## Contents

Molecular Nature of Energy, Temperature, and Pressure ..... 4
Classify KE and PE ..... 4
Molecular kinetic energy ..... 4
piston heating and thermal energy ..... 5
Energy changes upon isothermal condensation ..... 5
Identify regions of PT diagram ..... 6
PV diagram interpretation ..... 6
quality for tank scenarios ..... 8
single and double interpolation ..... 9
Steam quality calculation given T and V ..... 9
Calculate steam quality given P and H ..... 9
quality for tank scenarios using P ..... 9
Decide which steam table ..... 10
Entropy concepts for ideal gases ..... 10
Entropy concepts for liquids ..... 10
Identify purpose for process equipment ..... 11
Process equipment energy balances ..... 11
Delta H by various pathways ..... 12
create ideal gas enthalpy, internal energy, volume spreadsheet calculator ..... 13
Steam trap flash ..... 14
Carnot Cycle without using Entropy ..... 15
Routes for turbine and pump work ..... 16
compression in a piston/cylinder ..... 16
Adiabatic Reversible Pump ..... 17
turbine Ws given P2, T2 ..... 17
combustion reaction energy balance ..... 18
Rankine.problem ..... 19
Modified Rankine Cycle ..... 19
Ordinary Vapor Compression Problem for R-134a ..... 20
Refrigeration with economizer ..... 22
Virial equation of state ..... 23
Worksheet Excel excercise ..... 23
Find T where $\mathrm{Z}>0.95$ at 30 bar ..... 24
Find T where Z > 0.95 at 20 bar or 30 bar ..... 24
Peng Robinson select stable roots ..... 24
Particles with square well escaping ..... 26
Departure function concepts ..... 27
Departure functions simple practice ..... 27
compressor ..... 27
two stream heat exchanger ..... 27
one-phase steam turbine via Peng-Robinson equation of state ..... 28
two-phase steam turbine via Peng-Robinson equation of state ..... 28
Ternary Bubble Pressure ..... 29
Ternary Bubble Temperature ..... 29
Ternary Dew Pressure ..... 29
Ternary Dew Temperature ..... 30
Three component flash ..... 30
Fit Pxy point ..... 32
Class Excercise using Matlab and Modified Raoult's Law ..... 34
Bubble Temperature ..... 34
Dew Pressure Concepts ..... 35
Modified Raoults Law dew pressure ..... 36
Fit Pxy point ..... 37
Advantages of gammaModels folder ..... 37
Henry's law concepts ..... 38
Osmotic Pressure Concepts ..... 39
Place liquid gamma models in historical order ..... 40
van Laar ..... 40
Identify Flory as modeling excess entropy ..... 40
Concepts for models including excess entropy ..... 40
Polymer Models ..... 41
Scatchard-Hildebrand Theory ..... 41
Solubility parameter ..... 41
Models that use volume fraction ..... 41
Local Composition Concepts ..... 42
butanol plus water liquid-liquid equilibria ..... 43
Residue Curves for Methanol + Ethanol + Benzene option 1 ..... 44
Propane Cracking ..... 46
Styrene to Ethyl Benzene ..... 47
Haber Process equilibra ..... 48

## Introduction

The following problems are randomized for use in undergraduate chemical engineering thermodynamics. The problems offer immediate feedback to students if they are not getting correct answers. The problems are offered on the LONCAPA platform. The LONCAPA system (https://loncapa.org) is available at reasonable cost by EduCog.com (https://www.educog.com/) if your university does not have an installation. The system supports resource exchange between instructors. The LONCAPA platform can be used as a learning management system, or it can export scores and student performance data for use in other learning management systems.

The LONCAPA system provides a wide variety of problem seen in the examples below, including random labels on images. Other open source software has been integrated into LONCAPA to provide powerful options including real time graphing by gnuplot (http://gnuplot.info/) using values from scripts or student input, symbolic algebraic answer evaluation via Maxima (http://maxima.sourceforge.net/) or R (https://www.r-project.org/), and Geogebra (https://www.geogebra.org/) for drawing on plots. I have a variety of phase equilibria problems where conditions are randomly generated for each student. I have a the Peng-Robinson equation of state programmed for pure species in the calculation engine which can be used to broaden the randomization of EOS calculations for real fluids.

Please note that many of the randomized problems below are configured to show students one-part-at-a-time. This permits students to proceed with subsequent parts even if they have wrong answers to a single part. These problems will appear incomplete in the printing below; the first part of the problem statement will provide an overview of the content that is available. Some of the problems involve real time plot generation based on student input values, so they do not display properly here. Also the residue curve problem uses Geogebra (https://www.geogebra.org/) which displays properly online, but does not print below. All of the problems displayed here have been used with over 100 students, many for over 500 students. Many of the problems are based on similar problems from the textbook "Introductory Chemical Engineering Thermodynamics" (https://chethermo.net) by Richard Elliott and Carl Lira, Prentice Hall, 2012. If you join the LONCAPA network, please contact me to facilitate collaboration in problem development at lira@egr.msu.edu.

The following statements are related to the molecular nature of $\mathrm{T}, \mathrm{P}$, and U .
Choices: True, False.

- Heat transfer by conduction is due to the transfer of kinetic energy from a hotter region to a colder region.
- Ideal gas particles bounce off each other.
- Ideal gases have kinetic energy but no potential energy.
- Molar energy of a gas $(\mathrm{KE}+\mathrm{PE})$ can be equal to molar energy $(\mathrm{KE}+\mathrm{PE})$ of a liquid for the same substance.

Tries 0/99

Match the type of energy with the example.

## Choices: Kinetic Energy, Potential Energy, Both.

- Two positively charged ions that are placed near each other but are not moving.
- Flowing water in a river.
- A TV being held out a window on the fourth floor of an apartment complex.
- A car moving on a flat road at $10 \mathrm{~m} / \mathrm{s}$.
- A vibrating double bond between a carbon and oxygen atom.

Tries 0/99

Object 1 and Object 2 are both made up of the same type of molecules and the same number of molecules. Object 1 has a higher temperature than Object 2. Explain the difference in molecular kinetic energy between the two objects without using equations.


Tries 0/99

A variable-volume cylinder holds an ideal gas as shown below. The temperature of the gas is increased by heating. Explain the changes of the kinetic energy of the gas atoms without using equations.


Tries 0/99

A pure saturated vapor is condensed to a saturated liquid at constant temperature. The next three questions concern energy changes for this process.
A) For the condensation process at constant temperature, how does the kinetic energy of the fluid atoms change?
A. Increases
B. Stays the same
C. Decreases

Tries 0/2
Explain your answer using descriptions of molecular phenomena and without using equations.


Tries 0/2
B) For the condensation process at constant temperature, how does the potential energy between molecules change for the system of molecules?
A. Decreases
B. Stays the same
C. Increases

Explain your answer using descriptions of molecular phenomena and without using equations.


Tries 0/2
C) For the condensation process at constant temperature, how does the fluid's internal energy change?
A. Stays the same
B. Decreases
C. Increases

Tries 0/2
Explain your answer using descriptions of molecular phenomena and without using equations.


Tries 0/2


Match the following:
Choices: A, B, C, D, E, F, G, H.

- Melting Curve
- Solid, Liquid, and Gas
- Sublimation Pressure
- Liquid and Gas
- Solid and Liquid
- Solid
- Liquid Vapor Pressure
- Critical Point
- Gas
- Solid and Gas


On the PV diagram above there is one isobar with different points marked on it. Match the point with its correct state.

A Saturated Liquid
B Liquid
C Liquid and Vapor
D Saturated Vapor
E Vapor


Tries 0/99

Which of the points represent systems with a saturated phase or saturated phases?

## Choices: True, False.

- 1
- 3
- 5
- 4
- 2
- 6

Tries 0/99
Which of the point(s) have a quality of one?

## Choices: True, False.

- 5
- 4
- 3
- 1
- 2
- 6

Tries 0/99
Which state has highest quality of the following choices?
A. 4
B. 2
C. 3
D. 1

Tries 0/2

A tank is at a temperature of $185^{\circ} \mathrm{C}$ and has a quality of 0.5 . What is the enthalpy $(\mathrm{kJ} / \mathrm{kg})$ of the water in the tank? Use at least three significant figures.

Tries 0/99
What is the quality of steam inside a tank that has a volume of 510 L and a mass of 8 kg when it is at a temperature of $135^{\circ} \mathrm{C}$ ? Use at least three significant figures.


Tries 0/99
Suppose that a tank holds $6 \%$ liquid water by volume and $94 \%$ vapor water by volume at a temperature of $75^{\circ} \mathrm{C}$. What is the quality? Use at least three significant figures.

Tries 0/99

Complete the following enthalpy table (in $\mathrm{kJ} / \mathrm{kg}$ ), by using linear interpolation and the given values of $\mathrm{T}, \mathrm{P}$, and H .

|  | $0.1(\mathrm{MPa})$ | $0.19(\mathrm{MPa})$ | $0.2(\mathrm{MPa})$ |
| :---: | :---: | :---: | :---: |
| $900(\mathrm{C})$ | 4398 | $\mathbf{B}$ | 4519.1 |
| $925(\mathrm{C})$ | $\mathbf{A}$ | $\mathbf{D}$ |  |
| $950(\mathrm{C})$ | 4519.5 | $\mathbf{C}$ | 4642.3 |

The enthalpy that corresponds to letter $\mathbf{A},(\mathrm{kJ} / \mathrm{kg})$, is:

The enthalpy that corresponds to letter $\mathbf{B},(\mathrm{kJ} / \mathrm{kg})$, is:
The enthalpy that corresponds to letter $\mathbf{C},(\mathrm{kJ} / \mathrm{kg})$, is:
The enthalpy that corresponds to letter $\mathbf{D},(\mathrm{kJ} / \mathrm{kg})$, is:
Tries 0/99

Calculate the quality of water if it is at a temperature of $50^{\circ} \mathrm{C}$ and a overall specific volume of $9 \mathrm{~m}^{3} / \mathrm{kg}$.
Tries 0/99

Calculate the quality of water if it is at a pressure of 10 MPa and a enthalpy of $1970 \mathrm{~kJ} / \mathrm{kg}$.
$\square$
Tries 0/99

Suppose that a tank holds $10 \%$ liquid water by volume and $90 \%$ vapor water by volume at a pressure of 0.05 MPa . What is the quality? Use at least three significant digits in your answer.
$\square$
Tries 0/99
A tank is at a pressure of 0.08 MPa and has a quality of 0.52 . What is the enthalpy of the water $(\mathrm{kJ} / \mathrm{kg})$ in the tank?
Answer in $\mathrm{kJ} / \mathrm{kg}$.
$\square$

Tries 0/99
What is the quality of steam inside a tank that has a volume of 11070 L and a mass of 5.5 kg when it is at a pressure of 0.01 MPa ? Use three significant figures in your answer.
$\square$
Tries 0/99

Consider water as the fluid of interest. Given the conditions below, choose what steam table you would use to calculate the other variables?

