Final Examination

4 problems

Please start each problem on a separate sheet of paper.
Write your name, student ID number and the problem you are working on in the upper right hand corner of each page.

(200) 1. In the toluene hydrodealkylation process shown below in Figure 1, gaseous toluene and hydrogen are reacted to make benzene by the following reaction:

$$\underset{(T)}{C_7H_8(g)} + \underset{(H)}{H_2(g)} \rightarrow \underset{(B)}{C_6H_6(g)} + \underset{(M)}{CH_4(g)}$$

In this process, the reaction takes place at 700°C and 30 atm. The per pass conversion of the reaction is 50%, and the reactor effluent is flashed at 40°C to separate the hydrogen and methane from the benzene and toluene. Due to the high volatility of the benzene, 10% of the benzene in the reactor effluent exits the flash with the vapor. This benzene is recovered (at 100% efficiency) from the vapor stream by contacting the vapor in a scrubber with the pure benzene product stream. Some of the vapor from the scrubber is purged, and the remaining vapor is recycled to the reactor feed. The liquid exiting the flash enters a distillation column where pure toluene and benzene are separated. All of the toluene is recycled to the reactor feed; as mentioned previously, the distillation column overhead benzene is used to scrub benzene vapor from the flash overhead and then exits as product. The flow sheet is shown below (the components in each stream are indicated in parentheses).

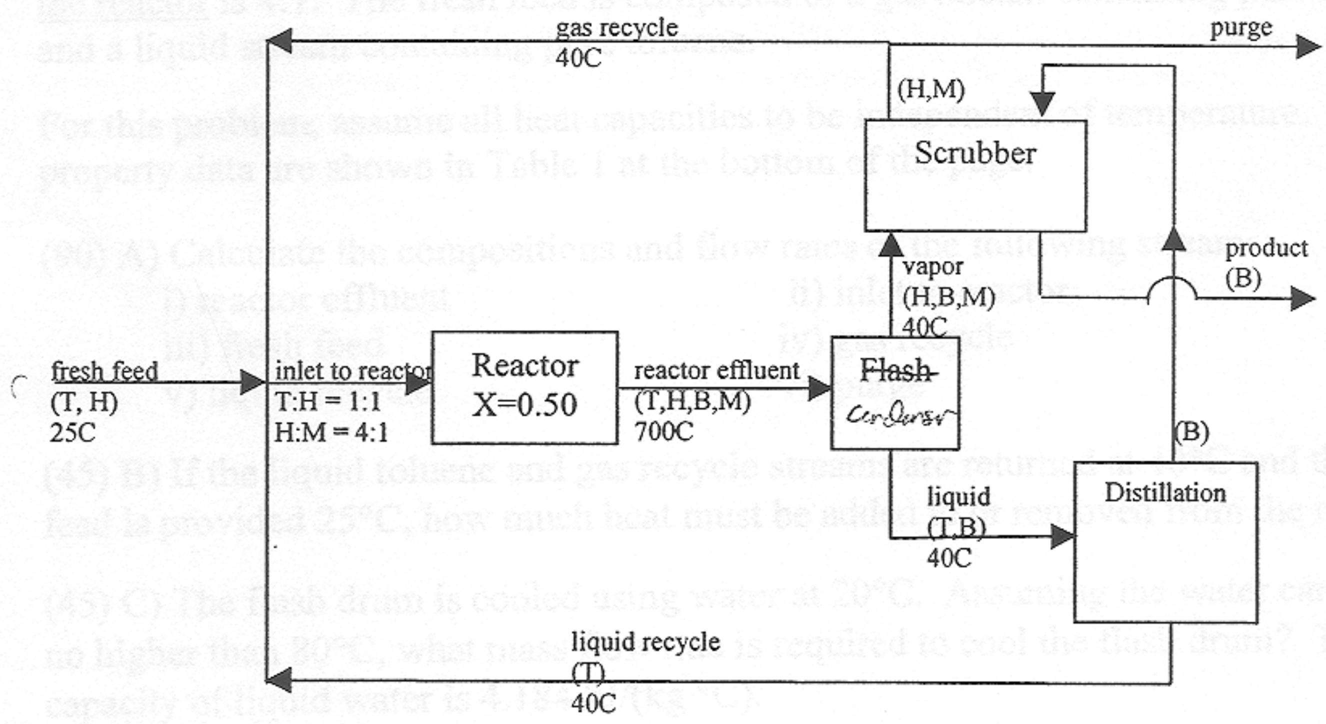

Figure 1: Toluene Hydrodealkylation Process Flow Sheet

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1. (continued)

