LAB2: Reactor design

Designing the hydrodealkylator

Process Systems Engineering A – Prof. Davide Manca

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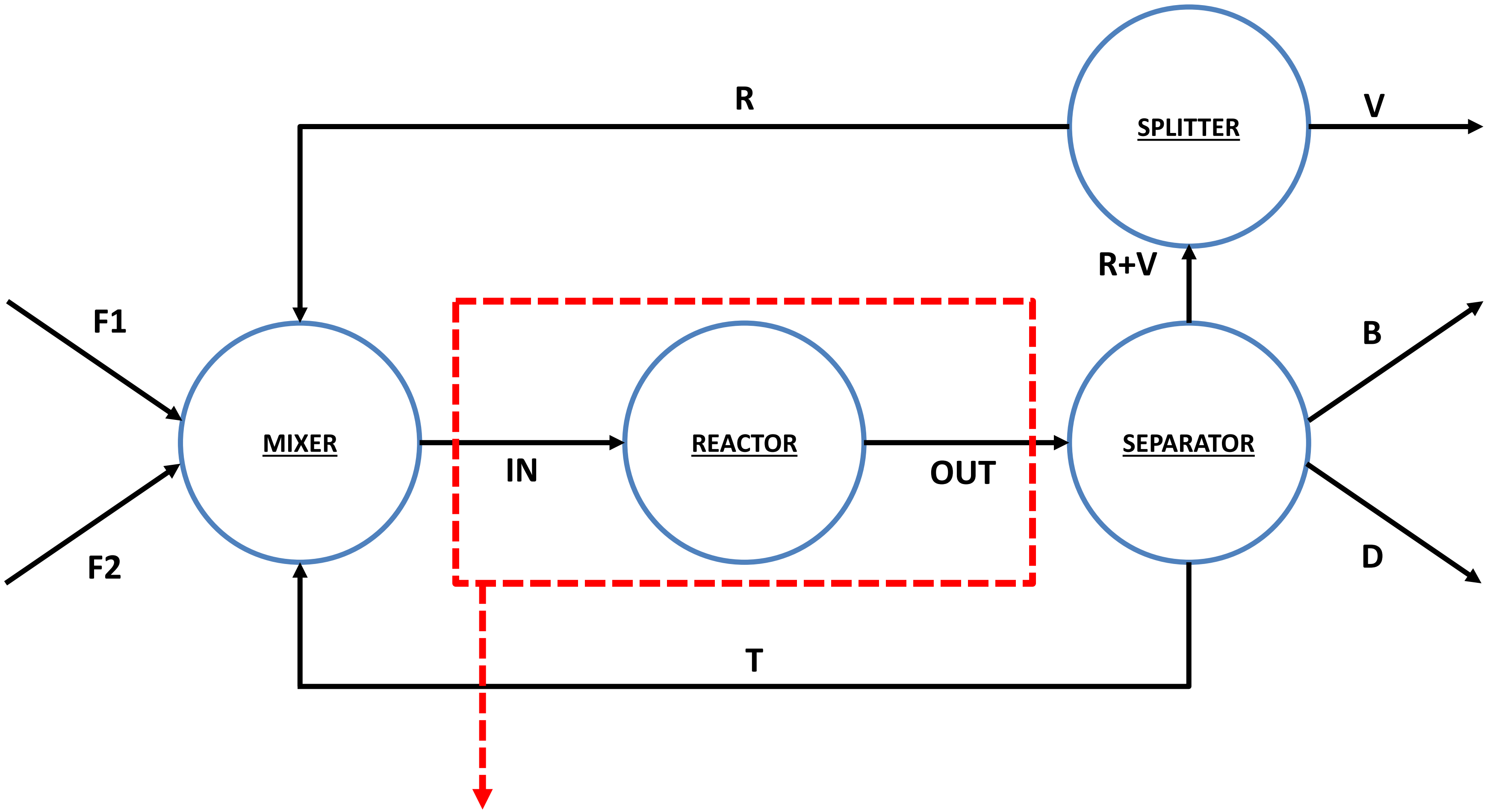


