

Appendix F

F.1 MICROSOFT EXCEL SOLVER FOR NON-LINEAR EQUATIONS

The *Solver* is an optimization package that finds a maximum, minimum, or specified value of a target cell by varying the values in one or several changing cells. It uses an iterative process, beginning with trial values of the coefficients. The value of each coefficient is changed by a suitable increment, the new value of the function is then calculated, and the change in the value of the function is used to calculate improved values for each of the coefficients. The process is repeated until the desired results are obtained. The *Solver* employs the gradient methods or the simplex method to find the optimum set of coefficients.

Constraints can be applied to the *Solver* using the Add button under the heading "Subject to the Constraints". The *Solver* is an Excel Add-in, a separate software package. To save memory, it may not automatically be opened whenever Excel is started. To install the *Solver*, choose Add-Ins from the Tools menu. Then select *Solver* Add-Ins from the resulting Add-Ins dialog box. Once the *Solver* feature has been installed, it will remain installed unless it is removed by reversing the above procedure.

To use the *Solver* to perform multiple non-linear least squares curve fitting, the procedure is as follows:

1. Start with a worksheet containing the data (independent variable X and the dependent variable Y_{obsd}) to be fitted.
2. Add a column containing Y_{calc} values, calculated by means of an appropriate formula, and involving the X -values and one or more coefficients to be varied.
3. Add a column to calculate the square of the residual ($Y_{\text{obsd}} - Y_{\text{calc}}$) for each data point.
4. Calculate the sum of squares of the residuals.
5. Use the *Solver* to minimize the sum of the squares of residuals (the target cell) by changing the coefficients of the function (the changing cells).

Since the *Solver* operates by a search routine, it will find a solution most rapidly and efficiently if the initial estimates that are provided are close to the final values. Conversely, it may not be able to find a solution if the initial estimates are far from the final values. To ensure that the *Solver* has found a global minimum rather than a local minimum, a solution is obtained using different sets of initial estimates.

The least-squares regression coefficients that are returned may be slightly different depending on the starting values being provided. The Excel spreadsheet prog6a.xls (Figures F-1a-f) uses the *Solver* to determine the outlet pressure P_2 of isothermal compressible fluid flow of Example 4-9 in the Chapter 4 of the book.

F.2 SOLVING EQUATIONS USING GOAL SEEK IN EXCEL

Microsoft Excel provides a built-in way to perform non-linear equations using the Goal Seek command in the Tools menu. Goal-Seek varies the value of a selected cell (the changing cell) to make the value of another cell (the target cell) reach a desired value. This feature permits rapid solutions of algebraic equations using iterative (i.e. trial and error) root-finding techniques based

on a series of successive refinements derived from an initial guess. For an adiabatic compressible fluid using the Excel spreadsheet (Example 4-11.xls) in Chapter 4 of the book, the implicit adiabatic equation in cell C53 is set to zero (Figures F-2a-f). The equation is expressed by

$$\frac{2}{Ma_1^2(\gamma+1)} \left[\left(\frac{\{\gamma+1\} Ma_1^2}{2 + \{\gamma-1\} Ma_1^2} \right)^{\frac{\gamma+1}{2}} - 1 \right] + 2 \ln \sqrt{\frac{2 + (\gamma-1) Ma_1^2}{(\gamma+1) Ma_1^2}} + K = 0 \quad (4-173)$$

The objective is to use Goal Seek to find the value of cell B44 that makes the function (in C53) equal to zero. The accuracy of the result depends on the magnitude of the Maximum Change parameter, which can be adjusted by choosing the Calculation tab in the Options command of the Tools menu. The default value is 0.001, and adjusting the Maximum Change parameter is critical when using Goal Seek. This allows Excel to stop iterating when the change in the result is less than the Maximum Change parameter. Therefore, the Maximum Change parameter needs to be adjusted to match the value of the function. For most calculations, the Maximum Change is set to 1E-12 or 1E-15.

The steps in using Goal Seek are as follows:

1. Select Goal Seek from the Tools menu as shown in Figure F-2a.
2. Enter \$C\$53 in the *Set cell* box.
3. Put the cursor in the *To value* box and enter the desired value, zero.
4. Put the cursor in the *By Changing cell* box and enter \$B\$44 by selecting the cell or by typing.
5. Then click on *OK* box.

After a few iteration cycles the *Status* dialog box Figure (F-2e) is displayed.

If a solution is obtained, the value of the root will appear in the cell originally containing the initial guess. The value in the cell containing the formula will show a value that is close to zero (or zero). This last value will appear within the Goal Seek status dialog box.

Cell \$B\$44 gives the root of the function cell (B44), which causes the target value to equal zero. The final value of the function depends to some extent on the starting value of Ma_1 . The likelihood of obtaining a converged solution will be enhanced, if the initial guess is as close as possible to the desired root.

For problems requiring the variation of two or more parameters, that is, varying the values of several cells to make the value of another cell reach a desired value involves the use of the *Solver*.

