P05 eLEAPS Problem Session Script

Problem Name: **P05 Adiabatic Reactor**
Problem Description: **Adiabatic Flame Temperature**

Date: _____ **Your Name:** _____

Problem Session Objectives

- To apply the five stages of the problem solving methodology.
- To apply material balances to solve a combustion problem.

- To apply the energy balance to find the adiabatic flame temperature.
- To use the heat-of-formation method to solve the energy balance.
- To find the molar enthalpy of mixtures, while accounting for chemical reactions.

Reference Readings

- Felder and Rousseau, 3rd Edition, Section 9.3, Standard Heats of Formation.
- Felder and Rousseau, 3rd Edition, Section 9.5, Energy Balances on Reactors.

- Felder and Rousseau, 3rd Edition, Section 9.1, Heats of Reactions.
- Felder and Rousseau, 3rd Edition, Section 9.2, Heats of Reactions: Hess's Law.
- Felder and Rousseau, 3rd Edition, Section 9.4, Heats of Combustion.

Review Materials

- Hanyak's "Energy Balance with No Chemical Reactions," CinChE Manual, Ch. 7.
- Hanyak's "Heat-of-Formation Method for Energy Balance," CinChE Manual, Ch. 7.
- Hanyak's "Derivation for the Heat-of-Reaction Method," CinChE Manual, Ch. 7.
- Hanyak's "Enthalpy Reference States: Why are They Arbitrary? ," CinChE Manual, Appendix F.

Interaction 1:

Topic: Adiabatic Reactor

Background: Welcome to the eLEAPS problem session about an adiabatic reactor. Save this script document to the desktop. Click here to open and save the solution template also to the desktop. Close all internet browser windows. Open the two saved documents with **Adobe Reader**.

In the solution template document, right click and select **Print**, choose "**Document and Markups**" under **Comments and Forms**, and print it to get a PAPER COPY. Print to a color printer for the best effect. You will fill-in this paper copy as you do the problem session. Close the template document and then delete it, since it is no longer needed.

P05 eLEAPS Problem Solution Template

Coaching Script and Solution Template

This coaching script contains two kinds of pages—script and template. They are arranged similar to the left and right pages in a book. The left page is an interaction in the coaching script. The right page is the current focus in the solution template that is associated with the left coaching script page.

How you navigate through the coaching script depends up the type of computer that you are using—a personal computer with a mouse or an Apple iPad with a stylus pen. In either case, you have opened this coaching script using the Acrobat Reader program that is installed on your computer and not the Acrobat Reader plug-in found in a web browser.

Please complete the first interaction in the first coaching script page. Then, proceed to navigate through the coaching script based upon your computer type, as describe below.

Personal Computer with a Mouse

The Acrobat Reader program should have displayed this coaching script in its two-page view mode. If not, then select the **View/Page Display/Two Page Scrolling** option from the menu bar.

In the two-page view mode, the left column of pages will be the coaching script, while the right column of pages will be the current focus in the solution template. You can magnify the view (i.e., zoom in) so that the coaching script page is readable. Then, you can use the horizontal scroll bar to move between the left page (the coaching script) and its right page (the template solution).

After you manually complete a portion of your PAPER COPY of the problem solution template (as directed by its associated coaching script interaction), you can then delete the boxes in the right page to view the correct answers. You can also view the popup notes found in the right page.

You proceed to the next script **Interaction** by scrolling down to the next set of two pages in the Acrobat Reader program.

Apple iPad with a Rubber-Domed Stylus Pen

The Acrobat Reader app for the iPad (downloaded from the App Store) does not support the two-page view mode. To simulate this viewing mode, select the **Single Page** option under **Document Modes** in the menu bar.

In the **Single Page** mode, you will be able to horizontally swipe between the left page (the coaching script) and its right page (the template solution).

After you manually complete a portion of your PAPER COPY of the problem solution template (as directed by its associated coaching script interaction), you can then delete the boxes in the right page to view the correct answers. You can also view the popup notes found in the right page.

You proceed to the next script **Interaction** by swiping pass the current right page in the Acrobat Reader app.

If you quickly tap the **Home** button on the iPad twice, you can conveniently switch between the Adobe Reader and any other apps.

Interaction 2:

Topic: Adiabatic Reactor

Background: An adiabatic reactor problem is used to illustrate how to find the outlet temperature for a combustion process.

The first step in the problem-solving methodology (PSM) is to analyze the problem statement and create a conceptual model composed of a labeled Diagram, Other Givens, Finds, and initial Assumptions.

Please examine the top portion of Page 1 in your PAPER COPY of the template document. As indicated by the yellow highlights to the right of this script page, you are to complete labeling the process state of each material stream and the FINDS quantity.

