A}=\mathbf{X}^{T} \mathbf{X}$ is the normal matrix, $\mathbf{X}=\left[\mathbf{x}_{0} \mathbf{x}_{1} \mathbf{x}_{2} \mathbf{x}_{3} \mathbf{x}_{4}\right]$ and $\hat{\boldsymbol{\beta}}=\left[\hat{\beta}_{0} \hat{\beta}_{1} \hat{\beta}_{2} \hat{\beta}_{3} \hat{\beta}_{4}\right]^{T}$.
The indicators (see, for example, Shacham et al. ${ }^{[6]}$ ) that can be used to check the appropriateness, accuracy and stability (conditioning) of the model are the residual plots,
variances, linear correlation coefficients, confidence intervals in addition to the eigenvalues and condition numbers of the normal matrices. The harmful effects of ill-conditioning can be demonstrated by carrying out the regression after removing a data point.

In this section the data and the problem definition are prepared in advance while the equations are developed in a live demonstration.

## Analysis of the Two Regression Models

The parameters of the various models and the quality of fit indicators can be calculated with Polymath and MATLAB in a live demonstration. Partial results of this analysis are presented in Figure 2 and Table 10. The random distribution of the residuals in Figure 2 shows that the linear model represents the data adequately. However, the results in Table 10 show that the regression model with the non-zero intercept is very unstable (ill-conditioned). The instability is reflected in the values of the $95 \%$ confidence intervals all of which are larger than the respective parameter values and the seven order of magnitude difference between the maximal and minimal eigevalues of the normal matrix ( condition number $=3.64 \mathrm{e} 7$ ). In contrast, the zero-intercept model is stable with much smaller values of the confidence intervals and the condition number.

The harmful effects of the instability can be demonstrated by carrying out the regression when the last data point is removed from the set. In this case the parameter values obtained for the nonzero intercept model are: $\hat{\beta}_{0}=36.2 ; \hat{\beta}_{1}=1.78 ; \hat{\beta}_{2}=0.80 ; \hat{\beta}_{3}=0.328$ and $\hat{\beta}_{4}=0.12$. These values are completely different than the parameter values in Table 10. For the case of $\hat{\beta}_{4}$, even the sign is different. The results for the zero intercept model match the results of Table 10 up to two decimal digits.

## Conclusions

A new approach for incorporating the computer in classroom teaching has been demonstrated. In the courses where this approach has been implemented the following educational benefits have been observed:

- The use of real-life problems for demonstration increases considerably the student motivation to study mathematical modeling and numerical methods as they understand better the need for learning these subjects.
- The development of the key algorithms and equations on the chalkboard (or the tablet PC) enables more extensive clarification of unclear points and gives the student more time to absorb and understand the new material.
- Students are very impressed with the live demonstrations that include solution of complex problems with a few key-presses using the various software packages. The conversion of a complex algorithm to a working program and the presentation of graphical and tabular results in a few minutes seems "amazing" to many of them. Consequently, their interest in the course and their appreciation of the instructor's expertise increase considerably.
- The proposed approach helped to retain or bring back the students to the classroom, and it provides many educational benefits in addition to avoiding "death by PowerPoint".


## Bibliography

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Table 1. Polymath Input File for the Multi-Component Diffusion Problem

```
Line Equation # Comment
    d(CA)/d}(\textrm{z})=(xA*NB-xB*NA)/DAB + (xA * NC - xC *NA)/DAC # Concentration of A (g-mol/L)
    d(CB)/d}(\textrm{z})=(\textrm{xB}*NA-xA*NB)/DAB + (xB*NC - xC *NB)/DBC # Concentration of B (g-mol/L)
    d(CC)/d}(\textrm{z})=(xC*NA - xA * NC) / DAC + (xC * NB - xB *NC) / DBC # Concentration of C (g-mol/L)
    NB = -0.0003363 # Molal flux of component B (kg-mol/m^2*s)
    NA = 2.396e-5 # Molal flux of component A (kg-mol/m^2*s)
    DAB = 1.47e-4 # Diffusivity of A through B (m^2/s)
    NC = 0 # Molal flux of stagnant component C (kg-mol/m^2*s)
    DAC = 1.075e-4# Diffusivity of A through C (m^2/s)
    DBC = 1.245e-4 # Diffusivity of B through C (m^2/s)
    CT = 0.2 / (82.057e-3 * 328) # Gas concentration g-mol/L
    xA = CA / CT # Mole fraction of A
    xB = CB / CT # Mole fraction of B
    xC = CC / CT # Mole fraction of C
    z(0) = 0 # Length coordinate at point 1
    CB}(0)=0 # Concentration of B at point 
    CA(0) = 0.0002229 # Concentration of A at point 1
    CC(0) = 0.007208 # Concentration of C at point 1
    z(f)=0.001 # Length coordinate at point 2 where at solution CA2 = 0 and CB2 = 0.002701
```