The Excel spreadsheet Prog6a.xls uses the Goal Seek routine to determine the friction factor of Colebrook-White implicit equation as defined by

$$F(f_D) = \frac{1}{f_D^{1/2}} + 0.8686 \ln \left\{ \frac{\varepsilon}{3.7D} + \frac{2.51}{Re \sqrt{f_D}} \right\} \quad (F-1)$$

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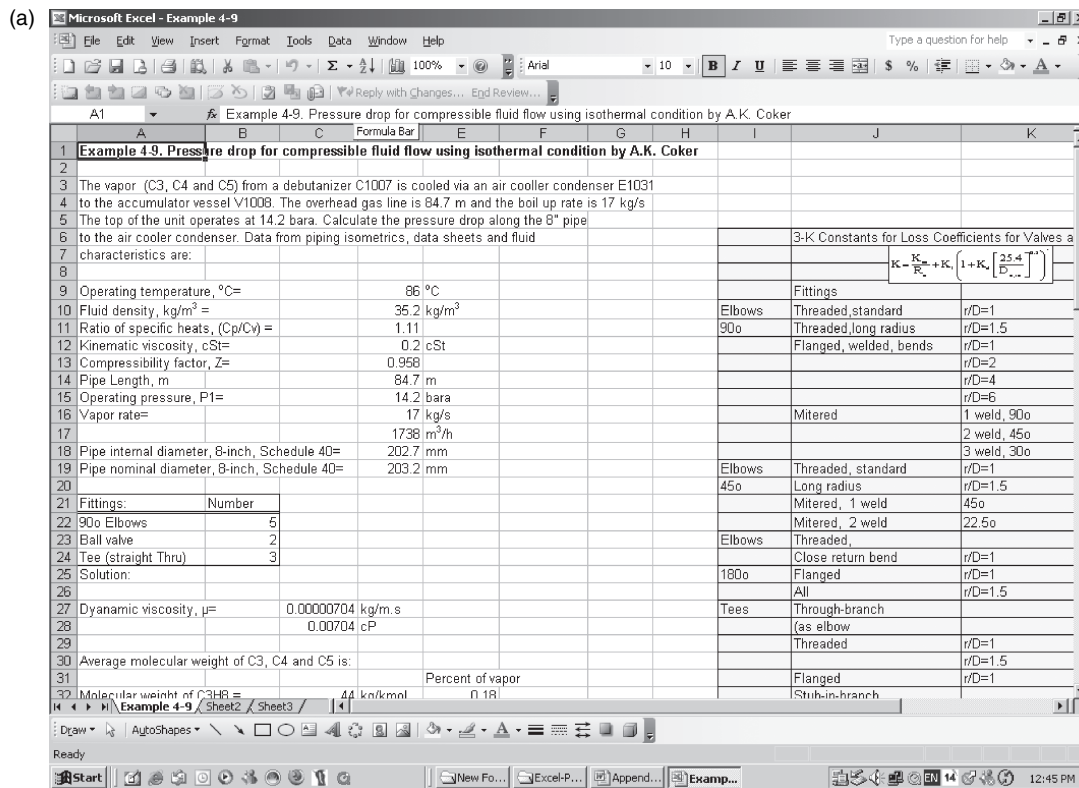


Figure F-1a Non-linear equation estimation using Solver from the tools menu of Microsoft Excel of Example 4.9.