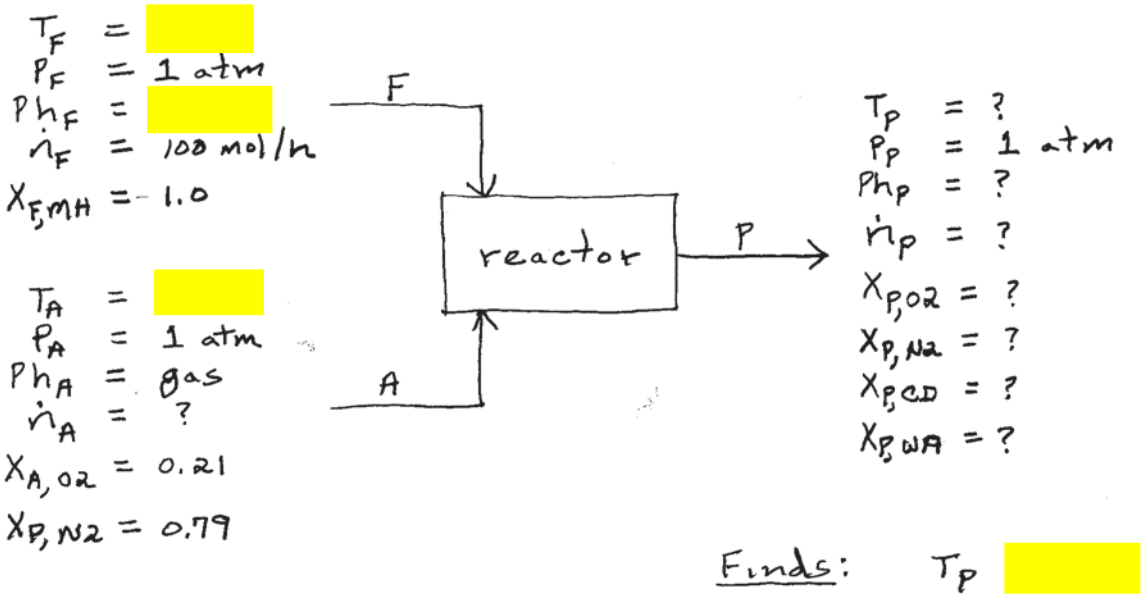
Conceptual Model Question:	Based on the information given in the diagram, which ONES of the following are valid assumptions?
Option 1:	☐ Steams F, A, and P are at 1 atm.
Option 2:	☐ Stream A has only 21/79 mol% O2/N2.
Option 3:	☐ Incomplete combustion of methanol occurs.
Option 4:	☐ Basis: Feed is at 100 mol/h.
Feedback 1:	Select the text of your first option and then highlight it. If necessary, select the text of additional options and highlight them. After selecting your option(s), click this yellow rectangle and then delete it to see the feedback for each option.
Feedback 2:	
Feedback 3:	
Feedback 4:	

Before continuing, close ALL browser and other windows that you opened during this interaction.

Problem Statement { Example 9.6-2 in Felder & Rousseau, 3rd Edition, 2005 }

Pure methanol at 25°C and 1 atm is to be fed to a furnace. Air in 100% excess at 100°C is also to be fed into the furnace. If you are to select the material of construction for the furnace, what is the highest temperature that the furnace walls will have to withstand?

Conceptual Model



Finds: T_P

Interaction 3:

Topic: Adiabatic Reactor

Background: To complete the conceptual model, you need to list any "Other Givens"; that is, additional information from the problem statement that was not placed on the diagram; for example, the percent excess air and the chemical reaction.

Please examine the bottom portion of Page 1 in your PAPER COPY of the template document. As indicated by the yellow highlights to the right of this script page under "Other Givens", you are to balance the chemical reaction and determine the standard heat of reaction at 25ºC and 1 atm.

You are ALWAYS to use whole numbers and NOT fractions for the stoichiometric coefficients in the chemical reaction. Furthermore, these whole numbers MUST be expressed using the lowest common denominator of one.

For the standard heat of reaction calculation, the heat of formation for each compound in the chemical reaction MUST be for its **STABLE** phase at 25ºC and 1 atm.

Use Table B.1 in the Felder and Rousseau textbook to observe the normal melting and boiling points for each compound at 1 atm, as well as the standard heat of formation at 25ºC, 1 atm, and stable phase.

Conceptual Model Question:	Based on your calculated value for the standard heat of reaction, which one of the following would probably be true about the temperature of Stream P?
Option 1:	○ Its temperature is less than 25ºC.
Option 2:	○ Its temperature is between 25 and 100ºC.
Option 3:	○ Its temperature is greater than 100ºC.
Feedback 1:	Select the text of only ONE option and then highlight it. After selecting your option, click this yellow rectangle and then delete it to see the feedback for each option.
Feedback 2:	
Feedback 3:	

Problem Statement { Example 9.6-2 in Felder & Rousseau, 3rd Edition, 2005 }

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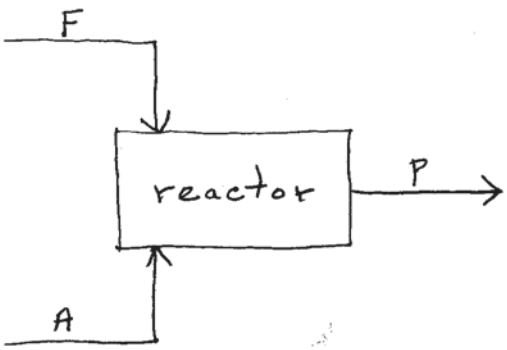
Conceptual Model

$T_F = 25°C$
$P_F = 1\ atm$
$Ph_F = liquid$
$\dot{n}_F = 100\ mol/h$
$X_{F,MH} = 1.0$

