

CADET _____ SECTION _____ TIME OF DEPARTURE _____

DEPARTMENT OF CHEMICAL & BIOLOGICAL SCIENCE & ENGINEERING

CH365 2025-2026
WRITTEN PARTIAL REVIEW III
24 November 2025, A-HourTEXT: Smith, Van Ness, & Abbott
SCOPE: Lessons 22-32
TIME: 55 Minutes

References Permitted: Open notes, book, internet, CHEMCAD, Mathematica, 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. There are 3 problems on 3 pages in this exam (not including the cover page). Write your name on the top of each sheet.
4. Solve the problems in Mathematica and the space provided. Show all work to receive full credit.
5. Laptops are authorized for referencing only. Desktop PCs must be used for all Mathematica calculations.
6. Save Mathematica and CHEMCAD files on your desktop and re-save frequently.
7. When finished, upload all electronic work files to CANVAS.

(TOTAL WEIGHT: 200 POINTS)

DO NOT WRITE IN THIS SPACE

PROBLEM	VALUE	CUT
A	40	
B	100	
C	60	
TOTAL CUT		
TOTAL GRADE	200	

Problem: Weight:
 A 40

Use Table C.1 on page 669 of the textbook with gas constant R=8.314 J/(mol·K) to calculate ΔH^{ig} and ΔS^{ig} for *ideal* gas-phase propane compressed and heated from 298.15 K and 1 bar to 600.0 K and 60.00 bar. Report your answers for ΔH^{ig} and ΔS^{ig} in J/mol and J/(mol·K), respectively.

Solution:

```
In[68]:= (*Propane*)
t = 600.0; (*K*)
p = 60.00; (*bar*)

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

a = 1.213;
b = 28.785 * 10^-3;
c = -8.824 * 10^-6;
Cp = a + b * T + c * T^2;

(*enthalpy*)
Hig = R * Integrate[Cp, {T, 298.15, t}] (*eq 2.21*)

(*entropy*)
Sig = R * (Integrate[Cp/T, {T, 298.15, t}] - Log[p/1]) (*eq 5.10*)

Out[75]= 30850.54 J/mol
          ANS,  $\Delta H^{\text{ig}}$ 
Out[76]= 35.30604 J/(mol·K)
          ANS,  $\Delta S^{\text{ig}}$ 
```

Problem: Weight:
 B 100

Use the Peng-Robinson (PR) equation of state to calculate the compressibility, residual enthalpy, and residual entropy (Z , H^R , and S^R) for propane at 600.0 K and 60.00 bar.

Use Table B.1 on pages 663-665 of the textbook for critical constants and acentric factor. Use gas constant $R=8.314 \text{ J}/(\text{mol}\cdot\text{K})$. Report your answers for H^R and S^R in J/mol and $\text{J}/(\text{mol}\cdot\text{K})$, respectively.

Solution:

```
In[122]:= (*Propane, Table B.1, p.663*)
  tc = 369.8; (*K*)
  pc = 42.48; (*bar*)
  omega = 0.152;

  (*Reduced t and p*)
  tr = t / tc; pr = p / pc;

  (*Table 3.1 page 100*)
  sigma = 1 + Sqrt[2];
  epsilon = 1 - Sqrt[2];
  Omega = 0.07780;
  Psi = 0.45724;
  alpha[x_] = (1 + (0.37464 + 1.54226 * omega - 0.26992 * omega^2) * (1 - Sqrt[x]))^2;

In[128]:= beta = Omega * pr / tr; (*eq 3.50*)
  q[x_] = Psi * alpha[x] / (Omega * x); (*eq 3.51*)
  eq1 = z == 1 + beta - q[tr] * beta * (z - beta) / ((z + epsilon * beta) * (z + sigma * beta)); (*eq 3.48*)
  Z = z /. Quiet[Solve[eq1, z, Reals]][[1]];
  I = 1/(sigma - epsilon) * Log[Z + sigma * beta / (Z + epsilon * beta)]; (*eq 13.72*)
  Hr[x_] = (Z - 1 + x * D[q[x], x] * I) * R * t; (*13.75*)
  Sr[x_] = (Log[Z - beta] + (q[x] + x * D[q[x], x]) * I) * R; (*13.76*)

In[135]:= Z
  Hr[tr]
  Sr[tr]

Out[135]= 0.9164279
ANS, Z

Out[136]= -2086.329
ANS, SR
J/mol

Out[137]= -2.69686
ANS, HR
J/(mol·K)
```

Problem: Weight:
C 60

(a) Using the results in the table below with standard heats of formation from Table C.4 on pages 671-672 of the textbook, calculate the total real-gas enthalpy and entropy of propane at 600.0 K and 60.00 bar. Report your answers for H and S in J/mol and J/(mol·K), respectively.

