LAB5: Simulation with HYSYS®/UniSim®

Modeling the HDA plant with the Process Simulator

Process Systems Engineering A – Prof. Davide Manca

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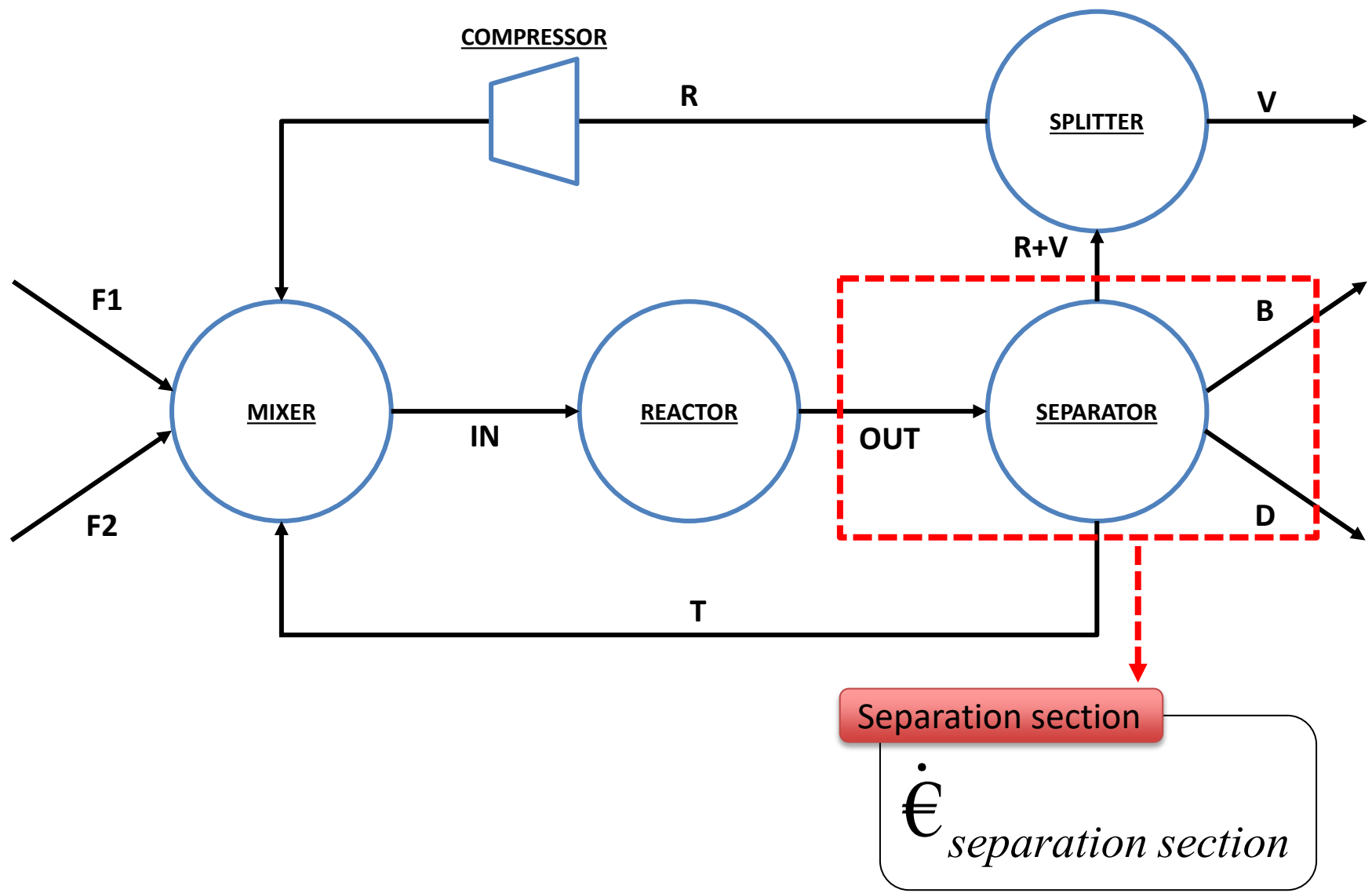
The economic potential of level-4 (EP_4) is defined as:

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

with EP_4 in [M€/y].

If the EP_4 is greater than zero, the process may be economically attractive; vice versa, the process is not economically interesting.

COMPRESSOR

SPLITTER

R

V

R+V

F1

MIXER

IN

REACTOR

OUT

SEPARATOR

B

F2

D

T

Separation section

$$\dot{\text{€}}_{separation\ section}$$

The equipment costs must account for:

- Capital expenditure (CapEx);

- Operative expenditure (OpEx).

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

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 considered at the EP_5 level.