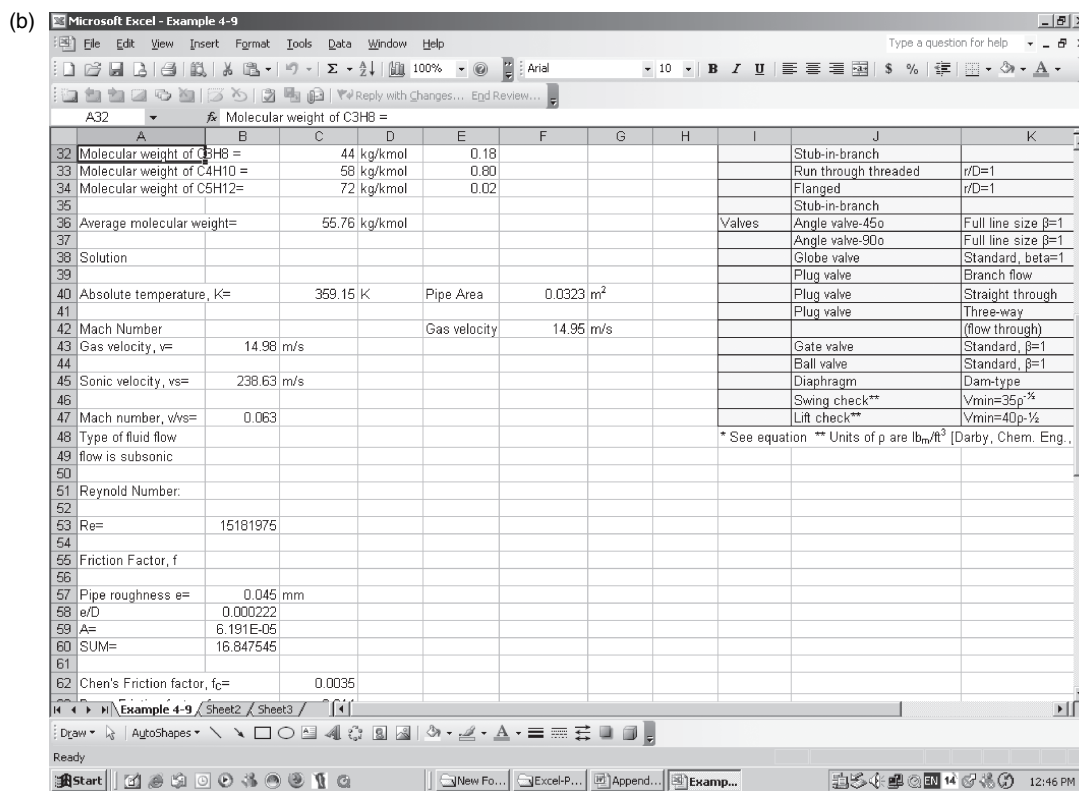


Figure F-1b—(continued).

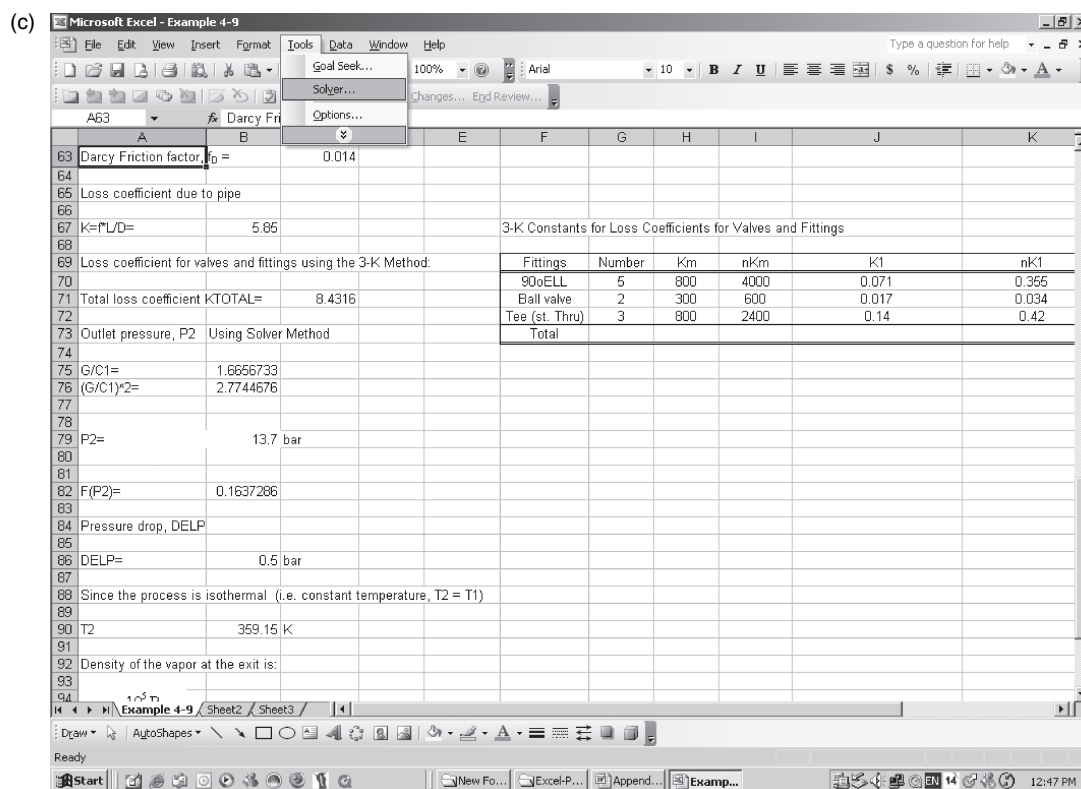


Figure F-1c—(continued).