Table 2. Concentration Values Obtained Using the Estimates: $N_{A}=-2.396 \times 10^{-5}$ and $N_{B}=-3.363 \times 10^{-4}$

| Variable | Initial value | Minimal value | Maximal value | Final value |
| :--- | ---: | ---: | ---: | ---: |
| $\boldsymbol{z}$ | 0 | 0 | 0.001 | 0.001 |
| $\boldsymbol{C}_{\boldsymbol{A}}$ | 0.0002229 | $-1.69 \mathrm{E}-05$ | 0.0002229 | $-1.69 \mathrm{E}-05$ |
| $\boldsymbol{C}_{\boldsymbol{B}}$ | 0 | 0 | 0.002284 | 0.002284 |
| $\boldsymbol{C}_{\boldsymbol{C}}$ | 0.007208 | 0.0051638 | 0.007208 | 0.0051638 |

Table 3. MATLAB Function for the Multi-Component Diffusion Problem.

| Line | Equation \% Comment |
| :---: | :---: |
| 1 | function dYfuncvecdz = ODEfun(z,Yfuncvec); |
| 2 | $\mathrm{CA}=\mathrm{Yfuncvec}(1)$; |
| 3 | $\mathrm{CB}=\mathrm{Y}$ funcvec(2); |
| 4 | $\mathrm{CC}=$ Yfuncvec(3); |
| 5 | NB $=-.0003363$; \% Molal flux of component $\mathrm{B}\left(\mathrm{kg}-\mathrm{mol} / \mathrm{m}^{\wedge} 2 * \mathrm{~s}\right)$ |
| 6 | NA $=.00002396 ; \%$ Molal flux of component A ( $\mathrm{kg}-\mathrm{mol} / \mathrm{m}^{\wedge} 2 * \mathrm{~s}$ ) |
| 7 | $\mathrm{DAB}=.000147$; \% Diffusivity of A through B ( $\mathrm{m}^{\wedge} 2 / \mathrm{s}$ ) |
| 8 | $\mathrm{NC}=0 ; \%$ Molal flux of stagnant component A ( $\mathrm{kg}-\mathrm{mol} / \mathrm{m}^{\wedge} 2 * \mathrm{~s}$ ) |
| 9 | DAC $=.0001075 ; \%$ Diffusivity of A through C ( $\mathrm{m}^{\wedge} 2 / \mathrm{s}$ ) |
| 10 | DBC $=.0001245 ; \%$ Diffusivity of B through C ( $\mathrm{m}^{\wedge} 2 / \mathrm{s}$ ) |
| 11 | $\mathrm{CT}=.2 /(.082057 * 328) ; \%$ Gas concentration g-mol/L |
| 12 | $\mathrm{xA}=\mathrm{CA} / \mathrm{CT}$; \% Mole fraction of A |
| 13 | $\mathrm{xB}=\mathrm{CB} / \mathrm{CT}$; \% Mole fraction of B |
| 14 | $\mathrm{xC}=\mathrm{CC} / \mathrm{CT}$; \% Mole fraction of C |
| 15 | $\mathrm{dCAdz}=(\mathrm{xA} * \mathrm{NB}-(\mathrm{xB} * \mathrm{NA})) / \mathrm{DAB}+(\mathrm{xA} * \mathrm{NC}-(\mathrm{xC} * \mathrm{NA})) / \mathrm{DAC} ; \%$ Concentration of A (g-mol/L) |
| 16 | $\mathrm{dCBdz}=(\mathrm{xB} * \mathrm{NA}-(\mathrm{xA} * \mathrm{NB})) / \mathrm{DAB}+(\mathrm{xB} * \mathrm{NC}-(\mathrm{xC} * \mathrm{NB})) / \mathrm{DBC} ; \%$ Concentration of B (g-mol/L) |
| 17 | $\mathrm{dCCdz}=(\mathrm{xC} * \mathrm{NA}-(\mathrm{xA} * \mathrm{NC})) / \mathrm{DAC}+(\mathrm{xC} * \mathrm{NB}-(\mathrm{xB} * \mathrm{NC})) / \mathrm{DBC} ; \%$ Concentration of C (g-mol/L) |
| 18 | dYfuncvecdz = [dCAdz; dCBdz; dCCdz]; |

