THE USE OF LOTUS 1-2-3 MACROS IN ENGINEERING CALCULATIONS

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There is a growing recognition of the potential usefulness of spreadsheet programs throughout the chemical engineering curriculum. This has been confirmed by the Education and Accreditation Committee of AIChE in its listing of the CACHE Corporation's recommendation of "Desired Computer Skills for Chemical Engineering Graduates" [1]. One of the desired skills is the use of the spreadsheet.

For educational use, the spreadsheet provides some appealing features:

- The student must have a complete understanding of the problem. He does not use a "canned" program which may hide the solution method.
- The spreadsheet allows the student to view the problem's solution directly without the need to print out iterations or look at an output file.
- The spreadsheet facility is generally available when other computational facilities may not be.

For industrial users, the spreadsheet is also of considerable interest:

- The user can use one system for a variety of problems. He need not learn multiple systems to carry out his job.
- There is a certain level of integration the user of the spreadsheet program can achieve by reading files from and sending files to other programs.

The use of the spreadsheet in chemical engineering calculations has been recently reviewed [2]. However, the use of macros was not indicated. Such macros extend the usefulness of the spreadsheet into a variety of applications which would be quite improbable without them. In this discussion, the macros of the popular spreadsheet program LOTUS 1-2-3 [3] will be used (Version 2.01).

MACROS

Macros were originally intended to simply allow the user to store a series of keystrokes so that they wouldn't have to be reentered in routine applications. Macros, however, allow programming in a broader sense. The early version of LOTUS 1-2-3 macros (/X commands) were difficult to use and to follow. However, with Release 2 the Advanced Macro Commands have become available. These are named in such a way as to be much more understandable, and one can follow a listing with comparative ease.

One of the limitations of the standard worksheet is that it doesn't allow for the use of "loop within loop" calculations which arise so often in chemical engineering. However, with macros, this limitation is removed and the capability to use subroutines, much as in FORTRAN, is possible.

A related limitation of the standard spreadsheet is the inability to jump to an arbitrary location as a result of a conditional evaluation. With macros, this is not only possible but also invaluable.

Since learning the macro language takes time and effort, it is fair to ask whether it is worthwhile to learn macros—especially if a calculation can be carried out in another way, say by using FORTRAN or BASIC. The answer certainly depends on system availability, accessibility, familiarity, and the time available for solution. However, it is worthwhile to note that the advanced macro capability of LOTUS 1-2-3 can be made useful with about one day's effort.
SUBROUTINES

There are differences in using subroutines in LOTUS 1-2-3 as compared to FORTRAN. The first is the ability in LOTUS 1-2-3 to address and manipulate any cell in the spreadsheet whether or not it is passed as an argument to the subroutine. Results from the subroutine cannot be placed in a relative location (i.e., the address cannot be passed on output). Instead the output must be picked up from locations designated by the subroutine.

These comments are illustrated in Figure 1 which shows the coding for a general purpose subroutine, ROOTX, based on Wegstein’s method [4] for solving a one dimensional equation in the form

\[ f(x) = x \]  

The subroutine operates in two modes. If ‘code’ (cell P6) is set to 0, then the working cells (P7 to P16) are cleared, and control is returned to the calling routine. If ‘code’ is set to 1, then ROOTX will return a new x for each pair of values x and f(x) supplied as arguments which are passed to cells P4 and P5 using the DEFINE keyword. Note that the upper and lower bounds on the slope in Wegstein’s method are set in cells P1 and P2.

The calling program is given in the macro \( \text{q} \). It is set up to solve either of two problems determined by cell H1 (Problem Selection). The arguments passed to the subroutine, H3, x, and H4, f(x), are specified in the call to the subroutine, i.e., \{ROOTX H3,H4\}. The new value of x generated by ROOTX is picked up from location P4 and passed to location H3 with the macro command \{LET H3,P4\}. The convergence criterion is given in the calling program and can be problem dependent.

\[
\begin{align*}
P1: & \quad \text{upper} \quad 0.8 \\
P2: & \quad \text{lower} \quad -9 \\
P3: & \quad x \quad 409.9927 \\
P4: & \quad f(x) \quad 409.9927 \\
P5: & \quad \text{code} \quad 1 \\
P7: & \quad \text{counter} \quad 4 \\
P8: & \quad x1 \quad 409.3356 \\
P9: & \quad f1 \quad 4.10 \times 10^{-9} \\
P10: & \quad x2 \quad 409.9942 \\
P11: & \quad f2 \quad 409.9927 \\
P12: & \quad \text{slope} \quad -0.01 \times 10^{0} \\
P13: & \quad \text{t} \quad 0.998153 \\
P14: & \quad \text{delta} \quad -0.00151 \\
P15: & \quad \text{total} \quad 0.683556 \\
P16: & \quad \text{done} \quad 0.683556 \\
\end{align*}
\]

