Due April 29, 2016

Solve each problem on a separate sheets of Engineering Computation paper. Carefully and neatly document your answers. Box your final answer, reporting it with the correct number of significant figures and units. Use plotting software for all plots.

1 Hot acid in a closed container

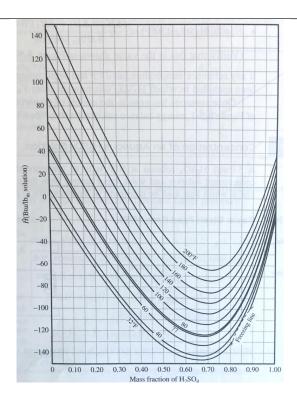
You are going to dilute 2.00 mol of 100% H₂SO₄ with enough water to make a 30%(mol/mol) solution. Both acid and H₂O are initially at 25 °C. Table B.11 is a convenient source of enthalpy of mixing data, and Perry's reports the specific heat of aqueous H₂SO₄ to be:

TABLE 2-174 Sulfuric Acid*

%H ₂ SO ₄	C _p at 20 °C, cal/(g·°C)	%H ₂ SO ₄	C _p at 20 °C, cal/(g·°C)
0.34	0.9968	35.25	0.7238
0.68	0.9937	37.69	.7023
1.34	0.9877	40.49	.6770
2.65	0.9762	43.75	.6476
3.50	0.9688	47.57	.6153
5.16	0.9549	52.13	.5801
9.82	0.9177	57.65	.5420
15.36	0.8767	64.47	.5012
21.40	0.8339	73.13	.4628
22.27	0.8275	77.91	.4518
23.22	0.8205	81.33	.4481
24.25	0.8127	82.49	.4467
25.39	0.8041	84.48	.4408
26.63	0.7945	85.48	.4346
28.00	0.7837	89.36	.4016
29.52	0.7717	91.81	.3787
30.34	0.7647	94.82	.3554
31.20	0.7579	97.44	.3404
33.11	0.7422	100.00	.3352

Vinal and Craig, Bur. Standards J. Research, 24, 475 (1940).

- 1. (4 pts) How much cooling (kJ) is necessary to maintain the final solution at 25 °C?
- 2. (4 pts) Suppose you do this mixing in a well-insulated 150 g flask that has a heat capacity of $3.30 \,\mathrm{J}\,\mathrm{g}^{-1}\,\mathrm{^{\circ}}\mathrm{C}^{-1}$. What is the final temperature of the solution?
- 3. (4 pts) In a separate experiment, you have an $\rm H_2SO_4$ solution of unknown compositionBelow is an enthalpy-concentration chart for $\rm H_2O/H_2SO_4$. Draw an appropriate line on it to estimate the final temperature if the mixing is done adiabatically.



2 Trying to concentrate

A 0.1%(mol/mol) caustic soda (NaOH) solution is to concentrated in a continuous evaporator. The solution enters the evaporator at 25 °C at a rate of 150 mol min⁻¹ and exits at 5%(mol/mol) and 60 °C. Hot dry air is bubbled into the evaporator at 200 °C and 1.1 bar absolute and leaves as saturated air at 60 °C and 1 atm. Because the liquid solutions are fairly dilute, you can assume their heat capacities to be the same as that of pure $\rm H_2O$.

- 1. (4 pts) Sketch a process diagram for this unit operation, labeling all inputs and outputs.
- 2. (2 pts) What is the composition of the exiting saturated air?
- 3. (4 pts) What are the molar flow rates of all streams? (Recall that dry air can be treated as a single compound with an effective MW).
- 4. (4 pts) What is the volumetric flow rate of dry air?
- 5. (8 pts) Create an enthalpy table (kJ/mol) for all inlet and exit species. Take as your enthalpy references the inlet caustic acid solution, dry air at $25\,^{\circ}$ C, and H_2O at $25\,^{\circ}$ C. Identify the tables from the text you use for each calculation.
- 6. (4 pts) Use an enthalpy balance to determine the required heat or cooling to maintain the target temperature.