Table 4. MATLAB "Main Program" for the Multi-Component Diffusion Problem

```
Line Command % Comment
    function MultDiffusB
    clear, clc, format short g, format compact
    tspan = [0 0.001]; % Range for the independent variable
    y0 = [0.0002229; 0;0.007208]; % Initial values for the dependent variables function
    disp(' Variable values at the initial point ');
    disp(['t = ' num2str(tspan(1))]);
    disp(' y dy/dt ');
    disp([y0 ODEfun(tspan(1),y0)]);
    [t,y]=ode45(@ ODEfun,tspan,y0);
    for i=1:size(y,2)
        disp([' Solution for dependent variable y' int2str(i)]);
        disp([' t y' int2str(i)]);
        disp([t y(:,i)]);
        plot(t,y(:,i));
        title([' Plot of dependent variable y' int2str(i)]);
        xlabel(' Independent variable (t)');
        ylabel([' Dependent variable y' int2str(i)]);
        pause
    end
```

Table 5. MATLAB Implementation of the NR Method for the Multi-Component Diffusion Problem

```
Line Command
    NAB(:,1)=[2.396e-5; 3.363e-4];
    disp([y0 ODEfun(tspan(1),y0,NAB(1,1),NAB(2,1))]);
    err=1;
    it=0;
    while (err>1e-10) & (it<20)
        it=it+1;
        itno(it)=it;
        [t,y]=ode45(@ODEfun,tspan,y0,[],NAB(1,it),NAB(2,it));
        f(:,it)=[y(end,1); y(end,2)-2.701e-3];
        err=sqrt(f(:,it)'*f(:,it));
        for j=1:2
            delj=abs(NAB(j,it))*0.01;
            NAB(j,it)=NAB(j,it)+delj;
            [t,yp]=ode45(@ODEfun,tspan,y0,[],NAB(1,it),NAB(2,it));
            fp=[yp(end,1); yp(end,2)-2.701e-3];
            for k=1:2
                    DF(k,j)=(fp(k)-f(k,it))/delj;
            end
            NAB(j,it)=NAB(j,it)-delj;
        end
        NAB(:,it+1)=NAB(:,it)-inv(DF)*f(:,it);
        end
        disp(' Iter. No. NA NB f1 f2 ');
        disp([itno' NAB(1,1:it)' NAB(2,1:it)' f(1,:)' f(2,:'']);
```