Desired reaction

$$C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4$$

Side reaction

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

Desired reaction

$$C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4$$

$$R_1 = k_1 C_{C_7H_8} \sqrt{C_{H_2}}$$

$$[\mathrm{kmol/(m^3 \cdot s)}]$$

$$k_1 = A_1 \exp\left(-\frac{E_1}{RT}\right) \; [\mathrm{m^{1.5}/(kmol^{0.5} \cdot s)}]$$

$$A_1 = 3.5 \cdot 10^{10} \; [\mathrm{m^{1.5}/(kmol^{0.5} \cdot s)}]$$

$$E_1 = 50900 \; [\mathrm{kcal/kmol}]$$

Side reaction

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

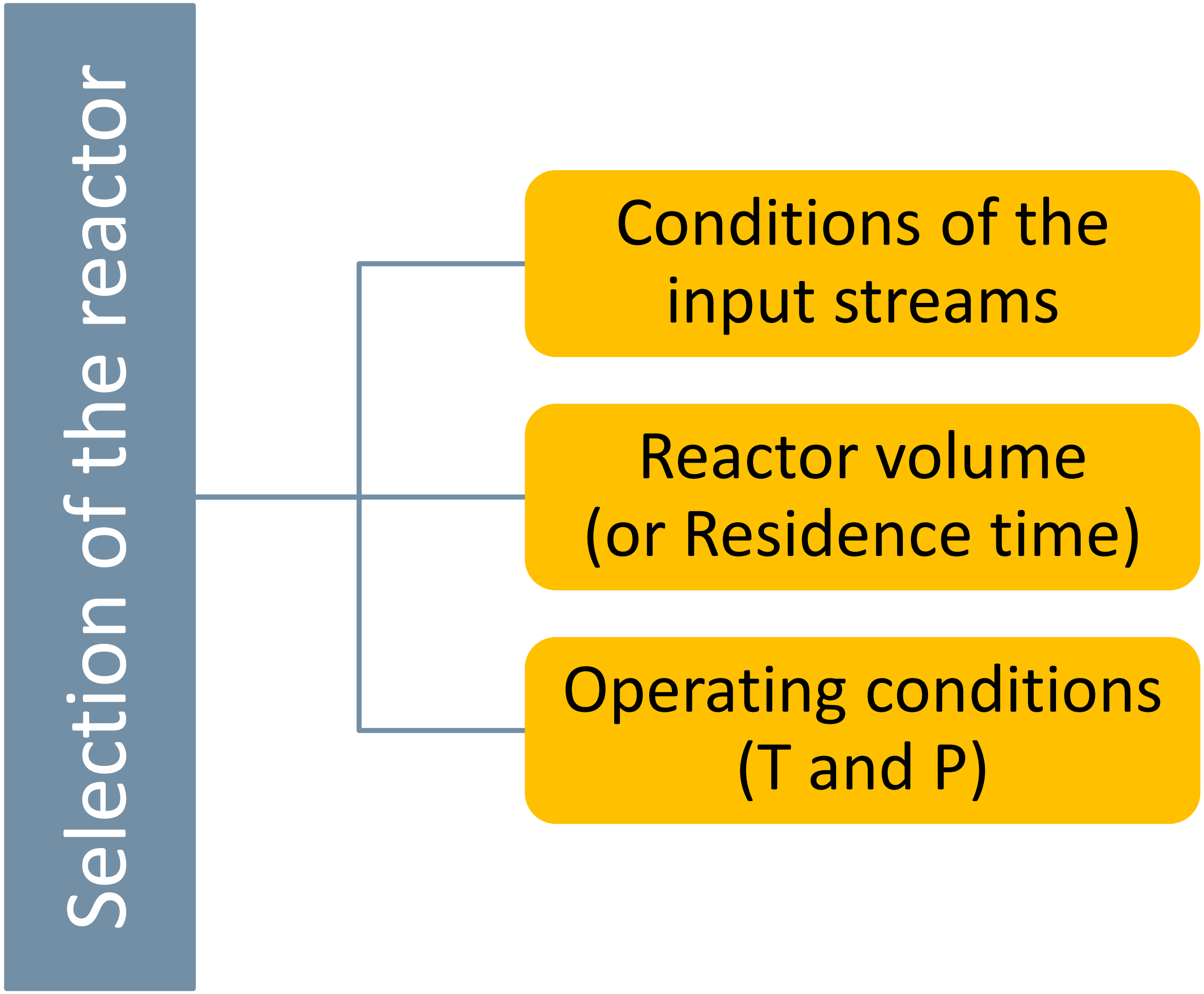
$$R_2 = k_2 C^2_{C_6H_6}$$

$$[\mathrm{kmol/(m^3 \cdot s)}]$$

$$k_2 = A_2 \exp\left(-\frac{E_2}{RT}\right) \; [\mathrm{m^3/(kmol \cdot s)}]$$

$$A_2 = 2.1 \cdot 10^{12} \; [\mathrm{m^3/(kmol \cdot s)}]$$

$$E_2 = 60500 \; [\mathrm{kcal/kmol}]$$


Selection of the reactor
Conditions of the input streams
Reactor volume (or Residence time)
Operating conditions (T and P)

Conditions of the input streams

- The stream of fresh hydrogen (F1) contains 5%$_{mol}$ of methane;
- The reactants are at ambient temperature;
- The Hydrogen-to-Toluene Ratio (HTR) at the inlet of the reactor must be equal to 5.

Reactor volume (and Residence time)

- Benzene selectivity must be ≥ 96%;
- Benzene productivity must be 265 kmol/h.

Operating conditions

Pressure

- Both reactions are equimolar.

⇒ P = 34 bar

Temperature

- No need for any catalyst;
- The desired reaction is exothermic;
- The side reaction is faster at high T (higher E_a).

