Simulation Training #2-Distributing the Chemicals

Statement

Using HYSYS, simulate the synthesis of a process to hydrodealkylate toluene. In this case, a product design alternative involves the conversion of toluene to benzene and, for this purpose, the principal reaction path is well defined. It involves

$$\mathrm{C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4}$$

which is accompanied by the side reaction to produce byphenil

$$2C_6H_6 \rightarrow \mathrm{C_{12}H_{10} + H_2}$$

Laboratory data indicate that the reactions proceed irreversibly without a catalyst at temperatures in the range of 1,200–1,270°F with approximately 75 mol% of the toluene converted to benzene and approximately 2 mol% of the benzene produced in the hydrodealkylation reaction converted to biphenyl. The final laboratory data was collected at an operating pressure of 494 psia and an operating temperature of 1,268ºF. The plant capacity is based on the target amount of benzene to be 250 MMlb/yr, assuming an operating factor of 90.4% of the year (or 330 days in operation in 365 days of the year). Here, the overall mass balance is carried out assuming that all of the unreacted toluene is recycled and consumed in the process to be synthesized.

Problem 1. Before inserting the reaction operation into a flowsheet, The first thing you must do is to determine the feasibility of the economic potential, EP (i.e., the sales minus the cost of raw materials, not including the cost of utilities and operating costs). Using the prices below from ICIS Chemical Business in late 2014 estimates, determined the economic potential (cents/lb of benzene) for the main reaction. Make sure to take into consideration inflation by using the following Cost Intext values $CEPCI_{2014}$=576 and $CEPCI_{2019}$=619.

Chemical	H_2	CH_4	C_6H_6	C_7H_8	$C_{12}H_{10}$
Cost in 2014 (cent/lb)	0.59	0.21	0.54	0.47	unavailable

Problem 2. As shown in Figure 1, one distribution of chemicals involves a large excess of hydrogen gas to prevent carbon deposition and absorb much of the heat of the exothermic hydrodealkylation reaction. Furthermore, to avoid an expensive separation of the product methane from the hydrogen gas, a purge stream is utilized in which methane leaves the process, unavoidably with a comparable amount of hydrogen (See Heuristic 5). Because the performance of the separation system, to be added in the next synthesis step, is unknown, the amount of hydrogen that accompanies methane in the purge stream is uncertain at this point in the synthesis. Hence, the distribution of chemicals in Figure 1 is known incompletely. Based on this information, determine a distribution of chemicals in HYSYS by using a conversion reactor and the Soave-Redlich-Kwong equation of state.