CH365 Chemical Engineering Thermodynamics

Lesson 20
Review

WPR 2

Lesson 21 – Thursday 12 October 2023

Coverage – Lessons 10-20 (Chapters 3 and 4) and Problem Sets 4, 5, 6, and 7

(1) Calculation of ideal ΔH, ΔU, W, and Q in a multi-step process. Sketching process path on PV axes.

(2) Real gases and cubic equations of state (RK, SRK, PR, virial)

(3) Correct enthalpy for temperature changes

a. Sensible Heat (direct integration of Cp, ICPH, MCPH)

b. Latent Heat / Heats of Reaction (IDCPH, MDCPH)

(4) Comparing CHEMCAD (to verify results of #2 and #3 above)

3 problems, (A-80, B-70, C-50 pts, 200 pts total), 55 minutes.

Make sure you have working Mathematica files for Problem 3.44 (c-e) 3.58 (c-f), 4.45, 4.55, and 4.83. Make sure you replicate approved solutions exactly or you have something wrong.

All WPR2 files uploaded to CANVAS (Mathematica, CHEMCAD)

Homework

Problem 4.6

If the heat capacity of a substance is correctly represented by an equation of the form

$$C_P = A + BT + CT^2,$$

show that the error resulting when $\langle C_P \rangle_H$ is assumed equal to C_P evaluated at the arithmetic mean of the initial and final temperatures is

$$C(T_2 - T_1)^2 / 12.$$

Problem 4.55

A natural-gas fuel contains 85mol-% methane, 10 mol-% ethane, and 5 mol-% nitrogen.

(a) What is the standard heat of combustion (kJ/mol) of the fuel at 25 deg C with H_2O(g) is a product?

(b) The fuel is supplied to a furnace with 50% excess air, both entering at 25 deg C. The products leave at 600 deg C. If combustion is complete and if no side reactions occur, how much heat (kJ per mole of fuel) is transferred in the furnace?

Problem 4.45

A process for the production of 1,3-butadiene results from the catalytic dehydrogenation at atmospheric pressure of 1-butene according to the reaction:

$$C_4H_8\ (g) \rightarrow C_4H_6\ (g) + H_2\ (g)$$

To suppress side reactions, the 1-butene feed is diluted with steam in the ratio of 10 moles of steam per mole of 1-butene. The reaction is carried out *isothermally* at 525 deg C, and at this temperature 33% of the 1-butene is converted to 1,3-butadiene. How much heat is transferred to the reactor per mole of entering 1-butene?

Problem 4.22

What is the standard heat of combustion of n-pentane gas at 25 deg C if the combustion products are H_2O(l) and CO_2(g)?

Problem 4.28

Natural gas (assume pure methane) is delivered to a city via pipeline at a volumetric rate of 150 million standard cubic feet per day. If the selling price of the gas is $5.00 per GJ of higher heating value, what is the expected revenue in dollars per day? Standard conditions are 60 deg F and 1 atm.

Problem 4.71

Locate your name in the list below and use the DIPPR database to find the critical temperature and pressure for the compounds assigned to you. Report your results in units of bar and K. What does DIPPR stand for, who created it, and when?

Baldwin	sodium chloride	chlorine dioxide	isoquinoline
Behr	bisphenol A	cyanogen chloride	acetoacetanilide
Benson	chlorine	chlorine trifluoride	p-cymene
Cianfaglione	piperazine	anisole	triethyl phosphate
Ibrahimi	pyridine	trans-2-hexene	naphthalene
Milanesa	acetone	sulfur dichloride	benzonitrile
Morrall	ethyl acetate	benzonitrile	camphor
Mossman	sodium hydroxide	silicon dioxide	cumene
Murray	1,3 dioxane	2-butanol	carbon monoxide
Onaga	ethanol	anethole	dibenzyl ether
Weaver	benzene	trans-3-hexene	cetane

Bennett, S	cis-3-hexene	acetaldoxime	phosgene
Cesarski	methyl methacrylate	2-chloroethanol	diethyl sulfide
Dolin	allyl alcohol	diethanolamine	ammonium sulfide
Goulet	iodine	crotyl glycol ether	methyl mercaptan
Johnson	quinoline	2-mercaptoethanol	pyrazine
Kotkin	acridine	ethylthioethanol	pyrazole
Patel	niacin	thiodiglycol	isoxazole
Sullivan	acrylonitrile	triethanolamine	caprolactam
Weathers	fluorine	triethylene glycol	cetyl methacrylate
Williams	n-tricosane	allyl methacrylate	graphite

Problem 4.83

Hydrocarbon fuels such as methanol are used to store energy in liquid form. Flow calorimeters are frequently used to measure standard heats of reaction for liquid fuels. An example is shown in Slide 5 from Lesson 17. Use CHEMCAD to construct a simulation of a flow calorimeter that is designed to combust methanol in a stoichiometric amount of air.

