

CADET _____ SECTION _____ TIME OF DEPARTURE _____

DEPARTMENT OF CHEMISTRY & LIFE SCIENCE

CH365 2023-2024

WRITTEN PARTIAL REVIEW II

12 October 2023, A-Hour

TEXT: Smith, Van Ness, Abbott & Swihart

SCOPE: Lessons 10-20

TIME: 55 Minutes

References Permitted: Open notes, book, internet, Mathematica, and Excel.

INSTRUCTIONS

1. Do not mark this exam or open it until “begin work” is given.
2. You have 55 minutes to complete the exam.
3. Solve the problems in the space provided. Show all work to receive full credit.
4. There are 3 problems on 3 pages in this exam (not including the cover page). Write your name on the top of each sheet.
5. Save Mathematica files on your desktop and re-save frequently.
6. When finished, upload all Mathematica files to Canvas.

(TOTAL WEIGHT: 200 POINTS)

DO NOT WRITE IN THIS SPACE

PROBLEM	VALUE	CUT
A	80	
B	70	
C	50	
TOTAL CUT		
TOTAL GRADE	200	

Problem: Weight:
A 80

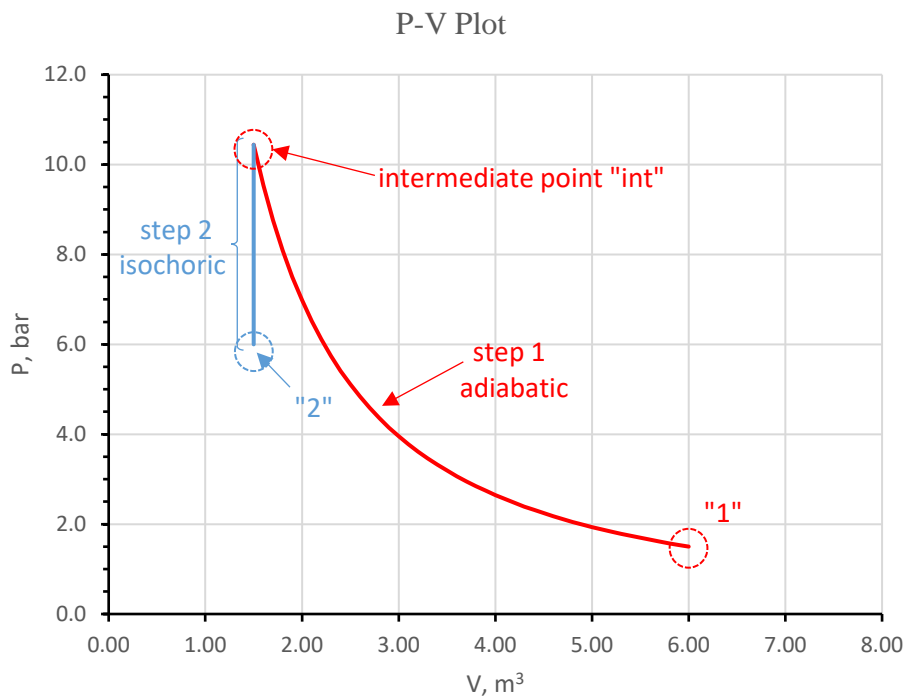
0.100 kmol of an ideal gas in a closed system initially at 6.0 m³, 1.5 bar and 1082.5 K undergoes a two-step process consisting of an adiabatic compression followed by cooling at constant volume to a final state of 1.5 m³, 6.0 bar, and 1082.5 K. (a) Sketch the process path on the PV axes below. (b) Calculate Q, W, ΔU and ΔH for the overall process in units of kJ. (c) Calculate the intermediate temperature after the first step in the process.

$$R = 8.314 \text{ J/(mol} \cdot \text{K)} = 0.08314 \text{ (bar} \cdot \text{m}^3\text{)/(kmol} \cdot \text{K)}$$

$$C_P = (7/2) \cdot R, \text{ and}$$

$$C_V = (5/2) \cdot R$$

Solution, part (a):



Solution, part (b):

The overall process is isothermal ($T_2=T_1$), so $\Delta H_{\text{Overall}} = \Delta U_{\text{Overall}} = 0 \text{ kJ}$
ANS

Equation 3.23c gives the P-V relation for an adiabatic process. Let the intermediate state be denoted with subscript “int” with $V_{\text{int}} = V_2$ since the second step is at constant volume.

Also $\gamma = C_P/C_V = (7R/2)/(5R/2) = (7/5) = 1.4$ from equation 3.24.

Solve for intermediate pressure, P_{int} , using the un-numbered equation 3.23c:

$$P_{\text{int}} = P_1 \left(\frac{V_1}{V_{\text{int}}} \right)^\gamma = 1.5 \text{ bar} \cdot \left(\frac{6.0 \text{ m}^3}{1.5 \text{ m}^3} \right)^{1.4} = 10.447 \text{ bar}$$

Once P_{int} is known, the adiabatic work for step 1 is given by equation 3.26:

$$W_{\text{Step1}} = \frac{P_{\text{int}} \cdot V_{\text{int}} - P_1 \cdot V_1}{\gamma - 1} = \frac{10.447 \text{ bar} \cdot 1.5 \text{ m}^3 - 1.5 \text{ bar} \cdot 6.0 \text{ m}^3}{1.4 - 1} = 16.675 \text{ bar} \cdot \text{m}^3$$

Step 2 is at constant volume, so work is zero since $\Delta V = 0$:

$$W_{\text{Step2}} = -P \cdot \Delta V = 0.$$

The total overall work is the sum of the work of each step:

$$W_{\text{Overall}} = W_{\text{Step1}} + W_{\text{Step2}} = 16.675 \text{ bar} \cdot \text{m}^3 + 0 \text{ bar} \cdot \text{m}^3 = 16.675 \text{ bar} \cdot \text{m}^3$$

Now convert the units to kJ:

$$W_{\text{Overall}} = 16.675 \text{ bar} \cdot \text{m}^3 \left(\frac{1 \text{ J}}{10^{-5} \text{ bar} \cdot \text{m}^3} \right) \cdot \left(\frac{1 \text{ kJ}}{1000 \text{ J}} \right) = \underline{\underline{1667.5 \text{ kJ}}}_{\text{ANS}}$$