- To calculate the 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 introduced in the calculation of the EP_2). It is, therefore, necessary to consider the tray efficiencies in the separation section.
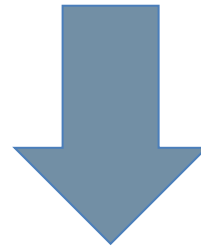
To simplify this complex operation, we can simulate the system through a process simulator (HYSYS or UniSim).
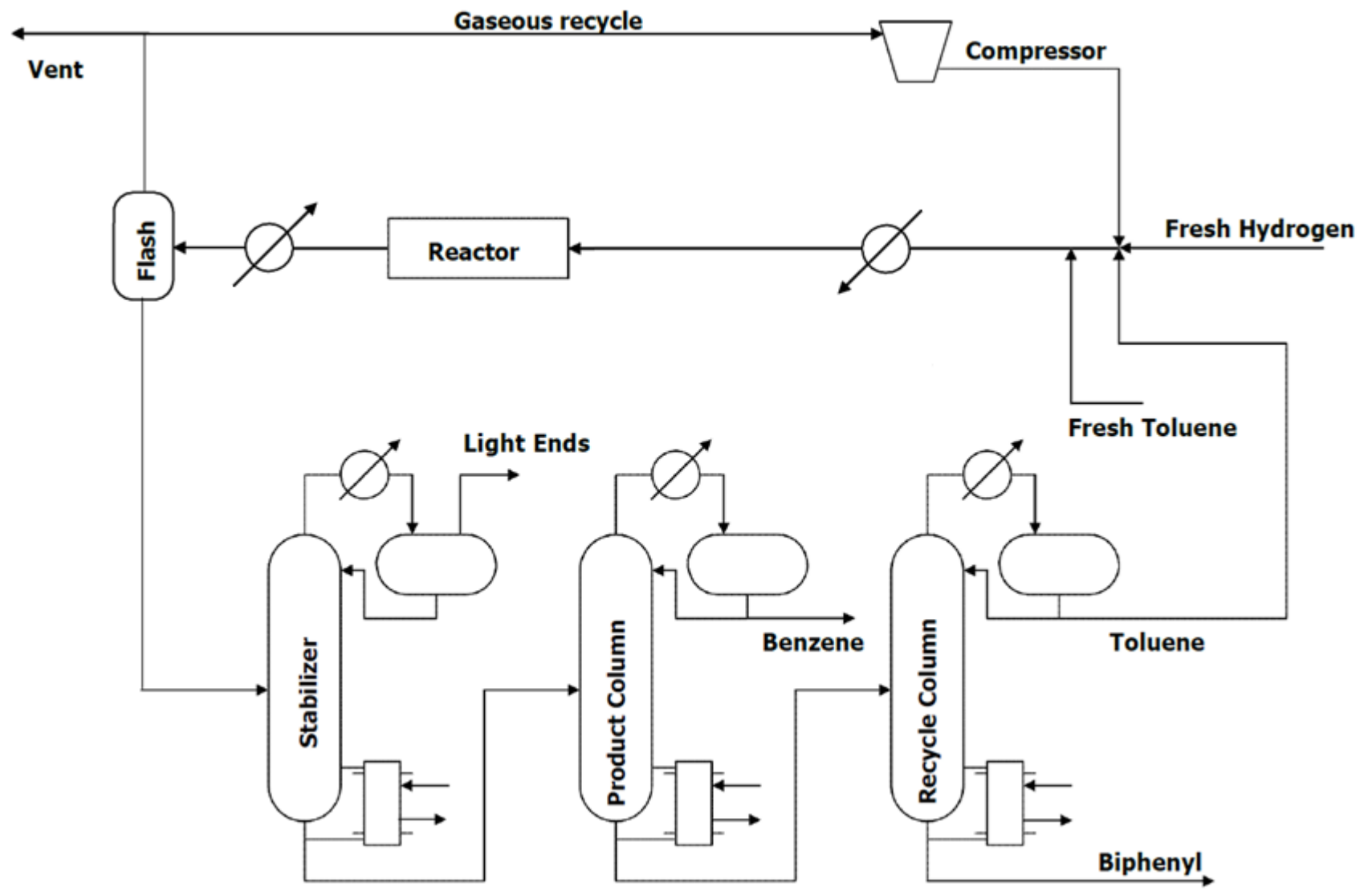
To set up a simulation with HYSYS/UniSim, we must proceed according to the following steps:

- 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 chemical species to the simulation by pressing "***View...***".

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

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 reaction's phase.

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

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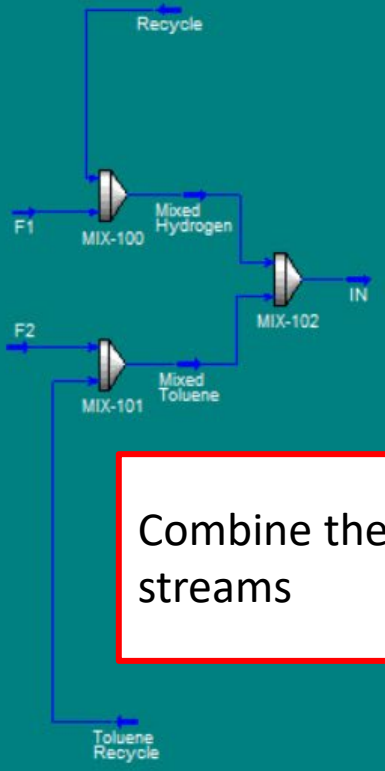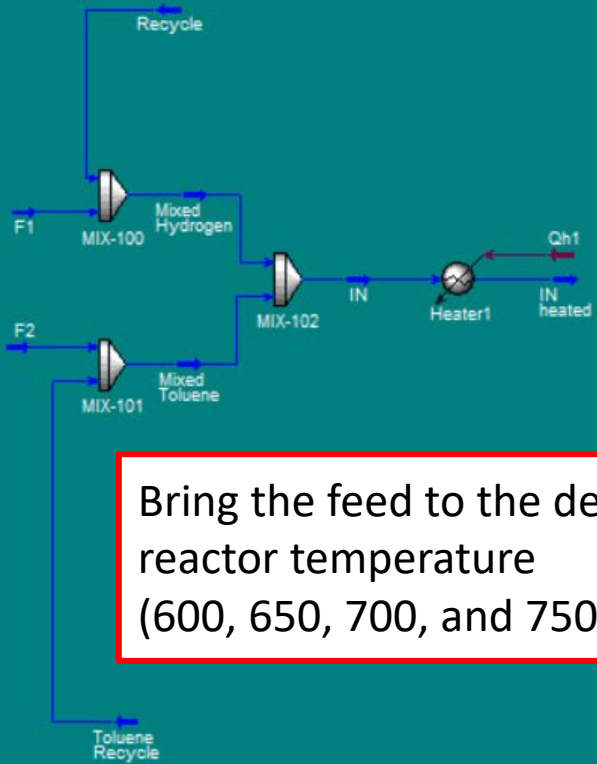
Recycle

