ChE 4133 **Homework #2** **Due: March 2, 2017**

Industrial Catalysis

Hydrogen and toluene are reacted over an acidic catalyst to form methane and benzene:

$$C_6H_5CH_3 + H_2 \rightarrow C_6H_6 + CH_4$$

$$or \qquad T + H_2 \rightarrow B + M$$

The following data were obtained.

Run	$-r_T \times 10^{10}$ $\left(\frac{g\ mol\ toluene}{g\ cat \cdot s}\right)$	Partial pressure (atm) Toluene P_T	Hydrogen (H_2), P_{H2}	Methane, P_M	Benzene, P_B
Set A					
1	71.0	1	1	1	0
2	71.3	1	1	4	0
Set B					
3	41.6	1	1	0	1
4	19.7	1	1	0	4
5	42.0	1	1	1	1
6	17.1	1	1	0	5
Set C					
7	71.8	1	1	0	0
8	142.0	1	2	0	0
9	284.0	1	4	0	0
Set D					
10	47.0	0.5	1	0	0
11	71.3	1	1	0	0
12	117.0	5	1	0	0
13	127.0	10	1	0	0
14	131.0	15	1	0	0
15	133.0	20	1	0	0
16	41.8	1	1	1	1

All runs were conducted at 10 atm total pressure and 600°C. Assume that the overall reaction is irreversible. Assume ideal gases.

1. Write two general LHHW rate expressions assuming that the surface reaction controls the rate, according to assumptions given below. After writing a full rate equation, examine the data qualitatively and eliminate any terms in the rate expression based upon the qualitative appraisal. Explain your simplifications by referring to run numbers in the first column of the data table.

   (a) For the first expression, assume H_2 adsorbs molecularly (i.e., does not disassociate).

   (b) For the second expression, assume H_2 does not adsorb and that it attacks from the gas phase (i.e., Eley-Rideal).

2. Linearize the rate expressions found in part 1 by taking the reciprocal, then multiplying through by $P_{H2} \bullet P_T$. Deduce which rate model gives the better fit to the data and find all constants in that rate expression using appropriate sets of data and linear regression.

3. Using the rate expression derived in part 2, design a packed-bed reactor to produce 10 moles of benzene per minute from a feedstock consisting of 20% toluene, 40% H_2, and 40% inerts at 10 atm and 600°C flowing at 400 lt/min. Keeping your units consistent, you will determine the mass of catalyst required to achieve the necessary conversion. Then, determine the volume of the reactor using $\rho_{BED} = 2.3$ gr/cm^3 (ρ_{BED} is the bulk or bed density of the catalyst).