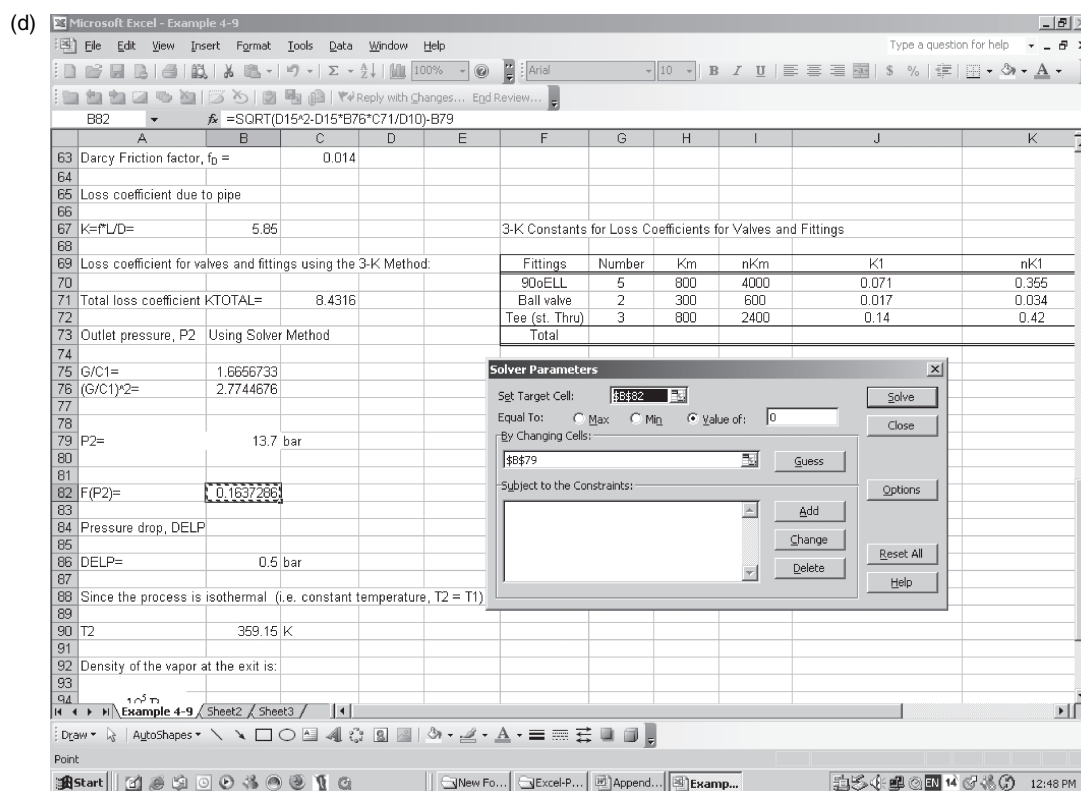


Figure F-1d—(continued).

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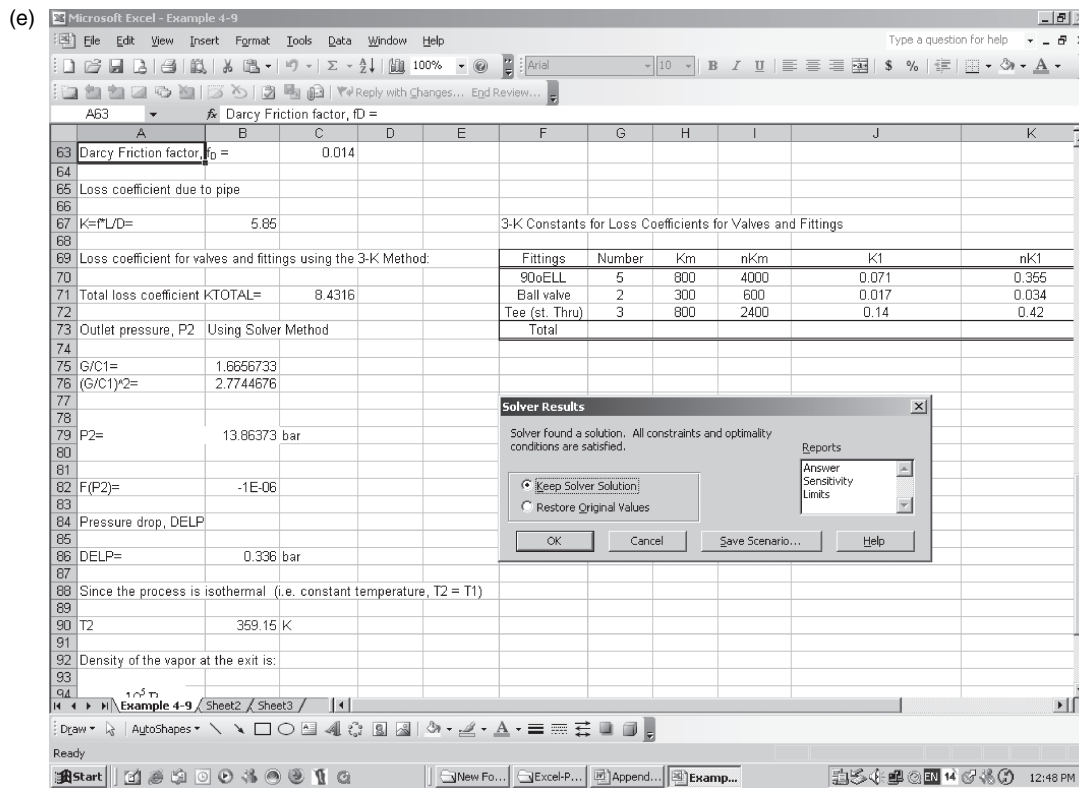


Figure F-1e—(continued).