Table 6. Shooting Method Iterations for $N_{A}$ and $N_{B}$

| Iter. No. | $\boldsymbol{N}_{\boldsymbol{A}}$ | $\boldsymbol{N}_{\boldsymbol{B}}$ | $\boldsymbol{f}_{\mathbf{1}}$ | $\boldsymbol{f}_{\mathbf{2}}$ |
| :---: | :---: | :---: | :---: | :---: |
| $\mathbf{0}$ | $2.3960 \mathrm{E}-05$ | $3.3630 \mathrm{E}-04$ | $3.35 \mathrm{E}-05$ | $-5.99 \mathrm{E}-03$ |
| $\mathbf{1}$ | $2.2076 \mathrm{E}-05$ | $-1.7614 \mathrm{E}-04$ | $7.53 \mathrm{E}-06$ | $-1.40 \mathrm{E}-03$ |
| $\mathbf{2}$ | $2.1252 \mathrm{E}-05$ | $-3.8575 \mathrm{E}-04$ | $8.52 \mathrm{E}-07$ | $-1.49 \mathrm{E}-04$ |
| $\mathbf{3}$ | $2.1150 \mathrm{E}-05$ | $-4.1375 \mathrm{E}-04$ | $1.77 \mathrm{E}-08$ | $-2.56 \mathrm{E}-06$ |
| $\mathbf{4}$ | $2.1149 \mathrm{E}-05$ | $-4.1424 \mathrm{E}-04$ | $7.05 \mathrm{E}-11$ | $-6.41 \mathrm{E}-09$ |
| $\mathbf{5}$ | $2.1149 \mathrm{E}-05$ | $-4.1425 \mathrm{E}-04$ | $1.67 \mathrm{E}-13$ | $-1.43 \mathrm{E}-11$ |

Table 7. Polymath Inputs for Carrying Out the First Jacobi and Gauss-Seidel Iterations for the Steady State Heat Conduction Problem

