CADET _____ SECTION _____TIME OF DEPARTURE _____

DEPARTMENT OF CHEMISTRY & LIFE SCIENCE

CH365 2024-2025   TEXT: Smith, Van Ness, Abbott & Swihart
WRITTEN PARTIAL REVIEW II   SCOPE: Lessons 10-20
15 October 2024, A-Hour   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. Use the back of the pages for extra workspace as needed.
5. Save Mathematica files on your desktop and re-save frequently.
6. When finished, upload all Mathematica files to Canvas.

(TOTAL WEIGHT: 200 POINTS)

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DO NOT WRITE IN THIS SPACE

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

Problem: Weight:
   A   50

Methanol ($CH_4O(g)$) is fed to a combustion reactor with 100% excess air.

(a) Balance the reaction on a basis of one mole of methanol in the feed.

(b) Calculate the heat of reaction at 25 °C and 1.0 bar in J/mol on a basis of one mole of methanol in the feed.

(c) Calculate the standard gas-phase isothermal heat of reaction at 300 °C and 1.0 bar for one mole of methanol in 100% excess air.

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

species	a	$b \times 10^3$	$c \times 10^6$	$d \times 10^{-5}$	$\Delta H^0_{f,298}$, J/mol
CH_4O	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, part (a):

Balanced reaction in 100% excess air:

$$CH_4O(g) + 3\ O_2(g) + 11.29\ N_2(g)$$
$$\rightarrow CO_2(g) + 2\ H_2O(g) + 1.50\ O_2(g) + 11.29\ N_2(g)$$
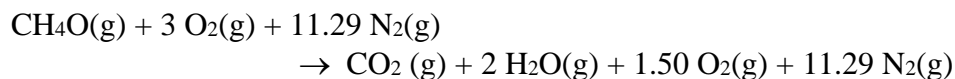
Solution of parts (b) and (c) in Mathematica are shown on the following page.

Solution, part (b):

```
(*List of stoichiometric coefficients*)
(*methanol, oxygen, nitrogen, carbon dioxide, water, oxygen, nitrogen*)
ν = {-1, -3, -11.29, 1, 2, 1.5, 11.29};

(*List of standard Heats of Formation*)
ΔHf298 = {-200 660, 0, 0, -393 509, -241 818, 0, 0};

(*Standard Heat of Reaction at 298 K*)
ΔH298 = Plus @@ (ν * ΔHf298)  (*J/mol*)

-676 485.
```

ANS, J per mole of methanol

Solution, part (c):

```
(*Heat Capacity polynomial coefficients, Given, from 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;

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

(*Temperatures, K*)
T = 300 + 273.15;
T0 = 25 + 273.15;

(*Gas constant*)
R = 8.314;  (* J/mol*K *)
```

```
(*Equation 4.21 for MDCPH*)
```
$$MDCPH = \Delta a + \frac{\Delta b}{2} * (T + T0) + \frac{\Delta c}{3} * (T^2 + T0^2 + T*T0) + \frac{\Delta d}{T*T0}$$

```
1.13391
```

```
(*Equation 4.22 for corrected heat of reaction*)
(*Gives molar heat of reaction in J/mol*)
ΔH573 = ΔH298 + MDCPH * R * (T - T0)

-673 892.5
```

ANS, J per mole of methanol

Problem: Weight:
   B   70

An engineering plan for a vinyl chloride plant includes a pipeline carrying ethylene (C_2H_4) at a volumetric flow rate of 25.750 MMSCFD (million standard cubic feet per day). Standard conditions are 519.67°R and 14.696 psia. At these conditions, the molar volume of C_2H_4 is 377.27 ft^3/lbmol.

(a) Calculate the molar flow rate of C_2H_4 in lbmol/sec.

(b) Use the van der Waals (vdW) equation of state (equations 3.41, 3.44, and 3.45), constants in Table 3.1, and gas constant R = 10.73 ft^3·psia/(lbmol·R) to determine the isothermal reversible work produced by increasing the molar volume of C_2H_4 by 5%. Report the work in hp.

From Appendix B, the critical temperature, pressure, and acentric factor for ethylene are T_C = 508.14 Rankine, and P_C = 730.99 psia, and ω = 0.087.

