Assignment 3 on Aspen Plus

Process to produce benzene by dehydrogenation of toluene

It is required to produce 265 mol/s of benzene by dehydrogenation of toluene. The reactor is operated isothermally at 6500C and 35 atm pressure. The following reactions occur in the reactor

Toluene + H2  Benzene + Methane

2Benzene <=> Diphenyl + H2

The fresh feed of toluene is pure while the fresh hydrogen feed contains 95 mol% hydrogen and the rest methane. Both the feed streams are at 25 deg C and 1 atm pressure and the molar feed rate of hydrogen stream is five times that of toluene. Assume that 70% of toluene fed to reactor is converted, and assume that the second reaction reaches equilibrium in the reactor. The reactor product stream is first sent to a flash drum which operates at 35 atm pressure and 300 C (isothermal flash), to obtain a vapour and liquid stream. 95% (mole basis) of the vapour stream from the flash is recycled back to the reactor and the rest purged. The liquid stream from the flash drum is further let down through an isenthalpic valve to 1 atm pressure and then flashed at 1 atm pressure and 90 deg C to recover benzene as a vapour product (usually this is done in a distillation column instead of a single stage flash unit), while the remaining stream containing most of the toluene, diphenyl and unrecovered benzene is recycled back to the reactor.

(a) Set up the flow sheet to model the feed compression, heating and reactor. (*Note: The reactor can be modeled in Aspen as a sequence of two reactors both operating at the same temperature and pressure, where reaction 1 occurs in first reactor and reaction 2 occurs in the second reactor*).

Determine the work required for compressing the hydrogen feed stream, energy required to heat the hydrogen stream fed to reactor, energy required to heat the toluene stream fed to reactor, and total energy removed or added to the two reactors to maintain isothermal conditions.

(b) Extend the above flowsheet to include the model of the flash units and vapour recycle from the first flash to the reactor and liquid recycle from the second flash unit to obtain a converged solution. What is the composition of the vapour stream from the flash, the recycle stream flow rates and amount of energy added/removed to the flash units? Determine the fresh feed rate of toluene required for the desired production rate of benzene.

(c) Give reasons why hydrogen is not fed in stoichiometric ratio but in excess? If you have the time simulate for different feed ratios and infer from the results.

Use Peng-Robinson.