

Mathcad Lecture #7 In-class Worksheet

"Smart" Solve Block Techniques

At the end of this lecture, you will be able to:

- use *functions* in solve block equations to improve convergence
- construct solve blocks with *minimal number of equations* to improve convergence
- use *range variables* and *parametric* solve block to repeat implicit calculations many times.
- solve *engineering problem* using solve blocks

1. Using functions in Solve Blocks

Background

Often in engineering, the same mathematical relationships occur over and over. When these appear in a system of equations to be solved, functions should be defined before the solve block and the function named used inside the Given..Find to reduce the possibility for error and ensure consistency.

Demonstration

The flow of an incompressible fluid through a constant diameter, straight, horizontal pipe, from point 1 to point 2, is described by

$$\frac{P_2 - P_1}{\rho} = -f \frac{L}{D} \frac{v_{ave}^2}{2}$$

where P_i is the pressure at point i , ρ is the density of the fluid, L is the length of the pipe, D is the diameter of the pipe, v_{ave} is the average velocity along the section of the pipe from point 1 to point 2, and f is the friction factor. The friction factor can be determined from the Colebrook formula

$$\frac{1}{\sqrt{f}} = -2.0 \log \left(\frac{\varepsilon / D}{3.7} + \frac{2.51}{\text{Re} \sqrt{f}} \right)$$

where $\text{Re} = \frac{\rho D v_{ave}}{\mu}$ and ε is a value describing the roughness of the pipe.

Water flows through a section of horizontal copper piping 20 meters. If the pressure drop ($P_2 - P_1$) along this section is measured to be -70 kPa, **what is the average velocity of the fluid in the pipe?** For water, $\rho = 994 \text{ kg/m}^3$ and $\mu = 0.00087645 \text{ Pa}\cdot\text{s}$. For the copper piping, $D = 1.91 \text{ cm}$ and $\varepsilon = 1.524 \times 10^{-3} \text{ mm}$. (Note: Friction factors have values on the order of 10^{-3} and are always positive; $\text{Pa} = \text{N/m}^2$)

Step 1: Define all known quantities

$$\rho := 994 \frac{\text{kg}}{\text{m}^3} \quad \mu := 0.00087645 \text{ Pa}\cdot\text{s} \quad \varepsilon := 1.524 \cdot 10^{-3} \text{ mm} \quad D := 1.91 \text{ cm} \quad \Delta P := -70 \text{ kPa} \quad L := 20 \text{ m}$$

Step 2: Define a function for the Reynold's number.

Key Point: The Reynold's number is defined as a function of v because the velocity is unknown.

Step 3: Solve for f and v , the two unknowns.

Guesses $v_g := 2 \frac{\text{m}}{\text{s}}$ $f_g := 10^{-3}$

Given

$$\frac{\Delta P}{\rho} = -f_g \cdot \frac{L}{D} \cdot \frac{v_g^2}{2} \quad \frac{1}{\sqrt{f_g}} = -2.0 \cdot \log \left(\frac{\frac{\epsilon}{D}}{3.7} + \frac{2.51}{\text{NRe}(v_g) \cdot \sqrt{f_g}} \right)$$

$$\begin{pmatrix} v \\ f \end{pmatrix} := \text{Find}(v_g, f_g) \quad v = \blacksquare \quad f = \blacksquare$$

Key Point: When N_{Re} appears in the equations inside the Solve block, it is evaluated using the guess value for velocity v_g .

Practice

The heat, q , needed to change the temperature of a gas at low pressures from T_1 to T_2 is given by

$$q = n \left(\int_{T_1}^{T_2} c_p(T) dT \right)$$

where c_p is the heat capacity of the gas. If 10,000 BTU is removed from 500 moles of ethane initially at 800 °F, calculate the final temperature of the gas. The heat capacity for ethane is given below. Please report your answer in Rankine.

