

Exercise 1: Reactors

Styrene can be produced by the catalytic dehydrogenation of ethylbenzene according to the following reaction:



- The reaction is carried out at temperatures ranging from 600°C to 650°C.
- To avoid undesirable side reactions, the reaction is carried out at reduced pressure (0,1 - 0,5 bar).

Given data:

- **$T_{\text{in}} = 600 \text{ °C}$**
- **$p_{\text{Reactor}} = 0,5 \text{ bar}$**
- **$F_{\text{in}} = 200 \text{ mol/sec}$**
- **Properties: RK-Soave**

Task 0

In which phase does the reaction occur? Create a p-T-diagram for the component ethylbenzene and mark the operating point in the diagram.

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Task 1

- 1) Model the reaction using a stoichiometric reactor (RStoic) with a 70% conversion of ethylbenzene.
 - a) What is the reactor outlet temperature under adiabatic operation?
 - b) What amount of heat must be supplied for isothermal operation?

- 2) Model the reaction using a Gibbs reactor (RGibbs). Plot the equilibrium conversion vs. Temperature in Excel for the two process pressures (0,5 bar and 1 bar). Vary the temperature between 500°C and 700°C.

- 3) What information do you obtain regarding the reactor type (e.g. CSTR, PFR).

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Task 2

The reaction kinetics for styrene production are as follows:

$$r_{EB} = k \cdot p_{EB} \quad \text{with} \quad k = k_0 \cdot e^{-\frac{E_A}{R \cdot T}}$$
$$k_0 = 89,22 \text{ kmol}/(\text{m}^3 \cdot \text{s} \cdot \text{Pa})$$
$$E_A = 21874 \text{ cal/mol}$$

Use the Power Law approach for implementation in Aspen Plus. Note that this is a first-order reaction.

- 1) Model the reaction using an isothermal plug flow reactor (RPLUG) with a length of 1m and a diameter of 0,25m.
- 2) Model the reaction using three adiabatic continuous stirred-tank reactors (CSTR) in series. Each stirred-tank reactor should have a volume of 100 liters.
- 3) Which measures can be taken to improve the conversions in the plug flow reactor and the CSTR cascade?