$T_A = 100°C$
$P_A = 1\ atm$
$Ph_A = gas$
$\dot{n}_A = ?$
$X_{A,O2} = 0.21$
$X_{P,N2} = 0.79$



$T_P = ?$
$P_P = 1\ atm$
$Ph_P = ?$
$\dot{n}_P = ?$
$X_{P,O2} = ?$
$X_{P,N2} = ?$
$X_{P,CO} = ?$
$X_{P,WA} = ?$

Finds: T_P in °C

other Givens: 100% excess air

Rxn I: $2\ CH_3OH + 3\ O_2 \rightarrow \square\ CO_2 + \square\ H_2O$

$\Delta\hat{H}^\circ_r = -2\,\Delta\hat{H}^\circ_{f,MH}(\square) - 3\,\Delta\hat{H}^\circ_{f,O2}(g) + \square\,\Delta\hat{H}^\circ_{f,CO}(g) + \square\,\Delta\hat{H}^\circ_{f,WA}(\square)$

$=$

$=$

Do this to determine if $T_P < T_A$ or $T_P > T_F$.

Assumptions

1. complete combustion of MeOH
2. Streams F, A, & P at 1 atm
3. Stream A is 21/79 mol % O_2/N_2
4. Continuous process; adiabatic
5. steady state
6. neglect ΔKE & ΔPE
7. no shaft work
8. Basis: $\dot{n}_F = 100\ mol/h$

Interaction 4:

Topic: Adiabatic Reactor

Background: The second step in the problem-solving methodology (PSM) is to review the conceptual model and create a mathematical model composed of first principle equations, additional equations, and a degrees-of-freedom analysis.

Please examine Page 2 in your PAPER COPY of the template document. As indicated by the yellow highlights to the right of this script page, you are to complete the fifteen equations in the math model and determine the final degrees of freedom.

Because of how the material and energy balances are written, five assumptions were added to the **List of Assumptions**, namely, continuous process, steady state, neglect changes in kinetic and potential energies, adiabatic, and no shaft work.

Math Model Question:	Based on your observation of your completed mathematical model, are the material balances necessary in order to find the temperature of Stream P?
Option 1:	○ yes.
Option 2:	○ no.
Feedback 1:	Select the text of only ONE option and then highlight it. After selecting your option, click this yellow rectangle and then delete it to see the feedback for each option.
Feedback 2:	

Mathematical Model

Material Balances:

① Total: $\dot{n}_F$ + [ ] + $\dot{R}_I = 0$

② MeOH: $\dot{n}_F - 2\dot{R}_I = 0$

③ O_2: $0.21\dot{n}_A - \dot{n}_{P,O2}$ [ ] $= 0$

④ N_2: $0.79\dot{n}_A - \dot{n}_{P,N2} = 0$

⑤ CO_2: $-\dot{n}_{P,CD} + 2\dot{R}_I = 0$

⑥ H_2O: $-\dot{n}_{P,WA}$ [ ] $= 0$

✓ mix P: $\dot{n}_P = \dot{n}_{P,O2} + \dot{n}_{P,N2} + \dot{n}_{P,CD} + \dot{n}_{P,WA}$

Click here for a definiton of % excess air.

⑦ $0.21\dot{n}_A = 2.0$ [ ]

# vars = 12
# eqns = 11
dof = 1

⑧-⑪ $\dot{n}_{P,j} = \dot{n}_P X_{P,j}$ for $j = O2, N2, CD, WA$

Energy Balance:

⑫ $\dot{n}_F \hat{H}_F$ + [ ] $= 0$

⑬ $\hat{H}_F = h_{mix}[T_F, P_F, \text{pure MeOH}]$

⑭ $\hat{H}_A = h_{mix}[T_A, P_A, \bar{X}_A]$

⑮ $\hat{H}_P = h_{mix}[T_P, P_P, \bar{X}_P]$

# vars = [ ]
# eqns = ___
dof = [ ]

Interaction 5:

Topic: Adiabatic Reactor

Background: The third step in the problem-solving methodology (PSM) is to transform the mathematical model into a mathematical algorithm. A math algorithm does not tell you how to solve, but it identifies the order in which the equations are to be solved.

Please examine Page 3 in your PAPER COPY of the template document. As indicated by the yellow highlights to the right of this script page, you are to complete the list of independent variables and the 12 steps in the math algorithm. When you are done, take some time and inspect your math algorithm. Remember that each variable that appears in the right-hand side of an assignment MUST be defined previously; that is, either it is known or it has been calculated earlier in the math algorithm.

In Step 12 of the math algorithm, the ITERATE-UNTIL construct is used to indicate that, in general, the temperature must be found by a trial-and-error technique or some other numerical technique like interval halving or the regula-falsi method [Felder and Rousseau, 3rd Ed., p.613]. The ITERATE-UNTIL construct could be replaced with the "**tmix**" functional form, as shown at the bottom of Page 3 in your PAPER COPY of the template document. Basically, this functional form means that the temperature can be found somehow once the pressure, molar enthalpy, and mole fractions of the Stream P are known.

Remember that any functional form can be represented one of four ways—by a graph, a table, a set of equations, or a computer program.