⇒ it is worth operating at low temperatures!

Range of interest: 600–750°C ⇒ carry out tests with ΔT=50°C

Reactor type

The reaction scheme is in series:

$$\text{Toluene} \xrightarrow{Reaction\ \#1} \text{Benzene} \xrightarrow{Reaction\ \#2} \text{Biphenyl}$$

The control of residence time is fundamental

($\sigma_{C_6H_6}$ must be kept ≥ 96%)

a **Plug Flow Reactor** (PFR) is needed

PFR: 5 species → 5 ODEs

$$\begin{cases} \dfrac{dF_{H_2}}{dV} = \nu_{1,H_2} R_1(T,P,\boldsymbol{x}) + \nu_{2,H_2} R_2(T,P,\boldsymbol{x}) \\ \dfrac{dF_{CH_4}}{dV} = \nu_{1,CH_4} R_1(T,P,\boldsymbol{x}) \\ \dfrac{dF_{C_7H_8}}{dV} = \nu_{1,C_7H_8} R_1(T,P,\boldsymbol{x}) \\ \dfrac{dF_{C_6H_6}}{dV} = \nu_{1,C_6H_6} R_1(T,P,\boldsymbol{x}) + \nu_{2,C_6H_6} R_2(T,P,\boldsymbol{x}) \\ \dfrac{dF_{C_{12}H_{10}}}{dV} = \nu_{2,C_{12}H_{10}} R_2(T,P,\boldsymbol{x}) \end{cases}$$

$$\begin{cases} F_{H_2}(V=0) = F_{H_2}^{IN} \\ F_{CH_4}(V=0) = F_{CH_4}^{IN} \\ F_{C_7H_8}(V=0) = F_{C_7H_8}^{IN} \\ F_{C_6H_6}(V=0) = 0 \\ F_{C_{12}H_{10}}(V=0) = 0 \end{cases}$$

$$\begin{cases} F_{H_2}(V=V_{tot}) = F_{H_2}^{OUT} \\ F_{CH_4}(V=V_{tot}) = F_{CH_4}^{OUT} \\ F_{C_7H_8}(V=V_{tot}) = F_{C_7H_8}^{OUT} \\ F_{C_6H_6}(V=V_{tot}) = F_{C_6H_6}^{OUT} \\ F_{C_{12}H_{10}}(V=V_{tot}) = F_{C_{12}H_{10}}^{OUT} \end{cases}$$

Also, remember:

$$\sigma_{C_6H_6} = \frac{F_{C_6H_6}}{F_{C_7H_8}^{IN} - F_{C_7H_8}^{OUT}}$$

Selectivity

$$\chi_{C_7H_8} = \frac{F_{C_7H_8}^{IN} - F_{C_7H_8}^{OUT}}{F_{C_7H_8}^{IN}}$$

Conversion

$$\tau = \frac{V}{\dot{V}}$$

Residence time