F1

F2

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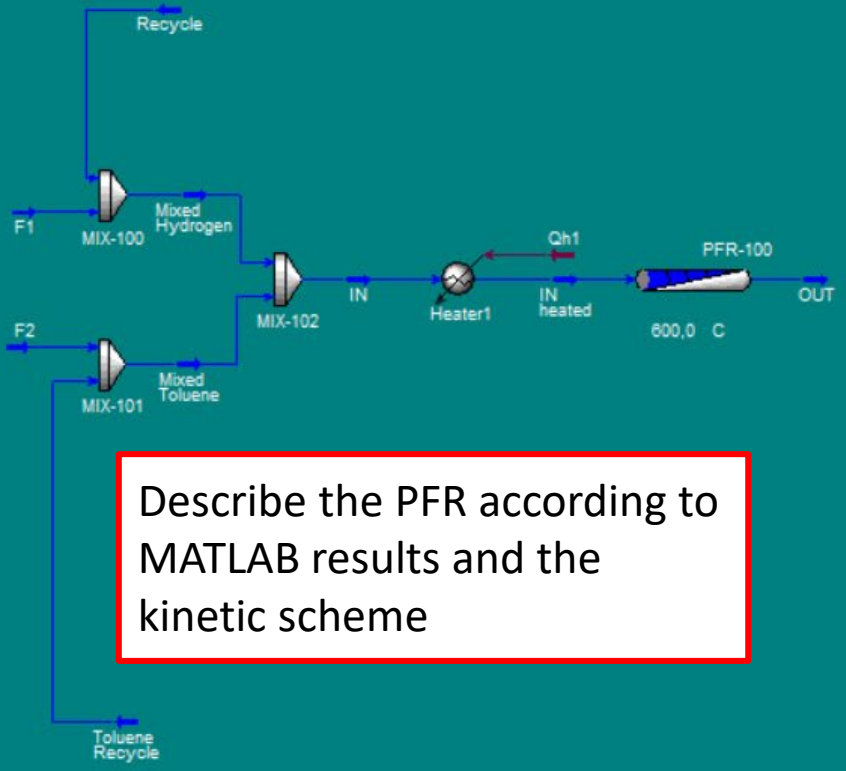to MATLAB results
(entering at 25°C, 34 bar)
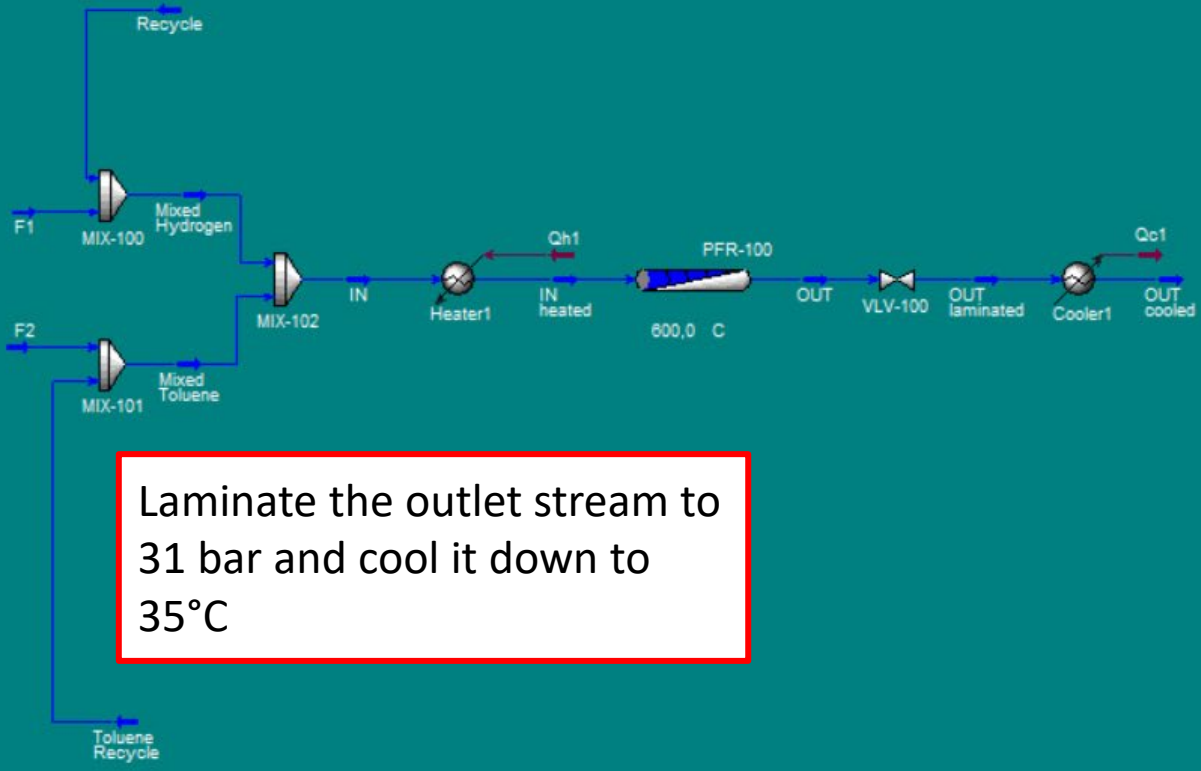
Toluene
Recycle