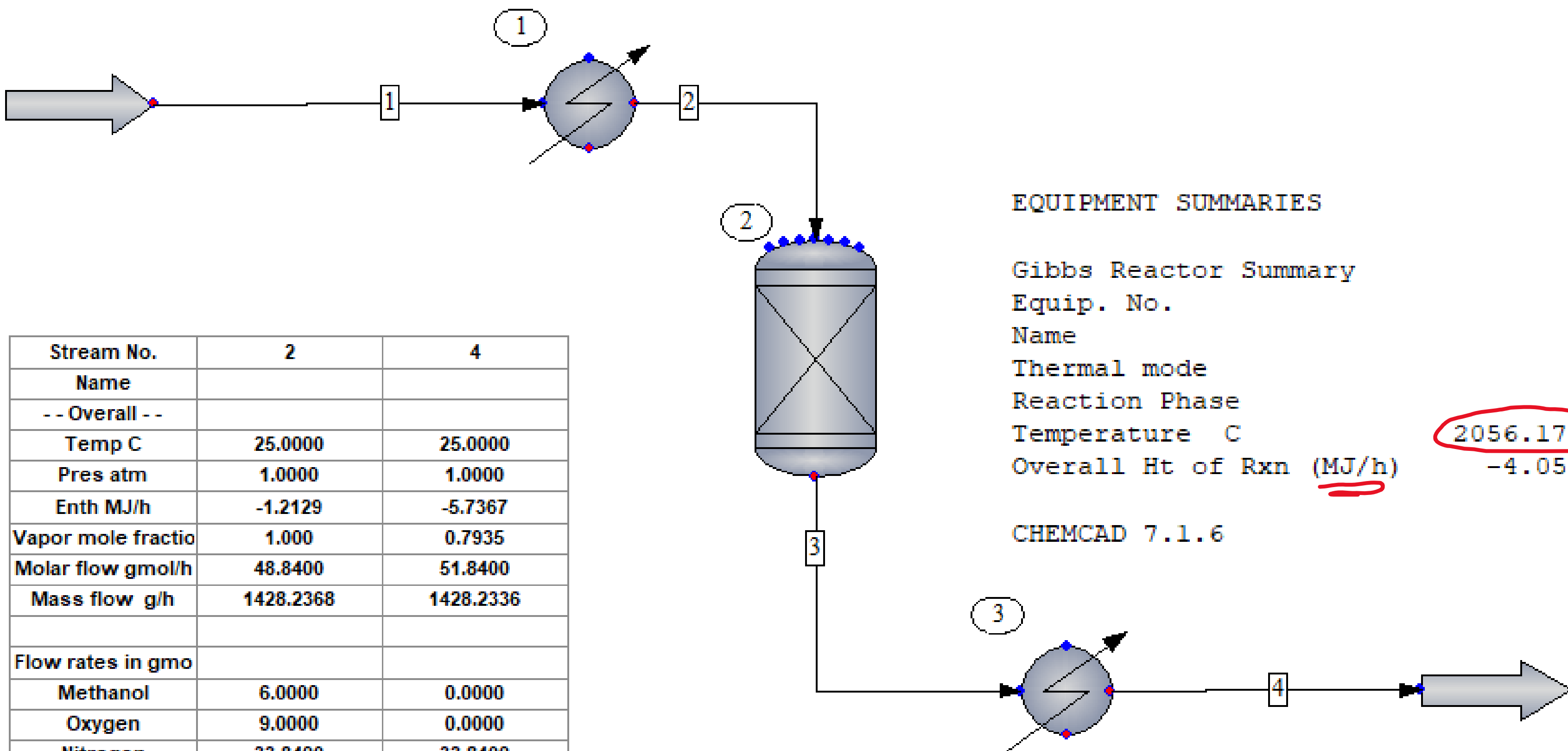
The feed mixture enters the process at 20 deg C and must be preheated to 25 deg C before entering the reactor. The reactor effluent must be cooled to 25 deg C before discharge to the atmosphere.

Compare the heat of reaction from CHEMCAD to the value obtained in Problem 4.20.

(Submit your CHEMCAD as a pdf inclusion to your other work)

Problem 4.83

Hydrocarbon fuels such as methanol are used to store energy in liquid form. Flow calorimeters are frequently used to measure standard heats of reaction for liquid fuels. An example is shown in page 54. Use CHEMCAD to construct a simulation of a flow calorimeter that is designed to combust methanol in a stoichiometric amount of air. The feed mixture enters the process at 20 deg C and must be preheated to 25 deg C before entering the reactor. The reactor effluent must be cooled to 25 deg C before discharge to the atmosphere. Compare the heat of reaction from CHEMCAD to the value obtained in Problem 4.20.



Stream No.	2	4
Name		
- - Overall - -		
Temp C	25.0000	25.0000
Pres atm	1.0000	1.0000
Enth MJ/h	-1.2129	-5.7367
Vapor mole fractio	1.000	0.7935
Molar flow gmol/h	48.8400	51.8400
Mass flow g/h	1428.2368	1428.2336
Flow rates in gmo		
Methanol	6.0000	0.0000
Oxygen	9.0000	0.0000
Nitrogen	33.8400	33.8400
Carbon Dioxide	0.0000	6.0000
Water	0.0000	12.0000

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EQUIPMENT SUMMARIES

Gibbs Reactor Summary
Equip. No.                          2
Name
Thermal mode                        1
Reaction Phase                      1
Temperature  C              2056.1731
Overall Ht of Rxn (MJ/h)      -4.0573

CHEMCAD 7.1.6
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The CHEMCAD Gibbs Reactor gives a calculated value of -4.0573 MJ per hour. Since the flow rates are specified in mol per hour, this is equivalent to -4.0573 MJ per 6 moles of CH_3OH. This is very close to the value of 4.0589 MJ per 6 moles of CH_3OH obtained in Problem 4.20. The difference is probably due to slight differences in the standard state gas phase heats of formation in the CHEMCAD database. We also note here that the heat duty on exchanger 3 is -4.5238 MJ. This accounts for the sensible heat contributions from Nitrogen, which are not included in the calculation of the standard heat of reaction.