Example numerical techniques are also presented by Felder and Rousseau:

Felder, R.M., & R.W. Rousseau. (1986). *Elementary Principles of Chemical Processes*, 2nd ed. New York: Wiley.

The following book is more of an advanced undergraduate/first-year graduate student text on numerical methods to solve chemical engineering problems. The emphasis is on FORTRAN subroutines to be used with the IMSL (FORTRAN-based) package.

Rameríz, W.F. (1989). *Computational Methods for Process Simulation*. Boston: Butterworths.

STUDENT EXERCISES

Single Variable Methods

1. Real gases do not normally behave as ideal gases except at low pressure or high temperature. A number of equations of state have been developed to account for the non-idealities (van der Waal's, Redlich-Kwong, Peng-Robinson, etc.). Consider the van der Waal's P$\hat{V}$ T relationship

$$\left(P + \frac{a}{\hat{V}^2}\right)(\hat{V} - b) = RT$$

where P is pressure (absolute units), R is the ideal gas constant, T is temperature (absolute units), $\hat{V}$ is the molar volume and a and b are van der Waal's constants. The van der Waal's constants are often calculated from the critical conditions for a particular gas.

Assume that a, b, and R are given. We find that if P and T are given, there is an iterative solution required for $\hat{V}$.

a. How many solutions for $\hat{V}$ are there? Why? (Hint: Expand the PVT relationship to form a polynomial.)

b. Recall that direct substitution has the form $\hat{V}_{k+1} = g\hat{V}_k$). Write three different direct substitution formulations for this problem (call these I, II, and III).

c. What would be your first guess for $\hat{V}$ in this problem? Why?

d. Write the MATLAB m-files to solve for $\hat{V}$ using direct substitution, for each of the three formulations developed in **b.**

Consider the following system: air at 50 atm and −100°C. The van der Waal's constants are (Felder and Rousseau, p. 201) a = 1.33 atm liter^2/gmol^2, b = 0.0366 liter/gmol, and R = 0.08206 liter atm/gmol K. Solve the following problems numerically.

e. Plot $\hat{V}$ as a function of iteration number for each of the direct substitution methods in **b.** Use 10 to 20 iterations. Also use the first guess that you calculated in **c.** Discuss the stability of each solution (think about the stability theorem).

f. Rearrange (1) to the form of $f(\hat{V}) = 0$ and plot $f(\hat{V})$ as a function of $\hat{V}$. How many solutions are there? Does this agree with your solution for **a**? Why or why not?

g. Use the MATLAB function `roots` to solve for the roots of the polynomial developed in **a**.

h. Write and use an m-file to solve for the equation in a using Newton's method. The numerical solution is considered converged when $\left|\frac{\hat{V}_k - \hat{V}_{k-1}}{\hat{V}_{k-1}}\right| < \varepsilon$. Let $\varepsilon = 0.0001$.

2. Consider the van der Waals relationship for a gas without the volume correction term ($b = 0$)

$$\left(P + \frac{a}{\hat{V}2}\right)\hat{V} = RT$$

a. How many solutions for $\hat{V}$ are there? Show the solutions analytically.

b. Which solution is correct?

3. A process furnace is heating 150 lbmol/hr of vapor-phase ammonia. The rate of heat addition to the furnace is 1.0×10^6 Btu/hr. The ammonia feedstream temperature is 550°R. Use Newton's method to find the temperature of the ammonia leaving the furnace. Assume ideal gas and use the following equation for heat capacity at constant pressure:

$$C_p = a + bT + cT^{-2}$$

$$a = 7.11\,\frac{\text{Btu}}{\text{lbmol °R}} \qquad b = 3.33 \times 10^{-3}\,\frac{\text{Btu}}{\text{lbmol °R}^2} \qquad c = -1.20 \times 10^5\,\frac{\text{Btu °R}}{\text{lbmol}}$$

and remember that $Q = \dot{n}\int_{T_{in}}^{T_{out}} C_p\,dT$

where $\dot{n}$ is the molar flowrate of gas and Q is the rate of heat addition to the gas per unit time. How did you determine a good first guess to use?

4. Consider Example 3.2 , $f(x) = -x^2 - x + 1 = 0$, with the direct substitution method formulated as $x = -x^2 + 1 = g(x)$, so that the iteration sequence is

$$x_{k+1} = g(x_k) = -x_k^2 + 1$$

Try several different initial conditions and show whether these converge, diverge, or oscillate between values. Discuss the stability of the two solutions $x^* = 0.618$ and $x^* = -1.618$, based on an analysis of $g'(x^*)$.

5. Show why the graphical Newton's method is equivalent to $x_{k+1} = x_k - f(x_k)/f'(x_k)$.

6. Develop an algorithm (sequence of steps) to solve an algebraic equation using interval halving (bisection).