Equation

$$c_p(t) := \left[\begin{aligned} &5.01696 \cdot 10^8 + 1.08753 \cdot 10^6 \cdot \left(\frac{t}{\text{K}} - 273.15 \right) + 863.337 \cdot \left(\frac{t}{\text{K}} - 273.15 \right)^2 - 1.9525 \cdot \left(\frac{t}{\text{K}} - 273.15 \right)^3 \dots \\ &+ 8.58038 \cdot 10^{-4} \cdot \left(\frac{t}{\text{K}} - 273.15 \right)^4 \end{aligned} \right] \cdot \frac{\text{erg}}{\text{mol} \cdot \text{K}}$$

Known Quantities:

$$T_1 := (800 + 459.67) \cdot \text{R}$$

$$q := -10000 \text{ BTU}$$

$$n := 500 \text{ mol}$$

Key Points:

1. Notice that the variable given to c_p is the variable of integration, not the guess.
2. By labeling the guess at T_g , you can use T_2 to label the final answer.
3. By using a function for the heat capacity, you can use c_p for later calculations.

2. Reducing the Number of Equations in a Solve Block.

Background

Numerical solvers, such as the solver in Excel or Given..Find Blocks in Mathcad, make use of numerical algorithms to find answers to systems of equations. When using solvers, it is best to reduce the number of equations and unknowns. It is generally easier to solve for two unknowns than three unknowns.

Techniques to Reduce Equations

1. Substitute simple relationships when possible. For example, mole fractions must sum to one, so instead of using x_1 and x_2 , use x_1 and $(1-x_1)$ in your equations.
2. Often, physical properties are correlated as a function of another variable such as temperature. In this case, define a function to reduce the number of equations.

Demonstration/Practice

Imagine mixing liquid benzene(species 1) and toluene(species 2) together in an initially empty container. At temperatures and pressures at equilibrium, some of the liquid from both species will evaporate into the vapor phase and some will be left liquid phase. Raoult's law may be used to describe the distribution of species in each phase for ideal cases. For the specific example mentioned above, Raoult's law gives the following two expression describing the equilibrium state

$$y_1 \cdot P = x_1 \cdot P_{sat1}$$

$$y_2 \cdot P = x_2 \cdot P_{sat2}$$

where y_i is the mole fraction of species i (either 1 or 2) in the vapor phase, x_i is the mole fraction of species i in the liquid phase, P_{sat_i} is the vapor pressure of species i at the system temperature T , and P is the system pressure. The vapor pressure of benzene and toluene can be found using the Antoine Equation

$$\ln(P_{sat}) = A - \frac{B}{T + C}$$

where P_{sat} is in kPa, T is in °C, and A , B , and C are found in the table below.

Antione Constants for Acetone and Methanol			
Compound	A	B	C
Benzene	13.7819	2726.81	217.572
Toluene	13.9320	3056.96	217.625

If a mixture of benzene and toluene has $y_1 = 0.33$ and $P = 120$ kPa, find x_1 .

Solution Method 1 (Poor)

Step 1: Define the knowns:

$$y_1 := 0.33 \quad P := 120$$

Step 2: List the unknowns:

$$y_2 \quad x_1 \quad x_2 \quad P_{sat1} \quad P_{sat2} \quad T$$

Step 3: Define guesses for each unknown:

$$y_{2g} := 0.5 \quad x_{1g} := 0.5 \quad x_{2g} := 0.5 \quad P_{sat1g} := 100 \quad P_{sat2g} := 100 \quad T_g := 50$$

Step 4: Use Given..Find to solve for six unknowns.

Given

$$x1_g + x2_g = 1$$

$$y1 + y2_g = 1$$

$$y1 \cdot P = x1_g \cdot Psat1_g$$

$$y2_g \cdot P = x2_g \cdot Psat2_g$$

$$\ln(Psat1_g) = 13.7819 - \frac{2726.81}{T_g + 217.572}$$

$$\ln(Psat2_g) = 13.9320 - \frac{3056.96}{T_g + 217.625}$$

$$\begin{pmatrix} x1 \\ x2 \\ y2 \\ Psat1 \\ Psat2 \\ T \end{pmatrix} := \text{Find}(x1_g, x2_g, y2_g, Psat1_g, Psat2_g, T_g)$$

$x1 = 0.173$	$x2 = 0.827$	$y2 = 0.67$
$Psat1 = 229.396$	$Psat2 = 97.175$	$T = 109.131$

Questions:

1. What don't you like about the above setup?
2. How can functions be used to improve the situation?
3. What simple relationships can be used to improve the situation?