A Saturated Pressure Table
B Saturated Temperature Table
C Superheated Steam
D Compressed Liquid Table
$\square \mathrm{T}=255^{\circ} \mathrm{C}$ and $\mathrm{S}=6.0243 \mathrm{~kJ} / \mathrm{kg}-\mathrm{K}$
$\mathrm{P}=.80 \mathrm{MPa}$ and $\mathrm{V}=.4356 \mathrm{~m}^{3} / \mathrm{kg}$
$\mathrm{P}=8 \mathrm{MPa}$ and $\mathrm{T}=275^{\circ} \mathrm{C}$
$\mathrm{T}=100^{\circ} \mathrm{C}$ and $\mathrm{S}=1.2506 \mathrm{~kJ} / \mathrm{kg}-\mathrm{K}$
$\square \mathrm{T}=120^{\circ} \mathrm{C}$ and $\mathrm{H}=1700 \mathrm{~kJ} / \mathrm{kg}$

Tries 0/99

For an ideal gas, does entropy increase, decrease, or stay about the same if:
Choices: Increases, Decreases, Stays about the same.

- The gas condenses at the vapor pressure?
- Two pure gas species are mixed at constant temperature?
- Temperature increases isobarically?
- Volume increases isothermally?
- Pressure increases isothermally?

Tries 0/99

For a liquid, does entropy increase, decrease, or stay about the same if:
Choices: Increases, Decreases, Stays about the same.

- Temperature increases isobarically?
- Two pure liquid species are mixed at constant temperature?
- Pressure increases isothermally?
- The liquid evaporates at the vapor pressure?
- The liquid freezes at the melting temperature?

Tries 0/99

Match the process equipment to the purpose.
A Compressors
B Nozzles
C Pumps
D Heat Exchangers
E Throttles
F Turbines
Either warms or cools one stream by using a nearby stream.
Lower the pressure of a flowing stream to control flow rate without producing work.
Puts work into a liquid by increasing the pressure.
Uses a difference in pressure to increase the velocity of fluid so it will be useful.
Uses a flowing stream to produce shaft work.

## Tries 0/99

Which of the following process equipment are isenthalpic?

## Choices: True, False.

- Valves
- Compressors
- Heat Exchangers
- Throttles
- Turbines
- Nozzles
- Pumps


## Tries 0/99

For which of the following equipment does the general energy balance simplify in steady-state flow to $\Delta \mathrm{H}=\mathrm{W}_{\mathrm{S}}$ ?

## Choices: True, False.

- Heat Exchangers
- Turbines
- Throttles
- Compressors
- Valves
- Pumps
- Nozzles

Tries 0/99

Which of the following process equipment cause a change in enthalpy of streams?

## Choices: True, False.

- Valves
- Throttles
- Pumps
- Heat Exchangers
- Compressors
- Nozzles
- Turbines

Tries 0/99

This problem asks for the change in enthalpy along different pathways. For all parts, consider carbon dioxide as an ideal gas and use the heat capacity polynomials that are found in Elliott and Lira Appendix E.
(a) Consider an isobaric change of carbon dioxide gas at a pressure of 0.2 MPa from a volume of $28000 \mathrm{~cm}^{3} / \mathrm{mol}$ to $9000 \mathrm{~cm}^{3} / \mathrm{mol}$ as an ideal gas. What is the change is enthalpy? The answer should be in $\mathrm{J} / \mathrm{mol}$. Remember to use the correct sign.
$\square$

Tries 0/99
(b) Consider an a isothermal change of 4 moles of carbon dioxide as an ideal gas from a volume of $17 \mathrm{~m}^{3}$ to $34 \mathrm{~m}^{3}$. What is the change in enthalpy from state 1 to state 2? The answer should be in Joules. Remember to use the correct sign.

Tries 0/99
(c) Consider an isothermal change of of 8 moles of carbon dioxide as an ideal gas from a pressure of 3 MPa to 20 MPa . What is the change in enthalpy from state 1 to state 2? The answer should be in Joules. Remember to use the correct sign.

Tries 0/99
(d) Consider an isobaric change at 0.1 MPa for 4 moles of carbon dioxide going from a temperature of 290 K to 440 K. What is the change in enthalpy? The answer should be in Joules. Remember to use the correct sign.

## Tries 0/99

(e) What is the change in enthalpy when 7 moles of carbon dioxide is taken from 348 K and 4 MPa to 279 K and 0.11 MPa. The answer should be in Joules. Remember to use the correct sign.
$\qquad$
Tries 0/99

The objective of this problem is to create your own spreadsheet calculator to calculate volume, enthalpy and internal energy changes between two states. A reference state is to be used as shown in the figure below. The spreadsheet should include the following features:

1. The layout below is an example. There is no need to make your sheet use the same layout. Consider that using cell names will help you debug your formulas more quickly.
2. Values entered in bold bordered cells are constants. All other numerical values are calculated from these constants.
3. The spreadsheet should be written so that the reference state can be changed by entering new values into the reference state cells.
4. The reference state should use $\mathrm{H}_{\mathrm{R}}=0$. Note the value of $\mathrm{U}_{\mathrm{R}}$ should be tabulated. (Consult a textbook for the relation between H and U ).
5. Heat capacity constants should be entered in tabular form.
6. The values of enthalpy at state 1 and state 2 should be calculated relative to the reference state using the integrated form of the Cp heat capacity polynomial. Use cell references to the Cp constants such that the when the constants are changed for a new fluid, all the dependent values automatically update. The Cp polynomial form and constants should be from the Elliott and Lira textbook, or the accompanying Props.xlsx spreadsheet, $\mathrm{Cp}(\mathrm{J} / \mathrm{mol}-\mathrm{K})=\mathrm{a}+\mathrm{b}^{*} \mathrm{~T}+\mathrm{c}^{*} \mathrm{~T}^{2}+\mathrm{d}^{*} \mathrm{~T}^{3}$, where T is in K .
7. Differences between state 1 and state 2 (in the column labeled 'Delta' in the example) should be calculated by simple subtraction rather than an integral.
8. Volumes $\left(\mathrm{cm}^{3} / \mathrm{mol}\right)$ are calculated using the ideal gas law.
9. With some thought, you will realize that to calculate U , no polynomial for Cv nor integral beyond that already calculated for H is necessary. (Consult a textbook for the relation between U and H .)
10. It may be helpful to test your spreadsheet using the fluid and conditions of the example. Then after your spreadsheet is debugged, change the fluid and heat capacity, and answer the questions below.

|  | A | B | C | D | E | F | G |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | Ideal Gas Property Calculator |  |  |  |  |  |  |
| 2 |  |  |  |  |  |  |  |
| 3 | Insert the appropriate values in the bold boxes. |  |  |  |  |  |  |
| 4 |  |  |  |  |  |  |  |
| 5 | Reference State (H, S = 0 in ref state) |  |  |  |  |  |  |
| 6 | T(K) | 298.15 | Fluid | propane |  |  |  |
| 7 | $\mathrm{P}(\mathrm{MPa})$ | 0.1 |  | a | b | C | d |
| 8 | U | -2478.96 | Cp | -4.224 | 0.3063 | -1.586E-04 | 3.215E-08 |
| 9 | H | 0 | Values at Tref |  |  |  |  |
| 10 | S | 0 | Cp | 73.85 |  | Cv | 65.54 |
| 11 |  |  |  |  |  |  |  |
| 12 | State | ref | state 1 | state2 | Delta |  |  |
| 13 | T(K) | 298.15 | 378.15 | 463.15 | 85 |  |  |
| 14 | P (MPa) | 0.1 | 0.5 | 2.5 | 2 |  |  |
| 15 | V(cm3/mol) | 24789.59 | 6288.23 | 1540.34 | -4747.89 |  |  |
| 16 | $\mathrm{U}(\mathrm{J} / \mathrm{mol})$ | -2478.96 | 3447.25 | 11145.26 | 7698.014 |  |  |
| 17 | $\mathrm{H}(\mathrm{J} / \mathrm{mol})$ | 0 | 6591.37 | 14996.11 | 8404.74 |  |  |
| 19 |  |  |  |  |  |  |  |

Create your spreadsheet with the indicated functionality. For the fluid METHYL ETHYL KETONE,

1. Insert the name.
2. Insert the Cp constants.
3. Set the reference state to 293.15 K , and 0.7 MPa .
4. Set state 1 to $448.15 \mathrm{~K}, 0.2 \mathrm{MPa}$, state 2 to $858.15 \mathrm{~K}, 8 \mathrm{MPa}$.
(a) What is $\mathrm{V} 1\left(\mathrm{~cm}^{3} / \mathrm{mol}\right)$ ?
$\square$

Tries 0/99
(b) What is V2 $\left(\mathrm{cm}^{3} / \mathrm{mol}\right)$ ?

Tries 0/99
(c) What is H1 $(\mathrm{J} / \mathrm{mol})$ ?

Tries 0/99
(d) What is $\mathrm{H} 2(\mathrm{~J} / \mathrm{mol})$ ?
$\square$

Tries 0/99
(e) What is $\mathrm{U} 1(\mathrm{~J} / \mathrm{mol})$ ?

Tries 0/99
(f) What is U2 $(\mathrm{J} / \mathrm{mol})$ ?

Tries 0/99
(g) What is $\Delta \mathrm{H}(\mathrm{J} / \mathrm{mol})$ ?

Tries 0/99
(h) What is $\Delta \mathrm{U}(\mathrm{J} / \mathrm{mol})$ ?

Tries 0/99
(i) Use Goal Seek or Solver to find the Temperature (K) where the enthalpy is $8.791 \times 10^{4} \mathrm{~J} / \mathrm{mol}$.