Math Algorithm Question:	In the ITERATE-UNTIL construct of Step 12, the molar enthalpy of Stream P was determined how?
Option 1:	○ It was given in the problem statement.
Option 2:	○ It was found by using a trial and error technique.
Option 3:	○ It was calculated through the energy balance.
Feedback 1:	Select the text of only ONE option and then highlight it. After selecting your option, click this yellow rectangle and then delete it to see the feedback for each option.
Feedback 2:	
Feedback 3:	

Mathematical Algorithm

$[T_P] = \text{flameT}[\quad, \bar{X}_A, \quad]$

② 1. $\dot{R}_I \leftarrow \dot{n}_F / 2$

⑤ 2. $\dot{n}_{P,CD} \leftarrow 2\dot{R}_I$

⑥ 3. $\dot{n}_{P,WA} \leftarrow 4\dot{R}_I$

⑦ 4. $\dot{n}_A \leftarrow \frac{2.0}{0.21}\dot{n}_F\left(\frac{3\ \text{mol}\ O_2}{2\ \text{mol}\ mH}\right)$

① 5. $\dot{n}_P \leftarrow \dot{n}_F + \dot{n}_A + \dot{R}_I$

③ 6. $\dot{n}_{P,O_2} \leftarrow 0.21\dot{n}_A - 3\dot{R}_I$

④ 7. $\dot{n}_{P,N_2} \leftarrow 0.79\dot{n}_A$

⑧-⑪ 8. $X_{P,j} \leftarrow \dot{n}_{P,j}/\dot{n}_P$ for $j = O_2, N_2, CO, WA$

⑬ 9. $\hat{H}_F \leftarrow \text{hmix}[T_F, P_F, \text{pure MeOH}]$

⑭ 10. $\hat{H}_A \leftarrow \text{hmix}[T_A, P_A, \bar{X}_A]$

⑫ 11. $\hat{H}_P \leftarrow (\dot{n}_F\hat{H}_F + \dot{n}_A\hat{H}_A)/\dot{n}_P$

12. Iterate T_P in

⑮ $f(T_P) \leftarrow$ [ ] $- \text{hmix}[T_P, P_P, \bar{X}_P]$

until $f(T_P) = 0$

Note that the Iterate-Until construct can be replaced with:

12. $T_P \leftarrow \text{tmix}[P_P, \hat{H}_P, \bar{X}_P]$

Interaction 6:

Topic: Adiabatic Reactor

Background: The fourth step in the problem-solving methodology (PSM) is to generate the Numerical Solution using the mathematical algorithm as a blueprint or guide.

Please examine Page 4 in your PAPER COPY of the template document. As indicated by the yellow highlights to the right of this script page, you are to complete the calculations, in order to find the temperature of Stream P. Do not forget to account for precision when writing the final answer for this temperature.

After you complete your numerical solution, we will next investigate how the enthalpy values in Steps 9 and 10 were determined for Streams F and A. Also, we will then examine how the temperature value of Stream P was found using the iteration technique of trial and error.

Numerical Solution

Basis: cgs system, $\dot{n}_F = 100$ mol/h

Knowns: $T_F = 25°C$, $P_F = 1$ atm, $P_p = 1$ atm
$T_A = 100°C$, $P_A = 1$ atm

1. $\dot{R}_I = \left(100 \frac{\text{mol MH}}{h}\right)\left(\frac{\text{g-rxn}}{2 \text{ mol MH}}\right) = 50$ g-rxn/h

2. $\dot{n}_{p,CD} = \left(2 \frac{\text{mol CD}}{\text{g-rxn}}\right)\left(50 \frac{\text{g-rxn}}{h}\right) = 100$ mol/h

3. $\dot{n}_{p,WA} = \left(\quad \frac{\text{mol WA}}{\text{g-rxn}}\right)\left(\quad \frac{\text{g-rxn}}{h}\right) =$

4. $\dot{n}_A = \frac{2.0}{0.21}\left(100 \frac{\text{mol}}{h}\right)\left(\frac{3 \text{ mol } O_2}{2 \text{ mol MH}}\right) = 1428.57$ mol/h

5. $\dot{n}_p = 100 + 1428.57 + \left(1 \frac{\text{mol}}{\text{g-rxn}}\right)\left(50 \frac{\text{g-rxn}}{h}\right) = 1578.57$ mol/h

6. $\dot{n}_{p,O_2} = 0.21(1428.57) - \left(3 \frac{\text{mol}}{\text{g-rxn}}\right)\left(50 \frac{\text{g-rxn}}{h}\right) = 150$ mol/h

7. $\dot{n}_{p,N_2} = 0.79\left(1428.57 \frac{\text{mol}}{h}\right) = 1128.57$ mol/h

8. $X_{p,O_2} = \left(150 \frac{\text{mol}}{h}\right) / \left(1578.57 \frac{\text{mol}}{h}\right) = 0.095023$

$X_{p,N_2} = \left(\quad \frac{\text{mol}}{h}\right) / \left(1578.57 \frac{\text{mol}}{h}\right) =$

$X_{p,CD} = \left(100 \frac{\text{mol}}{h}\right) / \left(1578.57 \frac{\text{mol}}{h}\right) = 0.063348$

$X_{p,WA} = \left(\quad \frac{\text{mol}}{h}\right) / \left(1578.57 \frac{\text{mol}}{h}\right) =$

9. $\hat{H}_F = -238.6$ kJ/mol, See Page 5

10. $\hat{H}_A = 2.19708$ kJ/mol, See Page 5

11. $\hat{H}_p =$

$=$

12. $T_p = 1256.2542\ °C$, see Page 6

$T_p =$

Interaction 7:

Topic: Adiabatic Reactor

Background: For each "hmix" function found in the math algorithm, we will use a set of equations to determine the molar enthalpy of the mixture. Click here to open the "**Mixture Enthalpy**" document and see the general math models for the mixture enthalpy when NO chemical reaction is occurring and when chemical reaction is occurring.