The flow sheet has been duplicated for your convenience

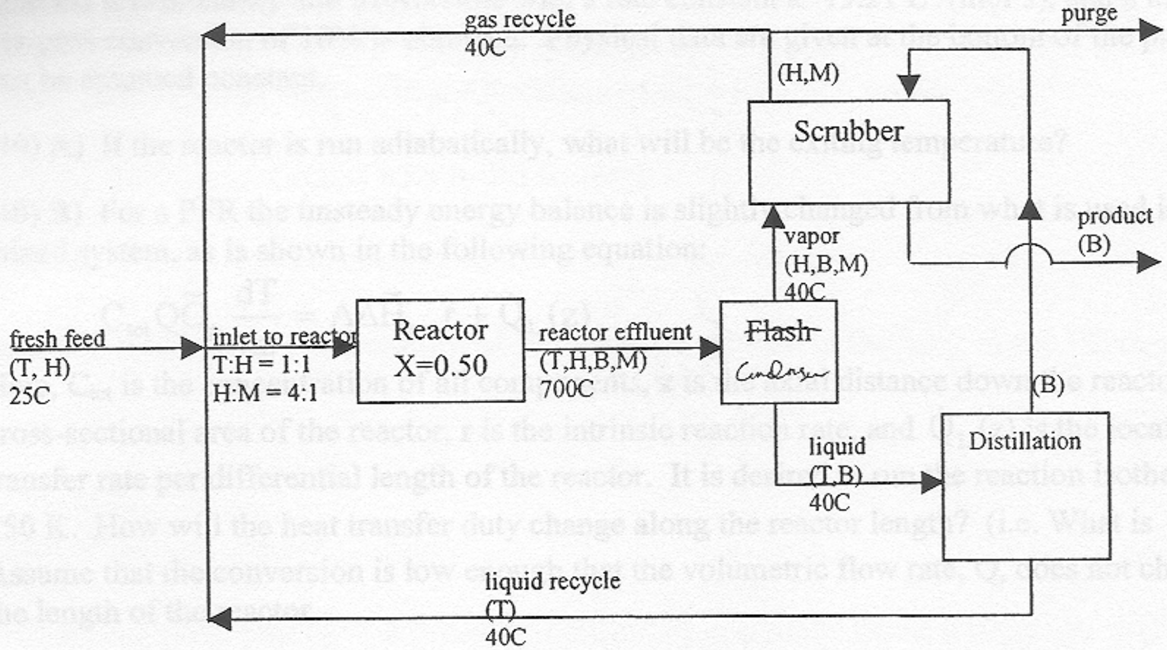

Figure 1: Toluene Hydrodealkylation Process Flow Sheet

The product (benzene) flow rate is 100 mol/hr. At the <u>inlet to the reactor</u>, toluene and hydrogen are fed in a stoichiometric ratio; the ratio of hydrogen to methane at the <u>inlet to the reactor</u> is 4:1. The fresh feed is composed of a gas stream containing pure hydrogen and a liquid stream containing pure toluene.

For this problem, assume all heat capacities to be independent of temperature. Thermal property data are shown in Table 1 at the bottom of the page.

(90) A) Calculate the compositions and flow rates of the following streams:

i) reactor effluent ii) inlet to reactor
iii) fresh feed iv) gas recycle
v) liquid recycle vi) purge

(45) B) If the liquid toluene and gas recycle streams are returned at 40°C and the fresh feed is provided 25°C, how much heat must be added to or removed from the reactor?

(45) C) The flash drum is cooled using water at 20°C. Assuming the water can leave at no higher than 80°C, what mass flow rate is required to cool the flash drum? The heat capacity of liquid water is 4.184 kJ/(kg °C).

(20) D) What is the overall conversion of the process with respect to toluene?

