Process Systems Engineering

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Exercise #2

The kinetic model relative to the main reactions that schematize the process of dealkylation is shown below.

Reaction #1:
$C_6H_5\text{-}CH_3 + H_2 \rightarrow C_6H_6 + CH_4$

$$A_1 = 3.5\text{E}+10 \qquad E_1 = 50900 \qquad k_1 = A_1 \exp\left(-\frac{E_1}{RT}\right) \qquad R_1 = k_1 c_T \sqrt{c_H}$$

Reaction #2:
$2\ C_6H_6 \rightarrow C_{12}H_{10} + H_2$

$$A_2 = 2.1\text{E}+12 \qquad E_2 = 60500 \qquad k_2 = A_2 \exp\left(-\frac{E_2}{RT}\right) \qquad R_2 = k_2 c_B^2$$

Activation energies are in kcal/kmol, and the rates of reaction are expressed in kmol/m^3/s. We

ask to:

- determine, via numerical integration of the plug-flow model of the reactor, the conversion, the selectivity and the residence time as a function of the operating temperature, by assuming isothermal the reactor, and neglecting the presence of recycles in the evaluation of initial concentrations
- evaluate the adiabatic ΔT of the reaction so to determine if the reactor can be considered isothermal

Carry out the following diagrams:

- conversion/selectivity as a function of reactor temperature
- temperature/conversion by imposing the selectivity of at least 96%
- temperature/residence time of imposing the selectivity of at least 96%
- residence time/flow rates of each of the input streams as a function of the reactor temperature

A suitable range of investigation for the working temperature of this unit is: 600-750 °C.