Finally, solve for Q:

$$\Delta U_{\text{Overall}} = Q_{\text{Overall}} + W_{\text{Overall}} = 0 \Rightarrow Q_{\text{Overall}} = -W_{\text{Overall}} = \underline{\underline{-1667.5 \text{ kJ}}}_{\text{ANS}}$$

Solution, part (c):

Let “int” designate the intermediate state, so $P_{\text{int}} = 10.447 \text{ bar}$ and $V_{\text{int}} = V_2 = 1.5 \text{ m}^3$:

$$PV = nRT \Rightarrow T_{\text{int}} = \frac{P_{\text{int}} \cdot V_{\text{int}}}{n \cdot R} = \frac{10.447 \text{ bar} \cdot 1.5 \text{ m}^3}{0.100 \text{ kmol} \cdot \left(0.08314 \frac{\text{bar} \cdot \text{m}^3}{\text{kmol} \cdot \text{K}} \right)} = \underline{\underline{1885 \text{ K}}}_{\text{ANS}}$$

Problem: Weight:
B 70

An engineering plan for a vinyl chloride plant includes a pipeline carrying chlorine (Cl₂) at a volumetric flow rate of 6.501 MMSCFD (million standard cubic feet per day). Standard conditions are 60 °F (519.67 °R) and 14.696 psia.

Use the Soave-Redlich-Kwong (SRK) equation of state, Table 3.1, and gas constant R = 10.73 ft³·psia/(lbmol·°R) to determine the molar flow rate of Cl₂ in lbmol/d. From Appendix B, the critical temperature, pressure, and acentric factor for Cl₂ are ω = 0.069, T_C = 750.96 °R, and P_C = 1118.24 psia.

Solution:

```

P = 14.696; (*psia*)
T = 519.67; (*Rankine*)
R = 10.73; (* $\frac{\text{ft}^3 \cdot \text{psia}}{\text{lbmol} \cdot \text{R}}$ , given*)
ω = 0.069; (*App. B, p.665*)
Tc = 750.96; (*p.665, converted K to R*)
Pc = 1118.24; (*p. 665 converted bar to psia, App A*)
Tr1 = T / Tc; (*reduced temperature*)

In[8]:= σ = 1; (*Table 3.1, p.100*)
ε = 0;
Ω = 0.08664;
Φ = 0.42748;
α = (1 + (0.480 + 1.574 * ω - 0.176 * ω2) * (1 - √Tr1))2;
a = Φ *  $\frac{\alpha * R^2 * Tc^2}{Pc}$ ; (*eq.3.45, p.98*)
b = Ω *  $\frac{R * Tc}{Pc}$ ; (*eq.3.44, p.98*)

In[15]:= eq1 = P ==  $\frac{R * T}{V - b} - \frac{a}{(V + ε * b) * (V + σ * b)}$ ; (*eq.3.41 p.97*)

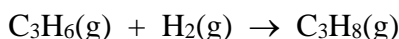
In[16]:= ans = Quiet[Solve[eq1, V]]
Out[16]= {{V → 0.8629639}, {V → 3.9380242}, {V → 374.62601}}
```

Use V and molar flow rate to solve for volumetric flow rate (V^t):

$$\frac{6.501 \times 10^6 \text{ ft}^3}{\text{day}} \cdot \frac{1 \text{ lbmol}}{374.626 \text{ ft}^3} = 17,353 \frac{\text{lbmol}}{\text{day}} \quad \underline{\underline{\text{ANS}}}$$

Problem: Weight:
C 50

Hydrogenation refers to the treatment of substances with hydrogen, H₂. Hydrogenation is important in the petrochemical and food processing industries. For example, hydrogenation of polyunsaturated fatty acids in vegetable oils reduces most of the carbon-carbon double bonds, making the oil safer and healthier for consumption. Hydrogenation reactions of hydrocarbons typically involve the reaction of alkenes with hydrogen to form alkanes at high temperatures and pressures, usually over a supported metal catalyst such as Raney nickel. Steam is often used as a diluent to control the temperature in the reactor. In this problem, you will consider the hydrogenation of propylene to form propane:



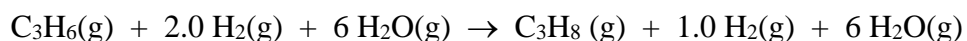
Calculate the standard gas-phase heat of hydrogenation of propylene at 535 °C and 1.00 bar in 100% excess hydrogen, with 6.00 moles of steam added per mole of propylene as a diluent to control the reactor temperature. The process is isothermal with reactants and products at 535 °C. Report your answer in J/mol.

The following table contains ideal gas heat capacity polynomial coefficients and standard heats of formation at 298 K from Appendix C:

species	a	b×10 ³	c×10 ⁶	d×10 ⁻⁵	ΔH _{f,298} ⁰ , J/mol
C ₃ H ₆	1.637	22.706	-6.915	0.000	19,710
H ₂	3.249	0.422	0.000	0.083	0
H ₂ O	3.470	1.450	0.000	0.121	-241,818
C ₃ H ₈	1.213	28.785	-8.824	0.000	-104,680

Solution:

Balanced Reaction:



Solution in Mathematica is shown on the following page.