Tries 0/99

Valves on steam lines are commonly encountered and you should know how they work. For most valves, the change in velocity of the fluid flow is negligible. Apply this principle to solve for the outlet of a steam trap.

Steam traps are common process devices used on the lowest points of steam lines to remove condensate. By using a steam trap, a chemical process can be supplied with so-called dry steam, i.e., steam free of condensate. As condensate forms due to heat losses in the supply piping, the liquid runs downward to the trap. As liquid accumulates in the steam trap, it causes a float mechanism to move. The float mechanism is attached to a valve, and when the float reaches a control level, the valve opens to release accumulated liquid, then closes automatically as the float returns to the control level. Most steam traps are constructed in such a way that the inlet of the steam trap valve is always covered with saturated liquid when opened or closed. Consider such a steam trap on a 2 MPa (absolute) line that vents to 0.4 MPa (absolute).
(a) What is the enthalpy of the inlet $(\mathrm{kJ} / \mathrm{kg})$ ?

Tries 0/99
(b) What is the enthalpy of the outlet $(\mathrm{kJ} / \mathrm{kg})$ ?

Tries 0/99
(c) What is the value of enthalpy for saturated liquid at the outlet condition $(\mathrm{kJ} / \mathrm{kg})$ ?
$\square$
Tries 0/99
(d) What is the value of enthalpy for saturated vapor at the outlet condition $(\mathrm{kJ} / \mathrm{kg})$ ?
Tries $0 / 99$
(e) What is the quality for the exiting stream at 0.4 MPa ?
$\square$
(f) What is the temperature of the outlet stream (C)?
$\square$
Tries 0/99

One mole of methane gas is held within a Carnot heat engine at an initial state of 544 K and 5 MPa . Assume the gas is ideal. The heat capacity $(\mathrm{Cp})$ is $35.8 \mathrm{~J} / \mathrm{mol}-\mathrm{K}$. The goal of this problem is to calculate $\mathrm{Q}, \Delta \mathrm{U}$, and Wec for the cycle as well as the thermal efficiency of the cycle. The cycle consists of 4 steps, with the last step returning the gas to the initial state. You will perform the calculations on each step individually, then tabulate the values for the cycle. Each step continues from the previous state to the new state.

There are 16 parts to this problem presented one-at-a-time.
Step 1: The gas is expanded isothermally from the initial state to State 2 which is at 3.34 MPa , absorbing a quantity of heat Qh1.
a) What is $\Delta U$ for this step? (in J) $\qquad$
Tries 0/3
Step 2: The gas is expanded adiabatically and reversibly from State 2 to State 3 which is at 0.889 MPa .
Step 3: The gas is compressed isothermally from State 3 to State 4 which is at 1.330 MPa .
Step 4: The gas is compressed adiabatically and reversibly from State 4 to the initial state which is at 544 K and 5 MPa.

What is the easiest way to calculate the energy balance around an adiabatic, reversible turbine?
A. Using entropy from steam tables.
B. Using imaginary pathways.
C. Using $\int V d P$.

Tries 0/2
What is the easiest way to calculate the energy balance around an adiabatic, reversible pump?
A. Using $\int V d P$.
B. Using imaginary pathways.
C. Using entropy from steam tables.

## Tries 0/2

One mole of an ideal gas $(\mathrm{Cp}=(5 / 2) \mathrm{R})$ in a closed piston/cylinder is compressed from $\mathrm{T}^{\mathrm{i}}=298 \mathrm{~K}, \mathrm{P}^{\mathrm{i}}=0.1 \mathrm{MPa}$ to $P^{f}=0.25 \mathrm{MPa}$ by the following pathways. For each pathway, calculate the $\Delta \mathrm{U}, \Delta \mathrm{H}, \mathrm{Q}$ and W in $\mathrm{J} / \mathrm{mol}$.
(a) Isothermal
$\Delta \mathrm{U}$


Tries 0/99
$\Delta \mathrm{H}$
$\square$
Tries 0/99
Q

Tries 0/99
W

Tries 0/99
(b) Isochoric (constant volume)
$\Delta \mathrm{U}$

Tries 0/99

Energy Balance
$\Delta \mathrm{H}$
$\square$
Tries 0/99
Q
Tries 0/99
W

| Tries $0 / 99$ |
| :--- |

(c) Adiabatic
$\Delta \mathrm{U}$
Tries 0/99
$\Delta \mathrm{H}$
$\square$
Tries 0/99
Q

Tries 0/99
W

Tries 0/99

An adiabatic reversible pump is designed to take saturated water at 0.01 MPa and compress it to 7.5 MPa . What is the change in enthalpy of the water?
(Answer in $\mathrm{kJ} / \mathrm{kg}$ )
Tries 0/99
What is enthalpy of the water exiting the pump?
(Answer in $\mathrm{kJ} / \mathrm{kg}$ )
$\square$

Tries 0/99

Water vapor at 7 MPa and $550^{\circ} \mathrm{C}$ is expanded through an adiabatic turbine to a a pressure of 0.5 MPa . A temperature probe is used to record to temperature of then outlet stream and it is found to be $222^{\circ} \mathrm{C}$. What is the amount of shaft work that can be produced from the turbine? Make sure to enter the correct sign. The work interaction of the turbine will be negative, but the work produced will be positive. (Answer in $\mathrm{kJ} / \mathrm{kg}$ )
$\square$
Tries 0/99
combustion E-bal
There are fourteen parts to this problem. In the final part, you will calculate the heat transfer for the reactor.
The following combustion reaction occurs:
$\mathrm{CH}_{4(\mathrm{~g})}+2 \mathrm{O}_{2(\mathrm{~g})} \rightarrow \mathrm{CO}_{2(\mathrm{~g})}+2 \mathrm{H}_{2} \mathrm{O}_{(\mathrm{g})}$
The reactants enter at a temperature of $566^{\circ} \mathrm{C}$, and products exit at a temperature of $852^{\circ} \mathrm{C}$
$180 \mathrm{~mol} / \mathrm{h}$ of CH 4 and $495 \mathrm{~mol} / \mathrm{h}$ of O 2 are fed to the reactor, with a 0.82 conversion of CH 4 .
Assume that only vapor is present throughout the reactor, for ease of calculation purposes
Use the heat capacity polynomial equation for ALL specific heat calculations (Elliott and Lira Appendix E).
(a) First calculate the gas phase standard state heat of reaction ( $\mathrm{kJ} / \mathrm{mol}$ ) and enter it below. (Use values from Elliott and Lira appendix E).
$\qquad$
Tries 0/99

$\mathrm{P} 3=10 \mathrm{MPa}, \mathrm{P} 4=0.01 \mathrm{MPa}, \eta_{\mathrm{E}}=0.82, \eta_{\mathrm{C}}=0.87$. The output of the plant is to be 77 MW.
This problem will solve the Rankine cycle by stepping around the cycle. The 19 parts to this problem will be presented one-at-a-time.
(a) $\mathrm{T} 3=580^{\circ} \mathrm{C}$. What is the value for $\mathrm{S} 3(\mathrm{~kJ} / \mathrm{kg}-\mathrm{K})$ ? (Provide only the numerical answer.) Your answer must be within +-0.02 .

Tries 0/99


This problem is designed to accompany Introductory Chemical Engineering Thermodynamics, Elliott and Lira, Prentice-Hall, 2012. Some of the hints reference parts of the textbook.

This modified Rankine power cycle involves three turbines, an open and a closed feed water preheater, a condenser, a boiler/superheater, two pumps and a throttle. The schematic is shown above and in the the text book on page 206 Figure 5.6. In this problem, all of the turbines and the pump between streams 5 and 6 are considered reversible. You should be able to do balances around them if were not ideal however. There are 18 parts to the problem shown one-at-a-time but many of the steps will not take very long to solve.

The pressures and temperatures are given are $\mathrm{P}_{1}=10 \mathrm{MPa}, \mathrm{P}_{2}=4 \mathrm{MPa}, \mathrm{P}_{3}=2 \mathrm{MPa} . \mathrm{T}_{1}=528^{\circ} \mathrm{C}, \mathrm{T}_{8}=217^{\circ} \mathrm{C}, \mathrm{T}_{9}=$ $300^{\circ} \mathrm{C}$. Streams $\mathrm{m} 2, \mathrm{~m} 3$, and m 4 go into the top of the respective preheater/condenser.
(a) What is $\mathrm{P}_{10}(\mathrm{MPa})$ ?

Tries 0/99


Process Thermo

Consider the cycle above for this problem. The evaporator and condenser are run at 0.1 MPa and 0.6 MPa respectively. Streams 1 and 3 can be considered saturated, and the efficiency of the compressor is 0.8 . Use the questions below as a guide to solve the problem.

There are nine parts to this problem displayed one-at-a-time.
A) Click on where stream 1 is located on the PH diagram.


Tries 0/99

An economizer is used in the refrigeration cycle shown below. HFC-134a is to be the refrigerant. For the desired application, the condenser outlet is saturated at $50 \& d e g C$ the evaporator outlet is saturated at $-50 \& d e g C$. In this problem you will determine the cooling capacity of the evaporator and the corresponding heat load of the condenser for this cycle using a P-H diagram. Assume that the economizer operates at 0.3 MPa . Also assume that both compressors are reversible. The flow through the evaporator is $185 \mathrm{~kg} / \mathrm{h}$. Use a straight edge against the computer screen to read values, or print the figure for part (a) for markup and use it during subsequent parts.

This problem will solve the cycle. There are 12 parts to this problem displayed one-at-a-time.

a) Let us begin with the conditions in the economizer. For the conditions given in the problem statement, locate state 8 on the P-H diagram. Click on the image to indicate the location of your answer, then click submit.
../images/PH_R-134a.GIF
Tries 0/99

This problem applies the virial equation using the second virial coefficient. There are six parts to the problem displayed one-part-at-a-time.

Given the reduced pressure, $\operatorname{Pr}=\mathbf{0 . 9 2}$ and the reduced temperature, $\operatorname{Tr}=\mathbf{1 . 2 4 9 8 8}$ with respect to Ethanol.
First calculate the temperature of the system, $\mathbf{T}$ (K)

Tries 0/99

This problem is an answer sheet for an accompanying handout. The problem will help you understand how to use the textbook software for the Peng-Robinson equation of state. Follow the preliminary instructions on the handout. When you reach a certain point indicating that LON-CAPA (LC) input is needed, enter the values here. Within the handout, LC1 means LC question 1, LC2 means LC question 2, etc.