| Line | Jacobi | Gauss-Seidel |
| :---: | :---: | :---: |
| 1 | $\mathrm{T} 12=(300+\mathrm{T} 22 \mathrm{i}+600+\mathrm{T} 22 \mathrm{i}) / 4$ | $\mathrm{T} 12=(300+\mathrm{T} 22 \mathrm{i}+600+\mathrm{T} 22 \mathrm{i}) / 4$ |
| 2 | $\mathrm{T} 22=(300+\mathrm{T} 12 \mathrm{i}+600+\mathrm{T} 32 \mathrm{i}) / 4$ | $\mathrm{T} 22=(300+\mathrm{T} 12+600+\mathrm{T} 32 \mathrm{i}) / 4$ |
| 3 | $\mathrm{T} 32=(300+\mathrm{T} 22 \mathrm{i}+\mathrm{T} 33 \mathrm{i}+\mathrm{T} 42 \mathrm{i}) / 4$ | $\mathrm{T} 32=(300+\mathrm{T} 22+\mathrm{T} 33 \mathrm{i}+\mathrm{T} 42 \mathrm{i}) / 4$ |
| 4 | $\mathrm{T} 42=(300+\mathrm{T} 32 \mathrm{i}+\mathrm{T} 43 \mathrm{i}+300) / 4$ | $\mathrm{T} 42=(300+\mathrm{T} 32+\mathrm{T} 43 \mathrm{i}+300) / 4$ |
| 5 | $\mathrm{T} 33=(\mathrm{T} 32 \mathrm{i}+600+\mathrm{T} 34 \mathrm{i}+\mathrm{T} 43) / 4$ | $\mathrm{T} 33=(\mathrm{T} 32+600+\mathrm{T} 34 \mathrm{i}+\mathrm{T} 43 \mathrm{i}) / 4$ |
| 6 | $\mathrm{T} 43=(\mathrm{T} 42 \mathrm{i}+\mathrm{T} 33 \mathrm{i}+\mathrm{T} 44 \mathrm{i}+300) / 4$ | $\mathrm{T} 43=(\mathrm{T} 42+\mathrm{T} 33+\mathrm{T} 44 \mathrm{i}+300) / 4$ |
| 7 | $\mathrm{T} 34=(\mathrm{T} 33 \mathrm{i}+600+\mathrm{T} 35 \mathrm{i}+\mathrm{T} 44 \mathrm{i}) / 4$ | $\mathrm{T} 34=(\mathrm{T} 33+600+\mathrm{T} 35 \mathrm{i}+\mathrm{T} 44 \mathrm{i}) / 4$ |
| 8 | $\mathrm{T} 44=(\mathrm{T} 43 \mathrm{i}+\mathrm{T} 34 \mathrm{i}+\mathrm{T} 45 \mathrm{i}+300) / 4$ | $\mathrm{T} 44=(\mathrm{T} 43+\mathrm{T} 34+\mathrm{T} 45 \mathrm{i}+300) / 4$ |
| 9 | $\mathrm{T} 35=(\mathrm{T} 34 \mathrm{i}+600+\mathrm{T} 34 \mathrm{i}+\mathrm{T} 45 \mathrm{i}) / 4$ | $\mathrm{T} 35=(\mathrm{T} 34+600+\mathrm{T} 34+\mathrm{T} 45 \mathrm{i}) / 4$ |
| 10 | $\mathrm{T} 45=(\mathrm{T} 44 \mathrm{i}+\mathrm{T} 35+\mathrm{T} 44 \mathrm{i}+300) / 4$ | $\mathrm{T} 45=(\mathrm{T} 44+\mathrm{T} 35+\mathrm{T} 44+300) / 4$ |
| 11 | $\mathrm{T} 12 \mathrm{i}=450$ | $\mathrm{T} 12 \mathrm{i}=450$ |
| 12 | $\mathrm{T} 22 \mathrm{i}=400$ | $\mathrm{T} 22 \mathrm{i}=400$ |
| 13 | T32i $=400$ | T32i $=400$ |
| 14 | $\mathrm{T} 42 \mathrm{i}=325$ | $\mathrm{T} 42 \mathrm{i}=325$ |
| 15 | $\mathrm{T} 33 \mathrm{i}=400$ | $\mathrm{T} 33 \mathrm{i}=400$ |
| 16 | $\mathrm{T} 43 \mathrm{i}=350$ | $\mathrm{T} 43 \mathrm{i}=350$ |
| 17 | $\mathrm{T} 34 \mathrm{i}=450$ | $\mathrm{T} 34 \mathrm{i}=450$ |
| 18 | $\mathrm{T} 44 \mathrm{i}=375$ | $\mathrm{T} 44 \mathrm{i}=375$ |
| 19 | $\mathrm{T} 35 \mathrm{i}=500$ | $\mathrm{T} 35 \mathrm{i}=500$ |
| 20 | $\mathrm{T} 45 \mathrm{i}=400$ | $\mathrm{T} 45 \mathrm{i}=400$ |
| 21 | err12=(T12-T12i)^2 | err12=(T12-T12i)^2 |
| 22 | err22=(T22-T22i)^2 | err22=(T22-T22i)^2 |
| 23 | err32=(T32-T32i)^2 | err32=(T32-T32i)^2 |
| 24 | err42=(T42-T42i)^2 | err42=(T42-T42i)^2 |
| 25 | err33=(T33-T33i)^2 | err33=(T33-T33i)^2 |
| 26 | err43=(T43-T43i)^2 | err43=(T43-T43i)^2 |
| 27 | err34=(T34-T34i)^2 | err34=(T34-T34i)^2 |
| 28 | err44=(T44-T44i)^2 | err44=(T44-T44i)^2 |
| 29 | err35=(T35-T35i)^2 | err35=(T35-T35i)^2 |
| 30 | err45=(T45-T45i)^2 | err45=(T45-T45i)^2 |