Solution, part (a):

$$\frac{25,750,000\,\text{ft}^3}{\text{day}} \cdot \frac{1\,\text{day}}{24\,\text{h}} \cdot \frac{1\,\text{h}}{3600\,\text{s}} \cdot \frac{1\,\text{lbmol}}{377.27\,\text{ft}^3} = 0.78997\,\frac{\text{lbmol}}{\underset{\text{ANS}}{\underline{\underline{\text{s}}}}}$$

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 = 0;
ε = 0;
Ω = 1 / 8;
Ψ = 27 / 64;
α = 1;
(*Equations 3.41, 3.44, and 3.45*)
```

$$b = \Omega * \frac{R * Tc}{Pc};$$

$$a = \Psi * \frac{\alpha * R^2 * Tc^2}{Pc};$$

$$P[V\_] = \frac{R * T}{V - b} - \frac{a}{(V + \epsilon * b) * (V + \sigma * b)};$$

$$W = -\int_{377.27}^{1.05*377.27} P[V]\,dV \quad (*\text{eq 1.4, units } \frac{\text{psia}*\text{ft}^3}{\text{lbmol}} *)$$

```
-270.5491
```

$$W = -\int_{377.27}^{1.05*377.27} P[V] \, dV \quad (*\text{eq } 1.4, \text{ units } \tfrac{psia*ft^3}{lbmol} *)$$

-270.5491

$$\frac{-270.5491 \, psia * ft^3}{lbmol} * \frac{\frac{lbf}{in^2}}{psia} * \left(\frac{12 \, in}{ft}\right)^2 * \frac{0.78997 \, lbmol}{s} * \frac{1.34102 \, hp}{737.562 \, \frac{ft*lbf}{s}}$$

$-55.95719 \, hp$

$\underline{\qquad\qquad}$ ANS

Problem: Weight:
  C   80

0.200 kmol of an ideal gas in a closed system is changed from an initial state of 1.5 m³, 5.0 bar and 451.0 K to a final state of 5.0 m³, 1.5 bar, and 451.0 K by a two-step process consisting of an adiabatic expansion followed by heating at constant pressure.
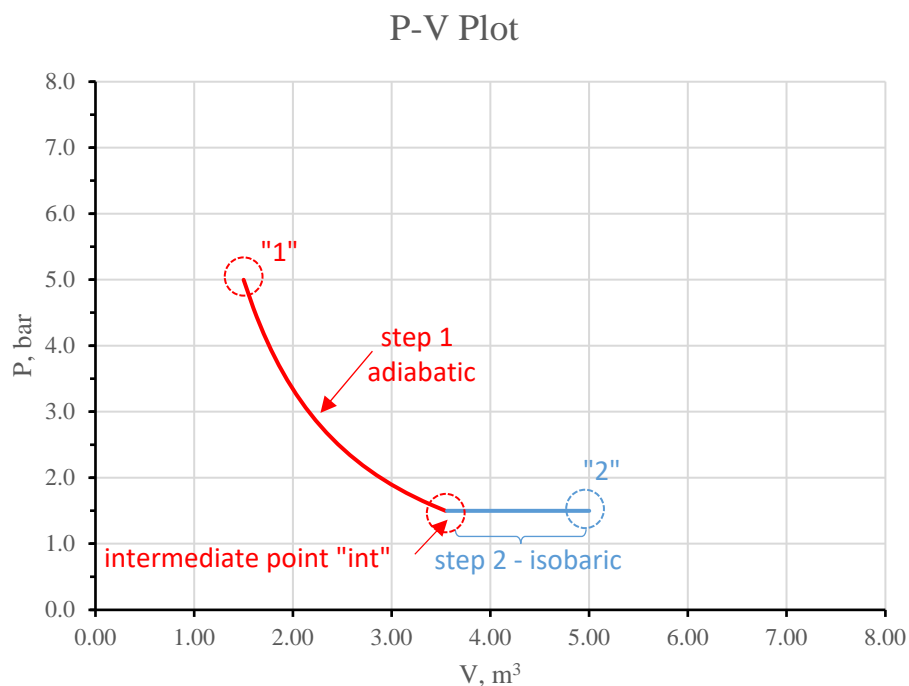
(a) Sketch the process path on the PV axes below.

(b) Calculate Q, W, ΔU and ΔH for the overall process <u>in units of kJ</u>.

(c) Calculate the intermediate temperature after step 1.

$$R = 8.314 \text{ J/(mol·K)} = 0.08314 \text{ (bar·m}^3\text{)/(kmol·K)}$$
$$C_P = (7/2)·R, \text{ and}$$
$$C_V = (5/2)·R$$

Solution, part (a):

P-V Plot

Solution, part (b):

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

ANS

Equation 3.23c gives the P-V relation for an adiabatic process. Let the intermediate state be denoted with subscript "int" with $P_{int} = P_2$ 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:

$$P_{int} V_{int}^{\gamma} = P_1 V_1^{\gamma} \Rightarrow V_{int} = \sqrt[\gamma]{\frac{P_1}{P_{int}} V_1^{\gamma}} = \sqrt[1.4]{\frac{5.0\,bar}{1.5\,bar}\left(1.5\,m^3\right)^{1.4}} = 3.544672\,m^3$$

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

$$W_{Step1} = \frac{P_{int} \cdot V_{int} - P_1 \cdot V_1}{\gamma - 1} = \frac{1.5\,bar \cdot 3.5446721\,m^3 - 5.0\,bar \cdot 1.5\,m^3}{1.4 - 1} = -5.457479\,bar \cdot m^3$$

Step 2 is at constant pressure, so work -PΔV:

$$W_{Step2} = -P \cdot \Delta V = -P \cdot \left(V_2 - V_{int}\right) = -1.5 \cdot \left(5.0\,m^3 - 3.544672\,m^3\right) = -2.18299\,bar \cdot m^3.$$

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

$$W_{Overall} = W_{Step1} + W_{Step2} = -5.45748\,bar \cdot m^3 + \left(-2.18299\right)bar \cdot m^3 = -7.64047\,bar \cdot m^3$$

Now convert the units to kJ:

$$W_{Overall} = -7.640471\,bar \cdot m^3 \left(\frac{1\,J}{10^{-5}\,bar \cdot m^3}\right) \cdot \left(\frac{1\,kJ}{1000\,J}\right) = \underline{\underline{-764.047\,kJ}}_{ANS}$$

Finally, for Q:

$$\Delta U_{Overall} = Q_{Overall} + W_{Overall} = 0 \Rightarrow Q_{Overall} = -W_{Overall} = \underline{\underline{764.047\,kJ}}_{ANS}$$

Solution, part (c):

$$PV = nRT \Rightarrow T_{int} = \frac{P_{int} \cdot V_{int}}{n \cdot R} = \frac{1.5\,bar \cdot 3.544672\,m^3}{0.200\,kmol \cdot \left(0.08314\dfrac{bar \cdot m^3}{kmol \cdot K}\right)} = \underline{\underline{319.8\,K}}_{ANS}$$

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

Problem: Weight:
   A   50

Ethanol ($C_2H_6O(g)$) is fed to a combustion reactor with 100% excess air.

(a) Balance the reaction on a basis of one mole of ethanol in the feed.

(b) Calculate the heat of reaction at 25 °C and 1.0 bar in J/mol on a basis of one mole of ethanol in the feed.

(c) Calculate the standard gas-phase isothermal heat of reaction at 30<u>0</u> °C and 1.0 bar for one mole of ethanol in 100% excess air.

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

species	a	$b \times 10^3$	$c \times 10^6$	$d \times 10^{-5}$	$\Delta H^0_{f,298}$, J/mol
C_2H_6O	3.518	20.001	-6.002	0.000	-235,100
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, part (a):

Balanced reaction in 100% excess air:

$C_2H_6O(g) + 6\ O_2(g) + 22.57\ N_2(g)$
$\rightarrow 2\ CO_2\ (g) + 3\ H_2O(g) + 3\ O_2(g) + 22.57\ N_2(g)$
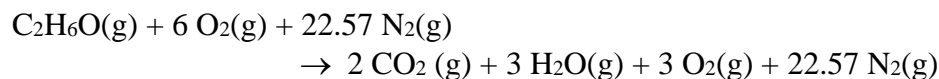
Solution of parts (b) and (c) in Mathematica are shown on the following page.

Solution, part (b):

```
(*List of stoichiometric coefficients*)
(*methanol, oxygen, nitrogen, carbon dioxide, water, oxygen, nitrogen*)
ν = {-1, -6, -22.57, 2, 3, 3, 22.57};

(*List of standard Heats of Formation*)
ΔHf298 = {-235100, 0, 0, -393509, -241818, 0, 0};

(*Standard Heat of Reaction at 298 K*)
ΔH298 = Plus @@ (ν * ΔHf298) (*J/mol*)
```

-1.277372×10^6

ANS, J per mole of ethanol

Solution, part (c):

```
(*Heat Capacity polynomial coefficients, Given, from Table C.1:*)
a = { 3.518,  3.639, 3.280,  5.457, 3.470,  3.639, 3.280};
b = {20.001,  0.506, 0.593,  1.045, 1.450,  0.506, 0.593} * 10^-3;
c = {-6.002,  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} * 10^5;