Please examine Page 5 in your PAPER COPY of the template document. As indicated by the yellow highlights to the right of this script page, you are to complete the equations and do the calculations to determine the molar enthalpies for Streams F and A.

You are to use the format illustrated on Page 5 to express YOUR SOLUTION to any "hmix" function on homeworks and exams.

Mixture Molar Enthalpy Question:	In a "**hmix**" function, why must the molar enthalpy of each pure chemical compound begin with its standard heat of formation and not any other arbitrarily-selected value like zero?
Option 1:	○ because chemical compounds are conserved during chemical reactions.
Option 2:	○ because the atoms of chemical compounds are conserved during chemical reactions.
Option 3:	○ because the mass of each chemical compound is conserved during chemical reactions.
Feedback 1:	Select the text of only ONE option and then highlight it. After selecting your option, click this yellow rectangle and then delete it to see the feedback for each option.
Feedback 2:	
Feedback 3:	

Before continuing, close ALL browser and other windows that you opened during this interaction.

$h_{mix}[T_F, P_F, \text{pure MeOH}]$

$$\hat{H}_F = \hat{H}^\circ_{MH} + \Delta\hat{H}_{MH}[25°C, 1\ atm, liq \leftarrow 25°C, 1\ atm, liq]$$

$$= \Delta\hat{H}^\circ_{f,MH} + \int_{25°C}^{25°C} c^L_{P,MH}\, dT + \int_{1\ atm}^{1\ atm} \left[\hat{V} - T\left(\frac{\partial \hat{V}}{\partial T}\right)_P\right] dP$$

↑ Table B.1

$$= \quad + 0 + 0$$

$$=$$

$h_{mix}[T_A, P_A, \bar{X}_A]$

Assumptions

1. ideal soln

$$\hat{H}_A = 0.21\,\hat{H}_{O2} + 0.79\,\hat{H}_{N2}$$

$$= 0.21(\quad) + 0.79(\quad)$$

$$= 2.19708\ kJ/mol$$

$$\hat{H}_{O2} = \hat{H}^\circ_{O2} + \Delta\hat{H}_{O2}[100°C, 1\ atm, gas \leftarrow 25°C, 1\ atm, gas]$$

$$= \Delta\hat{H}^\circ_{f,O2} + \int_{25°C}^{100°C} c^G_{P,O2}\, dT + \int_{1\ atm}^{1\ atm} \left[\hat{V} - T\left(\frac{\partial \hat{V}}{\partial T}\right)_P\right] dP$$

↑ Table B.1 — Table B.8

$$= 0 + \quad kJ/mol + 0 = \quad kJ/mol$$

$$\hat{H}_{N2} = \hat{H}^\circ_{N2} + \Delta\hat{H}_{N2}[100°C, 1\ atm, gas \leftarrow 25°C, 1\ atm, gas]$$

$$= \Delta\hat{H}^\circ_{f,N2} + \int_{25°C}^{100°C} c^G_{P,N2}\, dT + \int_{1\ atm}^{1\ atm} \left[\hat{V} - T\left(\frac{\partial \hat{V}}{\partial T}\right)_P\right] dP$$

↑ Table B.1 — Table B.8

$$= 0 + \quad kJ/mol + 0 = \quad kJ/mol$$

Interaction 8:

Topic: Adiabatic Reactor

Background: In general, the temperature of Stream P in the "tmix" function can be found manually by using an iteration technique called trial and error.

Please examine Page 6 in your PAPER COPY of the template document. As indicated by the yellow highlights to the right of this script page, you are to complete the table, equations, and calculations to determine the temperature for Stream P, knowing its pressure, molar enthalpy, and mole fractions.

Click here to open an Excel file in which you can do your trial-and-error iteration for the temperature. You will need a first estimate to get started. See the yellow popup note at the bottom of Page 6 to the right of this script page.

Mixture Molar Enthalpy Question:	Which value for the standard heat of formation of water makes the 4-th order polynomial equation less complicated to solve?
Option 1:	○ Its liquid value.
Option 2:	○ Its gas value.
Feedback 1:	Select the text of only ONE option and then highlight it. After selecting your option, click this yellow rectangle and then delete it to see the feedback for each option.
Feedback 2:	

Before continuing, close ALL browser and other windows that you opened during this interaction.

tmix [P_p, $\hat{H}_p$, $\bar{X}_p$]

Why all gases? Is this important?

