APPROVED SOLUTION

CADET ____________________ SECTION ______ TIME OF DEPARTURE ________

DEPARTMENT OF CHEMISTRY & LIFE SCIENCE

CH365 2022-2023
WRITTEN PARTIAL REVIEW III
17 November 2022, A-Hour

TEXT: 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. 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. Laptops are not authorized for this exam. You may use desktop PCs only.
6. Save all electronic work to your SharePoint directory.
7. Write the file name and file location on the exam.

(TOTAL WEIGHT: 200 POINTS)

DO NOT WRITE IN THIS SPACE

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

Cadet: **APPROVED SOLUTION**

Problem: A

Weight: 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 being compressed and heated from 298.15 K and 1 bar to 900 K and 30 bar. Report your answers for ΔH^{ig} and ΔS^{ig} in J/mol and J/(mol·K), respectively.

Solution:

```
p = 30.00; (*bar*)
t = 900.; (*K*)

R = 8.314;

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*)
```

$$Hig = R * \int_{298.15}^{t} Cp\, dT$$

$$Sig = R * \left(\int_{298.15}^{t} \frac{Cp}{T}\, dT - \text{Log}\left[\frac{p}{1}\right]\right)$$

Out[8]= 98142.1944246 J/mol

ANS, ΔH_{ig}

Out[9]= 140.031463151 J/(mol·K)

ANS, ΔS_{ig}

Cadet: **APPROVED SOLUTION**

Problem:	Weight:
B	100

Use the Peng-Robinson equation of state to calculate the compressibility, residual enthalpy, and residual entropy (Z, H^R, and S^R) for n-butane at 900 K and 30 bar.

Use Table B.1 on page 663 of the textbook for critical constants and acentric factor. Use gas constant R=8.314 J/(mol·K). Report your answers for H^R and S^R in J/mol and J/(mol·K), respectively.

Solution:

```
In[21]:= (*Table B.1, p.663*)
tc = 425.1; (*K*)
pc = 37.96; (*bar*)
ω = 0.200;

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

(*Table 3.1 page 100*)
ϵ = 1 - √2 ; σ = 1 + √2 ; Ω = 0.07780; Ψ = 0.45724;
α[x_] = (1 + (0.37464 + 1.54226 * ω - 0.26992 * ω^2) * (1 - √x))^2;

β = Ω * pr / tr; (*eq 3.50*)
q[x_] = (Ψ * α[x]) / (Ω * x); (*eq 3.51*)
eq1 = Z == 1 + β - q[tr] * β * (Z - β) / ((Z + ϵ * β) * (Z + σ * β)); (*eq 3.48*)
ans = Quiet[Solve[eq1, Z, Reals]];
Z1 = Z /. ans[[1]];
I = 1 / (σ - ϵ) * Log[(Z1 + σ * β) / (Z1 + ϵ * β)];  (*eq 13.72*)
Hr[x_] = (Z1 - 1 + x * ∂x q[x] * I) * R * t ; (*13.75*)
Sr[x_] = (Log[Z1 - β] + (q[x] + x * ∂x q[x]) * I) * R ; (*13.76*)


In[34]:= Z1
Hr[tr]
Sr[tr]

Out[34]= 0.99314832986
Out[35]= -736.617362747
Out[36]= -0.749348425478
```

Out[34]= 0.99314832986 — ANS, Z

Out[35]= -736.617362747 J/mol — ANS, H^R

Out[36]= -0.749348425478 J/(mol·K) — ANS, S^R

Cadet: **APPROVED SOLUTION**

Problem:	Weight:
C	60

(a) Using your results from Problems A and B and Table C.4 on page 671 of the textbook, calculate the total real-gas enthalpy and entropy for n-butane at 900 K and 30 bar. Report your answers for H and S in J/mol and J/(mol·K), respectively.

(b) Use CHEMCAD and the CHEMCAD file in your SharePoint directory calculate the enthalpy and entropy for n-butane at 900 K and 30 (same conditions as in Problem C.a).

(c) Give three reasons for the difference between the answers in C.a and C.b.

Solution, part (a):

$$\Delta Hfo = -125790;$$

$$\Delta Gfo = -16570;$$

$$\Delta Sfo = \frac{\Delta Hfo - \Delta Gfo}{298.15};$$

$$H = \Delta Hfo + Hig + Hr[tr] \quad (*6.50*)$$

$$S = \Delta Sfo + Sig + Sr[tr] \quad (*6.51*)$$

Out[29]= $\underline{\underline{-28384.4229382}}$ J/mol //ANS

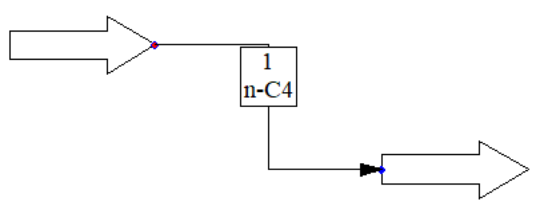
ANS, H

Out[30]= $\underline{\underline{-227.04356027}}$ J/(mol·K) //ANS

ANS, S

Solution, part (b):

Stream No.	1
Name	n-C4
- - Overall - -	
Temp K	900.0000
Pres bar	30.0000
Enth J/sec	-27152. //ANS
Molar flow mol/sec	1.0000
Entropy J/K/sec	-224.6 //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 standard-state enthalpy and entropy of formation. //ANS

APPROVED SOLUTION

CADET ____________________ SECTION ______ TIME OF DEPARTURE ________

DEPARTMENT OF CHEMISTRY & LIFE SCIENCE

CH365 2022-2023
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17 November 2022, B-Hour

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

Cadet: **APPROVED SOLUTION**

Problem: A Weight: 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-pentane being compressed and heated from 298.15 K and 1 bar to 800 K and 40 bar. Report your answers in J/mol and J/(mol·K).