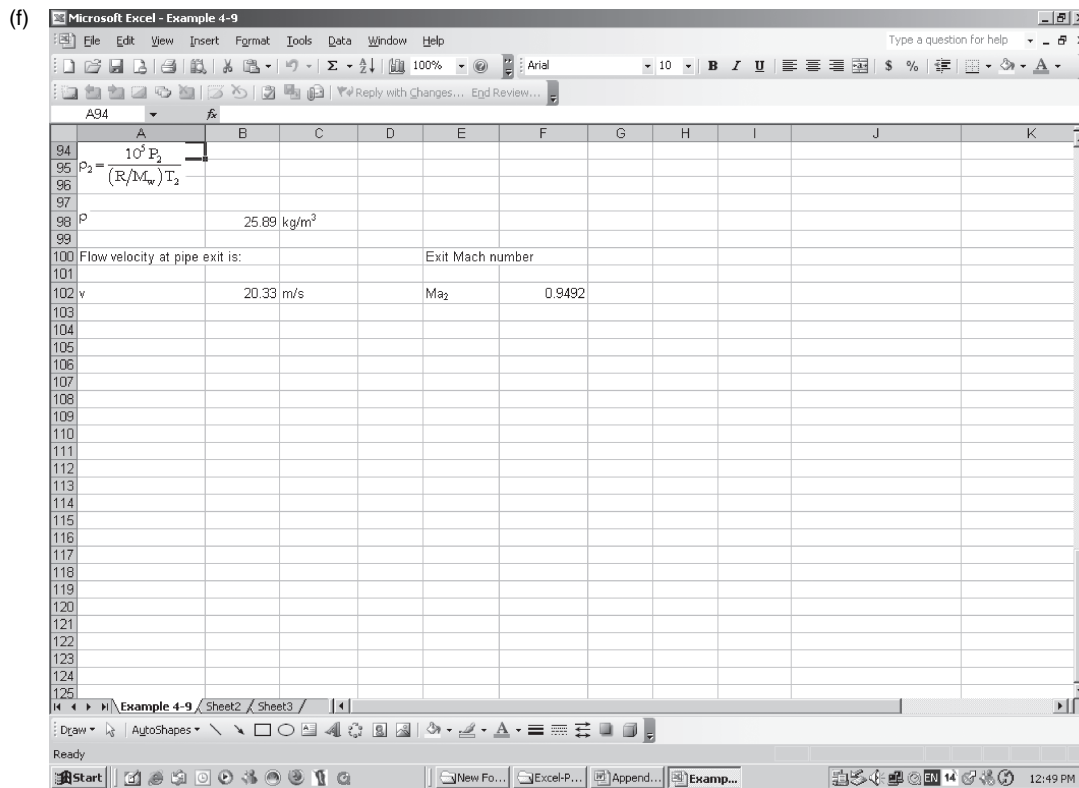


Figure F-1f—(continued).

(a) Microsoft Excel - Example 4-11

Example 4-11. Critical Flow of compressible fluid calculations by A.K. Coker

This is based upon Kumar's [68] method (Chem. Eng. Oct. 2002, p62) using thermodynamic principles to determine the status of flow (i.e. whether choking flow exists or not). This method removes the use of plots as generated in Crane Manual [3]. For an adiabatic compressible fluid flow.

$$\frac{2}{Ma_1^2(\gamma+1)} \left[\left(\frac{\gamma+1}{2+(\gamma-1)Ma_1^2} \right)^{\frac{\gamma+1}{2}} - 1 \right] + 2 \ln \sqrt{\frac{2+(\gamma-1)Ma_1^2}{(\gamma+1)Ma_1^2}} + K = 0 \quad (4-173)$$

$$r = \left(\frac{P_2}{P_0} \right)^\alpha = \frac{[0.5(\gamma+1)Ma_1^2]^{1/2}}{[1+0.5(\gamma-1)Ma_1^2]^{\frac{\gamma+1}{2(\gamma-1)}}} \quad (4-174)$$

$$Y_\alpha = \sqrt{\frac{K(1+r)}{2(K+2\ln[1/r])}} \quad (4-175)$$

$$W = 0.126D^2 Y_\alpha \sqrt{\frac{P_0 - P_2}{KV_0}} \quad (4-176)$$

Notations

D = Internal pipe diameter, mm.

K = Resistance or loss coefficient

L = Length of pipe, m.

Figure F-2a Solving implicit adiabatic compressible fluid flow equation of Example 4-11 using Goal Seek.

(b) Microsoft Excel - Example 4-11

PA =

27	$P_A =$	Ambient pressure, kPa abs
28	$P_0 =$	Stagnation upstream pressure, kPa abs
29	$P_1 =$	Pressure at inlet tip of the pipe, kPa abs
30	$P_2 =$	Pressure at outlet tip of the pipe, kPa abs
31	$Ma_1 =$	Mach number at inlet tip of the pipe
32	$Ma_2 =$	Mach number at outlet tip of the pipe
33	γ	Ratio of specific heat at constant pressure to specific heat at constant volume
34		at upstream conditions, dimensionless
35	$r =$	overall critical pressure ratio, dimensionless (P_2/P_0) _{cr}
36	$V_0 =$	Upstream specific volume, m^3/kg
37	$W =$	Mass flow rate, kg/h
38		
39	D	52.5 mm
40	P_A	200 kPaabs
41	P_1	6600 kPaabs
42	K	45
43	γ	1.55
44	Ma_1	0.12621
45	V_0	$0.01724 m^3/kg$
46	L	100 m
47		
48	Calculations	
49		
50	Using Goal Seek or Solver (from the Tools menu) by setting Eq. 4-173 = 0 (i.e. cell C53 = 0).	

