



**POLITECNICO**  
MILANO 1863

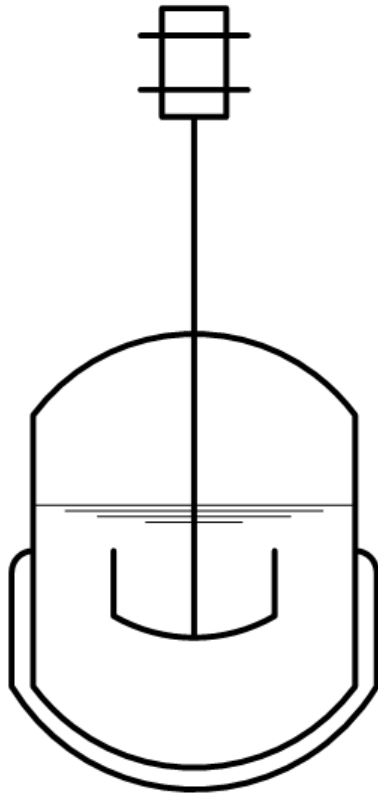
# LAB5: Simulation with HYSYS®/UniSim®

Simulation of the HDA process with the Process Simulator

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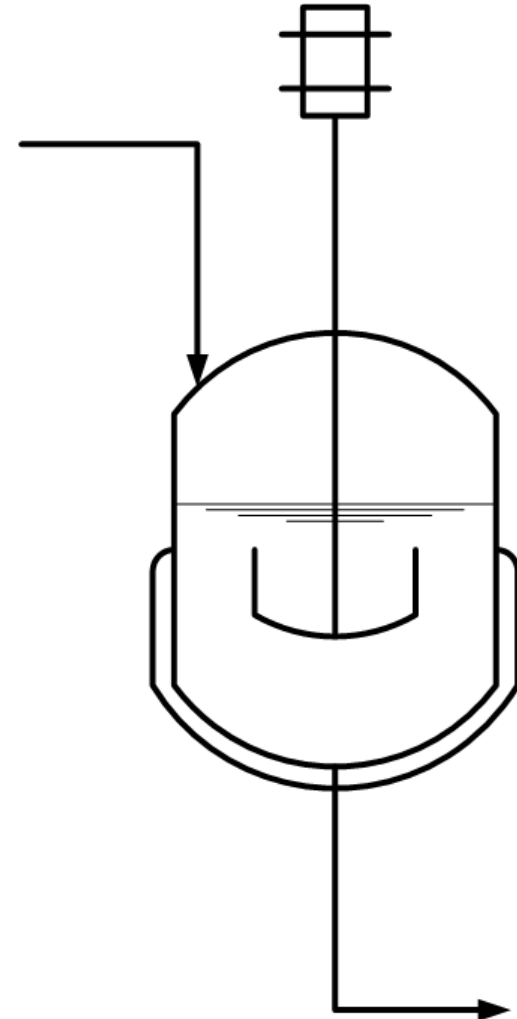