Solution:

```
p = 40.00; (*bar*)
t = 800.; (*K*)

R = 8.314;

a = 2.464;
b = 45.351 * 10^-3;
c = -14.111 * 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*)
```

$$Hig = R * \int_{298.15}^{t} Cp \, dT$$

$$Sig = R * \left(\int_{298.15}^{t} \frac{Cp}{T} \, dT - \text{Log}\left[\frac{p}{1}\right] \right)$$

Out[8]= 95191.6604796 J/mol
ANS, ΔH_{ig}

Out[9]= 146.444395848 J/(mol·K)
ANS, ΔS_{ig}

Cadet: **APPROVED SOLUTION**

Problem: B   Weight: 100

Use the Peng-Robinson equation of state to calculate the compressibility, residual enthalpy, and residual entropy (Z, H^R, and S^R) for n-pentane at 800 K and 40 bar.

Use Table B.1 on page 663 of the textbook for critical constants and acentric factor. Use gas constant R=8.314 J/(mol·K). Report your answers for H^R and S^R in J/mol and J/(mol·K), respectively.

Solution:

```
In[10]:= (*Table B.1, p.663*)
tc = 469.7; (*K*)
pc = 33.70; (*bar*)
ω = 0.252;

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

(*Table 3.1 page 100*)
ϵ = 1 - √2 ;  σ = 1 + √2 ;  Ω = 0.07780;  Ψ = 0.45724;
α[x_] = (1 + (0.37464 + 1.54226 * ω - 0.26992 * ω^2) * (1 - √x ))^2;

β = Ω * pr / tr; (*eq 3.50*)
q[x_] = (Ψ * α[x]) / (Ω * x); (*eq 3.51*)
eq1 = Z == 1 + β - q[tr] * β * (Z - β) / ((Z + ϵ * β) * (Z + σ * β)); (*eq 3.48*)
ans = Quiet[Solve[eq1, Z, Reals]];
Z1 = Z /. ans[[1]];
I = 1 / (σ - ϵ) * Log[(Z1 + σ * β) / (Z1 + ϵ * β)];  (*eq 13.72*)
Hr[x_] = (Z1 - 1 + x * ∂x q[x] * I) * R * t ; (*13.75*)
Sr[x_] = (Log[Z1 - β] + (q[x] + x * ∂x q[x]) * I) * R ; (*13.76*)


In[23]:= Z1
Hr[tr]
Sr[tr]

Out[23]= 0.954934272789
Out[24]= -1965.92751277
Out[25]= -2.03083124078
```

Out[23]= 0.954934272789 — ANS, Z

Out[24]= −1965.92751277 J/mol — ANS, H^R

Out[25]= −2.03083124078 J/(mol·K) — ANS, S^R

Cadet: **APPROVED SOLUTION**

<u>Problem:</u> <u>Weight:</u>
C 60

(a) Using your results from Problems A and B and Table C.4 on page 671 of the textbook, calculate the total real-gas enthalpy and entropy for n-pentane at 800 K and 40 bar. Report your answers for H and S in J/mol and J/(mol·K), respectively.

(b) Use CHEMCAD and the CHEMCAD file in your SharePoint directory calculate the enthalpy and entropy for n-pentane at 800 K and 40 bar (same conditions as in C.a).

(c) Give three reasons for the difference between the answers in C.a and C.b.

Solution, part (a):

In[26]:= (*Table C.4, p.671*)

$$\Delta Hfo = -146760;$$

$$\Delta Gfo = -8650;$$

$$\Delta Sfo = \frac{\Delta Hfo - \Delta Gfo}{298.15};$$

$$H = \Delta Hfo + Hig + Hr[tr] \quad (*6.50*)$$

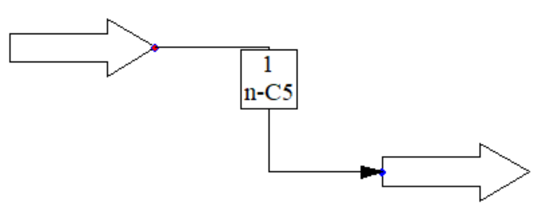
$$S = \Delta Sfo + Sig + Sr[tr] \quad (*6.51*)$$

Out[29]= $\underline{\underline{-53534.2670332}}$ J/mol //ANS
ANS, H

Out[30]= $\underline{\underline{-318.809645187}}$ J/(mol·K) //ANS
ANS, S

Solution, part (b):

Stream No.	1
Name	n-C5
- - Overall - -	
Temp K	800.0000
Pres bar	40.0000
Enth J/sec	-52242. //ANS
Molar flow mol/sec	1.0000
Entropy J/K/sec	-316.2 //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 standard-state enthalpy and entropy of formation. //ANS