P_p = 1 atm, H_p = -13.1265 kJ/mol, Find T_p in °C

Comp	Mol. Frac.	$\Delta\hat{H}^o_f$, kJ/mol		C_p, kJ/(mol Δ°C) a x 10^3	b x 10^5	c x 10^8	d x 10^{12}
O_2	0.095023	0.0	(g)	29.10	1.1580	-0.6076	1.311
N_2	0.714932	0.0	(g)	29.00	0.2199	0.5723	-2.871
CO_2	0.063348	-393.5	(g)	36.11	4.2330	-2.8870	7.464
H_2O	0.126697						
sum product:		-55.5666		30.0250		0.264874	-1.91039

$$\hat{H}_p = \sum_{j=1}^{4} X_{p,j}\,\hat{H}_j + \Delta\hat{H}^o_{mix} \qquad \text{ideal solution}$$

$$\hat{H}_j = \hat{H}_j^o + \Delta\hat{H}_j\,[T_p, 1\,atm, g \leftarrow 25°C, 1\,atm, g]$$

$$= \underbrace{\Delta\hat{H}^o_{f,j}}_{\text{Table B.1}} + \underbrace{\int_{25°C}^{T_p}[a_j + b_jT + c_jT^2 + d_jT^3]\,dT}_{\text{Table B.2}} + \underbrace{\int_{1atm}^{1atm}\left[\hat{V} - T\left(\frac{\partial\hat{V}}{\partial T}\right)_p\right]dP}_{\text{zero}}$$

$$= \Delta\hat{H}^o_{f,j} + a_j(T_p - 25) + \frac{b_j}{2}(T_p^2 - 25^2) + \frac{c_j}{3}(T_p^3 - 25^3) + \frac{d_j}{4}(T_p^4 - 25^4)$$

Thus,

$$\hat{H}_p = \sum_{j=1}^{4} X_{p,j}\,\Delta\hat{H}^o_{f,j} + (T_p - 25)[\quad] + \frac{1}{2}(T_p^2 - 25^2)\left[\sum_{j=1}^{4} X_{p,j}\,b_j\right] + \frac{1}{3}(T_p^3 - 25^3)\left[\sum_{j=1}^{4} X_{p,j}\,c_j\right] + \frac{1}{4}(T_p^4 - 25^4)\left[\sum_{j=1}^{4} X_{p,j}\,d_j\right]$$

$$-13.1265 = -55.5666 + 30.0250\times10^{-3}(T_p - 25) + 0.62257\times10^{-5}(T_p^2 - 25^2)/2 + 0.264874\times10^{-8}(T_p^3 - 25^3)/3 - 1.91039\times10^{-12}(T_p^4 - 25^4)/4$$

Using Excel and do trial and error (i.e., by iteration) on the temperature of the product stream, you get:

T_p =

For a first estimate of T_p, using linear relationship:

$-13.1266 = -55.5666 + 30.0250\times10^{-3}(T_p - 25)$, gives $(T_p)_{first}$ = 1438 °C

Interaction 9:

Topic: Adiabatic Reactor

Background: The fifth and final step in the problem-solving methodology (PSM) is to generate the Heuristic Observations about the numerical solution, the mathematical algorithm, the mathematical model, and the conceptual model.

Please examine the top half of Page 7 in your PAPER COPY of the template document and inspect the **heuristic observations** for the numerical solution and the mathematical algorithm. As indicated by the yellow highlights to the right of this script page, you are to complete writing the observations for the numerical solution.

Heuristic Observations Question:	A 4-th order polynomial equation was solved by iteration to find the temperature of Stream P. Which ones of the following options are plausible roots for the 4-th order polynomial?
Option 1:	☐ four real roots.
Option 2:	☐ three real roots and one imaginary root.
Option 3:	☐ two real roots and two imaginary roots.
Option 4:	☐ one real root and three imaginary roots.
Feedback 1:	Select the text of your first option and then highlight it. If necessary, select the text of additional options and highlight them. After selecting your option(s), click this yellow rectangle and then delete it to see the feedback for each option.
Feedback 2:	
Feedback 3:	
Feedback 4:	

Before continuing, close ALL browser and other windows that you opened during this interaction.

Heuristic Observations

1. Numerical Solution

Mat'l Bal check:

$$\dot{n}_{P,O2} + \dot{n}_{P,N2} + \dot{n}_{P,CD} + \dot{n}_{WA} = \dot{n}_P$$

$$X_{P,O2} + X_{P,N2} + X_{P,CD} + X_{P,WA} = 1.0$$

$$0.095023 + 0.714932 + 0.063348 + 0.126697 = 1.000000 \quad \text{OK!}$$

T_P check: $\Delta \hat{H}^\circ_r < 0$, thus exothermic rxn and temperature in stream P must higher for adiabatic reactor

$$\therefore \quad T_A < T_P < (T_P)_{first}$$

[redacted] < [redacted] < [redacted]

Interaction 10:

Topic: Adiabatic Reactor

Background: Please examine the bottom half of Page 7 in your PAPER COPY of the template document and inspect the **heuristic observations** for the mathematical model and the conceptual model.

The red-dashed rectangle on Page 7 indicates that an **EZ Setup** solution exists for this problem. You can examine that solution on Pages 8 and 9 in your PAPER COPY of the template document. Click here to view the Excel Worksheet "**flameT alg**" and iteratively solve the equations twice to find the temperature (TP) of Stream P. Use an initial estimate of 5000ºC and then 1438ºC for the variable named TP.