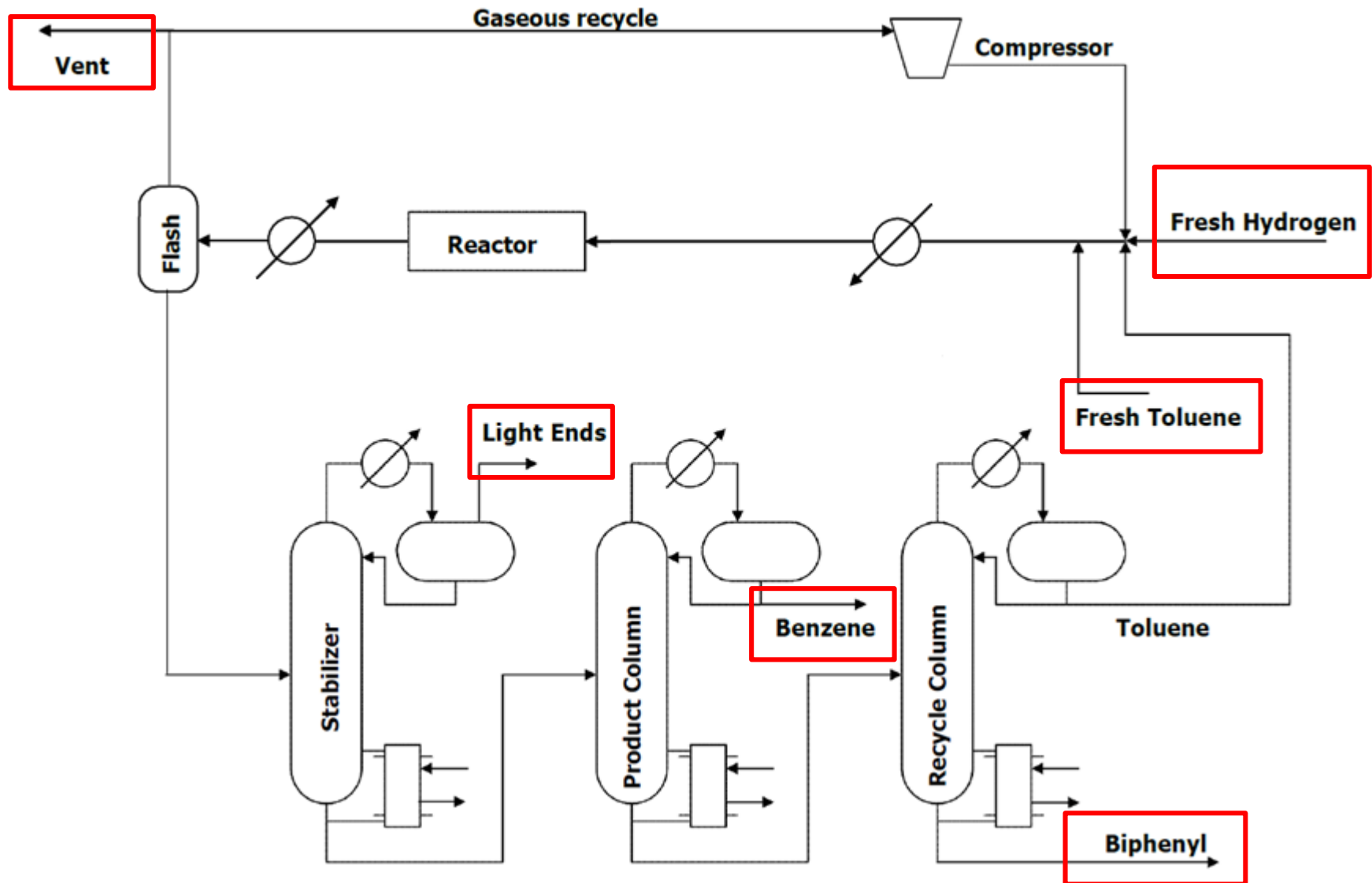
## BATCH PROCESS

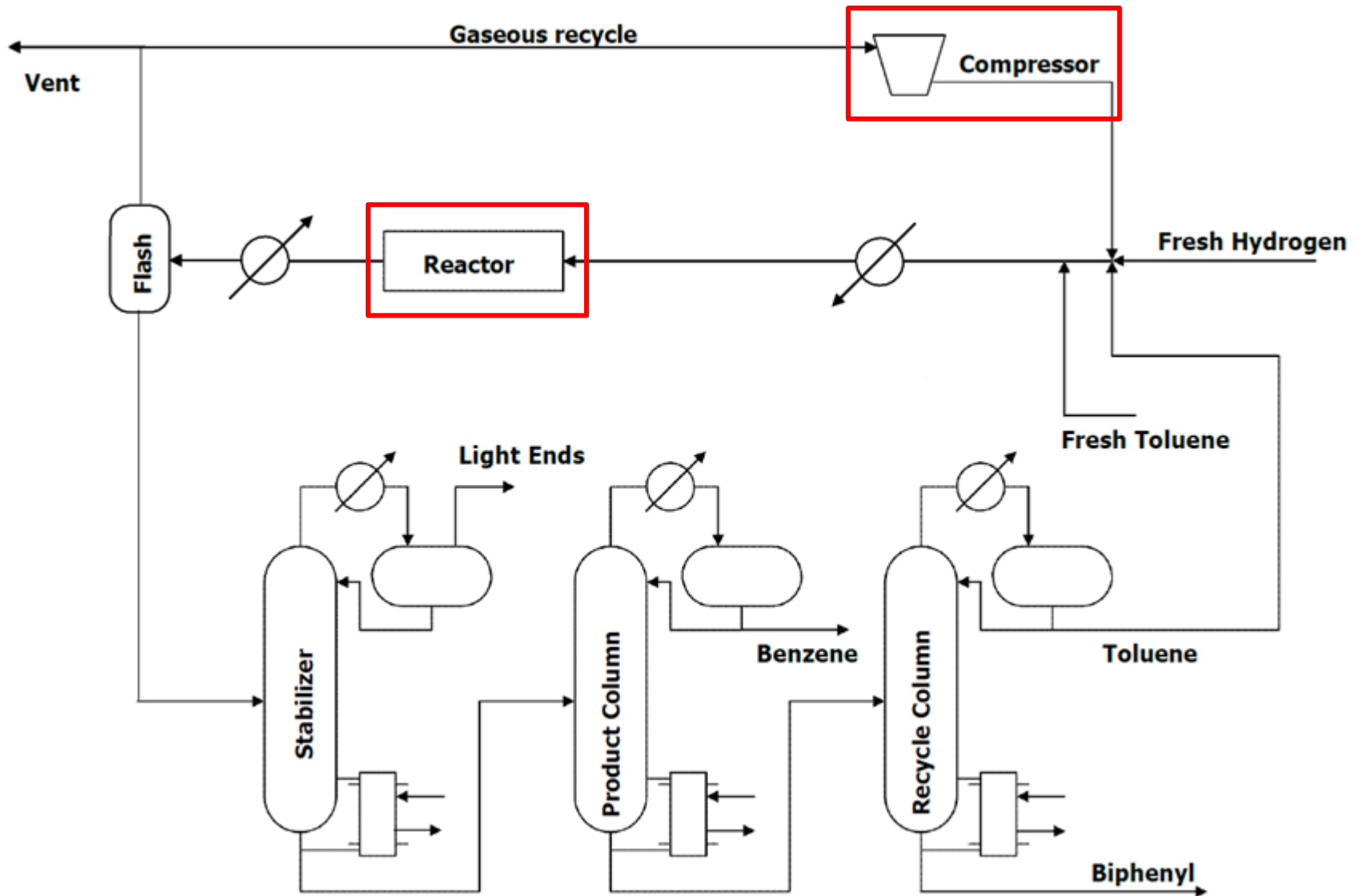


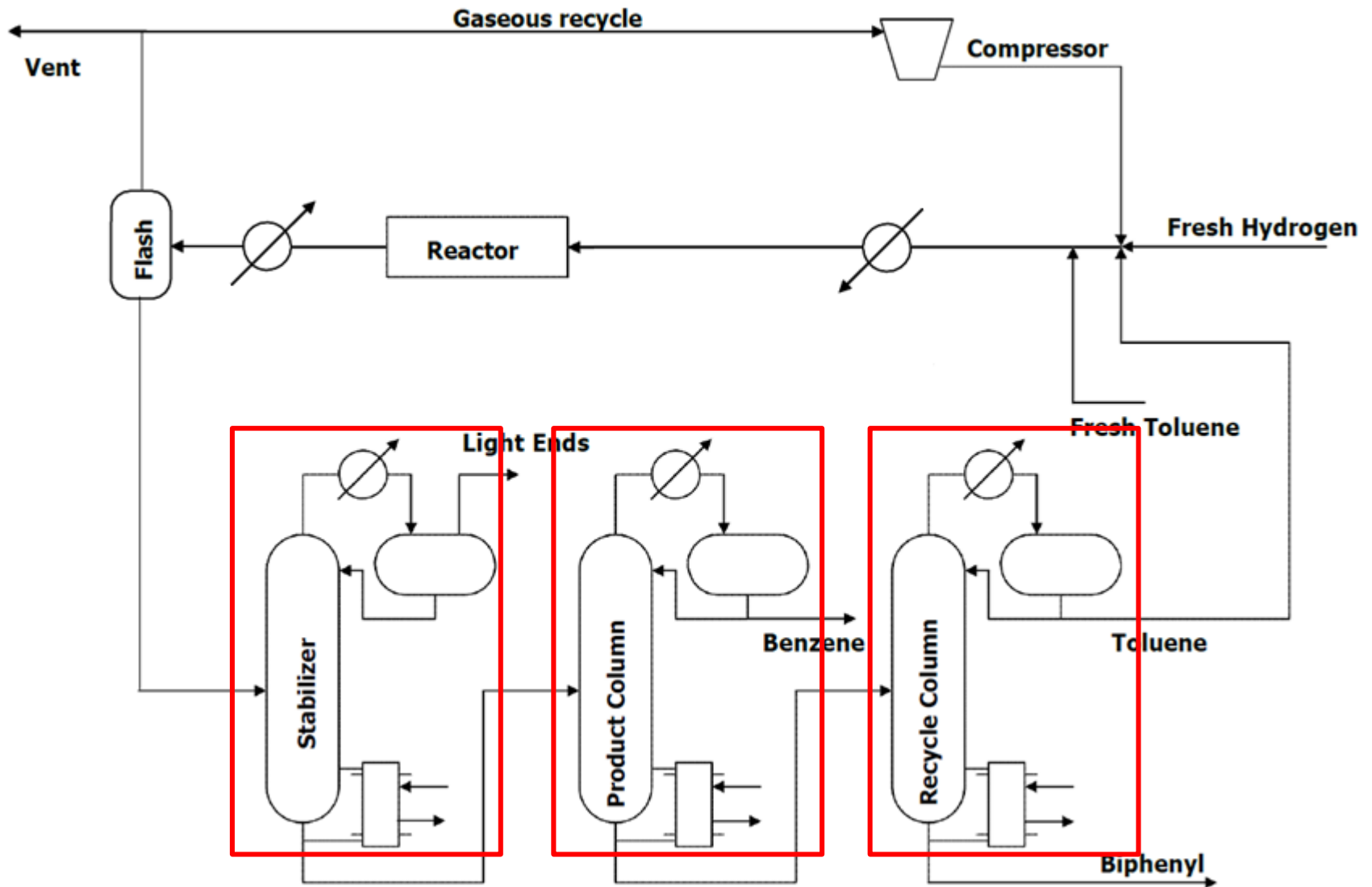
VS

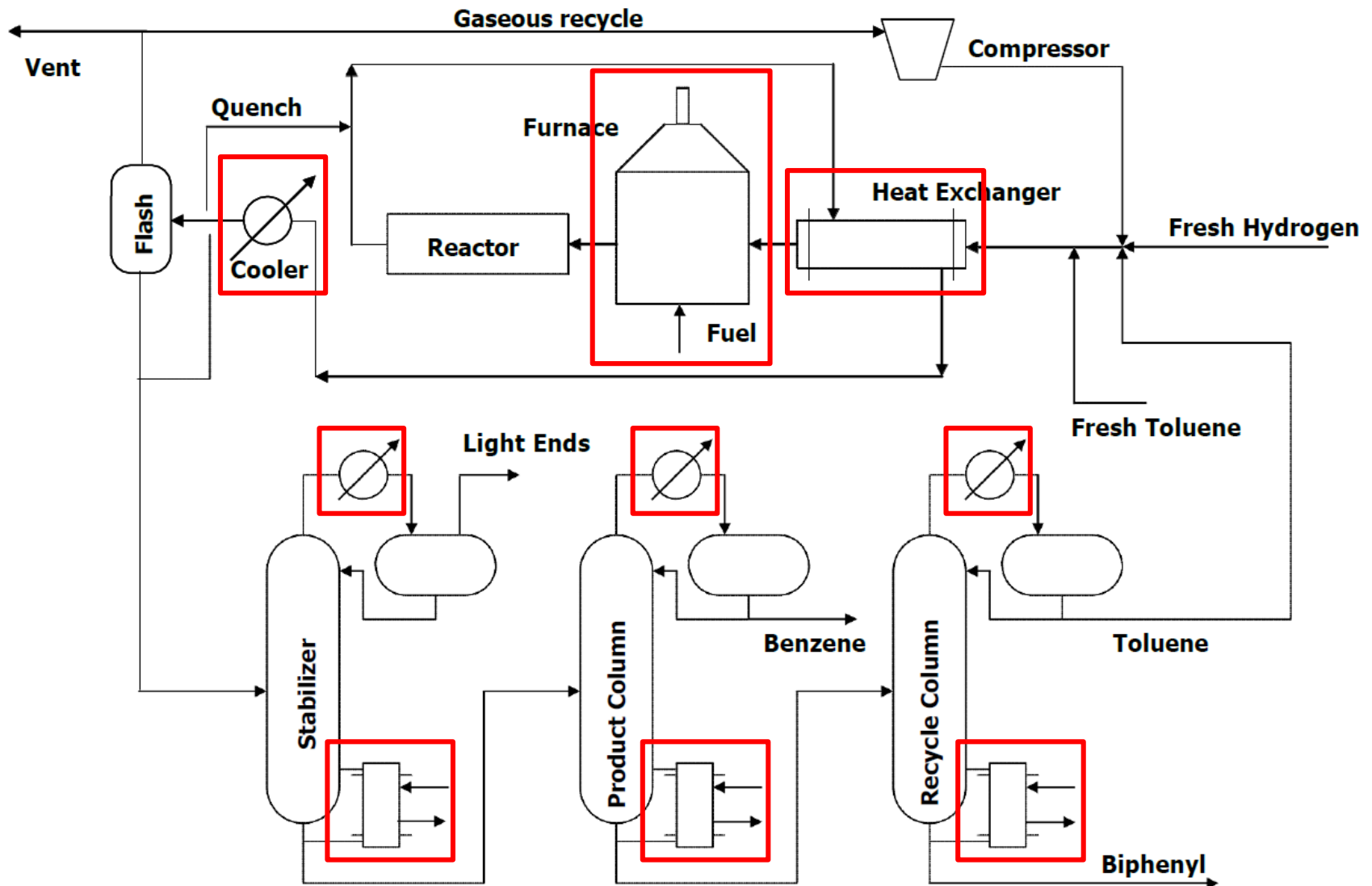
## CONTINUOUS PROCESS













The economic potential of the fourth level is defined as:

$$EP_4 = EP_3 - \text{€}_{\text{separation section}}$$

with  $EP_4$  in [M€/y].

If the potential of the fourth level is greater than zero, the process may be economically attractive; vice versa, the process is definitely not economically interesting.

Equipment costs are the sum of two contributions:

- the fixed costs of investment;
- operating costs.

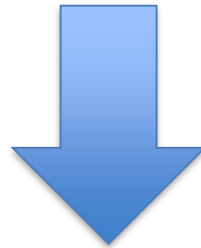
In the calculation of  $EP_4$ , the cost of columns and heat exchangers (*i.e.*, reboilers and condensers) is taken into account.

The cost of the flash is considered to be negligible, because it is much lower than that of a distillation column. Thus, it is not to be considered within the costs of the separation section.

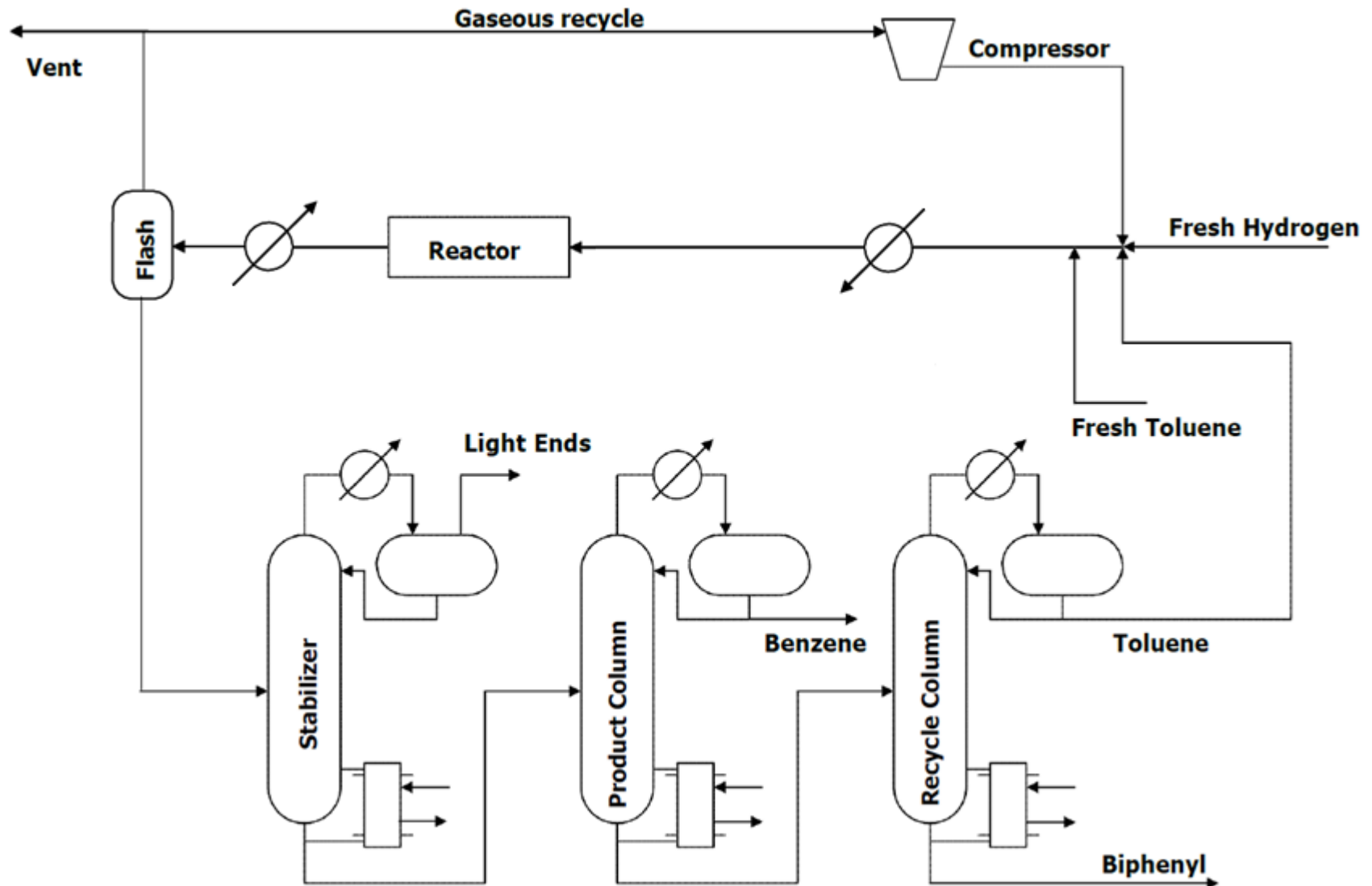
The cost of the furnace and other important process-to-process heat exchanges is taken into account at the  $EP_5$  level.



- To calculate investment and operating costs of a column it is necessary to know the diameter and the number of trays required for the separation.
- In this phase, the hypothesis of ideal separation of the components is removed (as it was introduced in the calculation of the  $EP_2$ ). It is therefore necessary to introduce the tray efficiencies in the separator section.