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

(*Temperatures, K*)
T = 300 + 273.15;
T0 = 25 + 273.15;

(*Gas constant*)
R = 8.314; (* J/(mol*K) *)

(*Equation 4.21 for MDCPH*)
```

$$MDCPH = \Delta a + \frac{\Delta b}{2} * (T + T0) + \frac{\Delta c}{3} * (T^2 + T0^2 + T * T0) + \frac{\Delta d}{T * T0}$$

0.7535926

```
(*Equation 4.22 for corrected heat of reaction*)
(*Gives molar heat of reaction in J/mol*)
ΔH573 = ΔH298 + MDCPH * R * (T - T0)
```

-1.275649×10^6

ANS, J per mole of ethanol

Problem: Weight:
   B   70

An engineering plan for a vinyl chloride plant includes a pipeline carrying ethylene (C_2H_4) 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 C_2H_4 is 376.68 ft^3/lbmol.

(a) Calculate the molar flow rate of C_2H_4 in lbmol/sec.

(b) Use the Peng-Robinson (PR) equation of state (equations 3.41, 3.44, and 3.45), constants in Table 3.1, and gas constant R = 10.73 ft^3·psia/(lbmol·R) to determine the isothermal reversible compression work required to reduce the molar volume of C_2H_4 by 10%. Report the work in hp.

From Appendix B, the critical temperature, pressure, and acentric factor for ethylene are T_C = 508.14 Rankine, and P_C = 730.99 psia, and ω = 0.087.

Solution, part (a):

$$\frac{7,175,000\,ft^3}{day} \cdot \frac{1\,day}{24\,h} \cdot \frac{1\,h}{3600\,s} \cdot \frac{1\,lbmol}{376.68\,ft^3} = 0.22046\,\underset{\text{ANS}}{\underline{\frac{lbmol}{s}}}$$

Solution, part (b):

```
T = 519.67; (*Rankine, given*)
R = 10.73; (* ft³*psia , given*)
              lbmol*R
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 + √2;
ε = 1 - √2;
Ω = 0.07780;
Φ = 0.45724;
α = (1 + (0.37464 + 1.54226 * ω - 0.26992 * ω²) * (1 - √Tr1));
(*Equations 3.41, 3.44, and 3.45*)
         R * Tc
b = Ω * ------- ;
           Pc