Solution Method 2 (Better)

$$\text{ORIGIN} := 1$$

$$A := \begin{pmatrix} 13.7819 \\ 13.9320 \end{pmatrix}$$

$$B := \begin{pmatrix} 2726.81 \\ 3056.96 \end{pmatrix}$$

$$C := \begin{pmatrix} 217.572 \\ 217.625 \end{pmatrix}$$

3. Constructing Solve Blocks for Multiple Calculations

Description

Often, we want to perform an implicit calculation many times. (An implicit calculation means we can't solve for the variable of interest such as volume in the van der Waals equation of state.) We do so by constructing solve blocks in a parametric way and then using matrices of range variables to repeat the calculation over and over.

Demonstration

In the UO lab, you use saturated steam on the shell side of a heat exchanger to heat water. The temperature of the steam is not directly measured, but the pressure is. However, since the steam is saturated, you can calculate the temperature from the pressure using a vapor pressure correlation. Such an equation is given below.

$$P_{\text{sat}_{\text{wtr}}}(t) := \exp \left[73.649 - \frac{7258.2}{\frac{t}{\text{K}}} - 7.3037 \cdot \ln \left(\frac{t}{\text{K}} \right) + 4.1653 \cdot 10^{-6} \cdot \left(\frac{t}{\text{K}} \right)^2 \right] \cdot \text{Pa}$$

Part a: Given the measured pressure of the saturated steam found in the matrix below, calculate the temperature of the steam.

M :=

	1
1	$2.299 \cdot 10^3$
2	$2.398 \cdot 10^3$
3	$2.503 \cdot 10^3$

$$P_{\text{exp}} := M \cdot \text{kPa}$$

Key Points:

1. Notice that the statement containing the find in the solve block is a function of p. This is telling Mathcad to solve for the temperature given any pressure.
2. We can perform solve block calculation many times given the input data in a matrix and using a range variable.
3. The range variable starts at the ORIGIN and ends at the number of rows in the matrix of data.

Part b: Plot $\ln P$ vs $1/T$ at saturation for water for saturation pressures from 1 atm to 130 atm.

Key Point: We can use range variables to define inputs for the parametric given block. This is often done when plotting or when you want to see the effect of a certain variable on the outcome or other trends.

Practice

Create a T-x-y diagram for $P = 130$ kPa for the benzene/toluene system described above. You do this by repeating the Raoult's Law calculation over and over. Remember, in the example above we were given a y and a P and were asked to find x and T . Now, you need to calculate x and T for all possible values of y at $P = 130$ kPa. For your reference, I have copied the Raoult's Law equations and the vapor pressure correlations below.

$$\text{ORIGIN} := 1 \quad A := \begin{pmatrix} 13.7819 \\ 13.9320 \end{pmatrix} \quad B := \begin{pmatrix} 2726.81 \\ 3056.96 \end{pmatrix} \quad C := \begin{pmatrix} 217.572 \\ 217.625 \end{pmatrix}$$

Raoult's Law

$$y_1 \cdot P = x_1 \cdot P_{\text{sat}_1}$$

$$y_2 \cdot P = x_2 \cdot P_{\text{sat}_2}$$

$$P_{\text{sat}}(i, t) := \exp \left(A_i - \frac{B_i}{\frac{t}{K} - 273.15 + C_i} \right) \cdot \text{kPa}$$

Extra Practice

The van der Waals equation of state, $P = \frac{R \cdot T}{v - b} - \frac{a}{v^2}$ describes the PVT behavior of real gases better than

the ideal gas equation of state. For butane, $a = 1.3701 \times 10^7 \text{ atm cm}^6 \text{ mol}^{-2}$ and $b = 116.4 \text{ cm}^3 \text{ mol}^{-1}$. Create a function (using a parametric give block) to calculate the the volume of butane for any T and P. Make the function versatile so that you can use it to calculate both liquid and vapor volumes (if they are present). Test your function by calculating the vapor and liquid volumes of butane at 100 °C and 15.41 bar. These volumes are 1611 and 212 cm³/mol respectively.