The blue-dashed rectangle on Page 7 indicates an Aspen HYSYS solution exists for this problem. Click here to see the HYSYS output, or click here to download the HYSYS file. Note that the HYSYS solution is 1239ºC for the temperature of Stream P. Why does it differ by about 1.4%? Hint, the heat capacity correlation for C_p in HYSYS is different from that used in **EZ Setup**. The correlation in **EZ Setup** is based on Table B.2 in the Felder and Rousseau textbook, 3rd Edition.

Heuristic Observations Question:	In the mathematical model on Page 2 in your PAPER COPY of the template document, the energy balance was expressed using the heat-of-formation method to solve Example 9.6-2 from the Felder and Rousseau textbook. A second method exists called the heat-of-reaction method, and it is used by Felder and Rousseau to solve Example 9.6-2 in their textbook. Are these two methods equivalent for the energy balance?
Option 1:	○ no.
Option 2:	○ yes.
Feedback 1:	Select the text of only ONE option and then highlight it. After selecting your option, click this yellow rectangle and then delete it to see the feedback for each option.
Feedback 2:	

Before continuing, close ALL browser and other windows that you opened during this interaction.

Heuristic Observations

1. Numerical Solution

Mat'l Bal check:

$$\dot{n}_{P,O2} + \dot{n}_{P,N2} + \dot{n}_{P,CD} + \dot{n}_{WA} = \dot{n}_P$$

$$X_{P,O2} + X_{P,N2} + X_{P,CD} + X_{P,WA} = 1.0$$

$$0.095023 + 0.714932 + 0.063348 + 0.126697 = 1.000000 \quad \text{OK!}$$

T_P check: $\Delta\hat{H}^\circ_r < 0$, thus exothermic rxn and temperature in stream P must higher for adiabatic reactor

$$\therefore \quad T_A < T_P < (T_P)_{first}$$

$$100°C < 1300°C < 1438°C$$

2. Mathematical Algorithm

What if T_P were given and not T_A?

Solve for $\hat{H}_A$ using energy balance; Iterate on T_A.

3. Mathematical Model

How would you solve problem using **EZ Setup?**

Code math model and enthalpy equations.

How would you solve problem using Aspen HYSYS?

Use general conversion reactor with PRSV e.o.s.

4. Conceptual Model

What if P_F, P_A, and P_P were 5 atm?

Then the pressure term $\int_{1atm}^{5atm} \left[\hat{V} - T\left(\frac{\partial \hat{V}}{\partial T}\right)_P\right] dP$

must be solved in all three enthalpy calculations.

An equation of state is needed like the modified Peng-Robinson (PRSV) model. Thus, solving this problem is best done using HYSYS.

Interaction 11:

Topic: Adiabatic Reactor

Background: Let's conclude with two more observations about the solution to this problem for the adiabatic flame temperature.

First, please examine the **EZ Setup** solution on Pages 8 to 9 in your PAPER COPY of the template document. You can also view Page 8 and 9 to the right of this script page. Note how a mixture enthalpy is modeled using the function "enthalpy" for Streams F, A, and P. This function automates the calculation for the sensible enthalpy change of $\int \hat{C}_P \, dT$. You could solve this problem in **EZ Setup** without using the function "enthalpy". Basically, you manually do the integration and substitute the resulting algebraic expression in place of the function. Click here to view the **EZ Setup** mathematical model that does not use the "enthalpy" function. If you would like to run this **EZ Setup** model, click here to open the Worksheet "**flameT2**" in the Microsoft Excel program.

Second, please examine Step 12 in the mathematical algorithm on Page 3 in your PAPER COPY of the template document. We can rewrite the ITERATE-UNTIL construct as follows:

$$\begin{aligned} &ITERATE \quad T_P \quad in \\ &\qquad \hat{H}'_P \;=\; hmix\left[T_P, P_P, \bar{X}_P,\right] \\ &\qquad f\left(T_P\right) \;=\; \hat{H}_P - \hat{H}'_P \\ &UNTIL \quad f\left(T_P\right) \;=\; 0 \end{aligned}$$

where $\hat{H}_P$ was calculated in Step 11 using the energy balance. If you plot $f(T_P)$ versus T_P, the curve would cross the x-axis twice, because the 4th-order polynomial express for *hmix* (as shown on Page 6 of your template document) has two real roots and two imaginary roots.

You can use **EZ Setup** to calculate and then plot $f(T_P)$ versus T_P by copying the **EZ Setup** solution given in the Worksheet "**flameT2 alg**". You would drop the ITERATE and UNTIL statements in the copied worksheet and then include the following statements:

```
fTP  =  HP – HP2
 TP  =  1256.2578
```

where HP2 is the molar enthalpy with a prime mark that appears in the above ITERATE-UNTIL construct.

Click here to view the plot $f(T_P)$ versus T_P. If you would like to view its **EZ Setup** algorithm, click here to open the Worksheet "**fTP**" in the Microsoft Excel program. This worksheet is used by the **SolverTable** command to generate the table given in Worksheet "**STS_1**".

Before continuing, close ALL browser and other windows that you opened during this interaction.