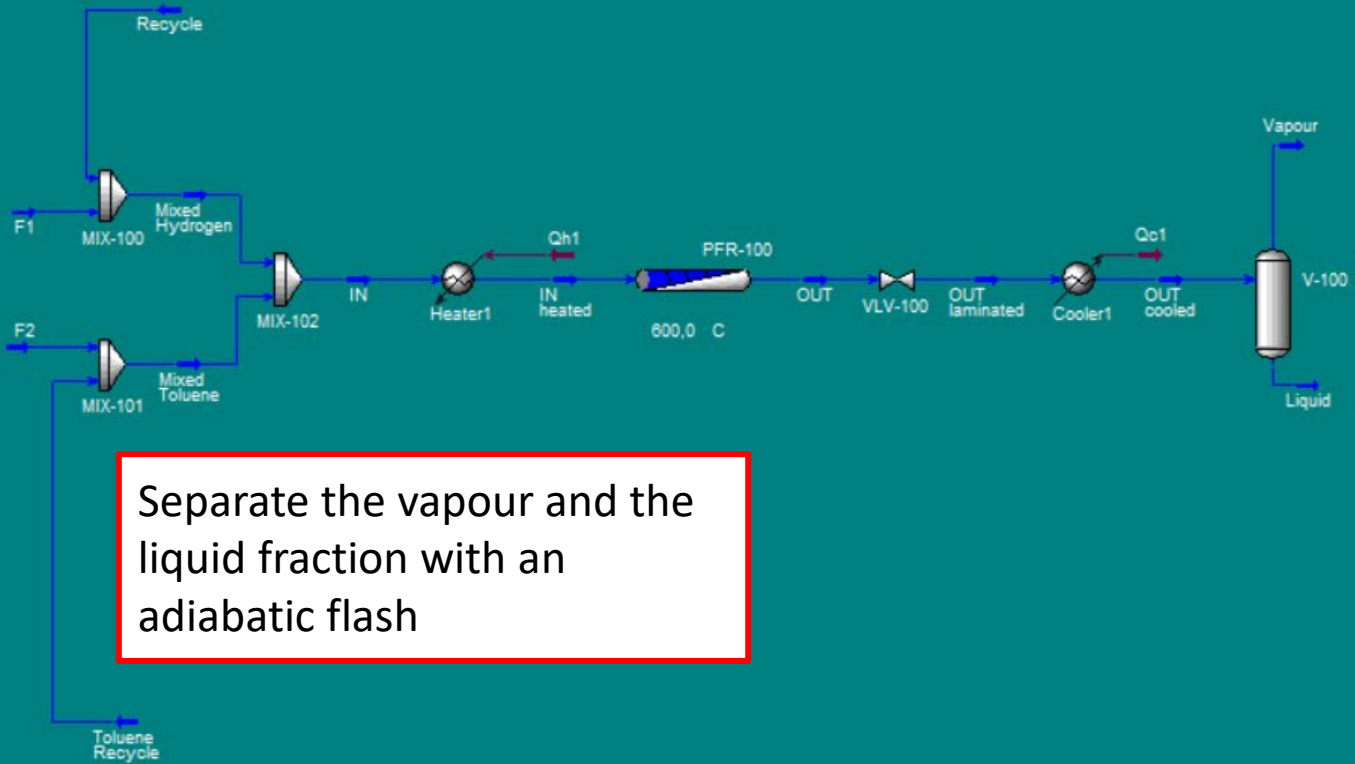Combine the inlet and recycle streams

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

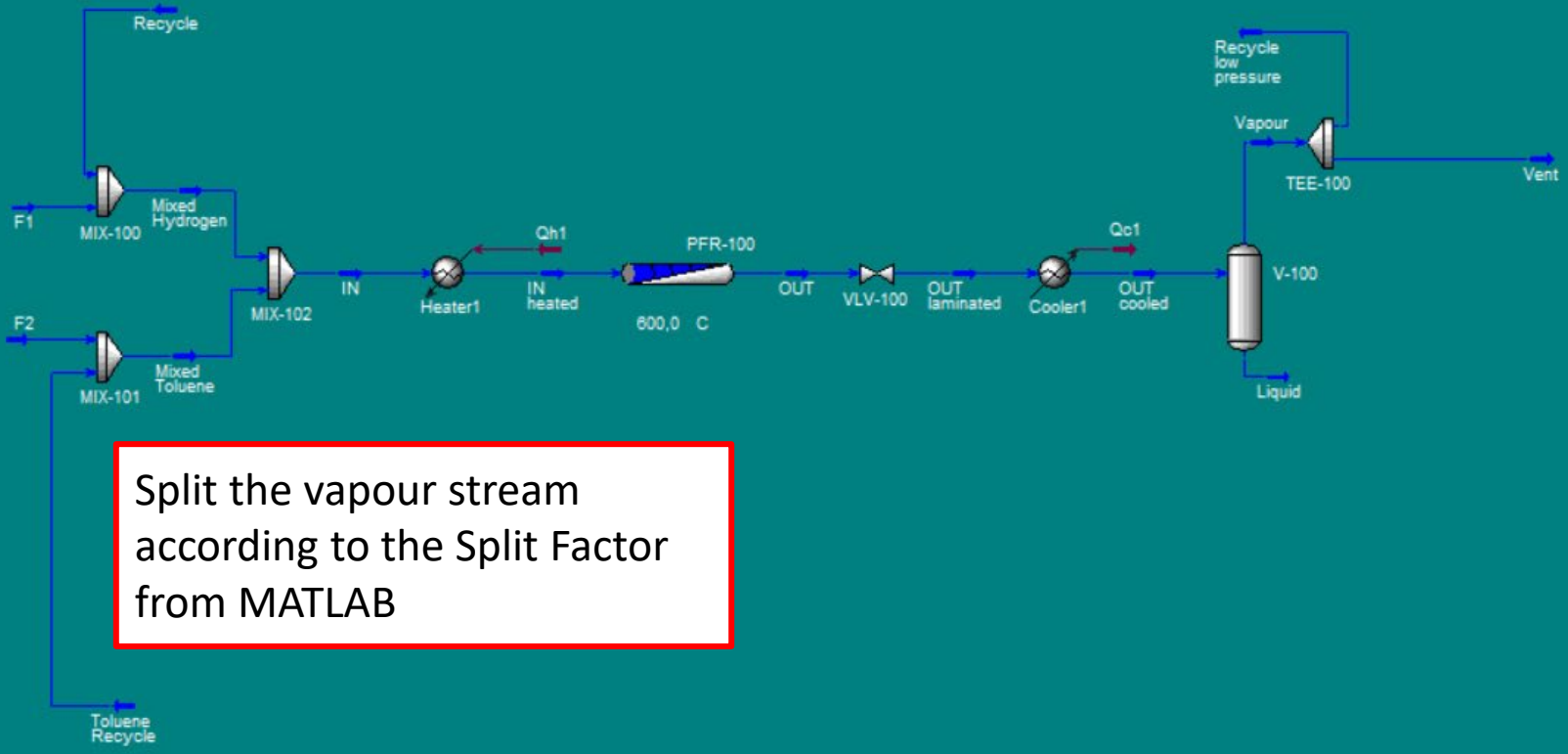Describe the PFR according to MATLAB results and the kinetic scheme