Mathematica Solution:

```

In[1]:= (*Stoichiometric coefficients*)
(*Propylene, hydrogen, water, ethane, hydrogen, water*)
v = {-1, -2.0, -6, 1, 1.0, 6};
(*Standard Heats of Formation*)
ΔHf298 = {19710, 0, -241818, -104680, 0, -241818};
(*Heat of Reaction at 298 K*)
ΔH298 = Plus@@ (v*ΔHf298) (*J/mol*)

Out[3]= -124390.

In[4]:= (*Heat Capacity polynomial coefficients, Table C.1:*)
a = {1.637, 3.249, 3.470, 1.213, 3.249, 3.470};
b = {22.706, 0.422, 1.450, 28.785, 0.422, 1.450} * 10-3;
c = {-6.915, 0.000, 0.000, -8.824, 0.000, 0.000} * 10-6;
d = {0.000, 0.083, 0.121, 0.000, 0.083, 0.121} * 105;

Δa = Plus@@ (v*a);
Δb = Plus@@ (v*b);
Δc = Plus@@ (v*c);
Δd = Plus@@ (v*d);

(*Gas constant*)
R = 8.314; (*  $\frac{\text{J}}{\text{mol}\cdot\text{K}}$  *)
(*Temperatures, K*)
T = 535 + 273.15; (*708.15 K*)
T0 = 298.15;
(*Equation 4.21 for MDCPH*)
MDCPH = Δa +  $\frac{\Delta b}{2} * (T + T0) + \frac{\Delta c}{3} * (T^2 + T0^2 + T * T0) + \frac{\Delta d}{T * T0}$ 

Out[15]= -1.2037611

(*Equation 4.22 for corrected heat of reaction at 808 K*)
(*Gives molar heat of reaction in J/mol*)
ΔH808 = ΔH298 + MDCPH * R * (T - T0)

Out[16]= -129494.12
          ANS, J per mole C3H6

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Problem: Weight:
A 80

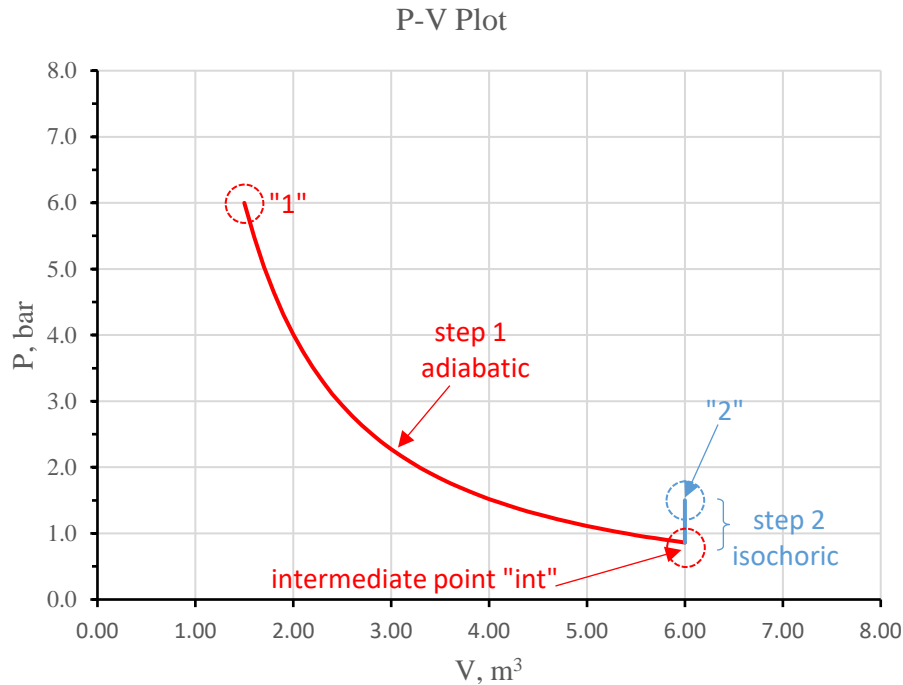
0.200 kmol of an ideal gas in a closed system initially 1.5 m³, 6.0 bar and 541.3 K undergoes a two-step process consisting of an adiabatic expansion followed by heating at constant volume to a final state of 6.0 m³, 1.5 bar, and 541.3 K. (a) Sketch the process path on the PV axes below. (b) Calculate Q, W, ΔU and ΔH for the overall process in units of kJ. (c) Calculate the intermediate temperature after the first step on the process.

$$R = 8.314 \text{ J/(mol} \cdot \text{K)} = 0.08314 \text{ (bar} \cdot \text{m}^3\text{)/(kmol} \cdot \text{K)}$$

$$C_P = (7/2) \cdot R, \text{ and}$$

$$C_V = (5/2) \cdot R$$

Solution, part (a):



Solution, part (b):

The overall process is isothermal ($T_2 = T_1$), so $\Delta H_{\text{Overall}} = \Delta U_{\text{Overall}} = 0 \text{ kJ}$
ANS

Equation 3.23c gives the P-V relation for an adiabatic process. Let the intermediate state be denoted with subscript “int.” Thus $V_{\text{int}} = V_2$ since the second step is at constant volume.

Also $\gamma = C_P/C_V = (7R/2)/(5R/2) = (7/5) = 1.4$ from equation 3.24.

Solve for intermediate pressure, P_{int} , using equation 3.23c from lesson 11:

$$P_{\text{int}} = P_1 \left(\frac{V_1}{V_{\text{int}}} \right)^\gamma = 6.0 \text{ bar} \cdot \left(\frac{1.5 \text{ m}^3}{6.0 \text{ m}^3} \right)^{1.4} = 0.86152 \text{ bar}$$

Once P_{int} is known, the adiabatic work for step 1 is given by equation 3.26:

$$W_{\text{Step1}} = \frac{P_{\text{int}} \cdot V_{\text{int}} - P_1 \cdot V_1}{\gamma - 1} = \frac{0.86152 \text{ bar} \cdot 6.0 \text{ m}^3 - 6.0 \text{ bar} \cdot 1.5 \text{ m}^3}{1.4 - 1} = -9.5771 \text{ bar} \cdot \text{m}^3$$

Step 2 is at constant volume, so work is zero since $\Delta V = 0$:

$$W_{\text{Step2}} = -P \cdot \Delta V = 0.$$

The total overall work is the sum of the work of each step:

$$W_{\text{Overall}} = W_{\text{Step1}} + W_{\text{Step2}} = -9.5771 \text{ bar} \cdot \text{m}^3 + 0 \text{ bar} \cdot \text{m}^3 = -9.5771 \text{ bar} \cdot \text{m}^3$$

Now convert the units to kJ:

$$W_{\text{Overall}} = -9.5771 \text{ bar} \cdot \text{m}^3 \left(\frac{1 \text{ J}}{10^{-5} \text{ bar} \cdot \text{m}^3} \right) \cdot \left(\frac{1 \text{ kJ}}{1000 \text{ J}} \right) = \underline{\underline{-957.71 \text{ kJ}}}_{\text{ANS}}$$

Finally, for Q:

$$\Delta U_{\text{Overall}} = Q_{\text{Overall}} + W_{\text{Overall}} = 0 \Rightarrow Q_{\text{Overall}} = -W_{\text{Overall}} = \underline{\underline{957.71 \text{ kJ}}}_{\text{ANS}}$$

Solution, part (c):

$$PV = nRT \Rightarrow T_{\text{int}} = \frac{P_{\text{int}} \cdot V_{\text{int}}}{n \cdot R} = \frac{0.86152 \text{ bar} \cdot 6.0 \text{ m}^3}{0.200 \text{ kmol} \cdot \left(0.08314 \frac{\text{bar} \cdot \text{m}^3}{\text{kmol} \cdot \text{K}} \right)} = \underline{\underline{310.9 \text{ K}}}_{\text{ANS}}$$

Problem: Weight:
B 70

An engineering plan for a vinyl chloride plant includes a pipeline carrying ethylene (C₂H₄) at a volumetric flow rate of 15.350 MMSCFD (million standard cubic feet per day). Standard conditions are 60 °F (519.67 °R) and 14.696 psia.

Use the Soave-Redlich-Kwong (SRK) equation of state, Table 3.1, and gas constant R = 10.73 ft³·psia/(lbmol·°R) to determine the molar flow rate of C₂H₄ in lbmol/d. From Appendix B, the critical temperature, pressure, and acentric factor for C₂H₄ are ω = 0.087, T_C = 508.14 °R, and P_C = 730.99 psia.

Solution:

```

In[4]:= P = 14.696; (*psia*)
T = 519.67; (*Rankine*)
R = 10.73; (* ft³*psia / (lbmol*R), given*)
ω = 0.087; (*App. B, p.665*)
Tc = 508.14; (*p.665, convert K to R*)
Pc = 730.99; (*p. 665 convert bar to psia, App A*)
Tr1 = T / Tc; (*reduced temperature*)

In[11]:= σ = 1; (*Table 3.1, p.100*)
ε = 0;
Ω = 0.08664;
ϖ = 0.42748;
α = (1 + (0.480 + 1.574*ω - 0.176*ω²) * (1 - √Tr1))²;
a = ϖ * (α * R² * Tc²) / Pc; (*eq.3.45, p.98*)
b = Ω * (R * Tc) / Pc; (*eq.3.44, p.98*)

In[18]:= eq1 = P == (R * T) / (V - b) - a / ((V + ε * b) * (V + σ * b)); (*eq.3.41, p.97*)

In[19]:= ans = Quiet[Solve[eq1, V, Reals]]
Out[19]= {{V -> 376.98933}}

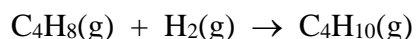
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Use V and molar flow rate to solve for volumetric flow rate (V^t):

$$\frac{15.350 \times 10^6 \text{ ft}^3}{\text{day}} \cdot \frac{1 \text{ lbmol}}{376.989 \text{ ft}^3} = \underline{\underline{40,717.4 \frac{\text{lbmol}}{\text{day}}}}_{\text{ANS}}$$

Problem: Weight:
C 50

Hydrogenation refers to the treatment of substances with hydrogen, H₂. Hydrogenation is important in the petrochemical and food processing industries. For example, hydrogenation of polyunsaturated fatty acids in vegetable oils reduces most of the carbon-carbon double bonds, making the oil safer and healthier for consumption. Hydrogenation reactions of hydrocarbons typically involve the reaction of alkenes with hydrogen to form alkanes at high temperatures and pressures, usually over a supported metal catalyst such as Raney nickel. Steam is often used as a diluent to control the temperature in the reactor. In this problem, you will consider the hydrogenation of 1-butene to form n-butane:



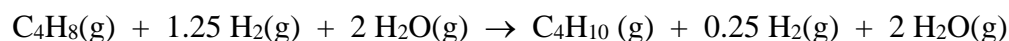
Calculate the standard gas-phase heat of hydrogenation of 1-butene at 475 °C and 1.00 bar in 25% excess hydrogen, with 2.00 moles of steam added per mole of propylene as a diluent to control the reactor temperature. The process is isothermal with reactants and products at 475 °C. Report your answer in J/mol.

The following table contains ideal gas heat capacity polynomial coefficients and standard heats of formation at 298 K from Appendix C:

species	a	b×10 ³	c×10 ⁶	d×10 ⁻⁵	ΔH _{f,298} ⁰ , J/mol
C ₄ H ₈	1.967	31.630	-9.873	0.000	-540
H ₂	3.249	0.422	0.000	0.083	0
H ₂ O	3.470	1.450	0.000	0.121	-241,818
C ₄ H ₁₀	1.935	36.915	-11.402	0.000	-125,790

Solution:

Balanced Reaction:



Solution in Mathematica is shown on the following page.

Mathematica Solution:

```

(*Stoichiometric coefficients*)
(*1-butene, hydrogen, water, butane, water*)
v = {-1, -1.25, -2, 1, .25, 2};
(*Standard Heats of Formation*)
ΔHf298 = {-540, 0, -241818, -125790, 0, -241818};
(*Heat of Reaction at 298 K*)
ΔH298 = Plus @@ (v*ΔHf298) (*J/mol*)

Out[3]= -125250.

In[4]:= (*Heat Capacity polynomial coefficients, Table C.1:*)
a = {1.967, 3.249, 3.470, 1.935, 3.249, 3.470};
b = {31.630, 0.422, 1.450, 36.915, 0.422, 1.450} * 10-3;
c = {-9.873, 0.000, 0.000, -11.402, 0.000, 0.000} * 10-6;
d = {0.000, 0.083, 0.121, 0.000, 0.083, 0.121} * 105;

Δa = Plus @@ (v * a);
Δb = Plus @@ (v * b);
Δc = Plus @@ (v * c);
Δd = Plus @@ (v * d);

(*Gas constant*)
R = 8.314; (*  $\frac{\text{J}}{\text{mol} \cdot \text{K}}$  *)
(*Temperatures, K*)
T = 475 + 273.15;
T0 = 298.15;
(*Equation 4.21 for MDCPH*)
MDCPH = Δa +  $\frac{\Delta b}{2} * (T + T0) + \frac{\Delta c}{3} * (T^2 + T0^2 + T * T0) + \frac{\Delta d}{T * T0}$ 

Out[15]= -1.2183988

In[16]:= (*Equation 4.22 for corrected heat of reaction at 748 K*)
(*Gives molar heat of reaction in J/mol*)
ΔH748 = ΔH298 + MDCPH * R * (T - T0)

Out[16]= -129808.4