Table 1: Thermal Properties

Component	H_2	CH_4	C_6H_6	C_6H_6	C_7H_8	C_7H_8
State	gas	gas	liquid	gas	liquid	gas
$\tilde{C}_p$ [kJ/(mol K)]	0.03	0.05	0.13	0.21	0.16	0.25
$\Delta\tilde{H}_f{}^\circ$ [kJ/mol]	0	-74.84	48.66	82.927	11.99	50.000

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(200) 2. Ammonia is made in a PFR as shown in Figure 2 below. Nitrogen and hydrogen are fed to the reactor in a 1:3 molar ratio at 300 atm and 750 K with no contaminants present. The reaction is elementary and irreversible with a rate constant k=19.21 $L^3/(mol^3 s)$, and a nitrogen per-pass conversion of 10% is obtained. Physical data are given at the bottom of the page and can be assumed constant.

(40) A) If the reactor is run adiabatically, what will be the exiting temperature?

(40) B) For a PFR the unsteady energy balance is slightly changed from what is used in a well mixed system, as is shown in the following equation:

$$C_{tot} Q \tilde{C}_p \frac{dT}{dz} = A \Delta \tilde{H}_{rxn} r + \dot{Q}_L(z)$$

Here, C_{tot} is the concentration of all components, z is the axial distance down the reactor, A is the cross-sectional area of the reactor, r is the intrinsic reaction rate, and $\dot{Q}_L(z)$ is the local heat transfer rate per differential length of the reactor. It is desired to run the reaction isothermally at 750 K. How will the heat transfer duty change along the reactor length? (i.e. What is $\dot{Q}_L(z)$?). Assume that the conversion is low enough that the volumetric flow rate, Q, does not change down the length of the reactor.

(25) C) If the exit stream from the reactor is sent directly to the condenser (bypassing the heat exchanger) what will be the heat duty of the condenser?

(25) D) How much heat will be saved by pre-cooling the reactor exit gases with the cold gases leaving the condenser as shown in the figure?

(40) E) The temperatures of the streams in the heat exchanger are changing all along the length, so when designing its area, the driving force for the heat transfer is not constant. Often, what is used is a log-mean temperature difference:

$$\Delta T_{lm} = \frac{\Delta T_1 - \Delta T_2}{\ln(\Delta T_1 / \Delta T_2)}$$

In this equation, ΔT_1 and ΔT_2 are the driving forces at each end of the heat exchanger. For the temperatures shown in the figure, what is the necessary heat transfer area? U = 10 $J/(s\,m^2 K)$

(30) F) What is the recycle molar flow rate?

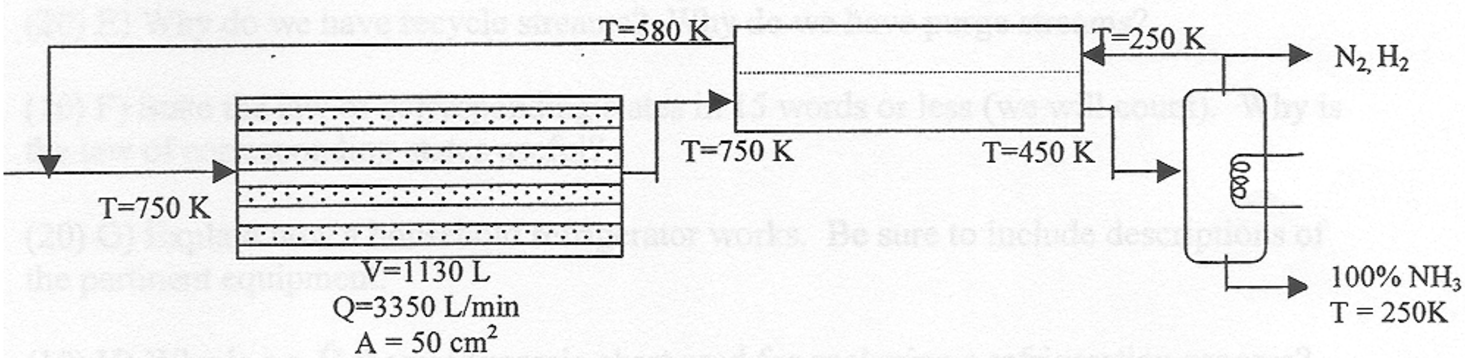

Figure 2: The Haber Process: $N_2 + 3H_2 \rightarrow 2NH_3$

$\Delta \tilde{H}_f^\circ (NH_3) = -67.2$ kJ/mol $\quad \Delta \tilde{H}_{vap} (NH_3) = 23.35$ kJ/mol