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

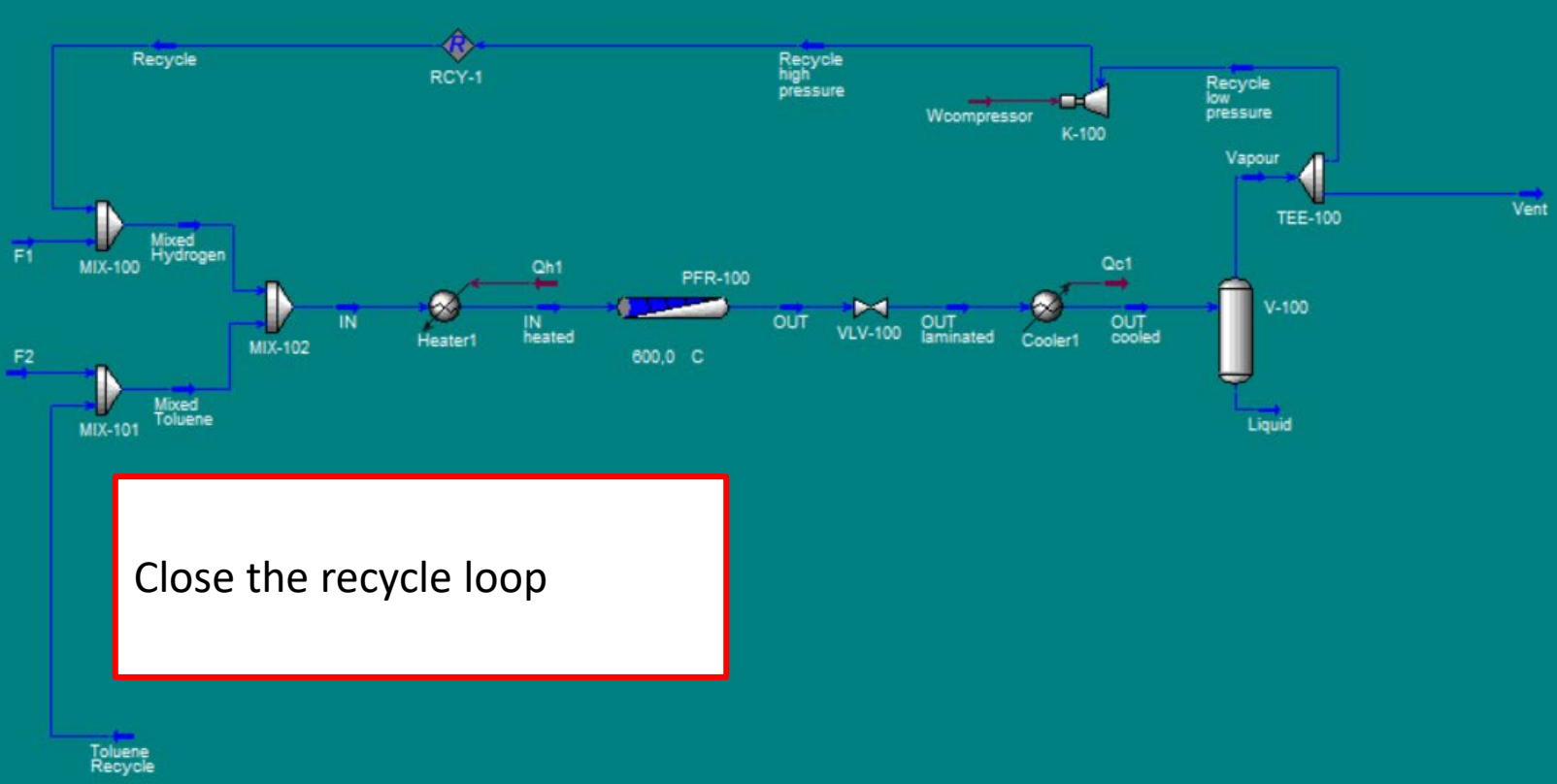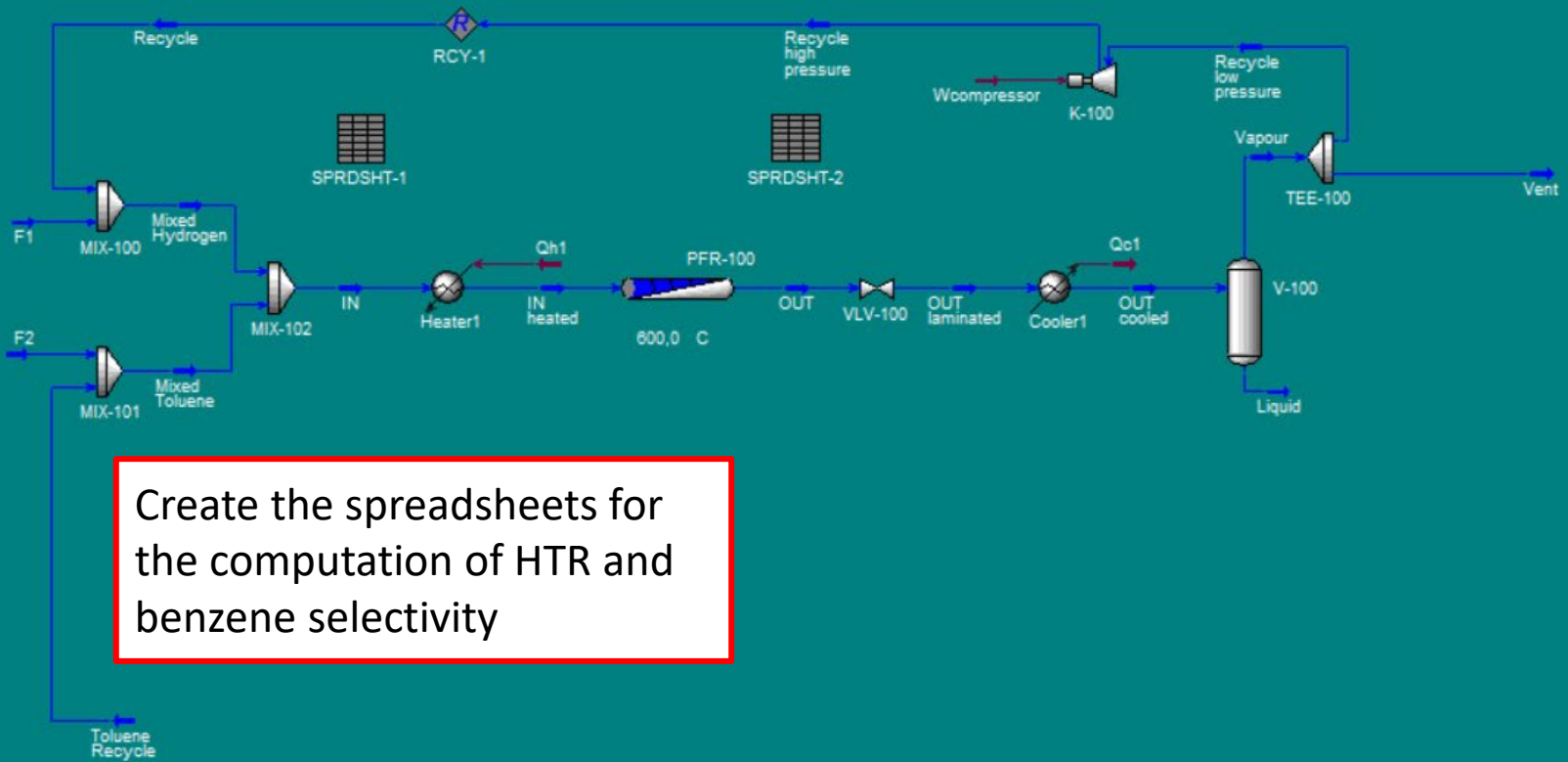Separate the vapour and the liquid fraction with an adiabatic flash

