Process Systems Engineering A

Prof. Davide Manca
Dipartimento di Chimica, Materiali e Ingegneria Chimica "G. Natta"
Politecnico di Milano

LAB 2

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

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

$$A_1 = 3.5\text{E}+10 \qquad E_1 = 50900$$

$$k_1 = A_1 \exp\left(-\frac{E_1}{RT}\right) \qquad R_1 = k_1 c_T \sqrt{c_H}$$

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

$$A_2 = 2.1\text{E}+12 \qquad E_2 = 60500$$

$$k_2 = A_2 \exp\left(-\frac{E_2}{RT}\right) \qquad R_2 = k_2 c_B^2$$

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, selectivity and residence time as a function of the operating temperature, by assuming the reactor isothermal (***HINT***: at this level of detail, the presence of recycles can be neglected in the evaluation of the initial molar flows/concentrations → Consider SF=100%).
- evaluate the adiabatic ΔT of the reaction so to determine if the reactor can be considered isothermal

Provide the following charts:

- Selectivity vs. Conversion, as a function of the reactor temperature
- Conversion vs. Temperature, by imposing a selectivity of at least 96%
- Volume/Residence time vs. Temperature, by imposing a selectivity of at least 96%
- Molar flows/concentrations vs. Volume/Residence time, as a function of the reactor temperature

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

Please note that you can generate your diagrams considering either the exact reactor volume values ***OR*** considering a very high volume/residence time (to depict the general evolution of the reaction).