1. What is the quality if 1 mole of argon is in a volume of $1200 \mathrm{~cm}^{3}$ at the given conditions? Enter your answer as a fraction, use 0.1 for $10 \%$.
$\square$

Tries 0/99
2. For each part of problem 2, for argon, enter the value only without units.
2. (a) What is the stable volume $\left(\mathrm{cm}^{3} / \mathrm{mol}\right)$ for $\mathrm{T}=0.7^{*} \mathrm{Tc} ; \mathrm{P}=0.5^{*} \mathrm{Pc}$ ?

Based on size of Z and V , the stable root is:
A. Liquid
B. Vapor

Tries 0/99
2. (b) What is the stable volume $\left(\mathrm{cm}^{3} / \mathrm{mol}\right)$ for $\mathrm{T}=0.7^{*} \mathrm{Tc}, \mathrm{P}=0.2^{*} \mathrm{Pc}$ ?

Based on size of Z and V, the stable root is:
A. Vapor
B. Liquid

Tries 0/99
2. (c) What is the stable volume $\left(\mathrm{cm}^{3} / \mathrm{mol}\right)$ for $\mathrm{T}=1.5^{*} \mathrm{Tc}, \mathrm{P}=0.5^{*} \mathrm{Pc}$ ?

Based on size of Z and V , the stable root is:
A. Liquid
B. Vapor

Tries 0/99
3. What is the value of Z for CO 2 at 298.15 K and 1 bar? $\square$
Tries 0/99
4. What is the maximum $\mathrm{P}(\mathrm{MPa})$ where $\mathrm{Z}>0.95$ at 298.15 K ? $\square$
Tries 0/99
5. What enthalpy value (after adjusting the reference state) is found at the state of problem $4(\mathrm{~J} / \mathrm{mol})$ ?
$\square$
Tries 0/99
6. For CO 2 at 0.8 MPa , at what $\mathrm{T}(\mathrm{K})$ is $\mathrm{H}=0$ ?

Tries 0/99
7. What CO 2 vapor pressure ( MPa ) is found at 170 K ? Enter the value only (no units). $\square$
Tries 0/99
8. What is the CO 2 saturation $\mathrm{T}(\mathrm{K})$ at 0.1 MPa ? Enter the value only (no units). $\square$
Tries 0/99

The compressibility factor provides a quick way to assess when the ideal gas law is valid. Modify the objective function calculation developed in the class excercise. Write a solver statement that find the minimum temperature where the fluid has a gas phase compressibility factor greater than 0.95 at 30 bar. Report the value in K , without units.
(a) Nitrogen
$\square$
Tries 0/99
(b) Carbon dioxide
Tries $0 / 99$
(c) Ethanol
$\square$
Tries 0/99

The compressibility factor provides a quick way to assess when the ideal gas law is valid. Use a solver to find the minimum temperature where the fluid has a vapor phase compressibility factor greater than 0.95 at 3 MPa . Report the value in ${ }^{\circ} \mathrm{C}$, without units.
(a) methane


Tries 0/99
(b) ethylene
$\square$
Tries 0/99
(c) ethanol
$\square$

Tries 0/99

Use the Peng-Robinson EOS to answer this problem.
What are the molar volumes $\left(\mathrm{cm}^{3} /\right.$ mole) for the physically realistic stable root of $n$-Hexane gas at the given conditions? Note: Some mathematical solutions to the cubic may not be physically realistic.
a) $\mathrm{T}=400 \mathrm{~K}$ and $\mathrm{P}=0.2 \mathrm{MPa}$

Tries 0/99
b) $\mathrm{T}=400 \mathrm{~K}$ and $\mathrm{P}=1 \mathrm{MPa}$
$\square$

Tries 0/99
b) $\mathrm{T}=400 \mathrm{~K}$ and $\mathrm{P}=100 \mathrm{MPa}$

Tries 0/99
b) $\mathrm{T}=400 \mathrm{~K}$ and $\mathrm{P}=130 \mathrm{MPa}$

Tries 0/99
b) $\mathrm{T}=400 \mathrm{~K}$ and $\mathrm{P}=150 \mathrm{MPa}$

Consider two identical moving particles interacting with square-well potential energy. Suppose they are in the potential energy well, moving away from each other. The minimum speed required for a successful well escape depends on the angle between the relative position and relative velocity. The minimum speed required for well escape occurs when the relative velocity is colinear with the vector between centers. In the cases below, the relative speed required to escape will be smaller for configuration (a) compared to (b). This problem asks you to quantify the behavior and calculate the velocity changes for the escape event.


We can develop the velocity vector using speed to denote magnitude together with a unit vector to denote direction. Then the relative velocity is $\mathrm{v}_{21}=\mathrm{v}_{21, \text { speed }}\left[\mathrm{v}_{\mathrm{x}}, \mathrm{v}_{\mathrm{y}}\right]$, where $1=\mathrm{v}_{\mathrm{x}}{ }^{2}+\mathrm{v}_{\mathrm{y}}{ }^{2}$. For case (a) above, $\mathrm{v}_{21}=\mathrm{v}_{21 \text {,speed }}[1,0]$. For case (b), if $\mathrm{v}_{21}$ is at $45^{\circ}$ relative to the x -axis, then $\mathrm{v}_{21}=\mathrm{v}_{21 \text {,speed }}[\cos (45), \sin (45)]=\mathrm{v}_{21 \text {,speed }}[0.7071,0.7071]$.

Parameters the particles are ( k is Boltzmann's constant):
$\sigma_{21}=3.9400 \times 10^{-10} \mathrm{~m}$
$\lambda_{21}=1.535$
$\mathrm{m}_{2}=\mathrm{m}_{1}=7.0905 \times 10^{-23} \mathrm{~g}$
$\epsilon_{21} / \mathrm{k}=121.6 \mathrm{~K}$
(a) The relative velocity is along the x-axis. What is the magnitude of the speed (Angstroms/ps) necessary for a well escape?
$\square$
Tries 0/99
(b) The relative velocity is oriented along the angle 40.2 degrees. What is the magnitude of the speed (Angstroms/ps) necessary for a well escape?

Tries 0/99
(c) For case (a), what is the change in velocity (Angstroms/ps) upon well escape for particle 2? Enter the answer as a vector with the components in the order $\mathrm{x}, \mathrm{y}$.

(d) For case (b), what is the change in velocity (Angstroms/ps) upon well escape for particle 2? Enter the answer as a vector with the components in the order $\mathrm{x}, \mathrm{y}$.
$\square$
Tries 0/99

Which statements are true?

## Choices: True, False.

- For a state change from 1 to 2 , the ideal gas state change is added to the departure of state 1 and the departure of state2 is subtracted.
- Quality calculations are probably no longer important because the equation of state calculates quality when three roots exist.
- The ideal gas calculation is a fundamental part of a state change calculation using departure functions.
- The departure for almost any equation of state would be evaluated using a density integral.


## Tries 0/99

A new experimental refigerant changes state from
$\mathrm{T}_{1}=305 \mathrm{~K}, \mathrm{P}_{1}=5 \mathrm{MPa}$ to
$\mathrm{T}_{2}=395 \mathrm{~K}, \mathrm{P}_{2}=5 \mathrm{MPa}$.
The departure functions at the two states are
$\left(\mathrm{H}-\mathrm{H}^{\mathrm{ig}}\right)_{1}=-2798 \mathrm{~J} / \mathrm{mol}$,
$\left(\mathrm{H}-\mathrm{H}^{\mathrm{ig}}\right)_{2}=-1477 \mathrm{~J} / \mathrm{mol}$.
Assuming a T-independent ideal gas heat capacity, $\mathrm{Cp}=4.456^{*} \mathrm{R}$, what value of $\Delta \mathrm{H}(\mathrm{J} / \mathrm{mol})(+-2 \%)$ results from a hand calculation? Give your answer without units.

Tries 0/99

This problem applies the Peng-Robinson equation of state to an adiabatic compressor.
(a) Using the Peng-Robinson equation of state, calculate the work needed in ( $\mathrm{kJ} / \mathrm{mol}$ ) for a reversible adiabatic compression of gaseous FREON-12, a refrigerant, from a pressure of 0.15 MPa and temperature of 450 K to a pressure of 2 MPa .
$\square$
Tries 0/99
(b) What is the work needed $(\mathrm{kJ} / \mathrm{mol})$ if the compressor efficiency is $\eta_{\mathrm{C}}=0.82$ ?

Tries 0/99

This problem uses the Peng-Robinson property calculator to evaluate the inlet/outlets of a heat exchanger and find the molar flow ratio of stream B to stream A. The stream A consists of water and is at a pressure of 0.24 MPa and it enters at 724 K and leaves at 526 K . Stream B is carbon dioxide at a pressure of 4.1 MPa and enters at a temperature of 415 K and exits at 451 K . The reference state is the real fluid equilibrium state of aggregation at $298.15 \mathrm{~K}, 0.1 \mathrm{MPa}$.

Note: One of your specified streams may be water. The Peng-Robinson EOS is not particularly accurate for water, but if you are assigned water, you are asked here to use the Peng-Robinson EOS as a learning tool for an approximate calculation.

A) What is the enthalpy of water entering the heat exchanger in stream $\mathrm{A}(\mathrm{J} / \mathrm{mol})$ ?
$\square$

Tries 0/99
B) What is the enthalpy of water exiting the heat exchanger in stream $A(\mathrm{~J} / \mathrm{mol})$ ?
$\square$
Tries 0/99
C) What is the enthalpy of carbon dioxide entering the heat exchanger in stream $\mathrm{B}(\mathrm{J} / \mathrm{mol})$ ?
$\qquad$
Tries 0/99
D) What is the enthalpy of carbon dioxide exiting the heat exchanger in stream $\mathrm{B}(\mathrm{J} / \mathrm{mol})$ ?
$\qquad$
Tries 0/99
E) Using an energy balance, what is the molar ratio of stream B to stream A?
$\square$
Tries 0/99

This problem considers a turbine/expander modeled with the Peng-Robinson equation of state.
(a) Using the Peng-Robinson EOS, calculate the change in enthalpy ( $\mathrm{kJ} / \mathrm{mol}$ ) for a reversible turbine/expander when nitrogen gas is expanded from a pressure of 5 MPa and temperature of 600 K to a pressure of 2 MPa . Remember to use the correct sign.