To simplify this complex operation, we can simulate the system by means of a process simulator (HYSYS or UniSim).



To set up a simulation with HYSYS, we must proceed according to the following steps:

- Select all the components involved in the simulation;
- Select the most appropriate Equation of State (EoS);
- Provide information on the chemical reactions involved in the simulation.

In the window "***Simulation Basis Manager***", the list of components can be entered by selecting the tab "***Components***". Add new components to the simulation by pressing "***View...***".

The components can be searched within the HYSYS database by entering the name or the chemical formula, and are added with the button " ***← Add Pure***".

In the tab "***Fluid Pkgs***", it is possible to select the most appropriate Equation of State (EoS).

For the simulation of the HDA plant, we use the "***SRK***" EoS.

Sets of chemical reactions can be added in the tab "**Reactions**".

Using the button "**Add Rxn...**", we can enter a single reaction in the kinetic scheme: at this point you need to select the type of information to be provided (*Conversion*, *Equilibrium*, **Kinetic**, ...).

Accordingly, it is possible to describe the reactor in different ways:

- "*Conversion*": providing the conversion (as a percentage) of the reactions with respect to the main reactant, using a conversion reactor;
- "*Equilibrium*": providing information about the reaction equilibrium, using an equilibrium reactor;
- "**Kinetic**": providing the kinetic parameters of the reactions (pre-exponential term and activation energy) in the tab "**Parameters**". Within the simulation environment, using a CSTR or a **PFR**.

Once we open the new window, in the menu "**stoichiometry**", insert chemical species taking part in the reaction, accompanied by their stoichiometric coefficients (note that those of the reactants are negative!). Then make sure that the mass balance is satisfied.

Within the tab "**Basis**" select the main component and the phase in which the reaction takes place.

Once we've entered all the reactions, add the thermodynamic package by selecting the "**Add to FP**".

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After completing all the above steps, we can enter the simulation by pressing "**Enter Simulation Environment**".

Recycle

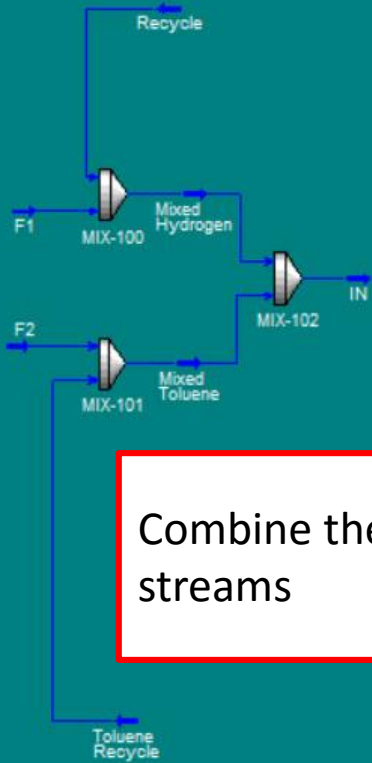
F1

F2

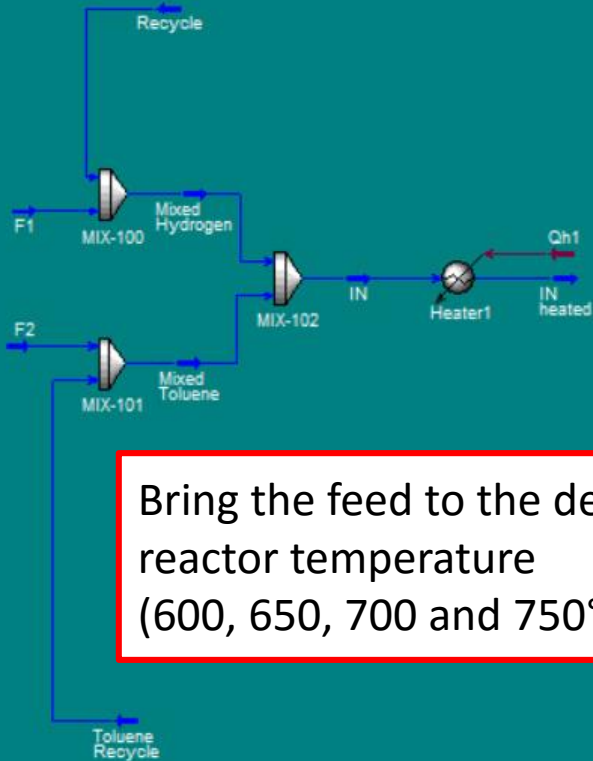
Define the streams according  
to MATLAB results  
(entering at 25°C, 34 bar)

Toluene  
Recycle

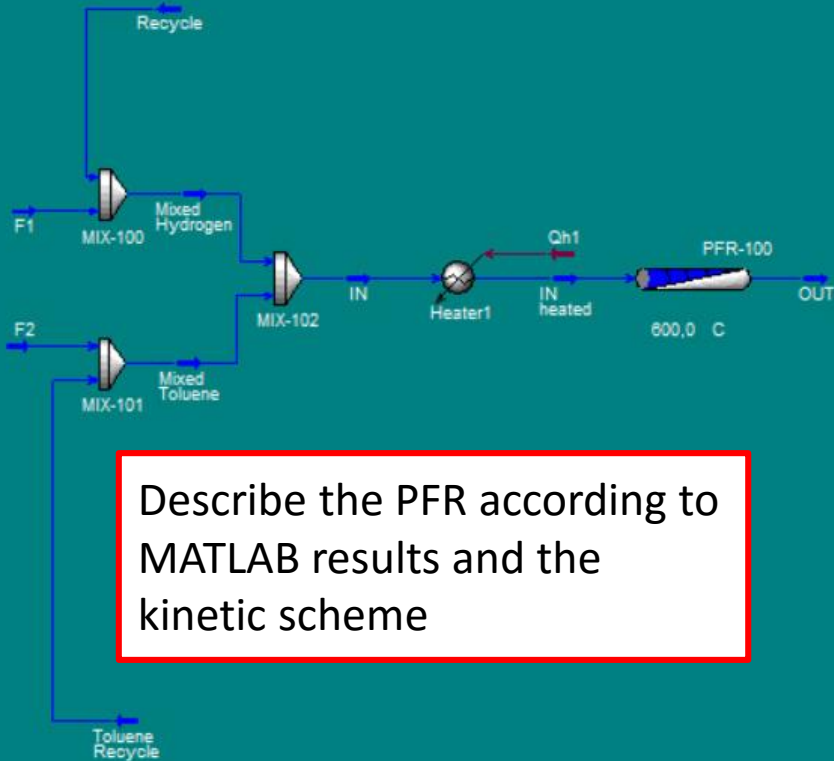




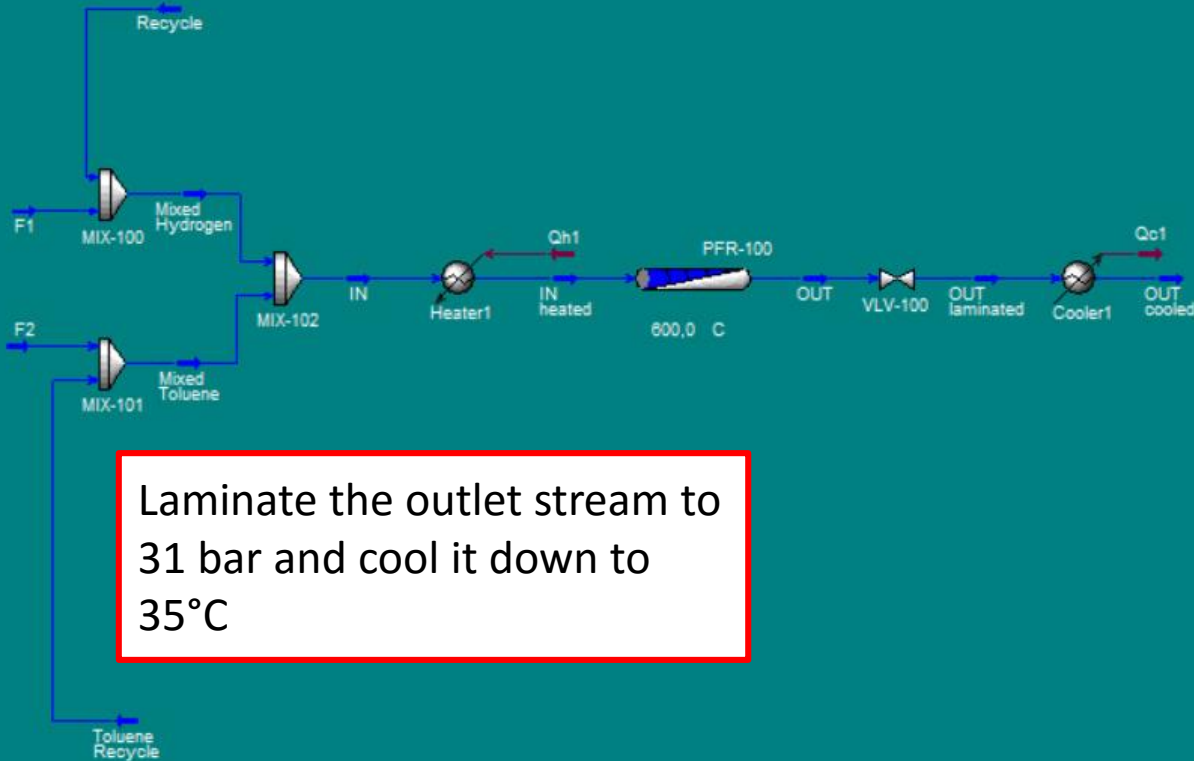
Combine the inlet and recycle streams



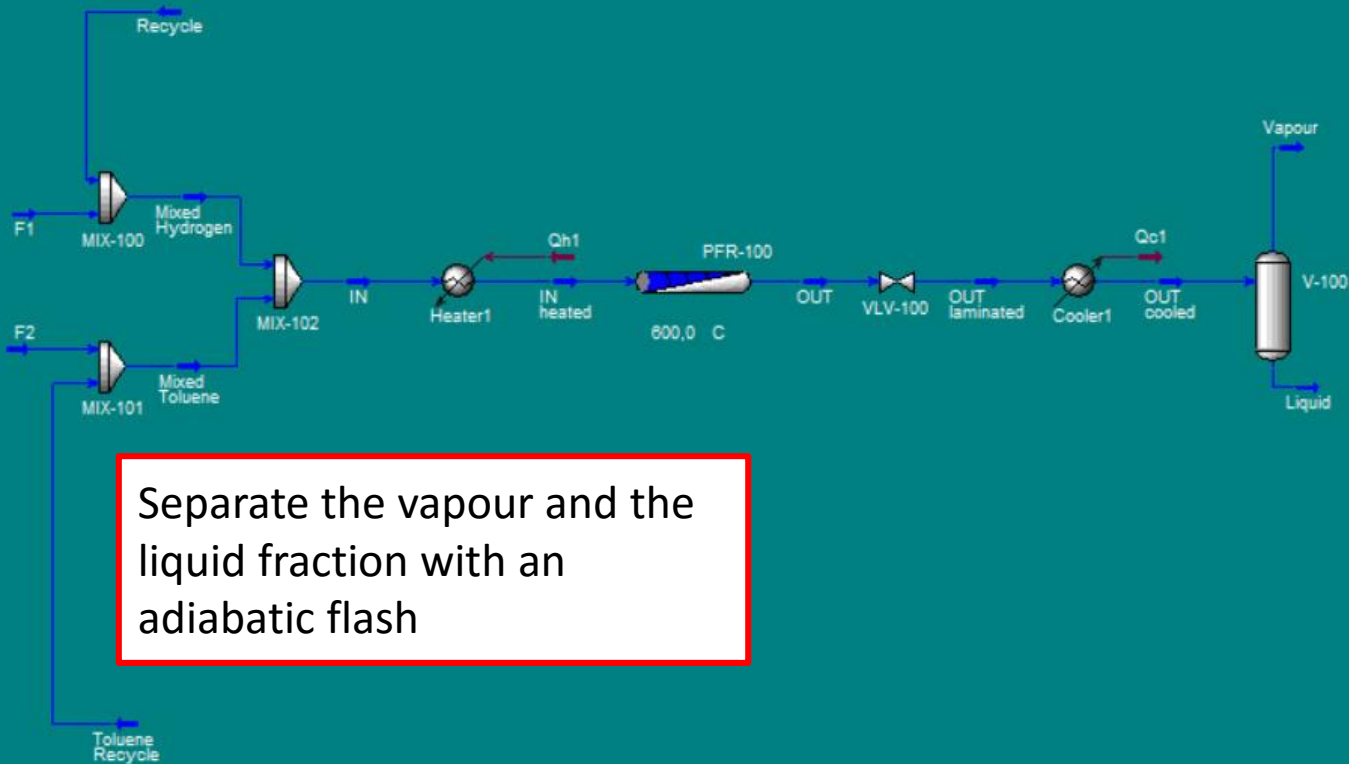
Bring the feed to the desired reactor temperature (600, 650, 700 and 750°C)