Split the vapour stream according to the Split Factor from MATLAB

Compress the recycle stream to 37 bar
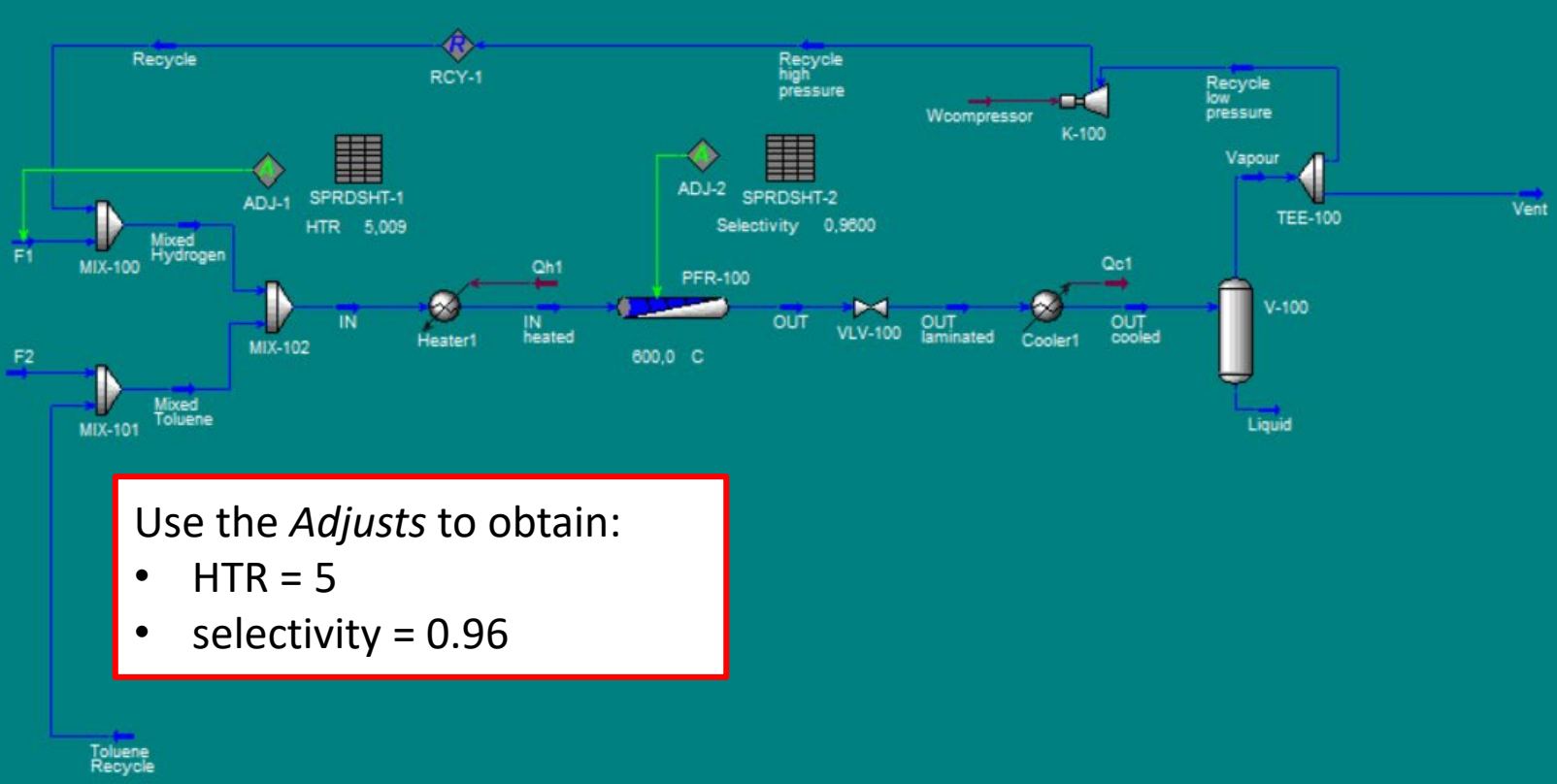
Close the recycle loop

