November 12, 2018

Styrene can be produced by the dehydrogenation of ethylbenzene:

$$C_8H_{10}$$
 (g) [ethylbenzene]  $\rightarrow C_8H_8$  (g) [styrene] +  $H_2$  (g)

However, styrene will polymerize once it is formed, so we wish to keep the temperature as low as possible to reduce polymerization. At the same time, the catalyst needs to have hydrogen present in as large a possible concentration to help keep carbon deposits from forming. Therefore, we would like to consider running the reaction starting with a 1/1 mole mixture of  $C_8H_{10}/H_2$  (no  $C_8H_8$  initially) and to run the reaction at  $700^{\circ}$ C and 5 bar absolute pressure. For this reaction:

a) 35 points

Calculate K<sub>a</sub> for the reaction at 700°C

b) 30 points

Set up a mole balance to give mole fractions (y's) of each species in terms of extent of reaction ( $\zeta$ ).

c) 35 points

Compute the mole fractions of each species at equilibrium at 700°C and 5 bar assuming the gas phase is a mixture of ideal gases.