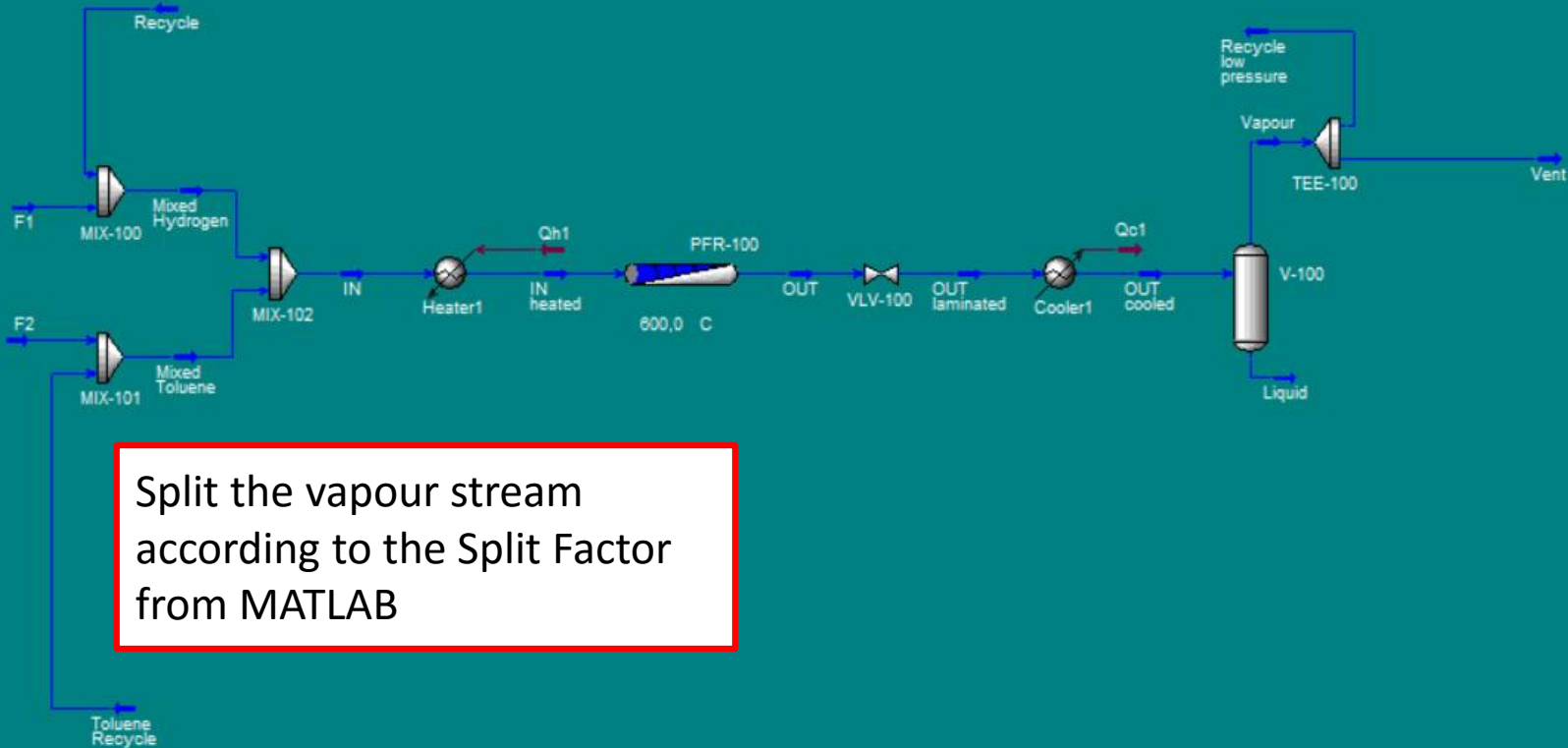
Describe the PFR according to MATLAB results and the kinetic scheme



Laminate the outlet stream to 31 bar and cool it down to 35°C



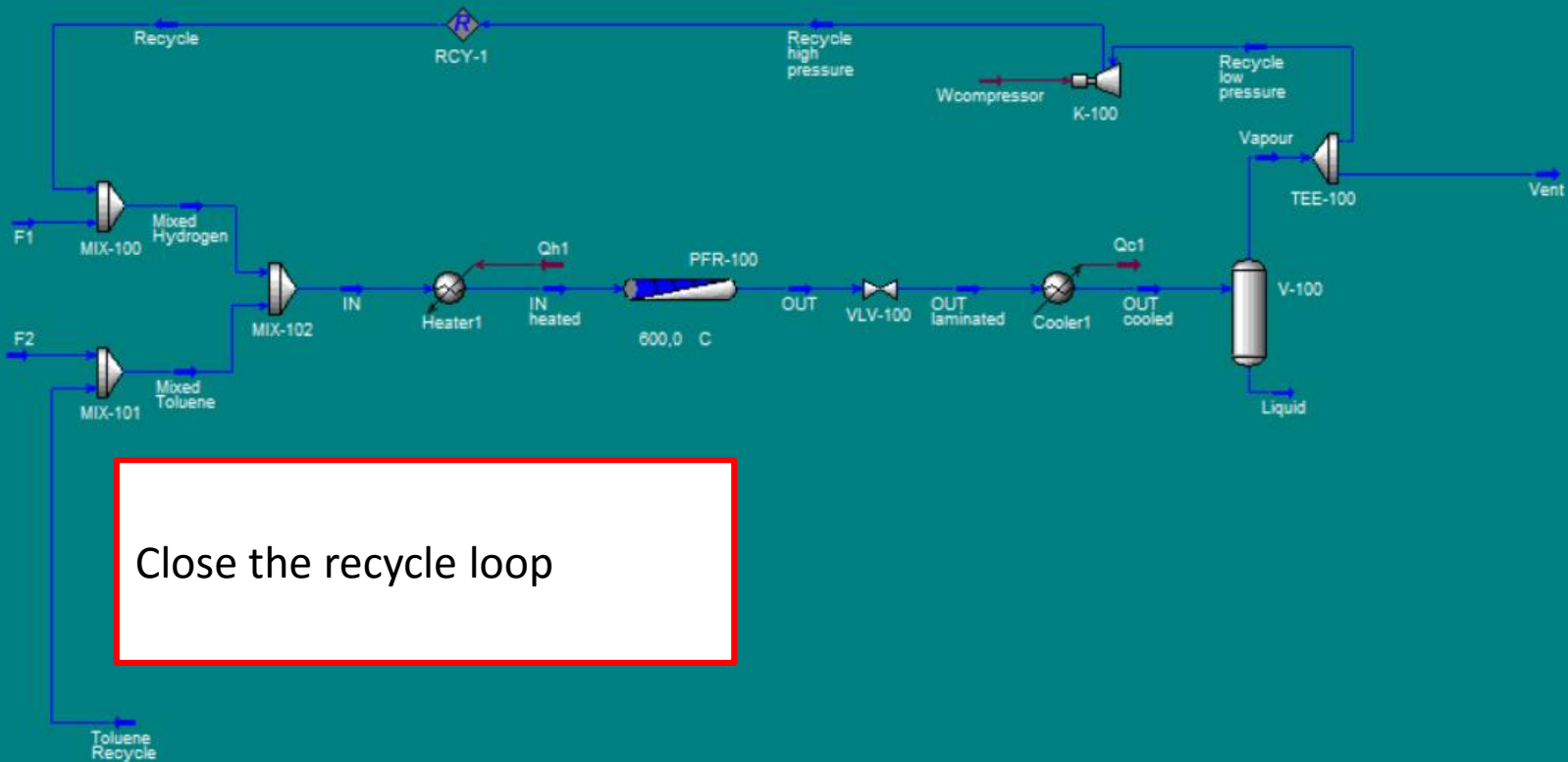
Separate the vapour and the liquid fraction with an adiabatic flash

