

Process Systems Engineering A

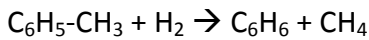
Prof. Davide Manca

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

LAB 2

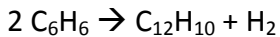
The kinetic model relative to the main reactions that schematize the process of dealkylation is shown below.

Reaction #1:



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

Reaction #2:



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

Activation energies are in [kcal/kmol], and the rates of reaction are expressed in [kmol/m³/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).