Process Systems Engineering

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Exercise #1

The Process Systems Engineering Laboratory lectures deal with the design and the economic assessment of a hydrodealkylation (**HDA**) plant for the production of benzene from toluene.

The chemical reactions involve radicals. The products have high molecular weight and are strongly dehydrogenated. For the sake of simplicity, we will deal with a kinetic scheme involving only two main reactions, where biphenyl is actually standing for the entire class of polyaromatic byproducts.

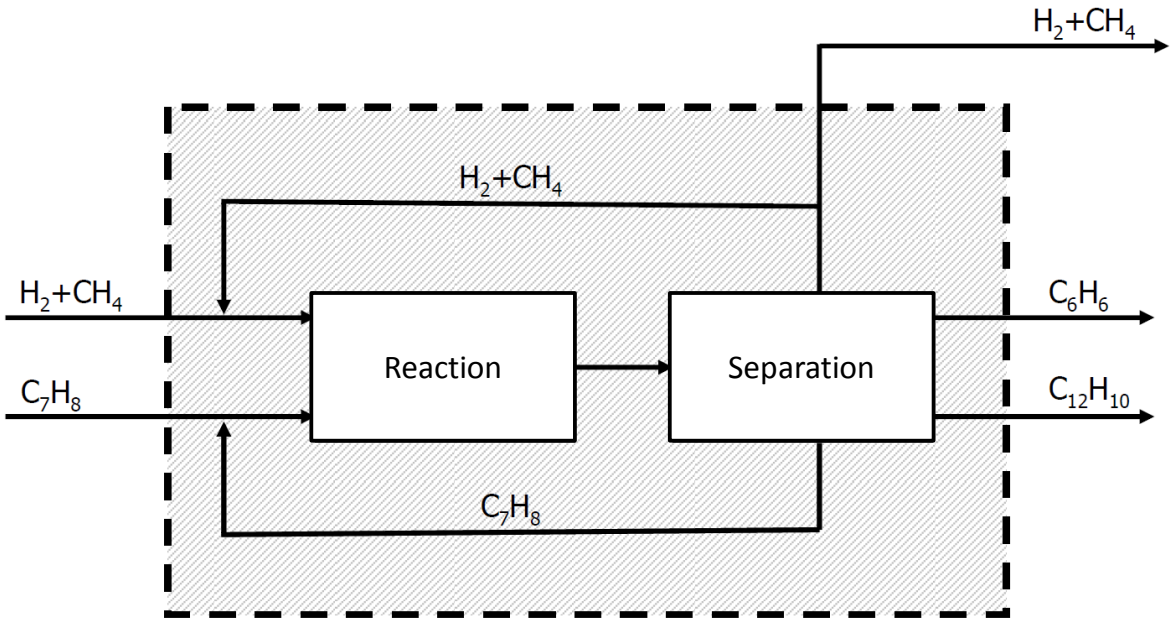
Reaction #1:
$C_6H_5\text{-}CH_3 + H_2 \rightarrow C_6H_6 + CH_4$

Toluene + Hydrogen → Benzene + Methane

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

2 Benzene → Biphenyl + Hydrogen

The Block Flow Diagram (BFD) of the process is shown in the following:



The design of the reactor calls for evaluating both conversion and selectivity.

Some specifications are given: operating pressure 34 bar, inlet H_2/C_7H_8 ratio to reactor section ≥ 5 to limit the formation of dehydrogenated products (coking), and to increase selectivity. At the same time an excess in H_2/C_7H_8 ratio would increase the recycle flow rate.

To make the plant economically feasible, selectivity has to be at least equal to 96%.

As far as the inlet streams to the plant are concerned, the toluene flowrate may be assumed pure, while the fresh hydrogen one contains a 5% impurity of methane. Both are fed at ambient temperature.

Benzene Specifications

- production capacity = 265 kmol/h
- purity = 0.9997 (molar)

Assignment

- Select the type of process: batch or continuous?
- Write explicit global mass balances, to estimate the inlet, outlet and recycle streams;
- Determine the Degrees of Freedom of the system;
- Determine the specific dependency of material fluxes from process variables (*e.g.*, temperature, conversion, selectivity, …).