4. Debugging Solve Blocks

Background

Solve blocks (Given...Find Blocks) are a very valuable tools to solve non-linear, simultaneous equations. You may solve for up to 400 unknowns. However, solve blocks are not forgiving of syntax errors or other mistakes, and debugging is often frustrating and time consuming. While experience and practice are the best teachers to improve your ability to debug solve blocks, some general tips can help facilitate the endeavor.

Debugging Techniques

- 1. Ensure that all function are defined before the solve block will work properly.** In engineering, we often define expressions, such as the Antoine Equation, which are later used in solve blocks. It is good practice to always check that your function works for some value before using it in a solve block.
- 2. Copy the LHS and RHS of each expression in a solve block to ensure correct: calculation, units, order of magnitude.** When a solve block is set up, you have to define everything, including guesses, before typing Given. This means that each side of each equation should evaluate to some numerical value. You should check to see if the units on each side of the equation are consistent and if the magnitudes of the numbers on each side are "close."
- 3. Ensure that each Solve block starts with a given and ends with a find.** Often, when working problems, you set up a solve block with a Given, but don't finish it with a find because you cannot figure out what equations to input. If you forget to finish the given block, and begin another one, you will have problems.
- 4. Double check that the correct variables are used.** Make sure the guess variables are the same before the given block, within the given block, and in the find statement.
- 5. Don't over/under specify the problem.** If a solve block has two equations, the given statement must have two unknowns. If the solve block has three equations, the find statement should have three unknowns.

Demonstration: Debug the following Solve Block

The van der Waals equation of state, $p = \frac{R \cdot T}{v - b} - \frac{a}{v^2}$ describes the PVT behavior of real gases better than

the ideal gas equation of state. For butane, $a = 1.3701 \times 10^7 \text{ atm} \cdot \text{cm}^6 \cdot \text{mol}^{-2}$ and $b = 116.4 \text{ cm}^3 \cdot \text{mol}^{-1}$. Using the van der Waals EOS, calculate the liquid and vapor volume of butane at 100°C and 15.41 bar .

$$R_g := 8.314 \frac{\text{J}}{\text{mol} \cdot \text{K}} \quad a := 1.3701 \cdot 10^7 \frac{\text{atm} \cdot \text{cm}^6}{\text{mol}} \quad b := 116.4 \frac{\text{cm}^3}{\text{mol}}$$

$$P := 15.41 \text{ bar} \quad t := (100 + 273.15) \cdot \text{K}$$

$$v_g := \frac{R_g \cdot T}{p} \quad \text{Given} \quad p = \frac{R_g \cdot T}{v_g - b} - \frac{a}{v_g^2} \quad v_{\text{gas}} := \text{Find}(v_g) \quad v_{\text{gas}} = \frac{\text{cm}^3}{\text{mol}}$$

$$v_g := 1.1 \cdot b \quad \text{Given} \quad p = \frac{R_g \cdot T}{v_g - b} - \frac{a}{v_g^2} \quad v_{\text{liq}} := \text{Find}(v_g) \quad v_{\text{liq}} = \frac{\text{cm}^3}{\text{mol}}$$