\[
\begin{align*}
P21: & \quad \text{ROOTX (DEFINE P4:VALUE,P5:VALUE)} \\
P22: & \quad \text{CALC} \\
P23: & \quad \{\text{IF P7=0}(\text{BRANCH P25}) \} \\
P24: & \quad \{\text{BRANCH P37} \} \\
P25: & \quad \{\text{IF P7<0.5}-,0.5-\} \\
P26: & \quad \{\text{RETURN} \} \\
P27: & \quad \{\text{LET P7,P7+1} \} \\
P28: & \quad \{\text{LET P9,P10} \} \\
P29: & \quad \{\text{LET P5,P9} \} \\
P30: & \quad \{\text{LET P10,P4} \} \\
P31: & \quad \{\text{LET P11,P5} \} \\
P32: & \quad \{\text{LET P15,ABS(P10-P8)} \} \\
P33: & \quad \{\text{IF P15<0}(\text{BRANCH P38}) \} \\
P34: & \quad \{\text{LET P16,P7} \} \\
P35: & \quad \{\text{BRANCH P37} \} \\
P36: & \quad \{\text{LET P6,P10-P8} \} \\
P37: & \quad \{\text{LET P12,P12+P10} \} \\
P38: & \quad \{\text{LET P13,P13+P11-P10} \} \\
P39: & \quad \{\text{LET P15,P13+P11-P10} \} \\
P40: & \quad \{\text{LET P4,P4+H14} \} \\
P41: & \quad \{\text{IF P7>1}(\text{LET P4,P5}) \} \\
P42: & \quad \{\text{RETURN} \} \\
\end{align*}
\]

FIGURE 1. Use of subroutine ROOTX in Macro q.
Depending on the problem specification given by HI(1 or 2) the macros EVAL or EVAL1 are used to evaluate \( f(x) \). Problem 1 (EVAL) is taken from Myers and Seider [5] in which the value of \( v \) is sought in the van der Waals equation in the form \( v = f(v) \). Problem 2 is taken from Reklaitis [6] in which a temperature is sought in an equation in the form \( T = f(T) \). The solutions found in each case agree with those given by the authors. Note that in each case (EVAL and EVAL1) the value of \( H_4, f(x) \), is calculated from the value of \( H_3, x \).

**PARTIAL DIFFERENTIAL EQUATIONS**

The use of the spreadsheet to solve the steady state Laplace equation in two dimensions and the simple parabolic equation in one dimension and time was discussed in [2]. In each of these cases the problem could be set up in a single two dimensional table and solved by an appropriate finite difference formulation using the standard spreadsheet. However, this is not possible in the following case.

Consider heat transfer in a cylinder of radius \( a \) and height \( L \):

\[
\rho c \frac{\partial T}{\partial \theta} = k \left( \frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial z^2} \right)
\]

where
- \( \rho \) = density
- \( c \) = heat capacity
- \( k \) = thermal conductivity
- \( T \) = temperature
- \( R \) = radial coordinate
- \( Z \) = height coordinate
- \( \theta \) = time

with boundary conditions

\[
\begin{align*}
\text{at } \theta = 0 & : T = T_i \text{ at } 0 < R < a \text{ and } 0 < Z < L \\
\text{at } \theta = \pi & : T = T_w \text{ at } R = 1 \text{ and } Z = 0 \text{ and } Z = L
\end{align*}
\]

In order to put Eq. (2) into dimensionless form, let

\[
r = \frac{R}{a}, \quad z = \frac{Z}{a}, \quad u = \frac{T - T_i}{T_w - T_i}, \quad \theta = \frac{k}{\rho c} \quad \text{where } \omega = \frac{k}{\rho c}
\]

Then

\[
\frac{\partial u}{\partial \theta} = \left( \frac{1}{r} \frac{\partial u}{\partial r} + \frac{\partial^2 u}{\partial r^2} + \frac{\partial^2 u}{\partial z^2} \right)
\]

with boundary conditions

\[
\begin{align*}
\text{at } t = 0 & : u = 0 \text{ at } 0 < r < 1 \text{ and } 0 < z < L/a \\
\text{at } t \geq 0 & : u = 1 \text{ at } r = 1 \text{ and } z = 0 \text{ and } z = L/a
\end{align*}
\]

Eq. (4) may be solved by finite differences using the stable Crank-Nicolson method [7,8]. Let

\[
\begin{align*}
i & = \text{index in the } r \text{ direction} \\
j & = \text{index in the } z \text{ direction} \\
n & = \text{index in time } t
\end{align*}
\]