3 Get oily clean

Trichloroethylene (TCE) is a common industrial cleaning solvent, produced by chlorinating ethylene:

$$C_2H_4(g) + 2Cl_2(g) \longrightarrow C_2H_2Cl_4(l) + H_2(g), \quad \Delta \hat{H}_r^{\circ} = -385.76 \,\text{kJ} \,\text{mol}^{-1}$$

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followed by dehydrochlorination of tetrachloroethane:

$$C_2H_2Cl_4(l) \longrightarrow C_2HCl_3(l) + HCl(g)$$

The standard heat of formation of TCE, $\Delta H_{\rm f,TCE}^{\circ} = -276.2\,{\rm kJ\,mol^{-1}}$, and other necessary standard heats are in Table B.1 of the text.

- 1. (2 pts) What is the standard heat of formation of $C_2H_2Cl_4(l)$?
- 2. (2 pts) What is the standard heat of the second reaction?
- 3. (2 pts) What is the standard enthalpy of the net reaction for making TCE from ethylene and Cl₂?
- 4. (2 pts) Suppose a process generates 300 mol/hr of TCE, with all reactants and products at 1 atm and 25 °C. How much heat must be added to or removed from the process?

4 A shifty reaction

Water-gas shift (WGS) is an important industrial reaction for generating H_2 from carbon monoxide:

$$CO(g) + H_2O(g) \longrightarrow CO_2(g) + H_2(g)$$

CO at 25 °C and steam at 150 °C are fed to a WGS reactor. The effluent contains 40.0% H₂, 40.0% CO₂, and balance steam at 500 °C and a flow rate of 3.50 standard cubic meters per hour. This effluent passes to a condenser to drop out the H₂O. Gas and liquid streams leave the condenser at 1 atm and 15 °C. The Henry's Law constants of H₂ and CO₂ are large enough to neglect their solubility in the liquid water.

- 1. (4 pts) Sketch and label the overall process.
- 2. (4 pts) Compute the inlet molar flow rates of CO and steam. If either is in excess, explain why the process is designed in such a way.
- 3. (4 pts) Compute the molar flow rate of exiting liquid water and of the vapor phase.
- 4. (4 pts) Do an enthalpy balance on the condenser and determine the rate at which it must be heated or cooled (kW).
- 5. (2 pts) What is the standard enthalpy of WGS?
- 6. (2 pts) What is the reaction advancement in the reactor?
- 7. (4 pts) Create an enthalpy table for the reactor based on the "heat of formation" method.
- 8. (4 pts) Do an enthalpy balance on the reactor and determine the rate at which it must be heated or cooled (kW).
- 9. (4 pts) It has been suggested that the inlet CO and reactor effluent could be passed through opposite sides of a heat exchanger before the effluent is sent to the condenser. Sketch such a process and explain why this might make sense. (This concept is called "heat integration.")

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5 BONUS BONUS BONUS

(For those of you looking for some extra points or an extra challenge.) Ammonia is oxidized to make nitric oxide in a well-insulated flow reactor:

$$4NH_3(g) + 5O_2(g) \longrightarrow 4NO(g) + 6H_2O(g), \quad \Delta H_r^{\circ} = -904.7 \text{ kJ mol}^{-1}$$

The feed stream enters at 200 °C with 4.00 and $6.00\,\mathrm{mol\,s^{-1}}$ NH₃ and O₂, respectively. The NH₃ conversion in 100%, and the products exit at some unknown temperature T.

- 1. (4 pts) Sketch and label a process flow chart for this process.
- 2. (6 pts) Perform a mass balance to determine the flow rates of all products and the reaction extent.
- 3. (2 pts) Now you need to perform an enthalpy balance. Which method do you choose, heat of reaction or heat of formation?
- 4. (4 pts) Compute the specific enthalpies of the reactants based on your choice.
- 5. (6 pts) Write expression for the specific enthalpies of the products based on your choice. Take advantage of the heat capacities in Table B.2.
- 6. (6 pts) Based on your enthalpy balance, what is the temperature of the exiting gases? This requires you to solve a non-linear equation. State the method you use and show intermediate results.
- 7. (4 pts) I'm pretty lazy at heart. Suppose I solved this problem using only the leading, constant terms for the heat capacities of the products. The problem is then much easier to solve. What temperature would I get, and how far off am I? Does it pay to be lazy?