Practice: Debug the following Solve Blocks

Problem A

$$\text{kmol} := 1000 \text{ mol} \quad \rho := 55.19 \frac{\text{kmol}}{\text{m}^3} \quad \mu := 0.00087645 \text{ Pa}\cdot\text{s} \quad \varepsilon := 1.524 \cdot 10^{-3} \text{ mm} \quad D := 1.91 \text{ cm} \quad \Delta P := -70 \text{ kPa} \quad \text{Len} := 20 \text{ m}$$

$$\text{Guesses} \quad v_g := 2 \frac{\text{m}}{\text{s}} \quad f_g := 10^{-3}$$

Given

$$\frac{\Delta P}{\rho} = -f_g \cdot \frac{L}{D} \cdot \frac{v_g^2}{2} \quad \frac{1}{\sqrt{f_g}} = -2.0 \cdot \log \left(\frac{\frac{\varepsilon}{D}}{3.7} + \frac{2.51}{\frac{\rho \cdot D \cdot v_g}{\mu} \cdot \sqrt{f_g}} \right)$$

$$\text{ans} := \text{Find}(v_g, f_g)$$

Problem B

$$f_g := .001 \quad \text{Re} := 25000$$

Given

$$\frac{1}{\sqrt{\frac{f_g}{2}}} = 2.5 \cdot \ln \left(\text{Re} \cdot \sqrt{\frac{f_g}{8}} \right) + 1.75$$

$$f := \text{Find}(f_g) \quad f = \blacksquare$$

Problem C

$$A := 4.0326 \cdot 10^4 \quad B := 1.3422 \cdot 10^5 \quad C := 1655.5 \quad D := 7.3223 \cdot 10^4 \quad E := 7.5287 \cdot 10^2$$

$$C_p(T) := \left[A + B \cdot \left(\frac{\frac{C \cdot K}{T}}{\sinh\left(\frac{C \cdot K}{T}\right)} \right)^2 + D \cdot \left(\frac{\frac{E \cdot K}{T}}{\cosh\left(\frac{E \cdot K}{T}\right)} \right) \right] \cdot \frac{J}{\text{kmol} \cdot \text{K}}$$

$$\text{Guess} \quad T_g := (600 + 459.67) \cdot \text{R} \quad n := 500 \text{ mol} \quad T_1 := 1300 \text{ R} \quad q := -10000 \text{ BTU}$$

$$\text{Given} \quad q = n \cdot \int_{T_1}^{T_2} C_p(T) \, dT \quad T_2 := \text{Find}(T_g) \quad T_2 = \blacksquare \cdot \text{R}$$

Problem D

$$x := -2$$

Given

$$\text{if}(x < 1, x^2 + 2 \cdot x - 1, \sqrt[3]{x} + \log(x) + 2) = 0$$

$$\text{ans} := \text{Find}(x) \quad \text{ans} = \blacksquare$$

Problem E

$$\gamma_0(x_0) := \exp[0.95 \cdot (1 - x_0)^2] \quad \gamma_1(x_0) := \exp(0.95 \cdot x_0^2)$$

$$\underline{A}_i := \begin{pmatrix} 8.04494 \\ 7.96681 \end{pmatrix} \quad \underline{B}_i := \begin{pmatrix} 1554.3 \\ 1668.21 \end{pmatrix} \quad \underline{C}_i := \begin{pmatrix} 222.63 \\ 228.0 \end{pmatrix}$$

$$\underline{P}_{\text{sat}}(i, t) := \frac{1}{760} \cdot 10^{\left(A_i - \frac{B_i}{\frac{t}{K} + C_i} \right)} \cdot \text{atm}$$

Define the known conditions

$$\underline{T} := 300\text{K} \quad y_0 := 0.5$$

Use a solve block to calculate the unknown quantities.

$$\text{Guesses} \quad P_g := 2\text{atm} \quad x_{0g} := 0.5$$

Given

$$x_{0g} \cdot \gamma_0(x_{0g}) \cdot P_{\text{sat}}(0, t) = y_0 \cdot P$$

$$(1 - x_{0g}) \cdot \gamma_1(x_{0g}) \cdot P_{\text{sat}}(1, t) = (1 - y_0) \cdot P$$

$$\begin{pmatrix} x_0 \\ P \end{pmatrix} := \text{Find}(x_{0g}, P_g)$$

$$x_1 := 1 - x_0$$

$$\gamma_0(x_0) = \blacksquare \quad \gamma_1(x_0) = \blacksquare \quad x_0 = \blacksquare \quad P = \blacksquare \cdot \text{atm} \quad x_1 = \blacksquare$$