	Ideal	Residual	Total
Enthalpy, J/mol	30,850.542	-2,086.329	-75,915.79 //ANS
Entropy, J/mol·K	35.306	-2.697	-237.02 //ANS

(b) Use CHEMCAD and the CHEMCAD file in Canvas to calculate the enthalpy and entropy of propane at 600.0 K and 60.00 bar using the Peng-Robinson (PR) equation of state and complete the following table:

CHEMCAD Enthalpy, J/mol	-75,876 //ANS
CHEMCAD Entropy, J/mol·K	-236.5 //ANS

(c) Give two reasons for the differences between the answers in parts (a) and (b).

Solution, part (a):

In[138]:= (*Propane, Table C.4, p.671*)

$$\Delta H_{f0} = -104\,680;$$

$$\Delta G_{f0} = -24\,290;$$

$$\Delta S_{f0} = \frac{\Delta H_{f0} - \Delta G_{f0}}{298.15};$$

$$H = \Delta H_{f0} + H_{ig} + H_r[tr] (*6.50*)$$

$$S = \Delta S_{f0} + S_{ig} + S_r[tr] (*6.51*)$$

Out[141]= -75\,915.79 J/mol //ANS

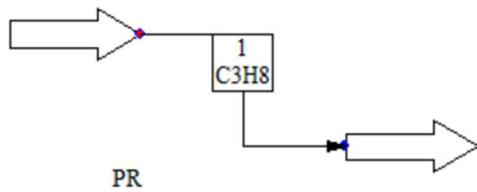
ANS, H

Out[142]= -237.0202 J/(mol·K) //ANS

ANS, S

Solution, part (b):**A-HOUR - C3H8**

Stream No.	1
Name	C3H8
-- Overall --	
Temp K	600.0000
Pres bar	60.0000
Enth J/sec	-75876. //ANS
Molar flow mol/sec	1.0000
Entropy J/K/sec	-236.5//ANS

**Solution, part (c):**

The answers are different because of the following: (1) different heat capacity polynomial, (2) different T_c , P_c , and ω , and (3) different numerical methods. //ANS

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PROBLEM	VALUE	CUT
A	40	
B	100	
C	60	
TOTAL CUT		
TOTAL GRADE	200	

Problem: Weight:
 A 40

Use Table C.1 on page 669 of the textbook with gas constant R=8.314 J/(mol·K) to calculate ΔH^{ig} and ΔS^{ig} for *ideal* gas-phase n-butane compressed and heated from 298.15 K and 1 bar to 800.0 K and 80.00 bar. Report your answers for ΔH^{ig} and ΔS^{ig} in J/mol and J/(mol·K), respectively.

Solution:

```
In[171]:= (*n-Butane*)
t = 800.0; (*K*)
p = 80.00; (*bar*)

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

a = 1.935;
b = 36.915 * 10^-3;
c = -11.402 * 10^-6;
Cp = a + b * T + c * T^2;

(*enthalpy*)
Hig = R * Integrate[Cp, {T, 298.15, t}] (*eq 2.21*)

(*entropy*)
Sig = R * (Integrate[Cp/T, {T, 298.15, t}] - Log[p/1]) (*eq 5.10*)

Out[178]= 77 302.9 J/mol
           ANS,  $\Delta H^{\text{ig}}$ 
Out[179]= 107.3486 J/(mol·K)
           ANS,  $\Delta S^{\text{ig}}$ 
```

Problem: Weight:
 B 100

Use the Peng-Robinson (PR) equation of state to calculate the compressibility, residual enthalpy, and residual entropy (Z , H^R , and S^R) for n-butane at 800.0 K and 80.00 bar.

Use Table B.1 on pages 663-665 of the textbook for critical constants and acentric factor. Use gas constant $R=8.314 \text{ J}/(\text{mol}\cdot\text{K})$. Report your answers for H^R and S^R in J/mol and $\text{J}/(\text{mol}\cdot\text{K})$, respectively.

