CADET	SECTION	TIME OF DEPARTURE	

DEPARTMENT OF CHEMISTRY & LIFE SCIENCE

CH365 2022-2023 TEXT: Smith, Van Ness, Abbott & Swihart

WRITTEN PARTIAL REVIEW III SCOPE: Lessons 22-31 10 November 2022, Practice 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 4 pages in this exam (not including the cover page). Write your name on the top of each sheet.
- 5. Save all electronic work to your SharePoint directory.
- 6. Write the file name and file location on the exam.

(TOTAL WEIGHT: 0 POINTS)

DO NOT WRITE IN THIS SPACE

PROBLEM	VALUE	CUT
A	0	
В	0	
С	0	
TOTAL CUT		
BONUS	0	
TOTAL GRADE	0	

Problem:	Weight:	
	40	

Syngas, or synthesis gas, is a mixture consisting primarily of hydrogen, carbon monoxide, carbon dioxide, and sometimes methane. A typical syngas composition is shown below:

Component	Mole fraction	Tc, K	Pc, bar	V _c , cm ³ /mol	ω
Hydrogen	0.300	33.27	12.9595	65.001	-0.220
Carbon Monoxide	0.600	132.95	34.9875	93.100	0.093
Carbon Dioxide	0.050	304.20	73.8152	92.863	0.231
Methane	0.050	190.63	46.0015	99.418	0.010

- (a) Use the information in the table to calculate T_c , P_c , and ω for syngas as a mixture of these four substances.
- (b) Check your answers in CHEMCAD. That is, define this mixture as a stream in CHEMCAD and compare the T_c and P_c of the stream to your calculated values.

Solution:

ANS

- (a) Use the generalized virial equation of state to calculate the residual enthalpy, residual entropy, and residual molar volume (H^R, S^R, and V^R) for syngas at (1) 1427 °C and 62 bar, (2) at 50 °C and 60 bar, and (3) the differences ΔH^R and ΔS^R between (1) and (2). Use the mixture critical temperature, pressure, and acentric factor of syngas from Problem A. Express your answers in the following units: enthalpy in J/mol, entropy in J/(mol·K), and molar volume in cm³/mol.
- (b) Repeat the three calculations in part (a) using the Peng-Robinson equation of state.

Solution, part (a.1):

Solution, part (a.2):

Solution, part (a.3):

In[8]:=
$$-209.365 - (96.4169)$$

 $-0.619844 - (-0.00854355)$
Out[8]= -305.782
ANS, ΔH^{R} , J/mol
Out[9]= -0.6113
ANS, ΔS^{R} , J/(mol·K)

Solution, part (b.1):

Solution, part (b.2):

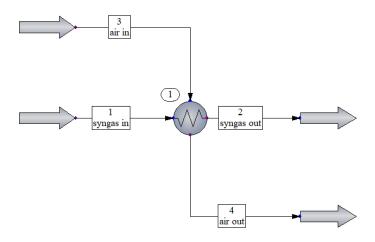
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 \begin{split} & \text{In}[15] = \text{Hr}[\text{tr}] \ (*//ANS, \ J/\text{mol*}) \\ & \text{Sr}[\text{tr}] \ (*//ANS, \ J/\text{mol*}K*) \\ & \text{Out}[15] = -\frac{265.898}{\text{ANS}, H^R, J/\text{mol}} \\ & \text{Out}[16] = -0.742927 \\ & \text{ANS}, S^R, J/\text{(mol·K)} \\ & \text{In}[17] = \left(*R = 83.14 \frac{\text{cm}^3 + \text{bar}}{\text{mol*}K} *\right) \\ & \text{Vr} = (83.14 * \text{t/p}) * (\text{Z-1}) \ (*//\text{ANS, cm}^3/\text{mol*}) \\ & \text{Out}[17] = -\frac{3.07207}{\text{ANS, V}^R, \text{cm}^3/\text{mol}} \end{aligned}
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Solution, part (b.3):

$$\begin{array}{c} \text{In[18]:=} & -265.89813 - 113.86994 \\ & -0.74292 - 0.00103 \\ \\ \text{Out[18]:=} & \frac{-379.768}{\text{ANS, } \Delta H^{\text{R}}, \text{J/mol}} \\ \\ \text{Out[19]:=} & -\frac{0.74395}{\text{ANS, } \Delta S^{\text{R}}, \text{J/(mol·K)}} \end{array}$$

Syngas leaving a coal gasifier at 1,427 °C and 62 bar is cooled and expanded to 50 °C and 60 bar in the tube-side of a counter-current heat exchanger. Compressed air used for cooling enters shell-side and is warmed and expanded from 25 °C and 2 bar to 50 °C and 1.013 bar. The CHEMCAD flowsheet and stream results are shown below. Heat losses from the exchanger to the surroundings may be considered negligible, and the temperature of the surroundings is 20 °C.

Stream No.	1	2	3	4
Name	syngas in	syngas out	air in	air out
Overall				
Temp C	1427.0000	50.0000	25.0000	40.0000
Pres bar	62.0000	60.0000	2.0000	1.0130
Enth kJ/sec	-4059.4	-8921.4	-144.31	4717.6
Molar flow gmol/sec	100.0000	100.0000	10924.8428	10924.8428
Entropy kJ/K/sec	8.195	2.543	-15.52	62.18



(a) Use CHEMCAD to calculate the entropy change of the syngas in kW/K. Is the entropy change of the syngas consistent with the Second Law of Thermodynamics? Why or why not?

Solution:
$$\Delta S_{12} = 2.543 - 8.195 = -5.652 \frac{kJ}{K \text{ sec}} = -5.652 \frac{kW}{K}$$

This result is negative, but the second law is not violated because the entropy change of the air stream is sufficiently positive to counteract the negative entropy change of the syngas. That is, total entropy generation across the flowing streams \dot{S}_G is positive:

$$\dot{S}_G = (2.543 - 8.195) + (62.18 - (-15.52)) = 72.048 \frac{kJ}{K \, sec}$$

(b) Calculate the lost work in the exchanger, \dot{W}_{lost} .

Solution:

Lost work is calculated from equation 5.29 on page 195:

The entropy generation was calculated in part (a) and T_{σ} is the surrounding temperature.

$$\frac{=21,121 \ kW}{\text{ANS}}$$

(c) What would happen to the lost work in the exchanger if the feed air pressure is increased and all other temperatures and pressures are unchanged? Would lost work increase, decrease, or stay the same? Explain.

Solution:

Lost work increases. The logic is outlined in the table below:

Property	Change $(\uparrow / \downarrow /)$
T ₃ (inlet)	
P ₃ (inlet)	
S ₃ (inlet)	
T ₄ (outlet)	
P ₄ (outlet)	
S ₄ (outlet)	
(S_4-S_3)	
T ₁ (inlet)	
P ₁ (inlet)	
S ₁ (inlet)	
T ₂ (outlet)	
P ₂ (outlet)	
S ₂ (outlet)	
S ₃ (inlet)	
(S_2-S_1)	
$(S_2-S_1) + (S_3-S_4)$	