Figure F-2b—(continued).

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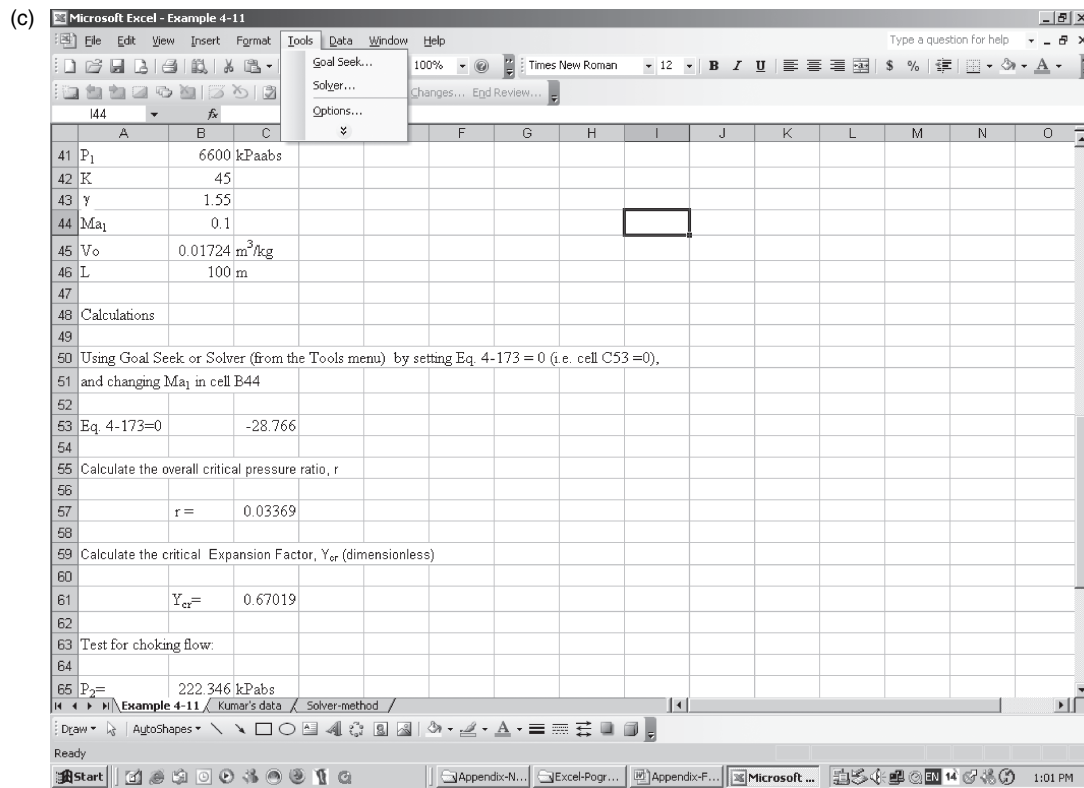


Figure F-2c—(continued).