$\tilde{C}_p (NH_3) = 0.659$ J/(mol K) $\quad \tilde{C}_p (H_2) = 0.392$ J/(mol K) $\quad \tilde{C}_p (N_2) = 0.413$ J/(mol K)

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(100) 3. A well-insulated and well-mixed tank of 100 ft^3 capacity is initially partially filled with 10 ft^3 of pure water at 160°F. A constant inlet flow of a 25 wt% aqueous caustic solution also at 160°F is then started. There is no outlet flow. The solutions are approximated as having constant densities of 62.4 lbm/ft^3. $\dot{Q}_{in} = 3.5\ ft^3/min$

(25) A) How long does it take to fill the tank?

(25) B) What is the concentration of caustic at the fill time?

(50) C) What is the temperature of the caustic solution in the tank at the fill time?

(200) 4. Short Answer Questions.

(10) A) Suppose you have a pressure-controlled container filled with water and ice at 1 atm. You begin heating it at a constant rate. Sketch the temperature profile (up to 200°C) with time assuming the vessel pressure is maintained at 1 atm.

(20) B) Suppose $A + B \leftrightarrow C$ is an exothermic and reversible gas-phase reaction. What happens to the reaction rate and the equilibrium conversion when:

i) T is increased
ii) P is increased
What if $\Delta H_{rxn} > 0$? (Answer above questions again.)

(15) C) Explain and contrast the meanings of unsteady state, steady state, and equilibrium.

(20) D) How is ammonia produced and from what raw materials? Be sure to list any pertinent reactions and why they are used.

(20) E) Why do we have recycle streams? Why do we have purge streams?

(10) F) State the law of corresponding states in 15 words or less (we will count). Why is the law of corresponding states useful?

(20) G) Explain how a household refrigerator works. Be sure to include descriptions of the pertinent equipment.

(10) H) Why is a p-$\hat{H}$ thermodynamic chart used for analyzing a refrigeration process? What governs the choice of a refrigerant?

(continued on next page)

4. (continued)

(15) I) Assume $y = f(x)$ and $y' = dy/dx$. Identify the order of the following ordinary differential equations. Classify them as linear or nonlinear, homogeneous or non-homogeneous, and initial-value or boundary-value problems.

i) $\dfrac{dy}{dx} + 2y - 3x = 0 \quad , \quad y(0) = 1$

ii) $\dfrac{d^2y}{dx^2} = 0 \quad , \quad y(0) = y'(0) = 1$

iii) $\left(\dfrac{dy}{dx}\right)^2 = \sin x \quad , \quad y(1) = 1$

iv) $\dfrac{d^2y}{dx^2} + y\dfrac{dy}{dx} + yx^2 = 0 \quad , \quad y(0) = 1, y'(1) = 1$

(20) J) How many stages are required for the distillation column shown in Figure 3 below. The equilibrium data are shown in Figure 4 on next page. Make sure you turn in Figure 4 with your exam!

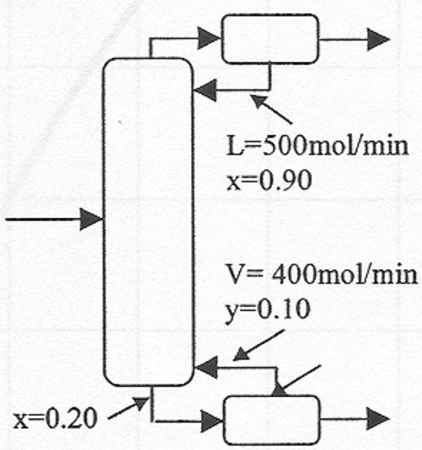

Figure 3: Distillation Column

(20) K) For a 4 component flash unit, how many variables must be fixed in order to specify the process completely?