Table 8．Jacobi Method Iterations for the Steady State Heat Conduction Problem

| Iter．No． | 0 | 1 | 2 | 3 | 4 | 5 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| T12 | 450 | 425 | 443.75 | 435.1563 | 440.625 | 438.5986 |
| T22 | 400 | 437.5 | 420.3125 | 431.25 | 427.1973 | 430.3192 |
| T32 | 400 | 356.25 | 381.25 | 373.6328 | 380.6519 | 378.8734 |
| T42 | 325 | 337.5 | 326.5625 | 336.7188 | 333.9844 | 337.1704 |
| T33 | 400 | 450 | 447.6563 | 454.6387 | 454.3121 | 456.8563 |
| T43 | 350 | 350 | 365.625 | 362.3047 | 368.0298 | 367.1471 |
| T34 | 450 | 468.75 | 475 | 475.5859 | 479.6265 | 479.554 |
| T44 | 375 | 375 | 375 | 380.7617 | 380.2917 | 383.485 |
| T35 | 500 | 475 | 479.6875 | 483.1055 | 483.6121 | 486.3842 |
| T45 | 400 | 381.25 | 382.4219 | 383.2764 | 386.2839 | 386.7419 |
| err12 |  | 625 | 351.5625 | 73.85254 | 29.90723 | 4.106164 |
| err22 |  | 1406.25 | 295.4102 | 119.6289 | 16.42466 | 9.746561 |
| err32 |  | 1914.063 | 625 | 58.02155 | 49.26696 | 3.162749 |
| err42 |  | 156.25 | 119.6289 | 103.1494 | 7.476807 | 10.15082 |
| err33 |  | 2500 | 5.493164 | 48.75422 | 0.106627 | 6.473016 |
| err43 |  | 0 | 244.1406 | 11.02448 | 32.77674 | 0.779196 |
| err34 |  | 351.5625 | 39.0625 | 0.343323 | 16.32586 | 0.005253 |
| err44 |  | 0 | 0 | 33.1974 | 0.220872 | 10.19706 |
| err35 |  | 625 | 21.97266 | 11.68251 | 0.256635 | 7.684763 |
| err45 |  | 351.5625 | 1.373291 | 0.730157 | 9.0451 | 0.20981 |
| $\underline{\left\\|\mathbf{x}_{k}-\mathbf{x}_{k-1}\right\\|}$ |  | 89.04879 | 41.27522 | 21.45657 | 12.72036 | 7.24675 |

Table 9．Data for the Multiple Linear Regression Example（Woods et al． 1 above ${ }^{7]}$ ）

| No． | $\mathbf{x}_{\mathbf{1}}$ | $\mathbf{x}_{\mathbf{2}}$ | $\mathbf{x}_{\mathbf{3}}$ | $\mathbf{x}_{\mathbf{4}}$ | $\mathbf{y}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 7 | 26 | 6 | 60 | 78.7 |
| 2 | 1 | 29 | 15 | 52 | 74.3 |
| 3 | 11 | 56 | 8 | 20 | 104.3 |
| 4 | 11 | 31 | 8 | 47 | 87.6 |
| 5 | 7 | 52 | 6 | 33 | 95.9 |
| 6 | 11 | 55 | 9 | 22 | 109.2 |
| 7 | 3 | 71 | 17 | 6 | 102.7 |
| 8 | 1 | 31 | 22 | 44 | 72.5 |
| 9 | 2 | 54 | 18 | 22 | 93.1 |
| 10 | 21 | 47 | 4 | 26 | 115.9 |
| 11 | 1 | 40 | 23 | 34 | 83.8 |
| 12 | 11 | 66 | 9 | 12 | 113.3 |
| 13 | 10 | 68 | 8 | 12 | 109.4 |

Table 10. Results of the Multiple Linear Regression Example

|  | Non-zero Intercept |  |  | Zero Intercept |  |
| :--- | ---: | :---: | :---: | :---: | :---: |
| Variable | Value | $\mathbf{9 5 \%}$ confidence | Value | 95\% confidence |  |
| $\hat{\beta}_{0}$ | 60.899 | 161.62 | - | - |  |
| $\hat{\beta}_{1}$ | 1.563 | 1.72 | 2.189 | 0.42 |  |
| $\hat{\beta}_{2}$ | 0.527 | 1.67 | 1.154 | 0.11 |  |
| $\hat{\beta}_{3}$ |  |  |  |  |  |
| $\hat{\beta}_{4}$ | 0.113 | 1.74 | 0.753 | 0.36 |  |
| $\mathbf{R}^{2}$ | -0.127 | 1.64 | 0.489 | 0.09 |  |
| Variance | 0.98 |  | 0.98 |  |  |
| Max. eigenvalue | 40402.00 |  | 5.82 |  |  |
| Min. eigenvalue | 0.0011 |  | 40402.00 |  |  |
| Condition number | $3.64 \mathrm{E}+07$ |  | 101.35 |  |  |



Figure 1 - Cross section of hollow chamber with square grid pattern for Example 2 (from Geankoplis ${ }^{[4]}$ )


Figure 2 - Residual Plot for the "Heat of Hardening" Example 3