```

ANS, J per mole of C₄H₈

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17 October 2023, Makeup v1

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BONUS	30	
TOTAL GRADE	200	

Problem: Weight:
A 80

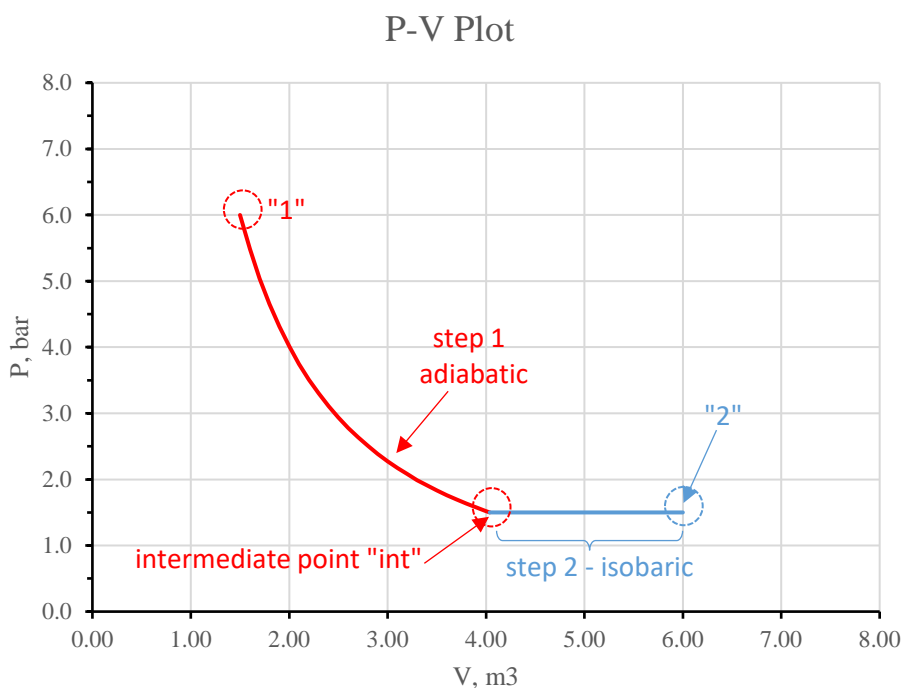
0.200 kmol of an ideal gas in a closed system is changed from an initial state of 1.5 m³, 6.0 bar and 541.3 K to a final state of 6.0 m³, 1.5 bar, and 541.3 K by a two-step process consisting of an adiabatic expansion followed by heating at constant pressure. (a) Sketch the process path in the PV axes below. (b) Calculate Q, W, ΔU and ΔH for the overall process in units of kJ. (c) Calculate the intermediate temperature after step 1.

$$R = 8.314 \text{ J}/(\text{mol} \cdot \text{K}) = 0.08314 \text{ (bar} \cdot \text{m}^3)/(\text{kmol} \cdot \text{K})$$

$$C_P = (7/2) \cdot R, \text{ and}$$

$$C_V = (5/2) \cdot R$$

Solution, part (a):



Solution, part (b):

The overall process is isothermal ($T_2 = T_1$), so $\Delta H_{\text{Overall}} = \Delta U_{\text{Overall}} = 0 \text{ kJ}$
ANS

Equation 3.23c gives the P-V relation for an adiabatic process. Let the intermediate state be denoted with subscript “int” with $P_{\text{int}} = P_2$ since the second step is at constant pressure.

Also $\gamma = C_P/C_V = (7R/2)/(5R/2) = (7/5) = 1.4$ from equation 3.24.

Solve for intermediate volume, V_{int} , using equation 3.23c from lesson 11:

$$P_{\text{int}} V_{\text{int}}^{\gamma} = P_1 V_1^{\gamma} \Rightarrow V_{\text{int}} = \sqrt[\gamma]{\frac{P_1}{P_{\text{int}}}} V_1^{\gamma} = \sqrt[1.4]{\frac{6.0 \text{ bar}}{1.5 \text{ bar}}} (1.5 \text{ m}^3)^{1.4} = 4.037701 \text{ m}^3$$

Once V_{int} is known, the adiabatic work for step 1 is given by equation 3.26:

$$W_{\text{Step1}} = \frac{P_{\text{int}} \cdot V_{\text{int}} - P_1 \cdot V_1}{\gamma - 1} = \frac{1.6 \text{ bar} \cdot 4.037701 \text{ m}^3 - 6.0 \text{ bar} \cdot 1.5 \text{ m}^3}{1.4 - 1} = -7.3586 \text{ bar} \cdot \text{m}^3$$

Step 2 is at constant pressure, so work $-P\Delta V$:

$$W_{\text{Step2}} = -P \cdot \Delta V = -P \cdot (V_2 - V_{\text{int}}) = -1.5 \cdot (6.0 \text{ m}^3 - 4.037701 \text{ m}^3) = -2.9434 \text{ bar} \cdot \text{m}^3.$$

The total overall work is the sum of the work of each step:

$$W_{\text{Overall}} = W_{\text{Step1}} + W_{\text{Step2}} = -7.3586 \text{ bar} \cdot \text{m}^3 + (-2.9434) \text{ bar} \cdot \text{m}^3 = -10.3021 \text{ bar} \cdot \text{m}^3$$

Now convert the units to kJ:

$$W_{\text{Overall}} = -10.3021 \text{ bar} \cdot \text{m}^3 \left(\frac{1 \text{ J}}{10^{-5} \text{ bar} \cdot \text{m}^3} \right) \cdot \left(\frac{1 \text{ kJ}}{1000 \text{ J}} \right) = \underline{\underline{-1030.21 \text{ kJ}}}_{\text{ANS}}$$

Finally, for Q:

$$\Delta U_{\text{Overall}} = Q_{\text{Overall}} + W_{\text{Overall}} = 0 \Rightarrow Q_{\text{Overall}} = -W_{\text{Overall}} = \underline{\underline{1030.21 \text{ kJ}}}_{\text{ANS}}$$

Solution, part (c):

$$PV = nRT \Rightarrow T_{\text{int}} = \frac{P_{\text{int}} \cdot V_{\text{int}}}{n \cdot R} = \frac{1.5 \text{ bar} \cdot 4.037701 \text{ m}^3}{0.200 \text{ kmol} \cdot \left(0.08314 \frac{\text{bar} \cdot \text{m}^3}{\text{kmol} \cdot \text{K}} \right)} = \underline{\underline{364.2 \text{ K}}}_{\text{ANS}}$$

Problem: Weight:
B 70

An engineering plan for a vinyl chloride plant includes a pipeline carrying ethylene (C₂H₄) at a volumetric flow rate of 15.350 MMSCFD (million standard cubic feet per day). Standard conditions are 519.67°R and 14.696 psia. At these conditions, the molar volume of C₂H₄ is 376.99 ft³/lbmol.

(a) Calculate the molar flow rate of C₂H₄ in lbmol/sec.