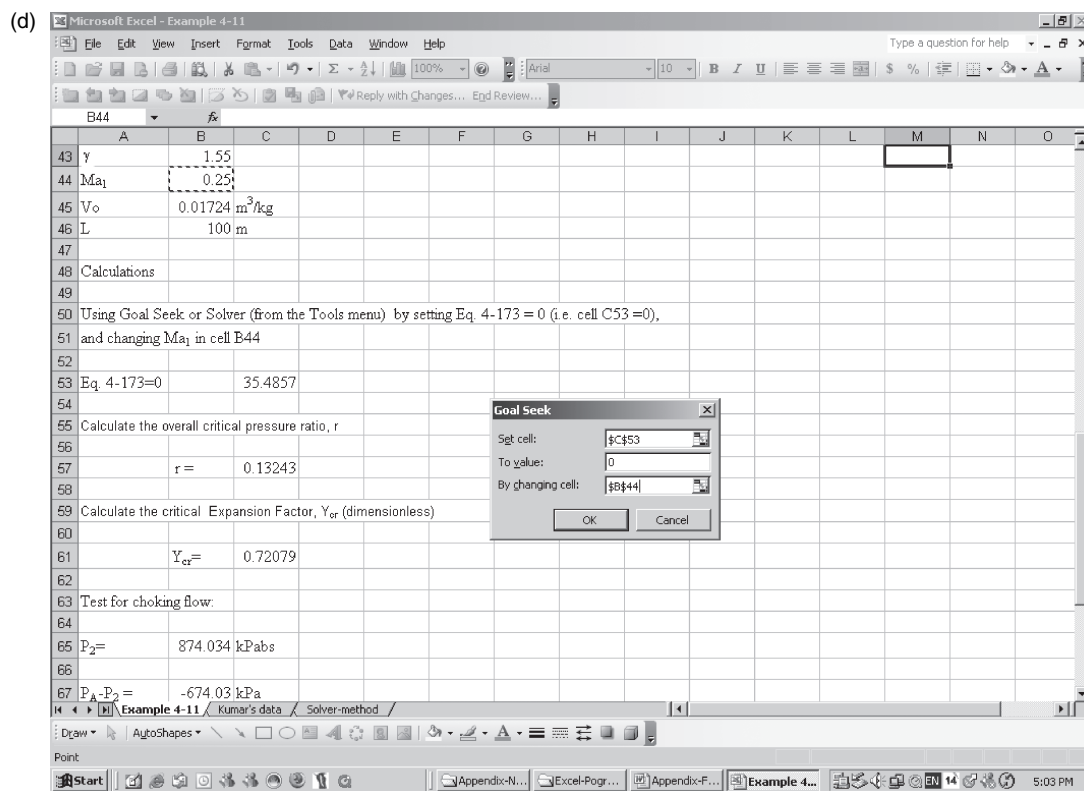


Figure F-2d—(continued).

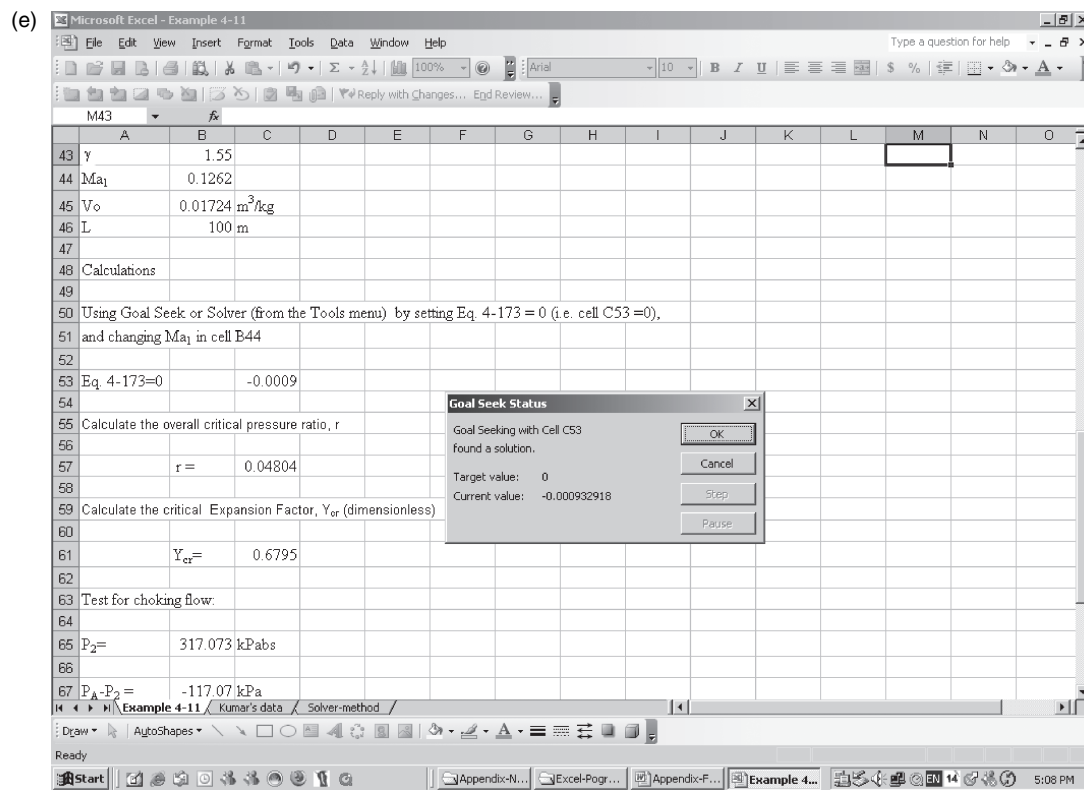


Figure F-2e—(continued).