Note: If you are assigned water, the Peng-Robinson is not particularly accurate, but use it as an approximate calculation.


Tries 0/99
(b) What is the change in enthalpy ( $\mathrm{kJ} / \mathrm{mol}$ ) if the turbine's efficiency is $\eta_{\mathrm{E}}=0.88$ ? Remember to use the correct sign.
$\qquad$
Tries 0/99

This problem considers a turbine/expander using the Peng/Robinson equation of state.
(a)Using the Peng-Robinson equation of state, calculate the change in enthalpy ( $\mathrm{J} / \mathrm{mol}$ ) for a reversible turbine/expander when steam is expanded from a pressure of 8 MPa and temperature of 700 K to a pressure of 1 MPa. Remember to use the correct sign. Use a reference state $H_{R}=0$ for a real fluid in the most stable state of aggregation at 298.15 K and 0.1 MPa . (Note that the Peng-Robinson is only semi-quantitative for water, so the results will differ slightly from steam table calculations.)
$\square$
Tries 0/99
What is the change in enthalpy in $(\mathrm{J} / \mathrm{mol})$ if the turbine/expander efficiency is $\eta_{\mathrm{E}}=0.8$ ? Remember to use the correct sign.

Tries 0/99

This problem asks you to calculate bubble pressure for a ternary mixture. There are three parts to this problem. Parts will be displayed one part at a time.

Concentrations: 1-propanol: 0.4 , ethanol: 0.3 , 1-butanol: 0.3
Antoine Coefficients:
1-propanol: A: 8.37895, B: 1788.02, C: 227.438
ethanol: A: 8.1122, B: 1592.864, C: 226.184
1-butanol: A: 7.81028 , B: $1522.56, \mathrm{C}: 191.95$
(a) Calculate the vapor pressures for 1-propanol, ethanol, and 1-butanol, respectively, using the Antoine Equation at $40^{\circ} \mathrm{C}$.

Psat for 1-propanol: $\qquad$
Psat for ethanol: $\square$
Psat for 1-butanol: $\square$
Tries 0/99

This problem asks for the bubble temperature and K-ratios using Raoult's law. There are three parts to this problem, displayed one part at a time.

Antoine Coefficients $\log 10(\operatorname{Psat}(\mathrm{mmHg}))=\mathrm{A}-\mathrm{B} /\left(\mathrm{T}\left({ }^{\circ} \mathrm{C}\right)+\mathrm{C}\right)$ :
1-butanol: A: 7.81028, B: 1522.56, C: 191.95
ethanol: A: 8.1122 , B: 1592.864, C: 226.184
1-propanol: A: 8.37895, B: 1788.02, C: 227.438
Using the Antoine coefficients given, check your programming of vapor pressure by calculating the VLE K-ratio for each component at at 700 mmHg and $95.4^{\circ} \mathrm{C}$. Provide three significant figures.

1-butanol: $\square$
ethanol: $\square$

1-propanol:
Tries 0/99

This problem asks you to determine dew pressure using Raoult's law. There are four parts to this problem, presented one-at-a-time.
(a) Using Antoine's equation, calculate the vapor pressures of methanol, 2-propanol, and 1-propanol at 45\&degC in mmHg . Use five significant digits.

Antoine Coefficients for Psat in mmHg :
methanol: A: 8.08097, B: 1582.271, C: 239.726
2-propanol: A: 8.87829, B: 2010.33, C: 252.636
1-propanol: A: 8.37895 , B: 1788.02 , C: 227.438
methanol: $\qquad$

2-propanol: $\qquad$
1-propanol: $\square$
Tries 0/99

This problem consists of three parts asked one-at-a-time.
(a) Using the Antoine coefficients given, calculate the dew temperature (\&degC) at 630 mmHg for 2-propanol, ethanol, and 1-propanol with their respective vapor compositions: $0.25,0.4$, and 0.35 . Use four significant figures.

Antoine Coefficients for Psat in ( mmHg ) :
2-propanol: A: 8.87829 , B: 2010.33, C: 252.636
ethanol: A: 8.1122, B: 1592.864, C: 226.184
1-propanol: A: 8.37895, B: 1788.02, C: 227.438
Dew temperature (\&degC): $\square$
Tries 0/99

This problem has two parts. The problem involves solving an isothermal flash drum. Ethyl Acetate, 1-Butanol, and Dichloroethane enter a flash drum maintained at $95^{\circ} \mathrm{C}$ and 1220.3 mm Hg with overall mole fractions of $0.288,0.181$, and 0.531 , respectively. Antoine coefficients A, B, C (for mmHg ) are:

Ethyl Acetate, 7.01461211 .9216 .01
1-Butanol, 7.47681362 .39178 .73
Dichloroethane, 7.08031138 .91231 .45
(a) What are the vapor pressures $(\mathrm{mmHg})$ at $95^{\circ} \mathrm{C}$ ? Use five significant figures.

Ethyl Acetate:
1-Butanol: $\square$
Dichloroethane:
Tries 0/99
(b) What is the VOF (vapor over feed) ratio in the drum? Use at least two decimal places.
$\square$
Tries 0/99

This problem concerns fitting the two-parameter Margules equation to a single measurement and then generating a predicted bubble pressure at a new composition. The problem has eight parts that will be asked one-at-a-time.

A phase equilibria experiment with chloroform (1) $+1,4$-dioxane (2) has been performed with the following measurements.
$\mathrm{P}=19.3 \mathrm{kPa}, \mathrm{x}_{1}=0.1757, \mathrm{y}_{1}=0.3302$.
Vapor pressures are $\mathrm{P}_{1}{ }^{\text {sat }}=69.36 \mathrm{kPa}, \mathrm{P}_{2}{ }^{\text {sat }}=15.79 \mathrm{kPa}$.
(a) At the given experimental measurements, what is $\gamma_{1}$ ?
$\square$
Tries 0/99

This excercise is to create a bubble pressure calculation first using Raoult's law and then generalize the result using Modified Raoult's law. This repeats the calculations of Example 11.2, and creates a figure like Figure 11.5.

These lines are for your reference, to remind you of the relations.
Raoult's Law - y_i * $\mathrm{P}=\mathrm{x} \_i$ * (Psat_i)
Modified Raoult's Law - y_i ${ }^{*} \mathrm{P}=\mathrm{x}$ _i ${ }^{*}$ (gamma_i) ${ }^{*}$ Psat_i
Open Excel/Actcoeff.xlsx and move to the 'Margules' tab.
Right-click the tab, select 'Move or Copy'. Create a new copy in a New workbook.
Save the new copy as 'Margules.xlsx' and close 'Actcoeff.xlsx'.
Clean up the variable names with the following procedure.
The spreadsheet holds many variables that had a Workbook scope. We won't need them anymore.
On Windows:
From the Formulas Ribbon->Name Manager dialog box, click the 'Refers To' header to sort and then delete all references that do not start with "=Margules...".
On Mac:
The steps depend on the excel version:
(1) PC and (MAC 2016): Formula $>$ Define Name
(2) MAC 2008 and 2011: Insert $>$ Name $>$ Define

You will need to scroll through the list. Look in the bottom 'Refers To:' text line, and delete all references that do not start with "=Margules...".
(Note that the original spreadsheet is quite old and some variables were created before Excel provided the capability to control variable scope. Even in Windows Excel 2013, there is not a good capability to edit the variable scope.)
Now, close all dialog boxes and use the name dropdown to browse through the remaining named ranges on the worksheet.

Copy the following table of Antoine Constants and paste into your sheet above the composition table. If the data don't paste in columns, convert the text to columns (Data Ribbon). Be careful to edit the values so that they are numerical. You must check each entry for white spaces before and after the digits. Though numbers are usually right-justified, this is not a sufficient criteria to evaluate if the digits have not white space surrounding them. The most common problem with vector mathematical formulas is that any single entry that is non-numeric will cause unexpected values, and not necessarily a !NUM error.

|  | 2-prop | water |
| :--- | :--- | :--- |
| A | 8.87829 | 8.07131 |
| B | 2010.33 | 1730.63 |

## C $\quad 252.636 \quad 233.426$

Next, we will set up name definitions that will permit us to us vectors for vapor pressure. Select both columns for row A, and name the cells 'A.' (with the period and without quotes). Select both columns for row B and C and name 'B.', 'C.' respectively. Thus A., B., and C. are vectors.

Create, label ( T will be in Celsius), and name ( T ) a cell to hold the temperature anywhere in the header space except directly below the Antoine table. Enter the temperature, 30, in Celsius.

Next we will create a vector of the vapor pressures in the row below the Antoine coefficient C.
Immediately below C, add the label 'Psat'.
Select BOTH cells below C..
Enter in the formula bar
$=10^{\wedge}$ (A. - B. $\left./(\mathrm{T}+\mathrm{C}).\right)$
and HOLD CNTL+SHIFT while you press enter.
The result should be vapor pressures of 58.3 and 31.7 mmHg respectively.

Now, let us create a Pxy plot for Raoult's law.
Select H10:H30.
Enter in the formula bar
$=\mathrm{x} 1 \_$* $\operatorname{INDEX}($ Psat, 1$)+\mathrm{x} 2 \_$* $\operatorname{INDEX}($ Psat, 2$)$
and use Cntrl+Shift+Enter because this is a vector/matrix equation. Notice how Psat(1) and Psat(2) are referenced as part of the Psat vector.

LON-CAPA, part (a), enter the Raoult's Law bubble pressure for $\mathrm{x} 1=0.7$.
Next calculate y1_RL for Raoult's law in I10:I:30. To use vector notation select I10:30 and enter, $=x 1 \_$*INDEX(Psat,1)/H10:H30, remembering to use Cntl+Shift+Enter.
At $\mathrm{x} 1=0.5$ you should get $\mathrm{y} 1=0.647$. (Note that you could name H10:H30 as P_RL and use the name instead of the vector reference.