(b) Use the Soave-Redlich-Kwong (SRK) equation of state (equations 3.41, 3.44, and 3.45), constants in Table 3.1, and gas constant R = 10.73 ft³·psia/(lbmol·R) to determine the isothermal reversible **compression** work required to increase the molar volume of C₂H₄ by 10%. From Appendix B, the critical temperature, pressure, and acentric factor for C₂H₄ are ω = 0.087, T_c = 508.14 Rankine, and P_c = 730.99 psia. Report the work in hp.

Solution, part (a):

$$\frac{15,350,000 \text{ ft}^3}{\text{day}} \cdot \frac{1 \text{ day}}{24 \text{ h}} \cdot \frac{1 \text{ h}}{3600 \text{ s}} \cdot \frac{1 \text{ lbmol}}{376.99 \text{ ft}^3} = 0.47126 \frac{\text{lbmol}}{\text{s}}$$

ANS

Solution, part (b):

```

T = 519.67; (*Rankine, given*)
R = 10.73; (* ft^3*psia / (lbmol*R), given*)
omega = 0.087; (*App. B, p.665*)
Tc = 508.14; (*Rankine, given*)
Pc = 730.99; (*psia, given*)
Tr1 = T / Tc; (*reduced temperature*)
(*Table 3.1, p.100*)
sigma = 1;
epsilon = 0;
Omega = 0.08664;
Psi = 0.42748;
alpha = (1 + (0.480 + 1.574*omega - 0.176*omega^2) * (1 - sqrt(Tr1)))^2;
(*Equations 3.41, 3.44, and 3.45*)
b = Omega * (R * Tc) / Pc;
a = Psi * (alpha * R^2 * Tc^2) / Pc;
P[V_] = (R * T) / (V - b) - (a / ((V + epsilon * b) * (V + sigma * b)));
    
```


Cadet: _____

$$\text{In[16]}:= W = \int_{376.99}^{1.1 \cdot 376.99} P[V] \, dV \quad (*eq \, 1.4, \text{ units } \frac{\text{psia} \cdot \text{ft}^3}{\text{lbmol}} *)$$

Out[16]= 528.19808

$$\text{In[17]}:= \frac{528.2 \text{ psia} \cdot \text{ft}^3}{\text{lbmol}} * \frac{\frac{\text{lbf}}{\text{in}^2}}{\text{psia}} * \left(\frac{12 \text{ in}}{\text{ft}} \right)^2 * \frac{0.47126 \text{ lbmol}}{\text{s}} * \frac{1.34102 \text{ hp}}{737.562 \frac{\text{ft} \cdot \text{lbf}}{\text{s}}}$$

Out[17]= 65.171571 hp

=====ANS

Problem: Weight:
C 50

Methanol ($\text{CH}_3\text{OH}(\text{g})$) is fed to a combustion reactor with 50% excess air. (a) Balance the reaction. (b) Calculate the heat of reaction at 25 °C and 1.01 bar in J/mol on a basis of one mole of methanol in the feed.. (c) Calculate the standard gas-phase heat of reaction at 30 °C and 1.01 bar in 50% excess air. The process is isothermal with reactants and products at 30 °C.

The following table contains ideal gas heat capacity polynomial coefficients and standard heats of formation at 298 K from Appendix C:

species	a	$b \times 10^3$	$c \times 10^6$	$d \times 10^{-5}$	$\Delta H_{f,298}^0$, J/mol
CH_3OH	2.211	12.216	-3.450	0.000	-200,660
O_2	3.639	0.506	0.000	-0.227	0
N_2	3.280	0.593	0.000	0.040	0
CO_2	5.457	1.045	0.000	-1.157	-393,509
H_2O	3.470	1.450	0.000	0.121	-241,818

Solution:

Balanced Reaction:



Solution in Mathematica is shown on the following page.

Mathematica Solution:

```
In[55]:= (*Stoichiometric coefficients*)
(*Methanol, oxygen, nitrogen, carbon dioxide, water, oxygen, nitrogen*)
v = {-1, -2.25, -8.46, 1, 2, .75, 8.46};
```

```
In[56]:= (*Standard Heats of Formation*)
ΔHf298 = {-200660, 0, 0, -393509, -241818, 0, 0};
```

```
In[57]:= (*Heat of Reaction at 298 K*)
ΔH298 = Plus@@(v*ΔHf298) (*J/mol*)
```

```
Out[57]= -676485.
```

```
In[58]:= (*Heat Capacity polynomial coefficients, Table C.1:*)
a = {2.211, 3.639, 3.280, 5.457, 3.470, 3.639, 3.280};
b = {12.216, 0.506, 0.593, 1.045, 1.450, 0.506, 0.593} * 10-3;
c = {-3.450, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000} * 10-6;
d = {0.000, -0.227, 0.040, -1.157, 0.121, -0.227, 0.040} * 105;
```

```
In[62]:= Δa = Plus@@(v*a);
Δb = Plus@@(v*b);
Δc = Plus@@(v*c);
Δd = Plus@@(v*d);
```

```
In[66]:= (*Temperatures, K*)
T = 303.15;
T0 = 298.15;
```

```
In[68]:= (*Gas constant*)
R = 8.314; (*  $\frac{\text{J}}{\text{mol}\cdot\text{K}}$  *)
```

```
In[69]:= (*Equation 4.21 for MCPH*)
MCPH = Δa +  $\frac{\Delta b}{2} * (T + T0) + \frac{\Delta c}{3} * (T^2 + T0^2 + T * T0) + \frac{\Delta d}{T * T0}$ 
```

```
Out[69]= 1.6888645
```

```
In[70]:= (*Equation 4.22 for corrected heat of reaction*)
(*Gives molar heat of reaction in J/mol*)
ΔH303 = ΔH298 + MCPH * R * (T - T0)
```

```
Out[70]= -676414.79
          ANS
```

CADET _____ SECTION _____ TIME OF DEPARTURE _____

DEPARTMENT OF CHEMISTRY & LIFE SCIENCE

CH365 2023-2024

WRITTEN PARTIAL REVIEW II

20 October 2023, Makeup v2

TEXT: Smith, Van Ness, Abbott & Swihart

SCOPE: Lessons 10-20

TIME: 55 Minutes

References Permitted: Open notes, book, internet, Mathematica, and Excel.