(20) L) How does the overall mass transfer coefficient, k_m relate to the single side mass transfer coefficients k_I and k_{II}?

(Figure 4 shown on next page)

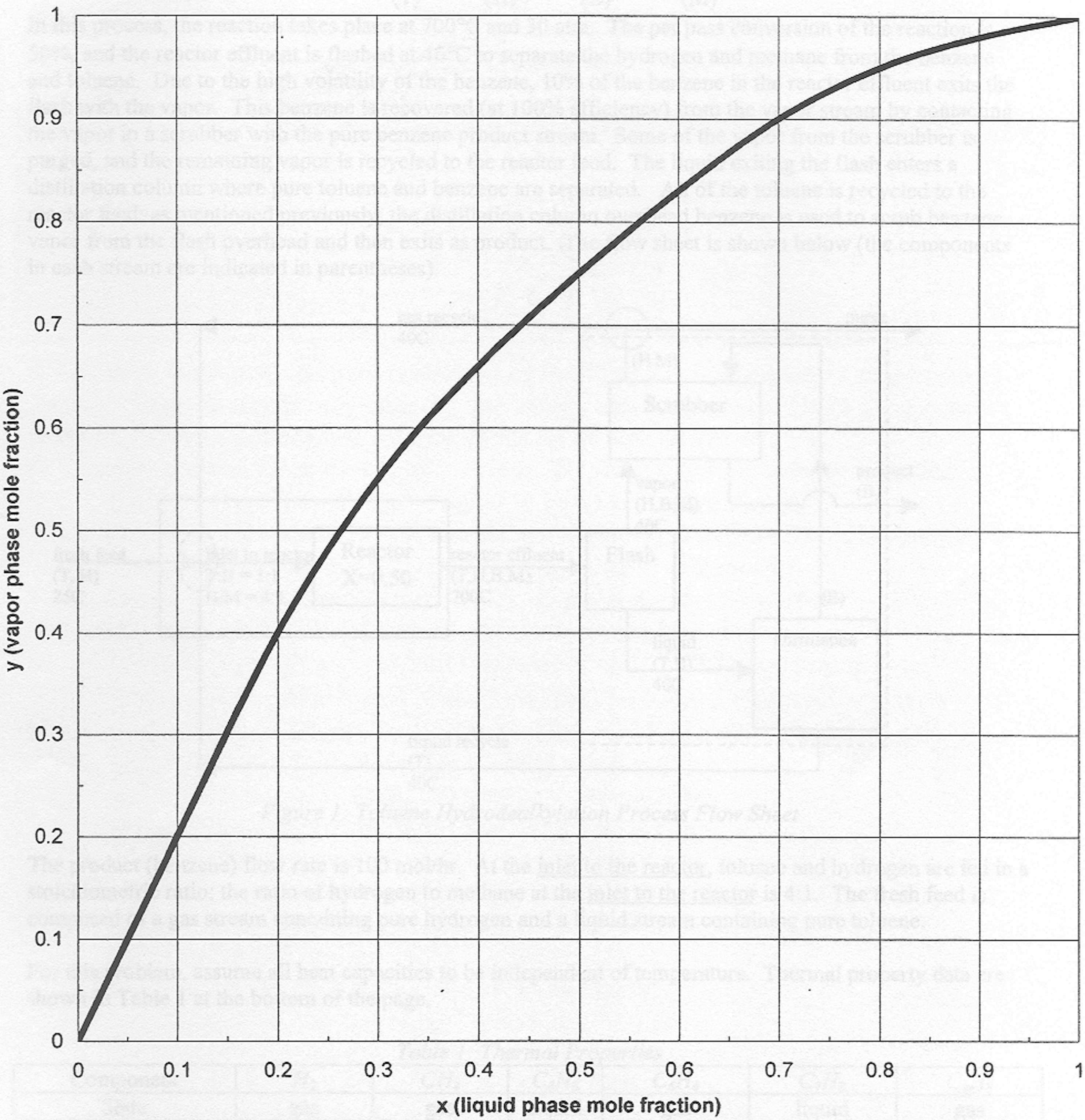

Figure 4: Equilibrium Data for Problem 4 (J)

Turn in with exam