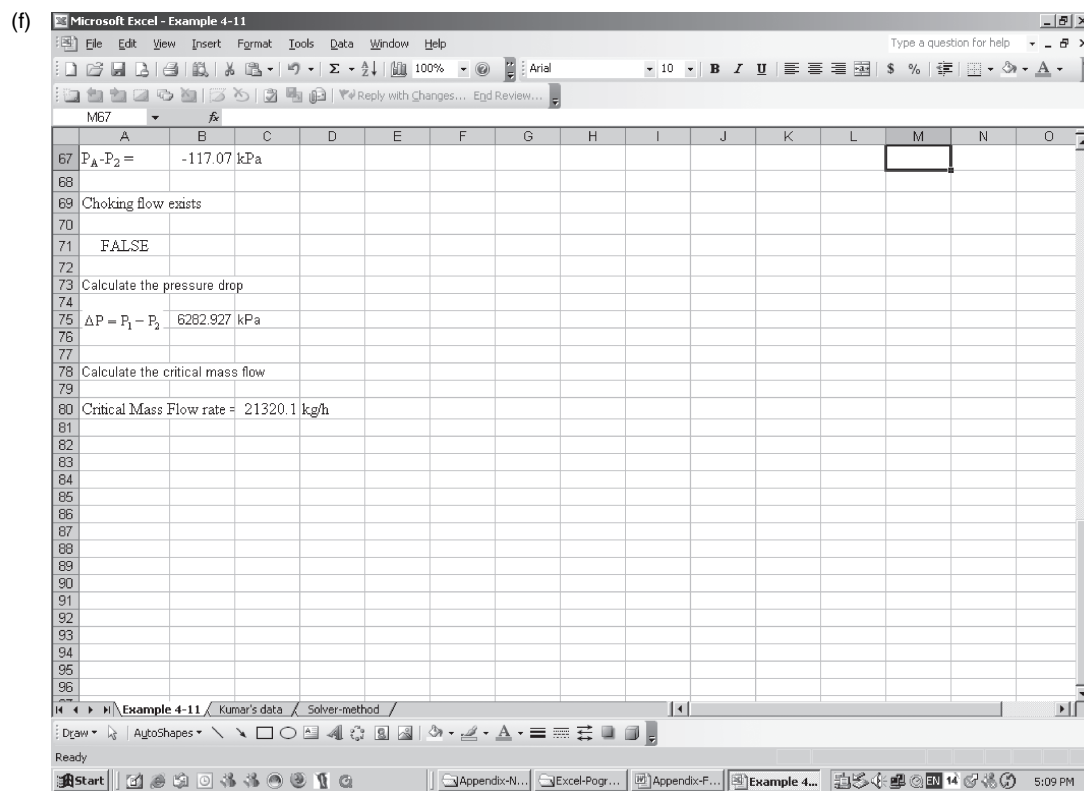


Figure F-2f—(continued).

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where

ε = Relative pipe roughness, in.

D = Pipe size, in.

f_D = Darcy friction factor

Re = number.

Re-arranging the friction factor equation in the form

$$F(f_D) = \frac{1}{f_D^{1/2}} + 0.8686 \ln \left\{ \frac{\varepsilon}{3.7D} + \frac{2.51}{Re \cdot f_D^{1/2}} \right\} \quad (\text{F-2})$$

The worksheet (Solution-1) in Excel spreadsheet program (Prog6a.xls) calculates the friction factor for given relative pipe roughness, pipe size, and Reynolds number. The Excel spreadsheet program Prog6a.xls and the Fortran program PROG6 show how the friction factor is determined. Table F-1 shows the computer results of a 2 in. (internal diameter=2.067 in.) stainless steel pipe size Sch 40, with pipe roughness of 0.0018 in. and Reynolds number of 184,000 (highly turbulent flow). The calculated friction factor $f = 0.02063$ with an initial guess of 0.015.

The worksheet (Solution-2) in Excel spreadsheet Prog6a.xls calculates the friction factor for flow of a suspension of fibrous particles to the Reynolds number given by an empirical equation of the form [5]:

$$\frac{1}{\sqrt{f}} = \left(\frac{1}{k} \right) \ln \left(Re \sqrt{f} \right) + \left(14.0 - \frac{5.6}{k} \right) \quad (\text{F-3})$$

where

f = friction factor

Re = Reynolds number

k = constant determined by the concentration of the suspension.

Re-arranging Eq. (F-3) gives

$$F(f) = \frac{1}{f^{1/2}} - \frac{1}{k} \ln \left(Re \cdot f^{1/2} \right) - 14.0 + \frac{5.6}{k} \quad (\text{F-4})$$

TABLE F-1 Newton-Raphson Method for a Non-Linear Equation

Initial Guess of the root $x = 0.0150$		
Iteration	x	$F(x)$
1	0.19423E-01	0.22078E+00
2	0.20577E-01	0.93463E-02
3	0.20630E-01	0.17983E-04
<i>Tolerance met in three iterations</i>		
Final root $x = 0.20630E-01$		
$F(x) = 0.17983E-04$		

FURTHER READING

1. Coker, A.K., *Fortran Programs For Chemical Process Design, Analysis and Simulation*, Gulf Publishing Co., Houston, TX, 1995.
2. Gottfield, B.S., *Spreadsheet Tools for Engineers Excel 5.0 Version*, The McGraw-Hill Co. Inc., 1996.
3. Billo, E.J., *Excel for Chemists - A Comprehensive Guide*, Wiley-VCH, Inc., 1997.
4. Gottfried, B.S., *Spreadsheet Tools for Engineers Excel 2000 Version*, McGraw-Hill's Best - Basic Engineering Series and Tools, 2000.
5. Lee and Duffy, "Relationships Between Velocity Profiles and Drag Reduction in Turbulent Fiber Suspension Flow", *AICHE J.*, 1976, pp. 750-753.