INSTRUCTIONS

1. Do not mark this exam or open it until “begin work” is given.
2. You have 55 minutes to complete the exam.
3. Solve the problems in the space provided. Show all work to receive full credit.
4. There are 3 problems on 3 pages in this exam (not including the cover page). Write your name on the top of each sheet.
5. Save Mathematica files on your desktop and re-save frequently.
6. When finished, upload all Mathematica files to Canvas.

(TOTAL WEIGHT: 200 POINTS)

DO NOT WRITE IN THIS SPACE

PROBLEM	VALUE	CUT
A	80	
B	70	
C	50	
TOTAL CUT		
BONUS	30	
TOTAL GRADE	200	

Problem: Weight:
A 80

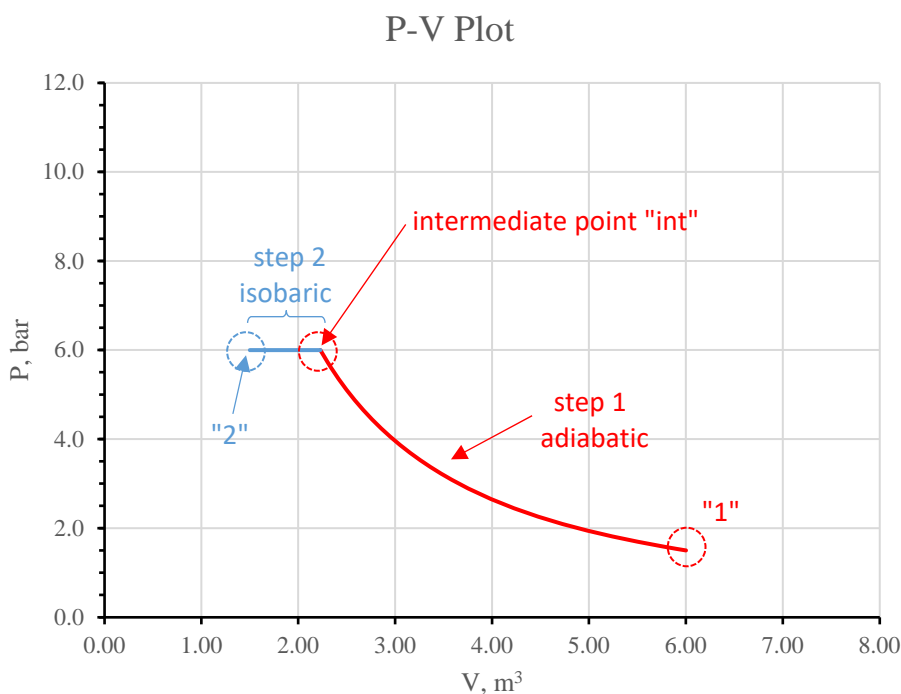
0.250 kmol of an ideal gas in a closed system is changed from an initial state of 6.0 m³, 1.5 bar and 433.0 K to a final state of 1.5 m³, 6.0 bar, and 433.0 K by a two-step process consisting of an adiabatic compression followed by cooling at constant pressure. (a) Sketch the process path in the PV axes below. (b) Calculate Q, W, ΔU and ΔH for the overall process in units of kJ. (c) Calculate the intermediate temperature after step 1.

$$R = 8.314 \text{ J/(mol} \cdot \text{K)} = 0.08314 \text{ (bar} \cdot \text{m}^3\text{)/(kmol} \cdot \text{K)}$$

$$C_P = (7/2) \cdot R, \text{ and}$$

$$C_V = (5/2) \cdot R$$

Solution, part (a):



Solution, part (b):

The overall process is isothermal ($T_2=T_1$), so $\Delta H_{\text{Overall}} = \Delta U_{\text{Overall}} = 0 \text{ kJ}$
ANS

Equation 3.23c gives the P-V relation for an adiabatic process. Let the intermediate state be denoted with subscript “int” with $P_{\text{int}} = P_2$ since the second step is at constant pressure.

Also $\gamma = C_P/C_V = (7R/2)/(5R/2) = (7/5) = 1.4$ from equation 3.24.

Solve for intermediate volume, V_{int} , using equation 3.23c from lesson 11:

$$P_{\text{int}} V_{\text{int}}^{\gamma} = P_1 V_1^{\gamma} \Rightarrow V_{\text{int}} = \sqrt[\gamma]{\frac{P_1}{P_{\text{int}}}} V_1^{\gamma} = \sqrt[1.4]{\frac{1.5 \text{ bar}}{6.0 \text{ bar}}} (6.0 \text{ m}^3)^{1.4} = 2.228991 \text{ m}^3$$

Once V_{int} is known, the adiabatic work for step 1 is given by equation 3.26:

$$W_{\text{Step1}} = \frac{P_{\text{int}} \cdot V_{\text{int}} - P_1 \cdot V_1}{\gamma - 1} = \frac{6.0 \text{ bar} \cdot 2.228991 \text{ m}^3 - 1.5 \text{ bar} \cdot 6.0 \text{ m}^3}{1.4 - 1} = +10.9349 \text{ bar} \cdot \text{m}^3$$

Step 2 is at constant pressure, so work $-P\Delta V$:

$$W_{\text{Step2}} = -P \cdot \Delta V = -P \cdot (V_2 - V_{\text{int}}) = -6.0 \cdot (1.5 \text{ m}^3 - 2.228991 \text{ m}^3) = +4.37395 \text{ bar} \cdot \text{m}^3.$$

The total overall work is the sum of the work of each step:

$$W_{\text{Overall}} = W_{\text{Step1}} + W_{\text{Step2}} = 10.9349 \text{ bar} \cdot \text{m}^3 + 4.3739 \text{ bar} \cdot \text{m}^3 = 15.3088 \text{ bar} \cdot \text{m}^3$$

Now convert the units to kJ:

$$W_{\text{Overall}} = 15.3088 \text{ bar} \cdot \text{m}^3 \left(\frac{1 \text{ J}}{10^{-5} \text{ bar} \cdot \text{m}^3} \right) \cdot \left(\frac{1 \text{ kJ}}{1000 \text{ J}} \right) = \underline{\underline{1530.88 \text{ kJ}}}_{\text{ANS}}$$

Finally, for Q:

$$\Delta U_{\text{Overall}} = Q_{\text{Overall}} + W_{\text{Overall}} = 0 \Rightarrow Q_{\text{Overall}} = -W_{\text{Overall}} = \underline{\underline{-1530.88 \text{ kJ}}}_{\text{ANS}}$$

Solution, part (c):

$$PV = nRT \Rightarrow T_{\text{int}} = \frac{P_{\text{int}} \cdot V_{\text{int}}}{n \cdot R} = \frac{6.0 \text{ bar} \cdot 2.228991 \text{ m}^3}{0.250 \text{ kmol} \cdot \left(0.08314 \frac{\text{bar} \cdot \text{m}^3}{\text{kmol} \cdot \text{K}} \right)} = \underline{\underline{643.44 \text{ K}}}_{\text{ANS}}$$

Problem: Weight:
B 70

An engineering plan for a vinyl chloride plant includes a pipeline carrying ethylene (C₂H₄) at a volumetric flow rate of 7.175 MMSCFD (million standard cubic feet per day). Standard conditions are 519.67°R and 14.696 psia. At these conditions, the molar volume of C₂H₄ is 376.99 ft³/lbmol.