Solution:

```
In[187]:= (*n-Butane, Table B.1, p.663*)
  tc = 425.1; (*K*)
  pc = 37.96; (*bar*)
  omega = 0.200;

  (*Reduced t and p*)
  tr = t / tc; pr = p / pc;

  (*Table 3.1 page 100*)
  sigma = 1 + Sqrt[2];
  epsilon = 1 - Sqrt[2];
  Omega = 0.07780;
  Psi = 0.45724;
  alpha[x_] = (1 + (0.37464 + 1.54226 * omega - 0.26992 * omega^2) * (1 - Sqrt[x]))^2;

In[193]:= beta = Omega * pr / tr; (*eq 3.50*)
  q[x_] = Psi * alpha[x] / (Omega * x); (*eq 3.51*)
  eq1 = z == 1 + beta - q[tr] * beta * (z - beta) / ((z + epsilon * beta) * (z + sigma * beta)); (*eq 3.48*)
  Z = z /. Quiet[Solve[eq1, z, Reals]][[1]];
  I = 1/(sigma - epsilon) * Log[Z + sigma * beta / (Z + epsilon * beta)]; (*eq 13.72*)
  Hr[x_] = (Z - 1 + x * D[q[x], x] * I) * R * t; (*13.75*)
  Sr[x_] = (Log[Z - beta] + (q[x] + x * D[q[x], x]) * I) * R; (*13.76*)

In[200]:= Z
  Hr[tr]
  Sr[tr]

Out[200]= 0.9639533 ANS, Z
Out[201]= -2409.272 J/mol ANS, SR
Out[202]= -2.588444 J/(mol·K) ANS, HR
```

Problem: Weight:
C 60

(a) Using the results in the table below with standard heats of formation from Table C.4 on pages 671-672 of the textbook, calculate the total real-gas enthalpy and entropy of n-butane at 800.0 K and 80.00 bar. Report your answers for H and S in J/mol and J/(mol·K), respectively.

	Ideal	Residual	Total
Enthalpy, J/mol	77,302.900	-2,409.272	-50,296.4 //ANS
Entropy, J/mol·K	107.349	-2.588	-259.6 //ANS

(b) Use CHEMCAD and the CHEMCAD file in Canvas to calculate the enthalpy and entropy of n-Butane at 800.0 K and 80.00 bar using the Peng-Robinson (PR) equation of state and complete the following table:

CHEMCAD Enthalpy, J/mol	-49,739 //ANS
CHEMCAD Entropy, J/mol·K	-259.2 //ANS

(c) Give two reasons for the differences between the answers in parts (a) and (b).

Solution, part (a):

In[203]:= (*n-Butane, Table C.4, p.671*)

$$\Delta H_{f\text{o}} = -125\,190;$$

$$\Delta G_{f\text{o}} = -16\,570;$$

$$\Delta S_{f\text{o}} = \frac{\Delta H_{f\text{o}} - \Delta G_{f\text{o}}}{298.15};$$

$$H = \Delta H_{f\text{o}} + H_{\text{ig}} + H_r[\text{tr}] \quad (*6.50*)$$

$$S = \Delta S_{f\text{o}} + S_{\text{ig}} + S_r[\text{tr}] \quad (*6.51*)$$

Out[206]= -50 296.37 J/mol //ANS

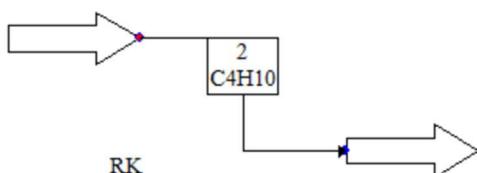
 ANS, H

Out[207]= -259.5532 J/(mol·K) //ANS

 ANS, S

Solution, part (b):**C-HOUR - C4H10**

Stream No.	2
Name	C4H10
-- Overall --	
Temp K	800.0000
Pres bar	80.0000
Enth J/sec	-49739. //ANS
Molar flow mol/sec	1.0000
Entropy J/K/sec	-259.2 //ANS

**Solution, part (c):**

The answers are different because of the following: (1) different heat capacity polynomial, (2) different T_c , P_c , and ω , and (3) different numerical methods. //ANS