LON-CAPA, part (b), enter the y 1 for $\mathrm{x} 1=0.7$.
Create a P-x-y plot for Raoult's law as a separate sheet. Label the coordinates.
Congratulations! you have completed Raoult's law.
Now we will use Modified Raoult's law. To mimic the textbook example, look at the top of the worksheet where the Margule parameters are tabulated. set the Margules paramters $\mathrm{A} 12=\mathrm{A} 21=1.42$. The value of gamma at the equimolar composition should be 1.426.

LON-CAPA part (c), what is gamma1 for $\mathrm{x} 1=0.7$ ?
Select J10:J30 and enter the following formula to calculate the bubble pressure for Modified Raoult's Law,
$=\mathrm{x} 1 \_$*gamma1_*INDEX $($Psat, 1$)+\mathrm{x} 2 \_{ }^{*}$ gamma $2 \_{ }^{*} \operatorname{INDEX}($ Psat, 2$)$
At the equimolar composition you should find $\mathrm{Pbub}=64.19 \mathrm{mmHg}$.
LON-CAPA part (d), what is Pbub for $\mathrm{x} 1=0.7$, Modified Raoult's Law?
Add a column to calculate y 1 . At the equimolar composition you should find $\mathrm{y} 1=0.6474$.
LON-CAPA part (e), for $\mathrm{x} 1=0.7$, what is y 1 for Modified Raoult's Law?
Add the MRL P-x-y lines to your plot. Your plot should look like the dashed line in Fig 11.5, except it is shifted slightly because the Antoine Psat for isopronaol does not agree exactly with the experimental data. If you want to override Antoine's equation use $\operatorname{Psat}(1)=60.7 \operatorname{Psat}(2)=32.1$.

Add experimental data to the plot by pasting the following table into excel.
$\begin{array}{lllllllllllllll}\mathrm{x} 1, \text { expt } & 0 & 0.0015 & 0.0111 & 0.0231 & 0.0357 & 0.0649 & 0.1168 & 0.197 & 0.2271 & 0.312 & 0.3958 & 0.4477 & 0.5009 & 0.6369\end{array} 0.7542 \quad 0$. $\begin{array}{llllllllllllllllll}\text { y1,expt } & 0 & 0.0254 & 0.1374 & 0.2603 & 0.3577 & 0.4604 & 0.5316 & 0.5547 & 0.5611 & 0.5659 & 0.5907 & 0.589 & 0.6098 & 0.6462 & 0.7296\end{array}$
$\begin{array}{lllllllllllllllllll}\text { Pexpt } & 32.1 & 33.8 & 37.1 & 42.3 & 47.2 & 55 & 60.3 & 62.9 & 63.5 & 64.4 & 65.1 & 65.8 & 66.6 & 66.9 & 66.8 & 65.7 & 63.2 & 60.7\end{array}$
Always follow conventions by using symbols for experimental data and lines for calculations.

This problem is a multipart problem for the in-class exercise to recreate Figure 11.5. The instructions indicate when to enter responses into LON-CAPA.
(a) What is the bubble pressure at $\mathrm{x} 1=0.7$ for Raoult's Law?

Tries 0/99
(b) What is y 1 at $\mathrm{x} 1=0.7$ for Raoult's Law?
$\square$

Tries 0/99
(c) What is gamma1 at $\mathrm{x} 1=0.7$ ?


Tries 0/99
(d) What is Pbub at $\mathrm{x} 1=0.7$ for Modified Raoult's law?
$\square$

Tries 0/99
(e) What is y 1 at $\mathrm{x} 1=0.7$ for Modified Raoult's law?
$\square$
Tries 0/99

This problem is going to walk you through using the Two-Parameter Margules equation to calculate the bubble temperature. Consider a binary mixture of component (1) + component (2). Vapor pressures using $\log 10(\mathrm{P}(\mathrm{mmHg}))$ $=\mathrm{A}-\mathrm{B} /(\mathrm{T}($ Celsius $)+\mathrm{C})$ for component (1) and component (2) are tabulated below.

|  | component (1) | component (2) |
| :--- | :--- | :--- |
| A | 7.20131 | 8.36605 |
| B | 1157 | 2170.24 |
| C | 168.279 | 205.921 |

(a) What is the vapor pressure $(\mathrm{mmHg})$ of component (1) at $24^{\circ} \mathrm{C}$ ?
$\square$
Tries 0/99
(b) What is the vapor pressure $(\mathrm{mmHg})$ of component (2) at $24^{\circ} \mathrm{C}$ ?
$\square$

Tries 0/99
(c) An experiment with a mixture of component (1) and component (2) was performed, resulting in $\mathrm{A}_{12}=-0.19$ and $\mathrm{A}_{21}=0.36$. At a mole fraction of component (1) of $\mathrm{x}(1)=0.94$, what is $\gamma_{1}$ ?
(d) At a mole fraction of component (1) of $\mathrm{x}(1)=0.94$, what is $\gamma_{2}$ ?
$\square$
Tries 0/99
(e) What is the bubble temperature $\left({ }^{\circ} \mathrm{C}\right)$ of a mixture of the two components if the mole fraction of component (1) is $\mathrm{x}(1)=0.94$, when the pressure of the system is 63.4 mm Hg ?

Tries 0/99
(e) What is the mole fraction of component (1) in the vapor phase, $\mathrm{y}(1)$ ?

Tries 0/99

This problem concerns dew pressure calculations.

## Choices: True, False.

- A good way to do a dew calculation is to use a 'while' loop and iterate until the liquid composition quits changing within an acceptable tolerance.
- A good way to do a dew pressure calculation is to write a 'while' loop and iterate until the vapor composition quits changing within an acceptable tolerance.
- For modified Raoult's Law, it is a good idea to set gamma_i $=1$ for both components for the first guess.


## Tries 0/99

## Choices: True, False.

- A good way to do a dew pressure calculation is to write a 'while' loop and iterate until the vapor composition quits changing within an acceptable tolerance.
- For Modified Raoult's Law, the dew pressure is iterative.
- A good way to do a dew calculation is to use a 'while' loop and iterate until the liquid composition quits changing within an acceptable tolerance.


## Tries 0/99

Choices: True, False.

- A good way to do a dew calculation is to use a 'while' loop and iterate until the liquid composition quits changing within an acceptable tolerance.
- For modified Raoult's Law, it is a good idea to set gamma_i = 1 for both components for the first guess.
- A good way to create an iterative loop for dew pressure is to write a 'for' loop and execute it a large number of times, e.g. 50.

Tries 0/99

## Choices: True, False.

- A good way to do a dew calculation is to use a 'while' loop and iterate until the liquid composition quits changing within an acceptable tolerance.
- For Modified Raoult's Law, the dew pressure is iterative.
- A good way to create an iterative loop for dew pressure is to write a 'for' loop and execute it a large number of times, e.g. 50.

This problem will walk you through a dew pressure calculation for a binary mixture of component (1) + component (2) using two parameter Margules equation. Antoine coefficients for $\log 10(\mathrm{P}(\mathrm{mmHg}))=\mathrm{A}-\mathrm{B} /(\mathrm{T}(\mathrm{Celsius})+\mathrm{C})$ are:

|  | component (1) | component (2) |
| :--- | :--- | :--- |
| A | 7.44 | 7.26475 |
| B | 1843.12 | 1434.148 |
| C | 230.22 | 246.721 |

(a)What is the vapor pressure ( mmHg ) of component (1) at a temperature of $114^{\circ} \mathrm{C}$ ?
$\square$
Tries 0/99
(b)What is the vapor pressure $(\mathrm{mmHg})$ of component (2) at $114^{\circ} \mathrm{C}$ ?
$\square$
Tries 0/99
(c) For a vapor mole fraction of $y(1)=0.02$ at $114^{\circ} \mathrm{C}$, what is the dew point pressure of the mixture assuming Raoult's law in mm Hg ?
$\square$
Tries 0/99
(d) We will use Raoult's law for an initial guess of the liquid phase compositions of components 1 and 2 . What is the liquid mole fraction of component 1 from Raoult's law dew pressure at $114^{\circ} \mathrm{C}$, if $\mathrm{y}(1)=0.02$ ?
$\qquad$
Tries 0/99
(e) In an experiment, the two-parameter Margules parameter values are determined to be $\mathrm{A}_{12}=0.69$ and $\mathrm{A}_{21}=0.29$.

Set up a loop to figure out the real liquid phase composition, until the change in current and previous values of x 1 is less than 0.0001 for two consecutive calculations.

For modified Raoult's law, for $\mathrm{y}(1)=0.02$, what is the dew point pressure at $114^{\circ} \mathrm{C} ?(\mathrm{~mm} \mathrm{Hg})$

Tries 0/99
(f) What is the composition of component $x(1)$ in the liquid phase at $114^{\circ} \mathrm{C}$ ?

Tries 0/99
(g) For the value of $x(1)$ above, what is $\gamma_{1}$ ?

Tries 0/99
(h) For the value of $\mathrm{x}(1)$ above, what is $\gamma_{2}$ ?
$\square$
Tries 0/99

This problem concerns fitting the two-parameter Margules equation to a single measurement and then generating a predicted bubble pressure at a new composition. The problem has eight parts that will be asked one-at-a-time.

A phase equilibria experiment with diethyl ketone (1) + n-hexane (2) has been performed with the following measurements.
$\mathrm{P}=62.95 \mathrm{kPa}, \mathrm{T}=338.15 \mathrm{~K}, \mathrm{x}_{1}=0.702, \mathrm{y}_{1}=0.368$.
Vapor pressures are $\mathrm{P}_{1}{ }^{\text {sat }}=29 \mathrm{kPa}, \mathrm{P}_{2}{ }^{\text {sat }}=90.15 \mathrm{kPa}$.
(a) At the given experimental measurements, what is $\gamma_{1}$ ?

Tries 0/99

Pick the best response. The primary advantage of providing activity model calculations in a single folder is:
A. It is a good idea to put a copy of the provided .m files into folders where gamma calculations are needed.
B. The example code in the provided folder can be copied and pasted into user .m files.
C. It is a good idea to write my own gamma calculations and use the provided examples to test my code.
D. By calling the routines in the provided folder properly from any Matlab routine anywhere on the computer, errors can be avoided in calculating gammas.

