ChE 3063 **Project 3** Due: December 4, 2020

There are numerous reactions that take place in a catalytic reformer. Let's take n-heptane as a typical paraffinic reactant and consider some of the reactions it undergoes:

C_7H_{16} n-heptane	⇆	C_7H_{14} + 1-heptene	H_2	dehydrogenation rxn 1)
C_7H_{16} n-heptane	⇆	C_7H_{16} 2-methylhexane		isomerization rxn 2)
C_7H_{16} n-heptane	⇆	C_3H_8 + propane	C_4H_8 1-butene	cracking rxn 3)
C_7H_{16} n-heptane	⇆	C_7H_8 toluene	+ $4H_2$	aromatization rxn 4)
C_7H_{16} n-heptane	⇆	C_6H_6 + benzene	CH_4 + $3H_2$ methane	aromatization with cracking rxn 5)
C_7H_{16} n-heptane	⇆	C_7H_{14} methylcyclohexane	+ H_2	cyclization rxn 6)

These reactions represent a very small fraction of the total number of reactions that naphtha, which is C_5 - C_8 or so paraffins, is converted to high octane components on a platinum catalyst. The thermodynamic features of the process are somewhat represented by the reactions given above. High temperatures are necessary to make the aromatization, dehydrogenation, and cyclization reactions, which are the desired reactions, thermodynamically favorable. In order to properly operate the catalyst, we need high hydrogen partial pressures to stop coke formation. Therefore, we usually co-feed hydrogen with the naphtha reactant even though the desired forward reactions are favored by low hydrogen partial pressures.

For these reactions, we need equilibrium data in the range 550-1050K at 10 bar and 20 bar total pressure. Using HYSYS for computing the equilibrium constants and compositions (plots may be prepared in Excel using the numbers imported from HYSYS):

A. Calculate and, <u>on a single graph</u>, plot $\ln(K_a)$ vs 1/T (ºK) for all reactions.

B. Calculate and plot the mole fraction of each species (n-heptane, propane, 1-butene, methane, 1-heptene, benzene, hydrogen, toluene, methylcyclohexane, and 2-

methylhexane) at equilibrium for each pressure as a function of temperature for an initial mixture which contains 1 mole n-heptane and 2 mole H_2 with no other species initially present. Put a single species on each graph comparing the 10 and 20 bar curves. Put 4 or 5 plots on a single page so you don't have too many printed pages to turn in.

Instructions for submitting the project: Turn in a paper solution with the ln(K) vs 1/T graph and all 10 of the individual species graphs. Be sure to annotate the plots and use captions and legends with big enough lettering to be legible. Save the HYSYS case as "Project3-FirstName-LastName.hsc" and email it to me *before* class the date it is due with the subject line: "ChE3063 Project 3 Solution". Submit your paper solution at the beginning of class the date it is due.

Some notes:

The reaction list as given is a set of independent reactions. Each one starts with n-heptane and the products are different in each case. Since the products are different, no reactions could be added or subtracted to give one of the other reactions; thus the reactions are independent.

Consider what would happen if you added this reaction to the set:

C_7H_{14}	⇆	C_7H_8	+	$3H_2$
1-heptene		toluene		

This is a totally acceptable reaction, and in fact is one of the routes toluene is formed in reformers. But if I take rxn 1) and subtract it from rxn 4) from the independent reaction set above, this reaction is the result. Therefore, these reactions are not independent. If you add this reaction to the reaction list in HYSYS, HYSYS will tell you that. Caution: it takes a little time for HYSYS to figure out the reactions are not independent, and I had HYSYS crash once while testing this, and I lost some of my work. Save your HYSYS file before you try it. Lesson learned: make sure all your reactions are independent when using this method to solve multi-reaction equilibrium problems.