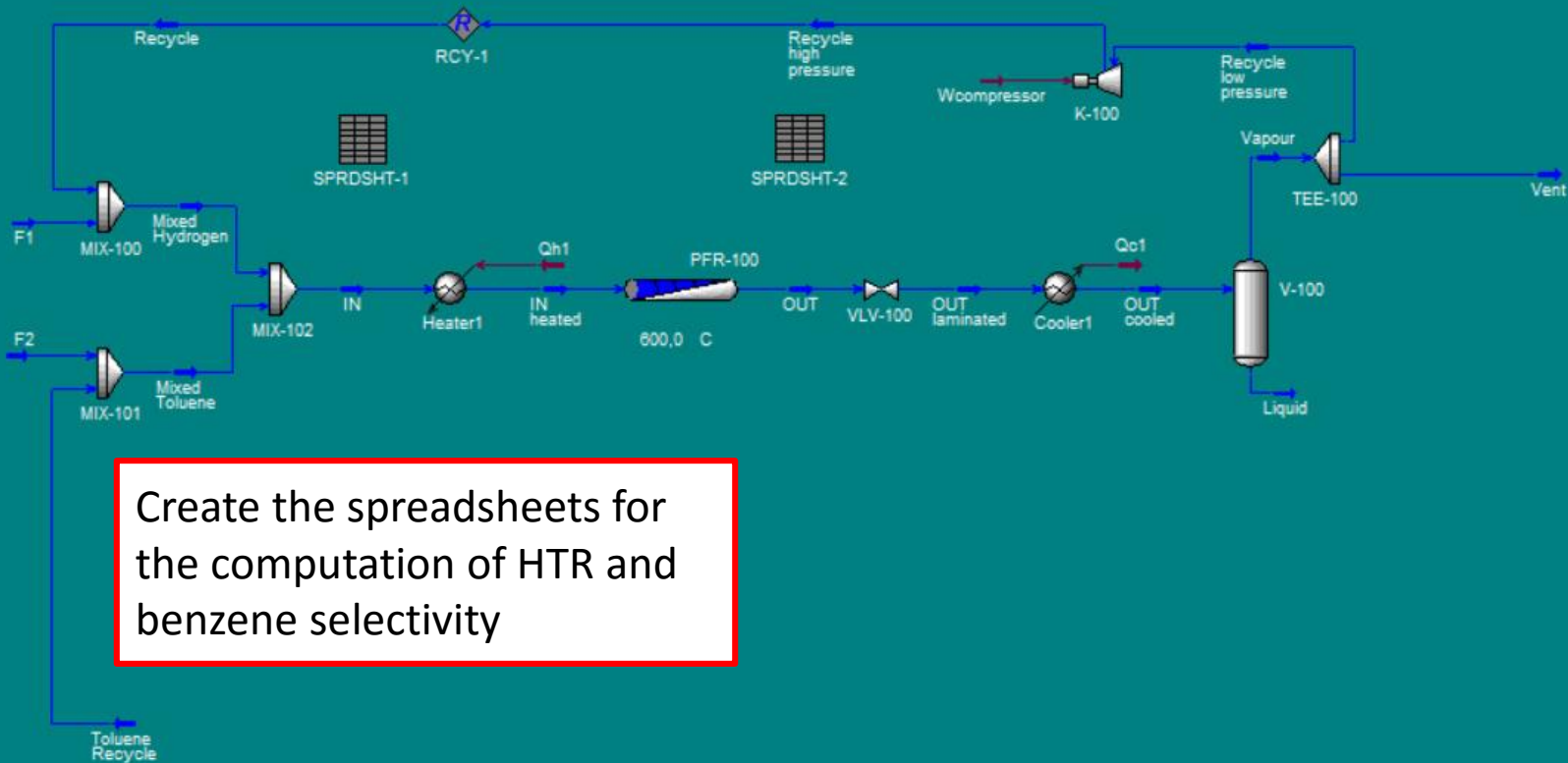


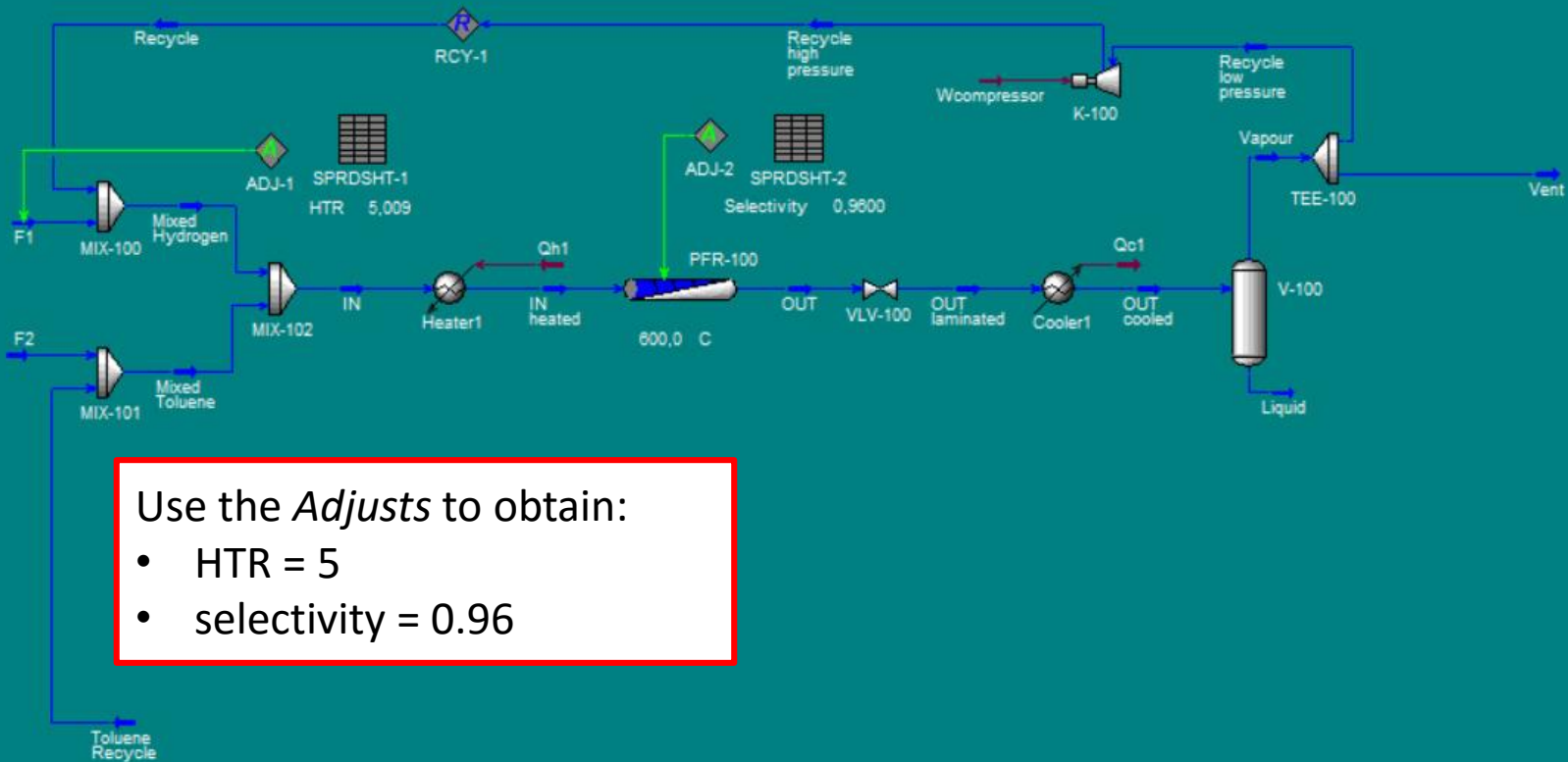
Split the vapour stream  
according to the Split Factor  
from MATLAB









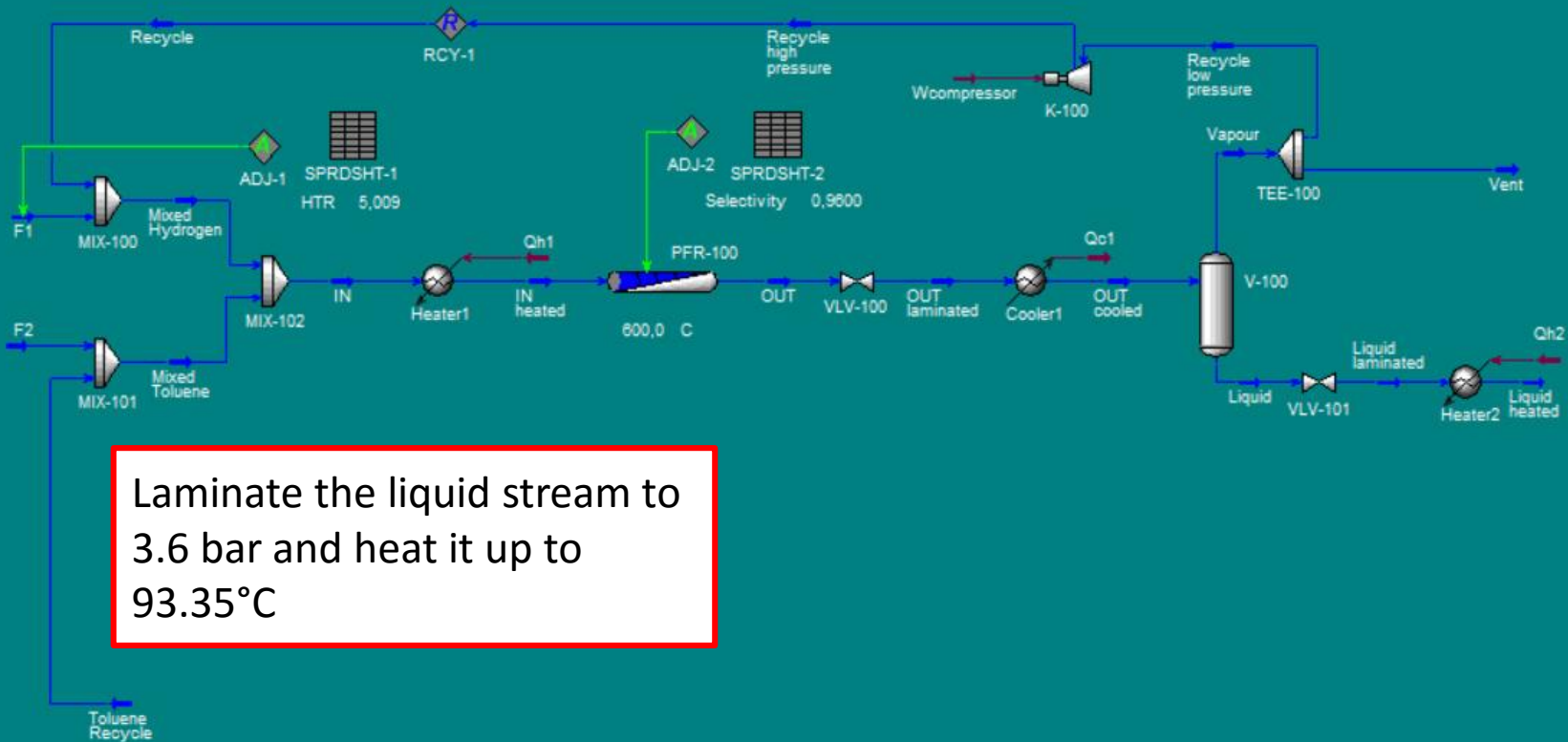


Use the *Adjusts* to obtain:

- HTR = 5
- selectivity = 0.96

**ADJ-1:**     *Target*     HTR  
                  *Adjusted*   F1 flow rate

**ADJ-2:**     *Target*     Benzene selectivity  
                  *Adjusted*   Reactor size



Laminate the liquid stream to 3.6 bar and heat it up to 93.35°C

Downstream of the flash, the liquid phase is sent to reach the specification on the purity of benzene (99.97% molar).

We have to design the separation section in order to separate the following streams:

- Benzene (main product)
- Light products (methane and hydrogen, to be burnt)
- Toluene (to be recycled to the reactor)
- Biphenyl (to be sold/burnt according to our decision made at level 2)

The desired separation can be performed with multiple sequences. However, there are guidelines to help you select the most appropriate one:

1. Remove the **corrosive** components first (in order to select **cheaper** material);
2. Remove **monomers** and **reactive** components (in order to avoid undesired **reactions** and **fouling**);
3. Remove components with **higher flow rates** (in order to use **smaller** equipment);
4. Remove **product and recycle** streams as **distillate** (in order to avoid thermal degradation of the product and to improve control of the purity specifications);
5. If **products and recycles** are obtained at the **bottom** of the column, it is better to collect them as vapour and then to condense them (in order to improve their purity specifications).