Tries 0/2

If a component has negative deviations from Raoult's law, then for the same component:
A. The Henry's law activity coefficient will be less than or equal to one.
B. The Henry's law activity coefficient will approach one when the Henry's law component is pure.
C. The Henry's law activity coefficient for will be greater than or equal to one.
D. Nothing can be assured about the size of the Henry's law activity coefficient.

Tries $0 / 2$
If the Lewis-Randall (L-R) activity coefficients are known for a binary system, then for the component to be modeled with Henry's law,
A. The Henry's law activity coefficient will differ from the L-R gamma for the same component in a complicated way.
B. The Henry's law activity coefficient will be the negative of the L-R gamma for the same component.
C. The slope of the Henry's law activity coefficient will be the same as the slope of the L-R gamma for the other component.
D. The curvature of the Henry's law activity coefficient will be exactly the same as the curvature of the L-R gamma for the same component.

Tries 0/2

Take this quiz after watching the screencasts on osmotic pressure.

## Choices: True, False.

- If a fluid is pure on one side of a semi-permeable membrane that only the fluid can pass through and a mixture is on the other side of the membrane, then at equilibrium, the pressure will be higher on the side with a mixture.
- Osmotic pressure occurs when at least one one component can not pass through a membrane but some other components can.
- Osmotic pressure occurs when all components can pass through a membrane, but some pass through faster than others.
- Water and a protein are on one side a semi-permeable membrane and pure water is on the other side. The sides are at equilibrium, and the pure water side is open to constant atmospheric pressure. Salt is added to the side initially with pure water and the pressure on the salt side is constant. Neither salt or protein can pass through the membrane. Some water will flow from the salt side to the protein side.


## Tries 0/99

## Choices: True, False.

- Fluid species (1) is pure on one side of a semi-permeable membrane that only species (1) can pass through. If a mixture with species (1) and (2) is on the other side of the membrane, then at equilibrium, the pressure will be higher on the side with a mixture.
- Water and a protein are on one side a semi-permeable membrane and pure water is on the other and the system is at equilibrium. The pure water side is open to constant atmospheric pressure. Salt is added to the side initially with pure water and the pressure on the salt side is constant. Neither salt or protein can pass through the membrane. Some water will flow from the salt side to the protein side.
- The ideal gas law can be used to calculate osmotic pressure.
- Osmotic pressure occurs when at least one one component can not pass through a membrane but some other components can.


## Tries 0/99

Which lists of models are in historical order (oldest first)?
Choices: True, False.

- van Laar, Scatchard-Hildebrand, Flory-Huggins
- Flory, Flory-Huggins, van Laar
- Scatchard-Hildebrand, Flory, van Laar
- Scatchard-Hildebrand, Flory, Flory-Huggins
- None of the other choices are true.
- Flory, van Laar, Scatchard-Hildebrand
- van Laar, Flory, Scatchard-Hildebrand

Tries 0/99

This model uses the van der Waals equation to develop the functional form, but uses two adjustable parameters instead of the values predicted by the van der Waals equation.

## Choices: True, False.

- Flory-Huggins
- van Laar
- Flory
- Scatchard-Hildebrand

Tries 0/99

This model was developed for mixtures of monomer plus polymer built from the same monomer. For such model, you would expect the energetic differences between species to be zero, and only size/shape effects to be important.

Choices: True, False.

- Flory
- van Laar
- Flory-Huggins
- Scatchard-Hildebrand

Tries 0/99

This model includes a term to represent excess entropy due to size differences.

## Choices: True, False.

- Flory
- van Laar
- Scatchard-Hildebrand
- None of the other choices are true.
- Flory-Huggins

Tries 0/99

This model is used frequently in the polymer field.
Choices: True, False.

- Flory
- Scatchard-Hildebrand
- Flory-Huggins
- van Laar
- None of the other choices are true.

Tries 0/99

This model uses the van der Waals equation to develop the functional form, but uses the experimental energy of vaporization and the liquid volume to predict the excess Gibbs energy.

## Choices: True, False.

- Flory
- van Laar
- Scatchard-Hildebrand
- Flory-Huggins

Tries 0/99

This model was the first to use solubility parameters.

## Choices: True, False.

- Flory
- Flory-Huggins
- Scatchard-Hildebrand
- van Laar

Tries 0/99

This model uses volume fractions in the calculation of the excess Gibbs Energy.

## Choices: True, False.

- van Laar
- Flory-Huggins
- Scatchard-Hildebrand
- Flory

Tries 0/99

Which model(s) use three adjustable parameters for each binary system?

## Choices: True, False.

- NRTL
- UNQUAC
- Wilson
- UNIFAC

Tries 0/99
Which model(s) provide activity coefficient predictions without fitting to experimental data?

Choices: True, False.

- UNIFAC
- NRTL
- UNQUAC
- Wilson

Tries 0/99
Which model(s) include the Flory equation as part of the activity coefficient expression?

## Choices: True, False.

- NRTL
- UNQUAC
- Wilson
- UNIFAC

Tries 0/99
Which model(s) are unable to model liquid-liquid equilibria?

## Choices: True, False.

- UNQUAC
- Wilson
- NRTL
- UNIFAC

Tries 0/99

This problem considers LLE for the butanol + water system. There are 13 parts to this problem presented one-at-atime.

N-butanol and water are partially miscible. One phase is approximately $96 \mathrm{~mol} \%$ water. The bubble temperature of a liquid mixture of n-butanol and water containing $96 \mathrm{~mol} \%$ water is $92.7^{\circ} \mathrm{C}$ at 1 bar.

At $92.7^{\circ} \mathrm{C}$ the vapor pressure of pure water is 0.776 bar and that of pure n-butanol is 0.380 bar. There are parts a m for this problem.
(a) Assuming the activity coefficient of water in the $96 \mathrm{~mol} \%$ water solution is near unity, what is the partial pressure of water (bar)?

Tries 0/99

This problem asks you to create and analyze the bow tie for preliminary distillation design using residue curves. The display should update with each submission. You should be able to drag and place the points when prompted. If the background image is not reloading properly on your browser, use a different browser.

Be patient because there is a delay while the Geogebra content loads after the page loads. Wait until Geogebra loads before clicking or scrolling.

Below is a residue curve diagram at 1 atm for methanol(1) + ethanol(2) + benzene(3). Temperature of the following points will be helpful: $(0.6,0), \mathrm{T}=59.85 \mathrm{C} ; ;(1,0), \mathrm{T}=64.5 \mathrm{C} ;(0,1), \mathrm{T}=78.3 \mathrm{C} ;(0,0), \mathrm{T}=80.1 \mathrm{C}$. You will be asked to analyze the diagram in several questions below. Drag the blue-dotted points on the diagram as instructed on each question and then click "Submit Answer" for each corresponding question. Instead of dragging the dots, you may enter digits in the numerical response boxes.

1. Based on the number of regions, how many azeotrope(s) are on the graph?

## Tries 0/99

2. Which of the following binaries have an azeotrope?

Choices: True, False.

- Ethanol - Methanol
- Benzene - Ethanol
- Methanol - Benzene

Tries 0/99
3. Drag point B to the origin of the residue curve lines and click 'Submit Answer.'

Point B Coordinates (x, y):


Tries 0/99
4. Using the given feed point F1 on the graph, what is the mole fraction of ETHANOL in the feed?


Tries 0/99
5. What is the mole fraction of BENZENE present in the same feed?


Tries 0/99
6. What is the mole fraction of METHANOL present in the same feed?
7. Using lines DE and FG, draw lines to connect the boundary of operation for the given feed composition. NOTE: Drag and drop the points one at a time and submit answer for each point dragged.

For the given feed, locate the highest boiling point in the region as one limit of operation. Point $\mathrm{D}(\mathrm{x}, \mathrm{y})$ : $\square$
$\square$
Tries 0/99
Locate the end of the line DE along which the other end of the column must operate. Point E ( $\mathrm{x}, \mathrm{y}$ ): $\square$
$\square$
Tries 0/99
For the given feed, locate the lowest boiling point in the region as one limit of operation. Point $\mathrm{F}(\mathrm{x}, \mathrm{y})$ : $\square$
$\square$
Tries 0/99
Locate the end of the line FG along which the other end of the column must operate. Point G (x, y): $\square$
$\square$ Tries 0/99
8. Use triangle KLM to identify the "top" region of operation. Start by placing point K on the feed and subsequent points alphabetically in a clockwise direction.


Tries 0/99
L $\qquad$
Tries 0/99
$\mathrm{M} \square \square$
Tries 0/99
9. Use triangle NOP to identify the "bottom" region of operation. Start by placing point N on the feed and subsequent points alphabetically in a clockwise direction.
$\mathrm{N} \square \square$
Tries 0/99
$\mathrm{O} \square \square$
Tries 0/99


Tries 0/99

In the cracking reaction below, propane is converted to ethylene and methane. Side reactions can be ignored at pressures up to 1 bar and assume ideal gas.
$\mathrm{C}_{3} \mathrm{H}_{8}<->\mathrm{C}_{2} \mathrm{H}_{4}+\mathrm{CH}_{4}$
a) Calculate the standard enthalpy of reaction in $\mathrm{kJ} / \mathrm{mol}$ at 298.15 K for the above reaction.

```
\(\Delta \mathrm{H}_{\mathrm{R}, 298.15}=\)
Tries 0/99
```