Then using finite difference approximations

\[
\begin{align*}
\frac{\partial^2 u}{\partial r^2} & \approx 0.5 \left( \frac{u_{i+1,j,n} - 2u_{i,j,n} + u_{i-1,j,n}}{(\Delta r)^2} \right) \\
\frac{\partial^2 u}{\partial z^2} & \approx 0.5 \left( \frac{u_{i,j+1,n} - 2u_{i,j,n} + u_{i,j-1,n}}{(\Delta z)^2} \right)
\end{align*}
\]

Substituting these approximations into Eq. (4) and solving for \( u_{i,j,n+1} \) there results

\[
u_{i,j,n+1} = \frac{1}{A - \frac{B}{i}} \left( \frac{(D + B/i)u_{i,j,n} + (B - B/i)(u_{i-1,j,n} + u_{i+1,j,n})}{A} + B(u_{i,j+1,n} + u_{i,j-1,n}) + C(u_{i,j-1,n} + u_{i,j,n} + u_{i,j+1,n}) \right)
\]

where

\[
\begin{align*}
A & = \frac{1}{\Delta t} + \frac{1}{(\Delta r)^2} + \frac{1}{(\Delta z)^2} \\
B & = \frac{1}{2(\Delta r)^2} \\
C & = \frac{1}{2(\Delta z)^2} \\
D & = \frac{1}{\Delta t} - \frac{1}{(\Delta r)^2} - \frac{1}{(\Delta z)^3}
\end{align*}
\]

Eq. (5) allows the computation of \( u \) at time \( n + 1 \) from the values at time \( n \). This permits the following scheme:

1. Set up a table to store the values of \( u \) at time \( n \). Initially this will be all zeros, except at the boundaries. Call this table the Storage Table (C100..AC125). It is shown in Figure 2 with the cells labeled.
Figure 2. Spreadsheet solution to Eq. (4) using Macro \( \lambda \).

Storage table after 50 iterations.

Center Line

| TIME HRS | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 |
|----------|---|---|---|---|---|---|---|---|---|---|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 00/1997  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 |
| 01/1998  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 |
| 02/1998  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 |
| 03/1998  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 |

S P R I N G 1 9 9 0  

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2. Set up a second table (the Calculate Table, C200..AC225) which will calculate the values of \( u \) at time \( n+1 \) from the formula of Eq. (5). Since the value of \( u_{ij,n+1} \) depends on the values at \( n+1 \) as well as at \( n \), iterate until convergence (say at least twelve iterations). The cells are labeled together with the cells for the Storage Table.

Figure 2 illustrates the spreadsheet setup for a cylinder of radius 0.5 meters and a height of 1 meter with the following physical properties:

\[
\begin{align*}
\rho &= 1000 \text{ kg/m}^3, & \text{density} \\
k &= 0.15 \text{ watts/(m deg C)}, & \text{thermal conductivity} \\
c &= 2500 \text{ J/(kg deg C)}, & \text{heat capacity}
\end{align*}
\]

The increments chosen (based on a table of 25 cells by 25 cells) were

\[
\begin{align*}
\Delta r &= 0.04 \\
\Delta z &= 0.04 \times \text{Height/Radius} = 0.08 \\
\Delta t &= 0.001
\end{align*}
\]

The macro \( \backslash \text{a} \) is set to run in two modes. If E4 is set to 1, then the tables are both set to zero (the Calculate Table is set to zero by having E93 set to zero as shown in the commands for cells D201 and E201) and the boundary values are set to 1. If E4 is set to 2, then the macro allows the Calculate Table to be generated from the Storage Table. The values are copied from the Calculate Table to the Storage Table after the temperatures at time \( n+1 \) are determined and the process is repeated until a fixed number of steps (i.e., time) is taken or a particular temperature is exceeded. The macro uses columns AY and AZ to record time and temperature at the location \( \alpha/2 \) and \( L/2 \). The results are shown in Figure 2. The computation stopped after 50 time steps (57.87 hrs) which was reached before the specified target temperature. Each of the time steps takes about 45 seconds on a Vectra ES/12 (80286) with a math coprocessor (80287).

The Calculate Table was constructed by copying the contents of cell D201 to cells D202..D224 and the contents of cell E201 to E202..AB224. By symmetry the values of column C were set to those of column E.