(a) Calculate the molar flow rate of C₂H₄ in lbmol/sec.

(b) Use the Soave-Redlich-Kwong (SRK) equation of state (equations 3.41, 3.44, and 3.45), constants in Table 3.1, and gas constant R = 10.73 ft³·psia/(lbmol·R) to determine the isothermal reversible compression work required to reduce the molar volume of C₂H₄ by 20%. From Appendix B, the critical temperature, pressure, and acentric factor for C₂H₄ are ω = 0.087, T_c = 508.14 Rankine, and P_c = 730.99 psia. Report the work in hp.

Solution, part (a):

$$\frac{7,175,000 \text{ ft}^3}{\text{day}} \cdot \frac{1 \text{ day}}{24 \text{ h}} \cdot \frac{1 \text{ h}}{3600 \text{ s}} \cdot \frac{1 \text{ lbmol}}{376.99 \text{ ft}^3} = 0.22028 \frac{\text{lbmol}}{\text{s}}$$

ANS

Solution, part (b):

```

T = 519.67; (*Rankine, given*)
R = 10.73; (* ft3*psia / (lbmol*R), given*)
ω = 0.087; (*App. B, p.665*)
Tc = 508.14; (*Rankine, given*)
Pc = 730.99; (*psia, given*)
Tr1 = T / Tc; (*reduced temperature*)
(*Table 3.1, p.100*)
σ = 1;
ε = 0;
Ω = 0.08664;
ϖ = 0.42748;
α = (1 + (0.480 + 1.574*ω - 0.176*ω2) * (1 - √Tr1))2;
(*Equations 3.41, 3.44, and 3.45*)
b = Ω * (R * Tc) / Pc;
a = ϖ * (α * R2 * Tc2) / Pc;
P[V_] = (R * T) / (V - b) - (a / ((V + ε * b) * (V + σ * b)));

```

Cadet: _____

$$W = - \int_{376.99}^{.8 \cdot 376.99} P[V] \, dV \quad (*eq \, 1.4, \, units \, \frac{psia \cdot ft^3}{lbmol} *)$$

1235.3086

$$\frac{1235.3086 \, psia \cdot ft^3}{lbmol} * \frac{\frac{lb_f}{in^2}}{psia} * \left(\frac{12 \, in}{ft} \right)^2 * \frac{0.22028 \, lbmol}{s} * \frac{1.34102 \, hp}{737.562 \, \frac{ft \cdot lb_f}{s}}$$

71.24423812 hp

===== ANS

Problem: Weight:
C 50

Methanol (CH₃OH(g)) is fed to a combustion reactor with 50% excess air. (a) Balance the reaction. (b) Calculate the heat of reaction at 25 °C and 1.01 bar in J/mol on a basis of one mole of methanol in the feed. (c) Calculate the standard gas-phase heat of reaction at 30 °C and 1.01 bar in 50% excess air. The process is isothermal with reactants and products at 30 °C.

The following table contains ideal gas heat capacity polynomial coefficients and standard heats of formation at 298 K from Appendix C:

species	a	b×10 ³	c×10 ⁶	d×10 ⁻⁵	ΔH _{f,298} ⁰ , J/mol
CH ₃ OH	2.211	12.216	-3.450	0.000	-200,660
O ₂	3.639	0.506	0.000	-0.227	0
N ₂	3.280	0.593	0.000	0.040	0
CO ₂	5.457	1.045	0.000	-1.157	-393,509
H ₂ O	3.470	1.450	0.000	0.121	-241,818

Solution:

Balanced Reaction:



Solution in Mathematica is shown on the following page.

Mathematica Solution:

```
In[55]:= (*Stoichiometric coefficients*)
(*Methanol, oxygen, nitrogen, carbon dioxide, water, oxygen, nitrogen*)
v = {-1, -2.25, -8.46, 1, 2, .75, 8.46};
```

```
In[56]:= (*Standard Heats of Formation*)
ΔHf298 = {-200 660, 0, 0, -393 509, -241 818, 0, 0};
```

```
In[57]:= (*Heat of Reaction at 298 K*)
ΔH298 = Plus @@ (v * ΔHf298) (*J/mol*)
```

```
Out[57]= -676485.
```

```
In[58]:= (*Heat Capacity polynomial coefficients, Table C.1:*)
a = {2.211, 3.639, 3.280, 5.457, 3.470, 3.639, 3.280};
b = {12.216, 0.506, 0.593, 1.045, 1.450, 0.506, 0.593} * 10-3;
c = {-3.450, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000} * 10-6;
d = {0.000, -0.227, 0.040, -1.157, 0.121, -0.227, 0.040} * 105;
```

```
In[62]:= Δa = Plus @@ (v * a);
Δb = Plus @@ (v * b);
Δc = Plus @@ (v * c);
Δd = Plus @@ (v * d);
```

```
In[66]:= (*Temperatures, K*)
T = 303.15;
T0 = 298.15;
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```
In[68]:= (*Gas constant*)
R = 8.314; (*  $\frac{\text{J}}{\text{mol}\cdot\text{K}}$  *)
```

```
In[69]:= (*Equation 4.21 for MCPH*)
MCPH = Δa +  $\frac{\Delta b}{2} * (T + T0) + \frac{\Delta c}{3} * (T^2 + T0^2 + T * T0) + \frac{\Delta d}{T * T0}$ 
```

```
Out[69]= 1.6888645
```

```
In[70]:= (*Equation 4.22 for corrected heat of reaction*)
(*Gives molar heat of reaction in J/mol*)
ΔH303 = ΔH298 + MCPH * R * (T - T0)
```

```
Out[70]= -676414.79
```

ANS, J per mole of methanol