b) Calculate the standard Gibbs energy of reaction in $\mathrm{kJ} / \mathrm{mol}$ at 298.15 K for the above reaction.
$\Delta \mathrm{G}_{\mathrm{R}, 298.15}=\square$
Tries 0/99
c) Calculate $\mathrm{K}_{\mathrm{a}, 298.15}$ for the above reaction.
$\mathrm{K}_{\mathrm{a}, 298.15}=$ $\square$
Tries 0/99
d) Develop an algebraic equation for the mole fraction of $\mathrm{C}_{3} \mathrm{H}_{8}$ at equilibrium. Use $E$ for the reaction coordinate.
$\mathrm{y}_{\mathrm{C}_{3} \mathrm{H}_{8}}=$
Tries 0/99
e) Develop an algebraic equation for the mole fraction of $\mathrm{C}_{2} \mathrm{H}_{4}$ at equilibrium. Use $E$ for the reaction coordinate.
$\mathrm{y}_{\mathrm{C}_{2} \mathrm{H}_{4}}=$
Tries 0/99
f) Develop an algebraic equation for the mole fraction of $\mathrm{CH}_{4}$ at equilibrium. Use E for the reaction coordinate.
$\mathrm{y}_{\mathrm{CH}_{4}}=$
Tries 0/99
Now for parts h-j will find the reaction temperature that gives the equilibrium propane conversion of 0.85 when starting with 1 mole of propane. The reaction pressure is 0.35 bar.
h) Calculate the reaction coordinate for the specified conversion of propane.
$\mathrm{E}=$ $\qquad$
Tries 0/99
i) Calculate the numerical value for $\mathrm{K}_{\mathrm{a}}$ at the temperature where the equilibrium propane conversion will be 0.85 when starting with 1 mole of propane. The reaction pressure is 0.35 bar.
$\mathrm{K}_{\mathrm{a}, \mathrm{T}}=\square$
Tries 0/99
j) Calculate the temperature (K) for the equilibrium propane conversion of 0.85 when starting with 1 mole of propane. The reaction pressure is 0.35 bar.
$\mathrm{T}=\square$
Tries 0/99
For parts k-r, you will be solving for the conversion for the given reaction at 600 K and a feed of 0.7 moles of propane and 0.3 moles of inerts. The pressure is 0.35 bar.
k) Develop an algebraic equation for the mole fraction of $\mathrm{C}_{3} \mathrm{H}_{8}$ at equilibrium. Use $E$ for the reaction coordinate.
$\mathrm{y}_{\mathrm{C}_{3} \mathrm{H}_{8}}=\square$
Tries 0/99
l) Develop an algebraic equation for the mole fraction of $\mathrm{C}_{2} \mathrm{H}_{4}$ at equilibrium. Use $E$ for the reaction coordinate. $\mathrm{y}_{\mathrm{C}_{2} \mathrm{H}_{4}}=\square$
Tries 0/99
$\mathrm{m})$ Develop an algebraic equation for the mole fraction of $\mathrm{CH}_{4}$ at equilibrium. Use E for the reaction coordinate. $\mathrm{y}_{\mathrm{CH}_{4}}=\square$
Tries 0/99
p) Calculate the numerical value for $\mathrm{K}_{\mathrm{a}}$ at 600 K using the short-cut method.
$\mathrm{K}_{\mathrm{a}, 600}=$
Tries 0/99
q) Using the value of the equilibrium constant for 600 K , solve for the reaction coordinate using Matlab or Excel.
$\mathrm{E}=$ $\qquad$
Tries 0/99
r) Solve for the conversion of propane at 600 K .

Conversion $=$ $\square$
Tries 0/99

The hydrogenation of styrene to produce ethylbenzene reaches equilibrium in the reaction below.
$\mathrm{C}_{6} \mathrm{H}_{5} \mathrm{CH}=\mathrm{CH}_{2}+\mathrm{H}_{2} \leftrightarrow \mathrm{C}_{6} \mathrm{H}_{5} \mathrm{C}_{2} \mathrm{H}_{5}$
The system initially contains 4 mol of $\mathrm{H}_{2}$ for each mole of styrene. Assume ideal gases. For styrene, $\Delta \mathrm{G}_{\mathrm{f}, 298.15}=$ $213.18 \mathrm{~kJ} / \mathrm{mol}$ and $\Delta \mathrm{H}_{\mathrm{f}, 298.15}=147.36 \mathrm{~kJ} / \mathrm{mol}$.
a) Calculate the standard Gibb's energy of the reaction at 298.15 K . ( $\mathrm{kJ} / \mathrm{mol}$ )
$\Delta \mathrm{G}_{\mathrm{f}, 298.15}=$ $\qquad$
Tries 0/99
b) Calculate the standard enthalpy of the reaction at $298.15 \mathrm{~K} .(\mathrm{kJ} / \mathrm{mol})$
$\Delta \mathrm{H}_{\mathrm{f}, 298.15}=$ $\qquad$
Tries 0/99
c) Calculate $K_{a R}$ at the reference temperature.
$\mathrm{K}_{\mathrm{a}, 298.15 \mathrm{~K}}=\square$
Tries 0/99
d) Calculate $\mathrm{K}_{\mathrm{a}}$ at $675^{\circ} \mathrm{C}$ using the shortcut van't Hoff equation.
$\mathrm{K}_{\mathrm{a}, 675^{\circ} \mathrm{C}}=$ $\qquad$
Tries 0/99
e) Assuming the system initially contains 4 mol of $\mathrm{H}_{2}$ for each mole of styrene, derive an algebraic expression for the total moles at reaction equilibrium using the reaction coordinate. Use E to represent the reaction coordinate.
$v_{\text {total }}=$ $\square$
Tries 0/99
f) Develop an algebraic expression for the mole fraction of styrene at equilibrium. Use $E$ for the reaction coordinate.
$\mathrm{y}_{\text {styrene }}=$
Tries 0/99
g) Develop an algebraic expression for the mole fraction of hydrogen at equilibrium. Use E for the reaction coordinate.
$\mathrm{y}_{\text {hydrogen }}=$
Tries 0/99
h) Develop an algebraic expression for the mole fraction of ethylbenzene at equilibrium. Use E for the reaction coordinate.
$\mathrm{y}_{\text {ethylbenzene }}=$ $\square$
Tries 0/99
j) Solve for the numerical value of the reaction coordinate using MATLAB or Excel at $675^{\circ} \mathrm{C}$ if the pressure is 1 bar. $\mathrm{E}=$ $\qquad$
Tries 0/99
k) Using the reaction coordinate calculated above, calculate the mole fractions of each species for reaction equilibrium at $675^{\circ} \mathrm{C}$.
$\mathrm{y}_{\text {styrene }}=\square$
$\mathrm{y}_{\text {hydrogen }}=\square$
$\mathrm{y}_{\text {ethylbenzene }}=\square$
Tries 0/99
l) If the pressure was raised to 9 bar, calculate the reaction coordinate at $675^{\circ} \mathrm{C}$.
$\mathrm{E}=\square$
Tries 0/99
m) Using the reaction coordinate calculated at 9 bar, calculate the mole fractions of each species for reaction equilibrium at $675^{\circ} \mathrm{C}$.
$\mathrm{y}_{\text {styrene }}=\square$
$\mathrm{y}_{\text {hydrogen }}=\square$
$\mathrm{y}_{\text {ethylbenzene }}=\square$
Tries 0/99

One of the most important reactions in the fixation of nitrogen for agriculture is known as the Haber Process for making ammonia shown below.
(1) $\mathrm{N}_{2}+\mathrm{bH}_{2} \rightarrow \mathrm{cNH}_{3}$
a) Balance to chemical equation.

b) Calculate the standard enthalpy of reaction at 298.15 K for the assigned stoichiometry. $(\mathrm{kJ} / \mathrm{mol})$
$\qquad$
Tries 0/99
c) Calculate the Standard Gibbs energy of reaction at 298.15 K for the assigned stoichiometry.(kJ/mol)
$\square$

Tries 0/99
d) Calculate $\mathrm{K}_{\mathrm{a}, 298.15 \mathrm{~K}}$, the equilibrium constant for the reaction at 298.15 K .
$\square$

Tries 0/99
e) Calculate $\mathrm{K}_{\mathrm{a}, 730}$ at 730 K using the short-cut van't Hoff equation.
$\square$
Tries 0/99
f) Enter the equation for the equilibrium constant using partial pressures of the components in algebraic form. The variables you should use are $\mathrm{pNH} 3, \mathrm{pH} 2, \mathrm{pN} 2$, are the partial pressures of $\mathrm{NH}_{3}, \mathrm{H}_{2}, \mathrm{~N}_{2}$ respectively.
$\mathrm{K}_{\mathrm{a}}=$
Tries 0/99
g) Enter the equation for the equilibrium constant using total pressure and mole fractions. The variables you should use are yNH3, yH2, yN2, for the mole fractions of $\mathrm{NH}_{3}, \mathrm{H}_{2}, \mathrm{~N}_{2}$ respectively and the total pressure, P .
$\mathrm{K}_{\mathrm{a}}=$ $\square$
Tries 0/99
h) Assuming that the moles fed into the reactor are 2 of nitrogen and 4 of hydrogen develop an algebraic equation for the total number of moles at reaction equilibrium using the reaction coordinate. Use E for the reaction coordinate.
Total moles $=$ $\square$
Tries 0/99
i) Now develop an algebraic equation for the mole fraction of $\mathrm{NH}_{3}$ at equilibrium. Use E for the reaction coordinate.
$\mathrm{y}_{\mathrm{NH} 3}=$ $\qquad$
Tries 0/99
j) Develop an algebraic equation for the mole fraction of $\mathrm{N}_{2}$ at equilibrium. Use E for the reaction coordinate.
$\mathrm{y}_{\mathrm{N} 2}=$
Tries 0/99
k) Develop an algebraic equation for the mole fraction of $\mathrm{H}_{2}$ at equilibrium. Use E for the reaction coordinate.
$\mathrm{y}_{\mathrm{H} 2}=\square$
Tries $0 / 99$
l) Insert the mole fractions that you submitted above to provide an algebraic representation of $K_{a}$ in terms of the reaction coordinate (use E for the reaction coordinate) and pressure, P .
$\mathrm{K}_{\mathrm{a}}=$
Tries 0/99
m) Using the value of the equilibrium constant from the short-cut method, solve for the reaction coordinate using Matlab or Excel at 730 K and $\mathrm{P}=23$ bar. What is the numerical value of the reaction coordinate?
$\mathrm{E}=$
Tries 0/99
n) Using the value of the equilibrium constant from the short-cut method, solve for the reaction coordinate using Matlab or Excel at 730 K and $\mathrm{P}=5$ bar. What is the numerical value of the reaction coordinate?
$\mathrm{E}=$ $\qquad$
Tries 0/99

Congratulations, you have completed the major steps for calculating reaction equilibria involving ideal gases. The major steps are to calculate the standard Gibbs energy and heat of reaction at 298.15 K , and correct for T. The reaction is balanced and a material balance is written to express the mole fractions in terms of the reaction coordinate. The equilibrium constant is first written in terms of partial pressures and then simplified in terms of the reaction coordinate and pressure. Other steps that you should know how to do are to calculate the final mole fractions and the conversion of the reactants using the reaction coordinate.