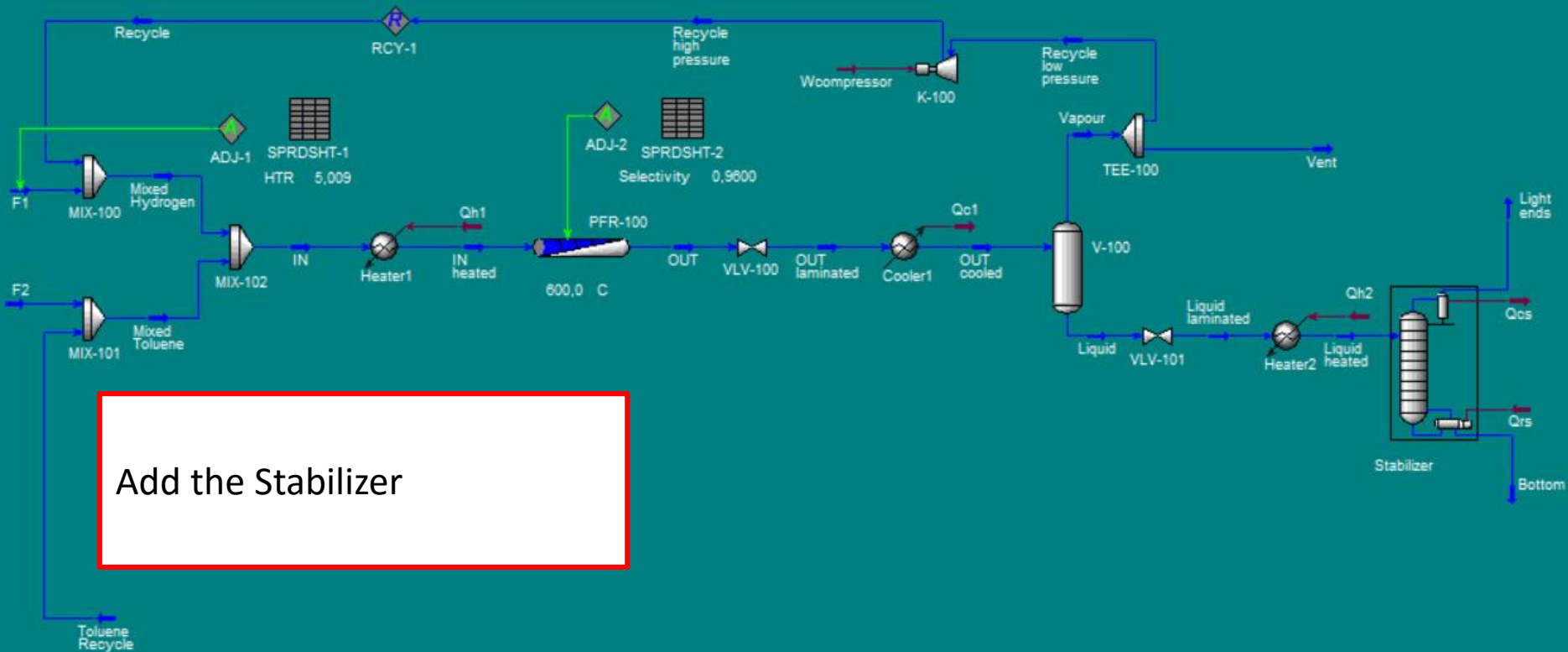
Following the guidelines, we can draw the following conclusions:

- Remove light-ends first, by using a column (Stabilizer), to avoid corrosion by hydrogen.
- To separate benzene, toluene and biphenyl, two different ways are possible:
  1. Separate first Benzene from Toluene+Biphenyl and then Biphenyl from Toluene;
  2. First separate Benzene+Toluene from Biphenyl and then Benzene from Toluene.

The first option is more convenient, since benzene is the most abundant compound.

Furthermore, using the first solution, the main product (benzene) and the recycle stream to the reactor (toluene) will be separated as distillates of the columns, facilitating their purity control.





Add the Stabilizer

The Stabilizer (full reflux) is made up of five real stages (**3 trays**): the feed tray is the **2<sup>nd</sup>** one. Both the top and bottom pressures are **3.573 bar**.

The refrigerant to be used is water: its inlet temperature is 30°C, whereas the maximum recommended outlet temperature is 38°C.

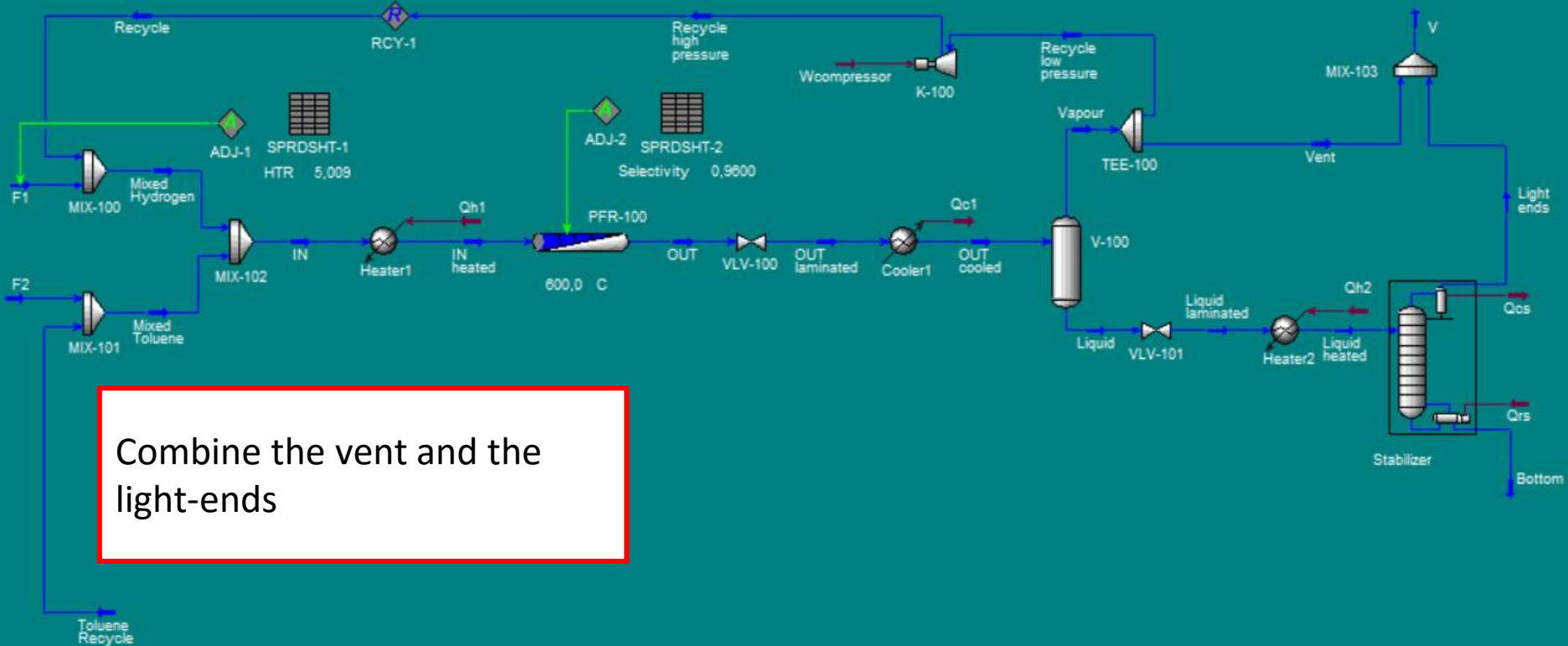
## Input data:

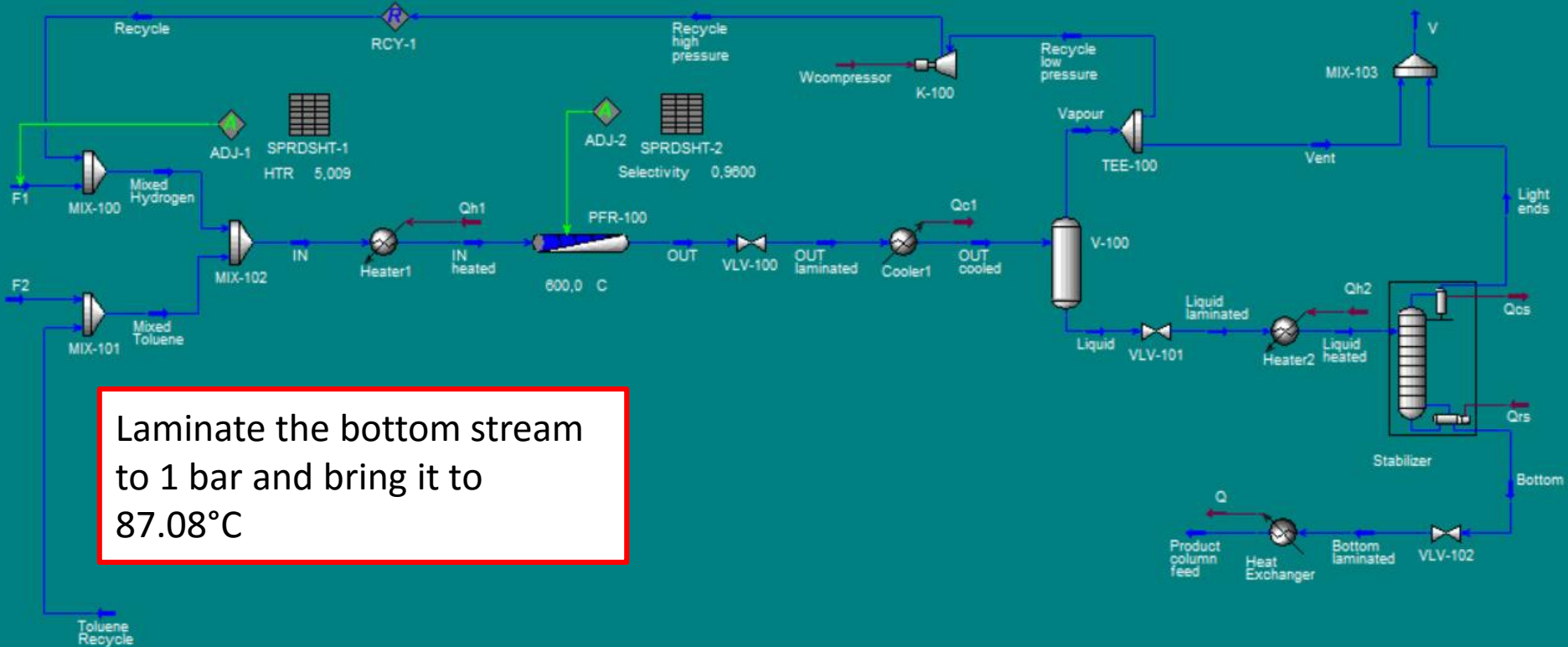
- Reflux Ratio =  $R/D = 0.619$ ;
- Temperature of the light-ends (to be calculated basing on a minimum required  $\Delta T_{\min} = 10^\circ\text{C}$ , with respect to the inlet water temperature).

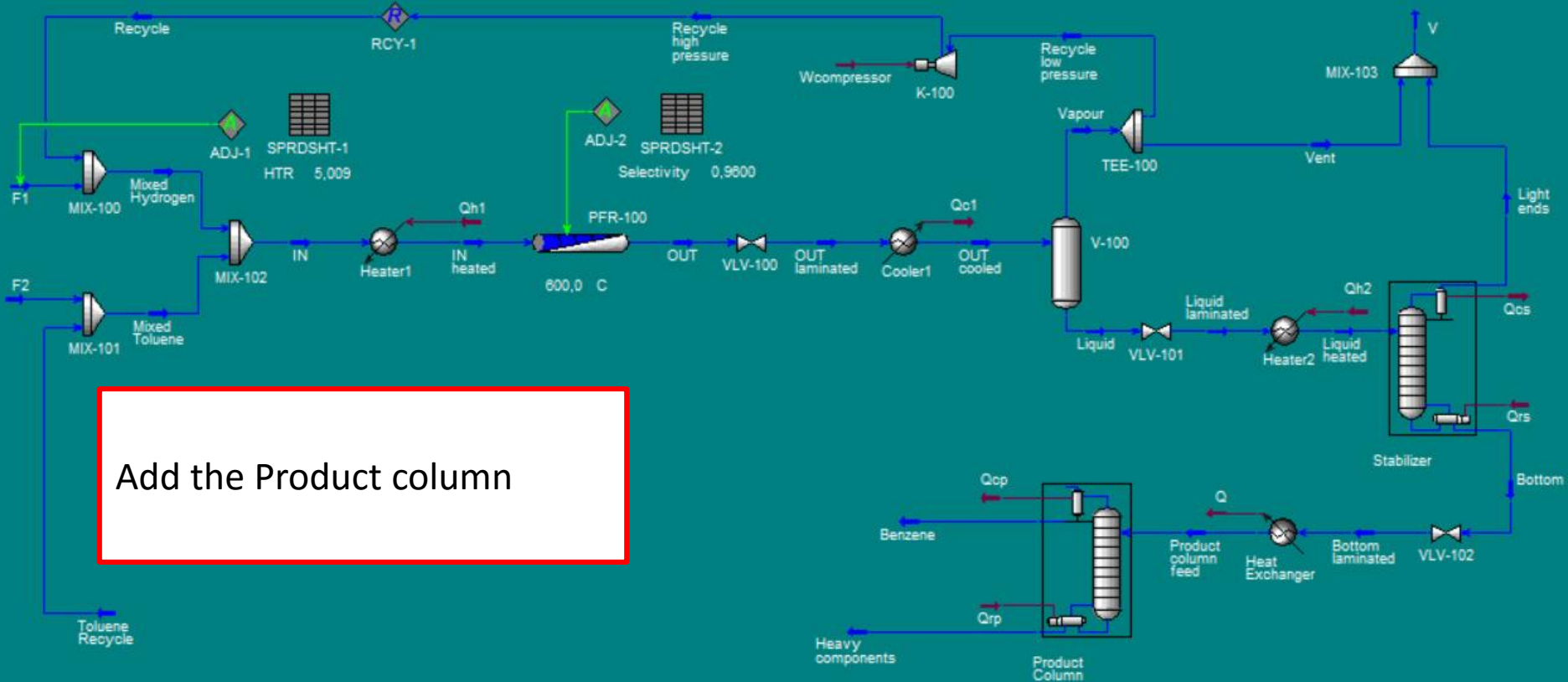
## Additional data: (at $T = 600^\circ\text{C}$ , just to check the results)

- Reboiler duty =  $2 \div 3 \cdot 10^6 \text{ kJ/h}$ ;
- $T_{\text{bottom}}$  estimated as  $130 \div 135^\circ\text{C}$ ;
- Light ends flowrate =  $15 \div 25 \text{ kmol/h}$ .