Create the spreadsheets for the computation of HTR and benzene selectivity

Use the *Adjusts* to obtain:
- HTR = 5
- selectivity = 0.96

ADJ-1:	*Target*	HTR	**ADJ-2**:	*Target*	Benzene selectivity
	Adjusted	F1 flow rate		*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 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.
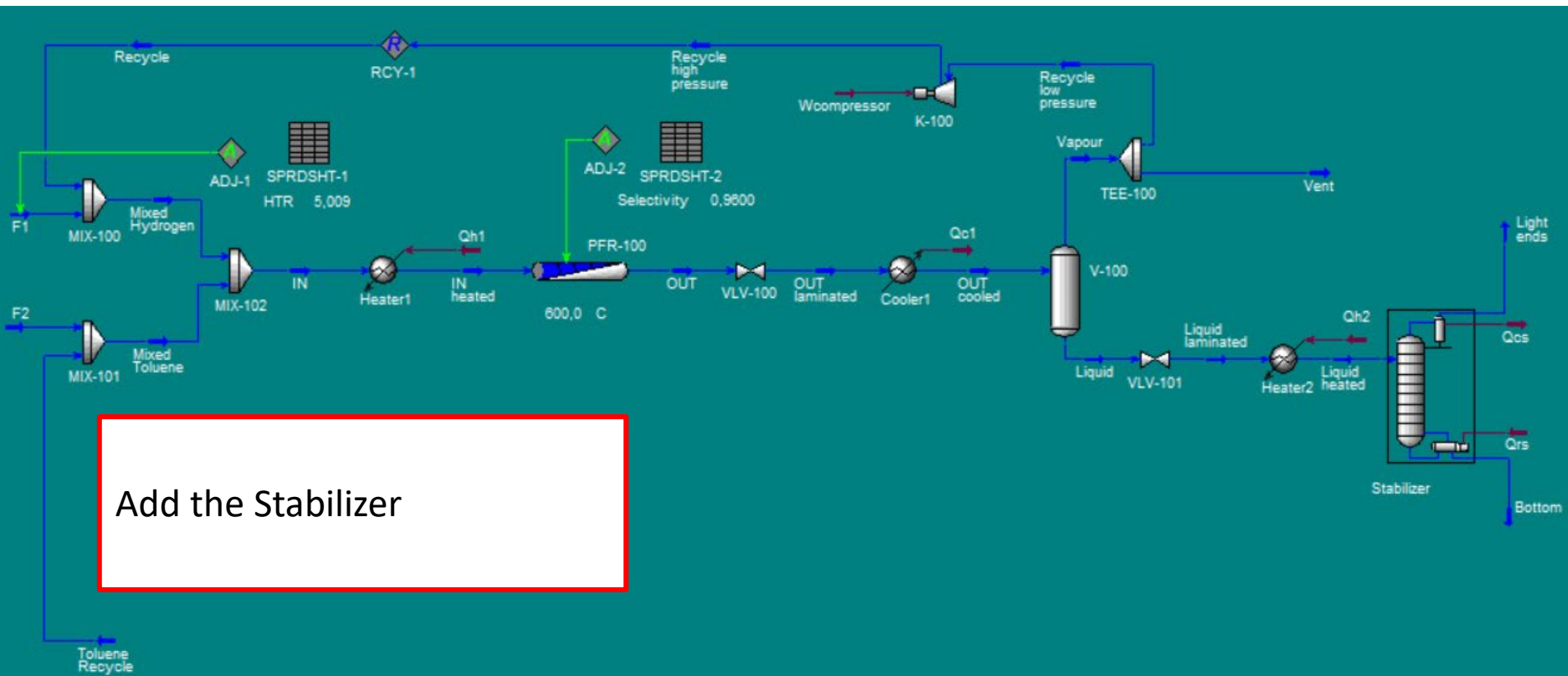
Add the Stabilizer