EZ Setup Mathematical Model and Solution

Adiabatic Flame Temperature, Example 9.6-2 in Felder & Rousseau, 3rd Edition, 2005

// Material Balances

/* Total */ nF + nA - nP + R1 = 0

/* MeoH */ nF - 2*R1 = 0

/* O2 */ 0.21*nA - nPO2 - 3*R1 = 0

/* N2 */ 0.79*nA - nPN2 = 0

/* CO2 */ - nPCD + 2*R1 = 0

/* WA */ - nPWA + 4*R1 = 0

/* % excess */ 0.21*nA = (1 + ex/100) * nF * (3 / 2) /* 3 mol O2 per 2 mol MeOH */

/* mol frac P */
nPO2 = nP * xPO2
nPN2 = nP * xPN2
nPCD = nP * xPCD
nPWA = nP * xPWA

// Givens

nF = 100 // mol per h
ex = 100 // % excess air
TF = 25 // C
TA = 100 // C
Tref = 25 // 25 C, 1 atm, stable phase of each element

// Energy Balance

nF * HF + nA * HA - nP * HP = 0

// hmix [TF = 25 C, PF = 1 atm, pure MeOH]

HF = dHfMH + enthalpy("methanol", Tref, TF, "C", "l")

// hmix [TA = 100 C, PA = 1 atm, xA = 0.21, 0.79]

HA = 0.21 * dHaO2 + 0.79 * dHaN2

dHaO2 = dHfO2 + enthalpy("oxygen", Tref, TA, "C", "g")

dHaN2 = dHfN2 + enthalpy("nitrogen", Tref, TA, "C", "g")

Page 9 referenced in Interaction11 =====➔

// hmix [TP = ____ C, PP = 1 atm, xP's from mat'l balances]

```
HP  = xPO2 * dHpO2  +  xPN2 * dHpN2  +  xPCD * dHpCD  +  xPWA * dHpWA

dHpO2  =  dHfO2  +  enthalpy("oxygen",          Tref, TP, "C", "g")

dHpN2  =  dHfN2  +  enthalpy("nitrogen",        Tref, TP, "C", "g")

dHpCD  =  dHfCD  +  enthalpy("carbon dioxide", Tref, TP, "C", "g")

dHpWA  =  dHfWA  +  enthalpy("water",           Tref, TP, "C", "g")
```

// Standard Heats of Formation, Table B.1, F&R, 3rd Ed., 2005

```
dHfMH  =   -238.6          //  (liquid)  kJ / mol,  Methanol
dHfO2  =     0.0           //  (gas)  kJ / mol,    Oxygen
dHfN2  =     0.0           //  (gas)  kJ / mol,    Nitrogen
dHfCD  =   -393.5          //  (gas)  kJ / mol,    Carbon Dioxide
dHfWA  =   -241.83         //  (gas)  kJ / mol,    Water
```

Numerical Solution as given by E-Z Solve

	nA	nP	nPCD	nPN2	nPO2	nPWA	R1
	1428.57	1578.57	100	1128.57	150	200	50
HF	HA	HP	xPCD	xPN2	xPO2	xPWA	
-238.6	2.19708	-13.1266	0.0633484	0.714932	0.0950226	0.126697	
TP	dHaN2	dHaO2	dHpCD	dHpN2	dHpO2	dHpWA	
1256.2	2.187	2.235	-330.08	39.4321	41.7603	-192.42	

P05 eLEAPS Problem Session Script

Interaction 12:

Topic: Adiabatic Reactor

Background: Thank you for completing this problem session. Please place your filled-in PAPER COPY of the template document in your technical journal. Click here for the correct solution to the template document.

If you so desire, you could print this eLEAPS script (two pages per sheet and on both side of a sheet) and place it also in your technical journal.

If you have any questions or concerns about the problem session, please contact your instructor.

Read the Important Observations below and consult the Reference Readings and Review Materials.

Problem Session Observations

- Apply the problem solving methodology to setup and solve problems.
- Apply material balances to solve for unknown compositions.

- Apply the energy balance to find the temperature of a process stream.
- Use the heat-of-formation method to find molar enthalpies of mixtures.
- Set the reference state when chemical reactions occur to be the pure elements at 25ºC, 1 atm, and stable phase, not the compounds.

Reference Readings

- Felder and Rousseau, 3rd Edition, Section 9.3, Standard Heats of Formation.
- Felder and Rousseau, 3rd Edition, Section 9.5, Energy Balances on Reactors.

- Felder and Rousseau, 3rd Edition, Section 9.1, Heats of Reactions.
- Felder and Rousseau, 3rd Edition, Section 9.2, Heats of Reactions: Hess's Law.
- Felder and Rousseau, 3rd Edition, Section 9.4, Heats of Combustion.

Review Materials

- Hanyak's "Energy Balance with No Chemical Reactions," CinChE Manual, Ch. 7.
- Hanyak's "Heat-of-Formation Method for Energy Balance," CinChE Manual, Ch. 7.
- Hanyak's "Derivation for the Heat-of-Reaction Method," CinChE Manual, Ch. 7.
- Hanyak's "Enthalpy Reference States: Why are They Arbitrary? ," CinChE Manual, Appendix F.