Trays are assumed to operate at 100% efficiency.







Add the Product column

For the design of the second column the **specifications** assigned are:

- purity of the recovered benzene of 99.97% molar;
- recovery of 99.5% with respect to benzene fed.

The column operates at  $P = 1$  bar and with a total condenser.

Since the column involves a multi-component distillation, it cannot be sized by the McCabe-Thiele method.

We can design it by the **Fenske-Underwood-Gilliland method**.

It is possible to assume a reflux ratio 1.3 times the minimum ratio.

- 1) Selection of light-key component and heavy-key component

**light-key (lk):** benzene

**heavy-key (hk):** toluene

$$\alpha_{Benzene} > \alpha_{Toluene} > \alpha_{Biphenyl}$$

(No distributed components between lk and hk components)

- 2)  $F$  and  $z_i$  come from HYSYS results. Methane traces (whose molar fraction is in the order of  $10^{-5}$ ) can be neglected.

- 3) From the specifications and the following material balances we calculate the composition and flowrates at the top and the bottom of the column:

$$\begin{cases} Fz_i \cong Dx_{i,D} & i < lk \\ Fz_i \cong Dx_{i,D} + Bx_{i,B} & i = lk, hk \\ Fz_i \cong Bx_{i,B} & i > hk \end{cases}$$



- 4) Calculation of relative volatilities at the top and the bottom of the column

$$\alpha_{i,hk} = \frac{P_0(T)_i}{P_0(T)_{hk}} \quad \text{relative volatility of component i respect to hk}$$

Coefficient for calculation of volatility:

$$\ln[P_0(T)] = C1 + \frac{C2}{T} + C3 \cdot \ln(T) + C4 \cdot T^{C5} \quad T \text{ [K]}, P \text{ [Pa]}$$

	C1	C2	C3	C4	C5
<b>Benzene</b>	83.918	-6517.7	-9.3453	7.12E-06	2
<b>Toluene</b>	80.877	-6902.4	-8.7761	5.80E-06	2
<b>Biphenyl</b>	76.811	-9878.5	-7.4384	2.04E-18	6

5)  $N_{\min}$  calculation by the *Fenske correlation*:

$$\left( \frac{Dx_{i,D}}{Bx_{i,B}} \right) / \left( \frac{Dx_{hk,D}}{Bx_{hk,B}} \right) = \bar{\alpha}_i^{N_{\min}} \xrightarrow{i=lk} N_{\min} = \frac{\ln \left( \frac{Dx_{i,D}}{Bx_{i,B}} \cdot \frac{Bx_{hk,B}}{Dx_{hk,D}} \right)}{\ln(\bar{\alpha}_{lk})}$$

6)  $R_{\min}$  calculation by the *Underwood equations*:

$$(I) \sum_{i=1}^{NC} \frac{\bar{\alpha}_i \cdot z_i}{\bar{\alpha}_i - \theta} = 1 - q \quad (II) \sum_{i=1}^{NC} \frac{\bar{\alpha}_i \cdot x_{i,D}}{\bar{\alpha}_i - \theta} = R_{\min} + 1$$

7)  $R$  calculation by the heuristic rule:  $R_{\text{opt}} = 1.3 R_{\min}$

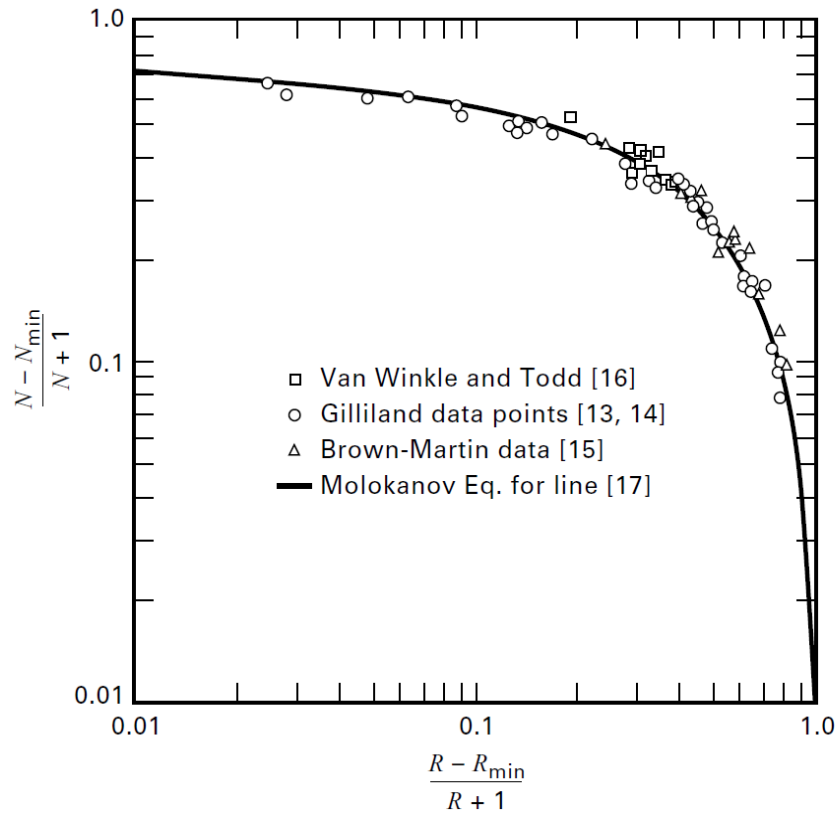
**PLEASE NOTE:**

$$\bar{\alpha} = \sqrt{\alpha_{\text{top}} \cdot \alpha_{\text{bottom}}}$$

$$q = \frac{h^V - h^F}{h^V - h^L}$$

( $h^{V/L/F}$  from HYSYS)

8) N calculation by *Gilliland diagrams* or by the following equations:



$$\phi(N) = \frac{N - N_{min}}{N + 1}$$

$$F(R) = \frac{R - R_{min}}{R + 1}$$

$$\phi = 0.75 - 0.75F^{0.5668} \quad \text{Eduljee}$$

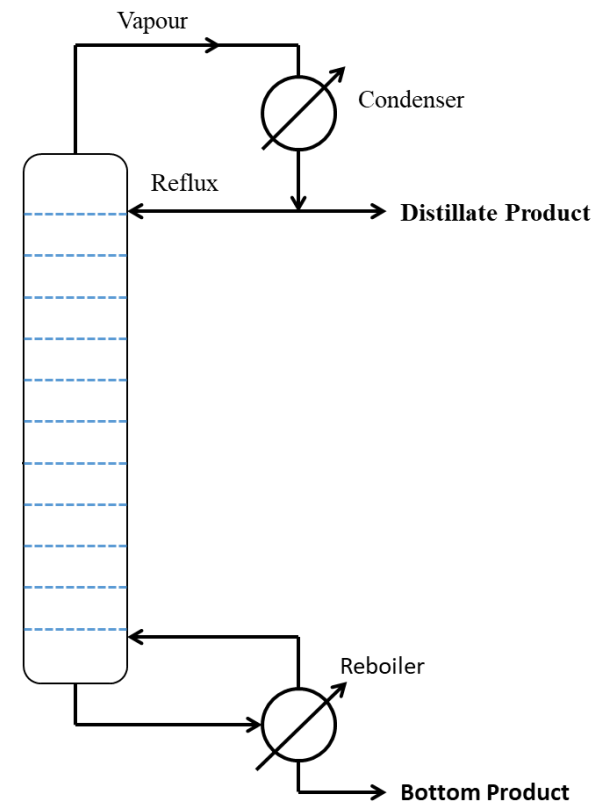
$$\phi = 1 - e^{\left( \frac{1+54.4F}{11+117.2F} \cdot \frac{F-1}{\sqrt{F}} \right)} \quad \text{Molokanov}$$

The FUG method is not able to provide us any information about the optimal feed tray: short-cut correlations can be used for this purpose.

Fenske correlation:

$$N_{min,INF} = \frac{\ln \left( \frac{z_{lk}}{z_{hk}} \cdot \frac{x_{hk,B}}{x_{lk,B}} \right)}{\ln(\alpha_{lk,INF})}$$

$$\frac{N_{INF}}{N_{min,INF}} = \frac{N}{N_{min}}$$



The efficiency is related to the mass transfer, which depends on the geometry and the design of the trays, on the flow rates, on the paths followed by the streams and on the compositions.

Different types of efficiencies can be defined:

- **Overall column efficiency:** a single value of efficiency to the entire column;
- Tray (or *Murphree*) efficiency: an efficiency defined differently for each tray;
- Local efficiency: an efficiency for each specific geometrical point of a tray.