         α * R² * Tc²
a = Φ * ------------- ;
             Pc

       R * T              a
P = ------- - ------------------------- ;
     V - b    (V + ε * b) * (V + σ * b)
```

$$W = -\int_{376.68}^{0.9*376.68} P \, dV \quad (* \text{eq 1.4, units } \frac{psia*ft^3}{lbmol} *)$$

583.0164

$$\frac{583.0164 \, psia * ft^3}{lbmol} * \frac{\frac{lbf}{in^2}}{psia} * \left(\frac{12 \, in}{ft}\right)^2 * \frac{0.22046 \, lbmol}{s} * \frac{1.34102 \, hp}{737.562 \, \frac{ft*lbf}{s}}$$

33.65192 hp
_____ ANS

Problem: Weight:
  C   80

0.500 kmol of an ideal gas in a closed system is changed from an initial state of 7.0 m³, 3.0 bar and 505.2 K to a final state of 3.0 m³, 7.0 bar, and 505.2 K by a two-step process consisting of an adiabatic compression followed by cooling at constant pressure.
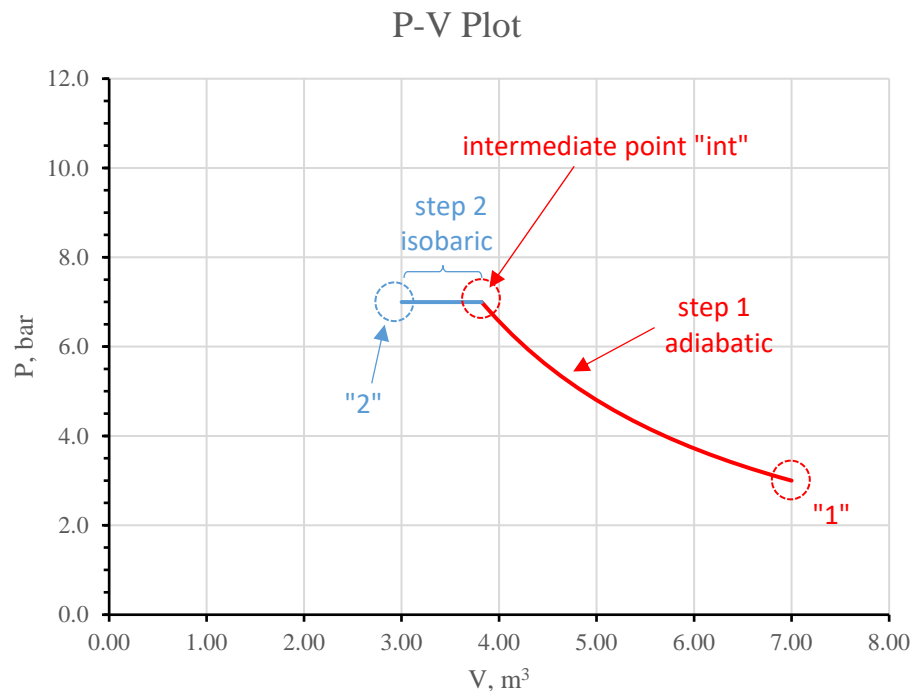
(a) Sketch the process path on the PV axes below.

(b) Calculate Q, W, ΔU and ΔH for the overall process <u>in units of kJ</u>.

(c) Calculate the intermediate temperature after step 1.

$$R = 8.314 \text{ J/(mol·K)} = 0.08314 \text{ (bar·m}^3\text{)/(kmol·K)}$$
$$C_P = (7/2)·R, \text{ and}$$
$$C_V = (5/2)·R$$

Solution, part (a):

P-V Plot

Solution, part (b):

The overall process is isothermal (T2=T1), so $\underline{\underline{\Delta H_{Overall} = \Delta U_{Overall} = 0 \, kJ}}$
ANS

Equation 3.23c gives the P-V relation for an adiabatic process. Let the intermediate state be denoted with subscript "int" with $P_{int} = P_2$ 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.

CH365, AY24-25   5
WPRII, C-Hour, Solution

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

$$P_{int} V_{int}^{\gamma} = P_1 V_1^{\gamma} \Rightarrow V_{int} = \sqrt[\gamma]{\frac{P_1}{P_{int}} V_1^{\gamma}} = \sqrt[1.4]{\frac{3.0\,\text{bar}}{7.0\,\text{bar}} (7.0\,\text{m}^3)^{1.4}} = 3.821708\,\text{m}^3$$

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

$$W_{Step1} = \frac{P_{int} \cdot V_{int} - P_1 \cdot V_1}{\gamma - 1} = \frac{7.0\,\text{bar} \cdot 3.8217081\,\text{m}^3 - 7.0\,\text{bar} \cdot 3.0\,\text{m}^3}{1.4 - 1} = +14.37989\,\text{bar} \cdot \text{m}^3$$

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

$$W_{Step2} = -P \cdot \Delta V = -P \cdot (V_2 - V_{int}) = -7.0 \cdot (3.0\,\text{m}^3 - 3.821708\,\text{m}^3) = +5.751956\,\text{bar} \cdot \text{m}^3.$$

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

$$W_{Overall} = W_{Step1} + W_{Step2} = 14.37989\,\text{bar} \cdot \text{m}^3 + 5.751956\,\text{bar} \cdot \text{m}^3 = 20.13184\,\text{bar} \cdot \text{m}^3$$

Now convert the units to kJ:

$$W_{Overall} = 20.1318\,\text{bar} \cdot \text{m}^3 \left(\frac{1\,\text{J}}{10^{-5}\,\text{bar} \cdot \text{m}^3} \right) \cdot \left(\frac{1\,\text{kJ}}{1000\,\text{J}} \right) = \underline{\underline{2013.18}}\,\text{kJ}_{\text{ANS}}$$

Finally, for Q:

$$\Delta U_{Overall} = Q_{Overall} + W_{Overall} = 0 \Rightarrow Q_{Overall} = -W_{Overall} = \underline{\underline{-2013.18}}\,\text{kJ}_{\text{ANS}}$$

Solution, part (c):

$$PV = nRT \Rightarrow T_{int} = \frac{P_{int} \cdot V_{int}}{n \cdot R} = \frac{7.0\,\text{bar} \cdot 3.821708\,\text{m}^3}{0.500\,\text{kmol} \cdot \left(0.08314 \dfrac{\text{bar} \cdot \text{m}^3}{\text{kmol} \cdot \text{K}} \right)} = \underline{\underline{643.54\,\text{K}}}_{\text{ANS}}$$