Carslaw and Jaeger [8] give an analytical solution for this case:

\[
u = 1 - \frac{8}{\pi a} \sum_{k=0}^{\infty} \sum_{m=1}^{\infty} \frac{(-1)^k J_0(Ra_m)}{(2k+1)\alpha_m J_1(\alpha_m)} \cos\left(\frac{(2k+1)\pi x}{2h}\right) \exp\left(-\alpha_m^2 + \frac{(2k+1)^2 \pi^2}{4h^2}\right)
\]  

where

\[
\begin{align*}
\alpha_m &= \frac{L/2}{a} \\
-h < x < h
\end{align*}
\]

and \( \alpha_m \) is calculated from the roots of the zero\(^{th}\) order Bessel function \( J_0 \); i.e.,

\[
\begin{align*}
\alpha_1 &= (1\text{st root})/a \\
\alpha_2 &= (2\text{nd root})/a \\
&\vdots \\
\alpha_m &= (m\text{th root})/a
\end{align*}
\]

The upper limit on \( m \) was taken as 40 and the upper limit on \( k \) was 50. The first forty roots of the zero\(^{th}\) order Bessel function were taken from Jahnke and Emde [10].

Table 1 compares Eq. (6) to the spreadsheet solution at \( L/2 \) (\( x = 0 \)) at a number of values of \( R \). Since the spreadsheet solution is not given exactly at \( L/2 \), the average value of the surrounding cells at a given \( r \) was used. The table also gives values found when the time increment was reduced to 0.0005 and the values of the coordinate increments were \( \Delta r = 0.025 \) and \( \Delta z = 0.050 \).

Reducing the values of \( \Delta r \) and \( \Delta z \) (a 40 x 40 table) improved the accuracy somewhat, but cutting the value of \( \Delta t \) did not. Eq. (3) may be used to convert the dimensionless solution to the scaled solution sought. An error of 0.005 in \( u \) corresponds to an error in \( T \) of 0.5 deg C if \( (T_w - T_1) = 100 \).

**CONCLUSIONS**

Macros allow the use of the spreadsheet for a greater variety of problems than can be done without
them. The LOTUS 1-2-3 advanced macro commands are relatively easy to learn and apply. Their use should be considered.

REFERENCES


REVIEW: Aerosols and Hydrosols

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In the third chapter, the author focuses on procedures for modeling granular media in filters. Rather than utilizing a "black box" approach to describe the filter (inherent in the methods described in Chapter Two) in order to determine concentration histories and pressure drops, the specifications of the collector's structure, geometry, size, size distribution, and the fluid flow fields around the particles are considered.

In Chapter Four, a variety of mechanisms for the deposition of particles on collectors from flowing suspensions are discussed. Expressions for collection efficiencies for these various deposition mechanisms are derived, utilizing the media modeling methods described in Chapter Three.

In the fifth chapter, the author illustrates that trajectory analysis, along with the media models described in the third chapter, can be used to estimate filtration rates. Because of complexities associated with representing fluid drag forces acting upon suspended particles and also representing particle surface geometry as deposition proceeds, the method of trajectory analysis is limited mainly to clean filters.

In Chapter Six we find that because of distinct differences in the particle deposition mechanisms, it becomes necessary for the author to depart from the integrated approach he has followed up to this point and to treat aerosols and hydrosols separately. In this chapter he focuses on prediction and measurement of initial collection efficiencies for the granular filtration of aerosols. Collection efficiencies are predicted using the trajectory analysis methods discussed in the fifth chapter. A variety of experimental methods for determining initial collection efficiencies are briefly discussed, and appropriate experimental results are provided. Empirical correlations and their relative merits are also discussed.

In the seventh chapter, the author describes the prediction of initial collection efficiencies for hydrosols using trajectory analysis. Results of these calculations are compared with experimental data. Limitations of the trajectory analysis approach and possibilities for improving it are discussed.

In Chapter Eight the author begins to look at the entire process of particle deposition, not just the initial stages which have been addressed up to this point. Dendrite growth of deposited particles and stochastic simulations of particle deposition are the focus of much of this chapter. The author points out that much of what is covered in this chapter is still in the developmental stage and, as such, is included to demonstrate general principles and the potential of the methods.

Finally, in Chapter Nine, the author focuses on a number of actual investigations (case studies) dealing with the granular filtration of aerosols and hydrosols. Topics discussed include filter ripening, effects of deposit morphology on filter performance, effects of deposition on aerosol filtration, aerosol deposition in fluidized filters, and the increase in hydrosol filter coefficient.

In summary, the author has done a nice job of writing about a sharply focused area of separations which, up to now, has been largely dealt with in scientific journals. A great deal of information has been brought together in a coherent, logical format. It is particularly useful because it tells you how to do things. The book is fairly easy to read, and the figures, graphs, and tables are clear and easy to understand. The author does not get bogged down in tedious mathematical derivation. That which is not shown directly is usually referenced adequately. The text is designed to bring someone who is interested in further work in the area "up to speed" in a reasonable period of time. The references are extensive and will be particularly helpful to anyone interested in the field. Since the subject matter of the book is admittedly narrow, it would only be useful as a course text or supplemental text for advanced, research oriented graduate courses.