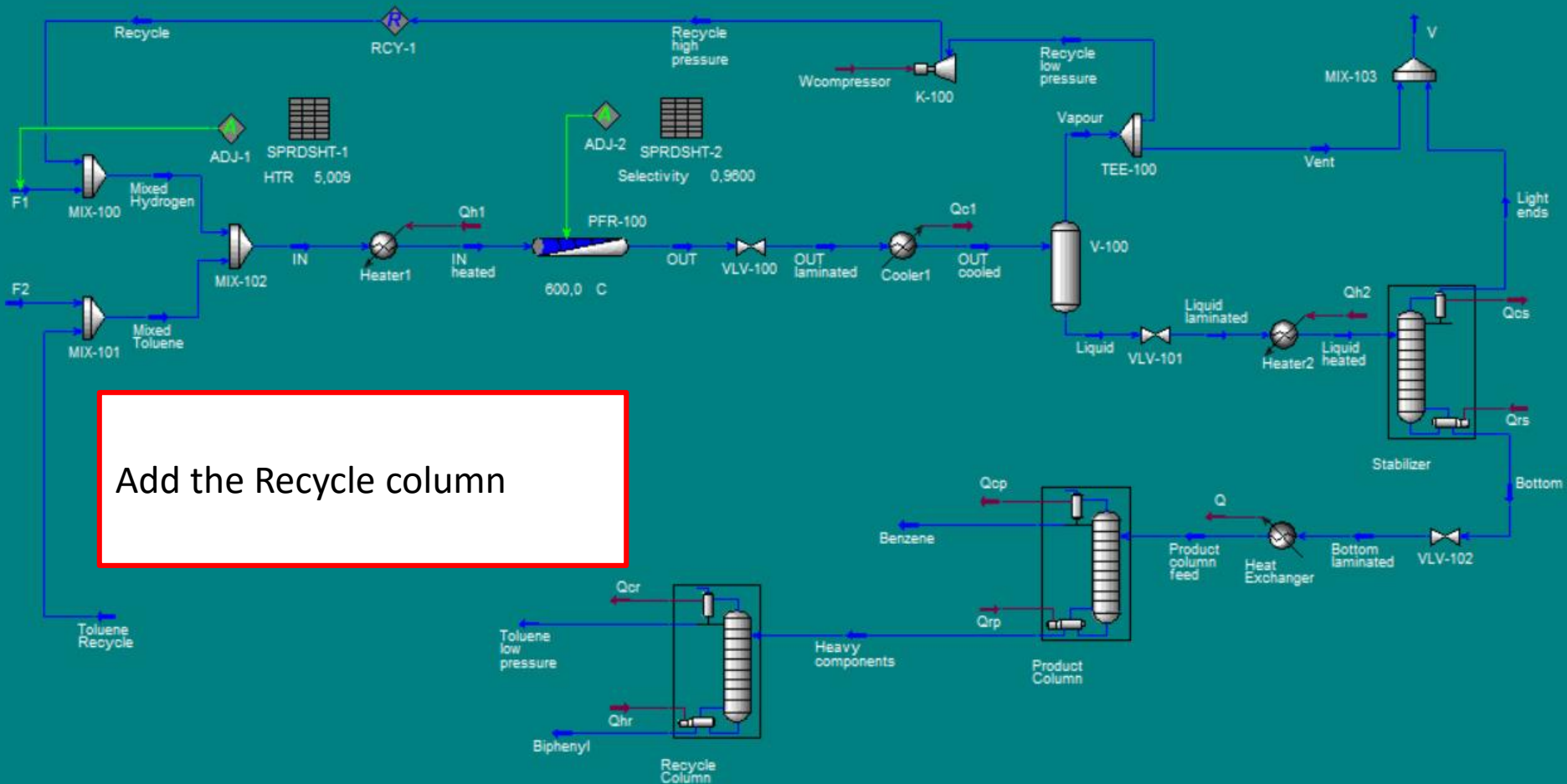
For the preliminary design of a column, we can use the overall efficiency:  $\eta = \frac{N_{ideal}}{N_{real}}$

For the calculation of the column efficiency, we use the **O'Connell correlation**:

$$\eta = \frac{0.5}{(\mu_F \cdot \alpha)^{0.25}}$$

Where  $\mu_F$  is the viscosity of liquid feed at bubble point (*measured in centipoise, cP*) and  $\alpha$  is the relative volatility of the two species to be separated.

The viscosity of the inlet stream is **0.3 cP**.



For the design of the third column the **specifications** assigned are:

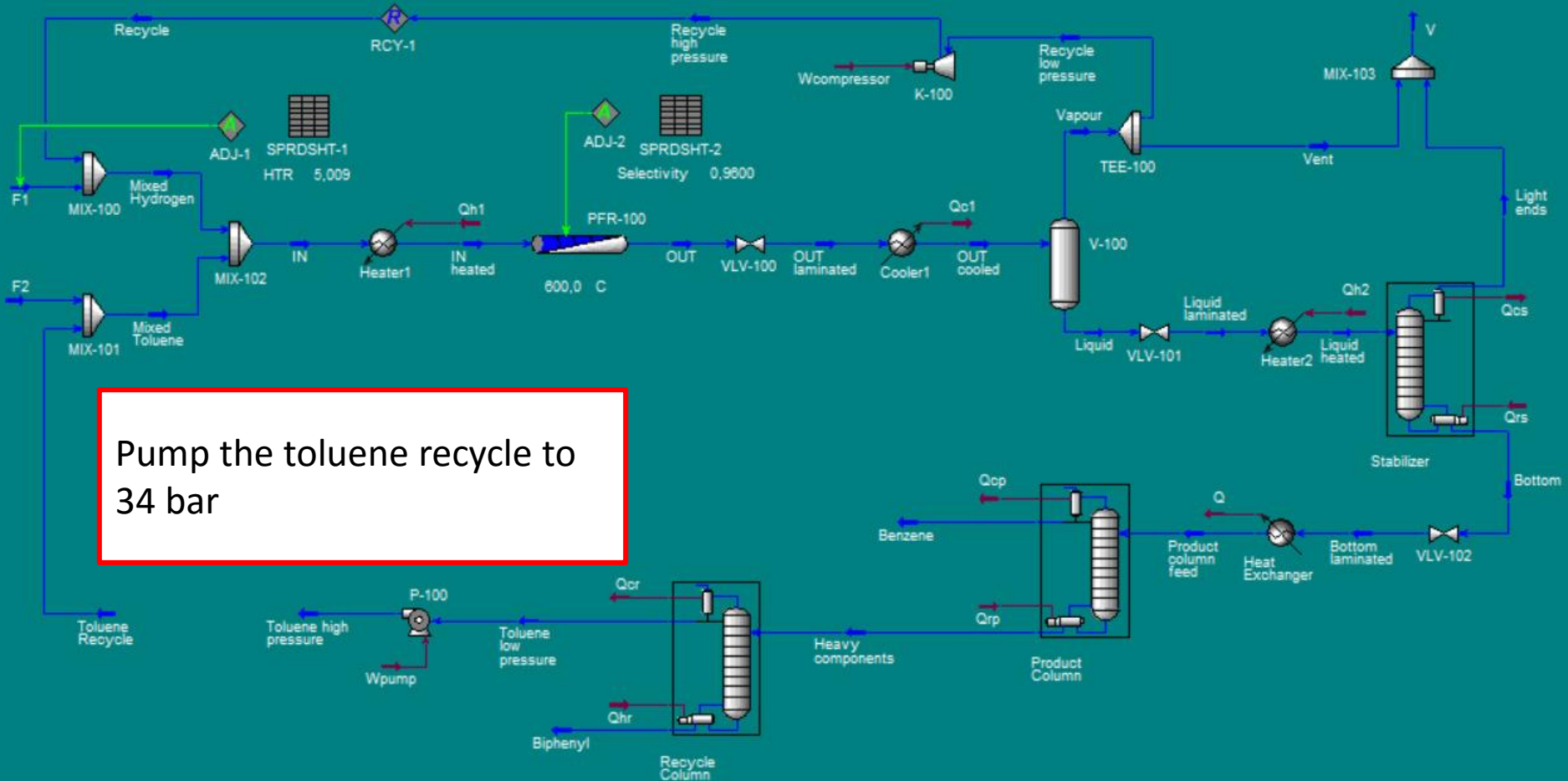
- Recovery of 99.5% with respect to toluene fed;
- Recovery of 99.5% with respect to biphenyl fed.

The column operates at  $P = 1$  bar and with a total condenser.

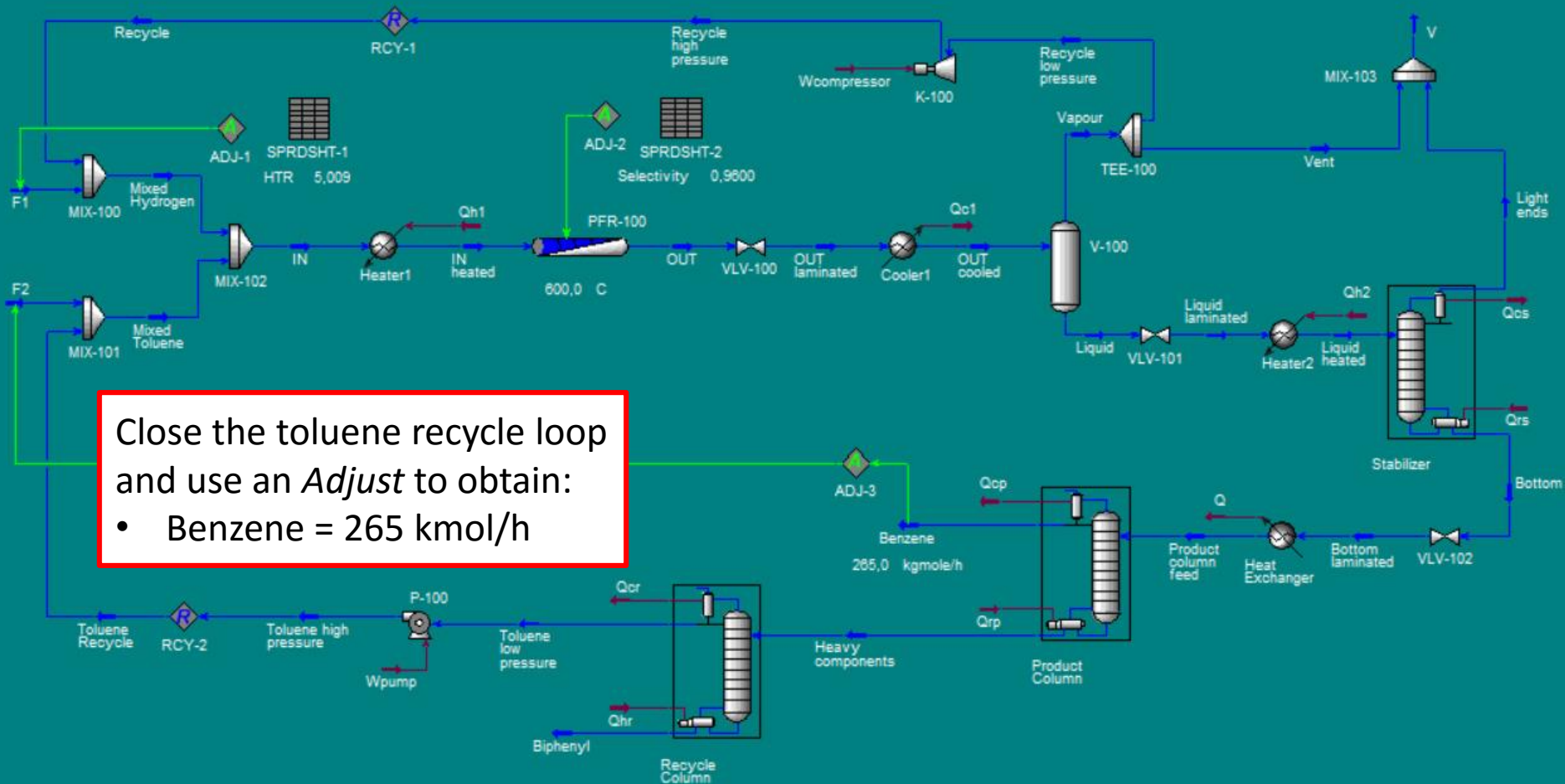
Preliminarily, use a **short-cut distillation column** in the process simulator to estimate the number of ideal trays and the optimal feed tray, assuming  $R_{\text{eff}} = 1.3 R_{\text{min}}$ .

Then, using the results of the short-cut design tool, **simulate** the distillation by means of a **standard distillation column**, using the "*Modified HYSIM Inside-Out*" solver.

Assume an overall O'Connell efficiency equal to 0.24.







**ADJ-3:**     **Target**     Benzene productivity  
                  **Adjusted**     F2 flow rate

In order to determine the size of the trays of each column, use the "**Tray Sizing**" utility of the process simulator.

Define a tray section which covers the entire column and perform the tray sizing evaluation:

- Three different **tray** spacings (12", 18" and 24") must be evaluated.

*LAB6: we will select the one which leads to the smallest column CAPEX.*

- If the diameter obtained is smaller than 2 ft, the column should be **packed**.

*LAB6: we will estimate its cost considering an equivalent tray column, whose tray spacing (12", 18" or 24") is the closest to the HETP (Height Equivalent of a Theoretical Plate).*