The Stabilizer (full reflux) is made up of five real stages (**3 trays**): the feed tray is the **2nd** 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.
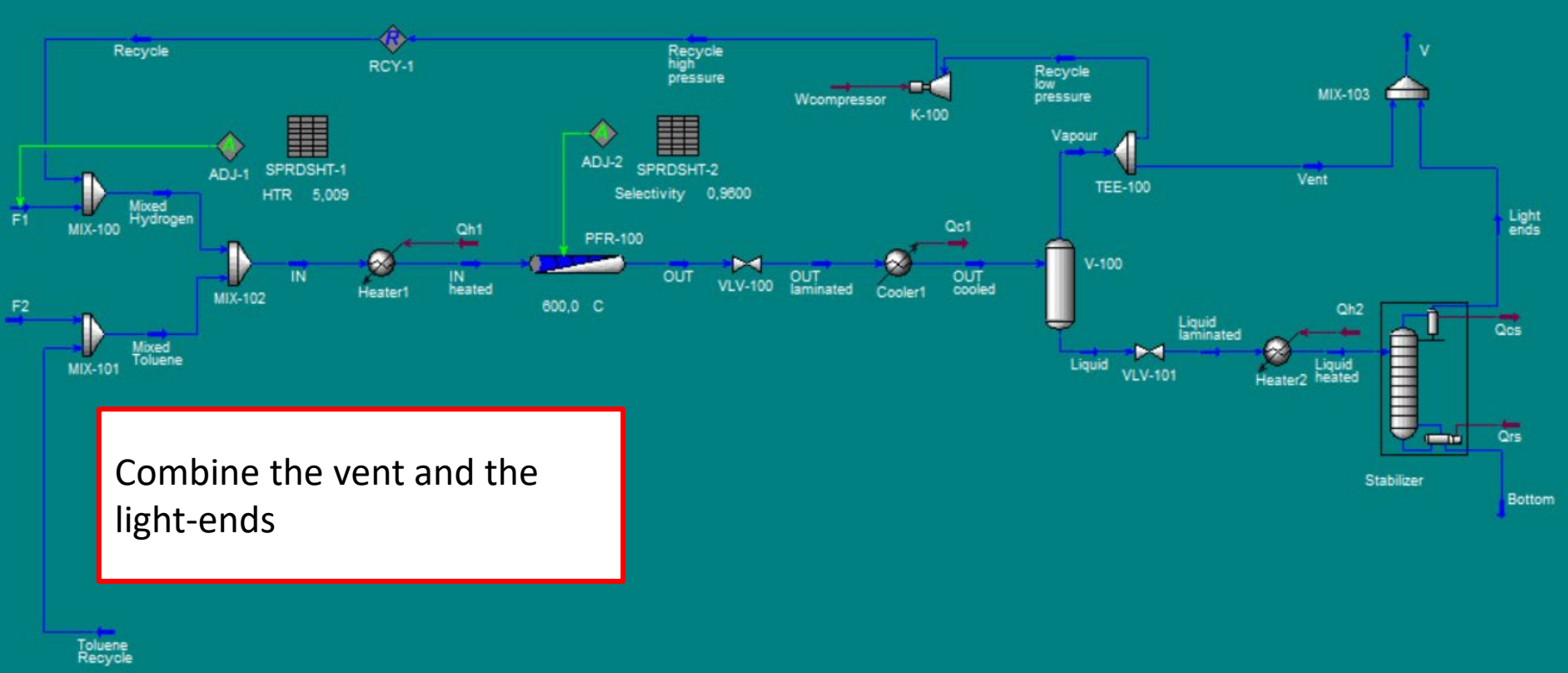
Input data:

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

Additional data: (at T = 600°C, just to check the results)

- Reboiler duty = 2÷3 · 10^6 kJ/h;
- T_{bottom} estimated as 130÷135°C;
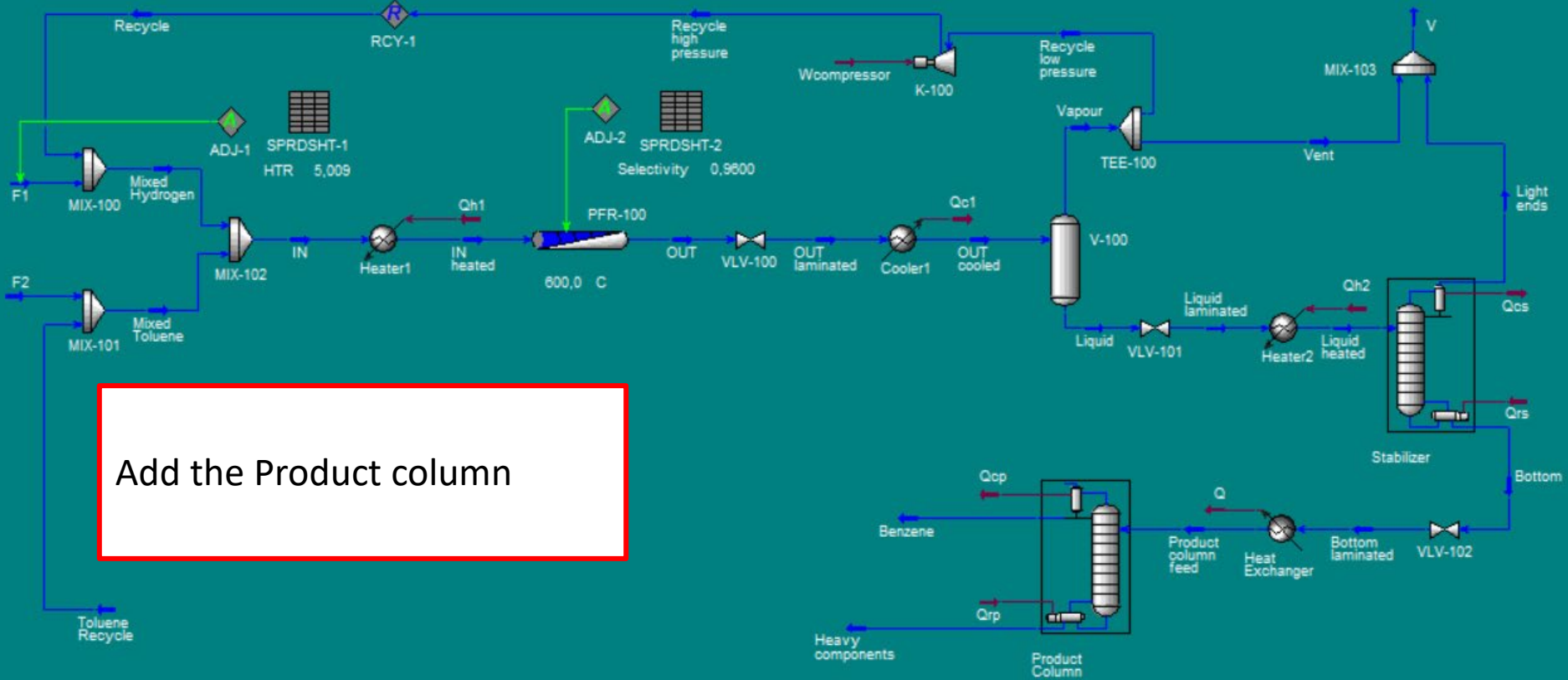- Light ends flowrate = 15÷25 kmol/h.

Trays are assumed to operate at 100% efficiency.

Combine the vent and the light-ends
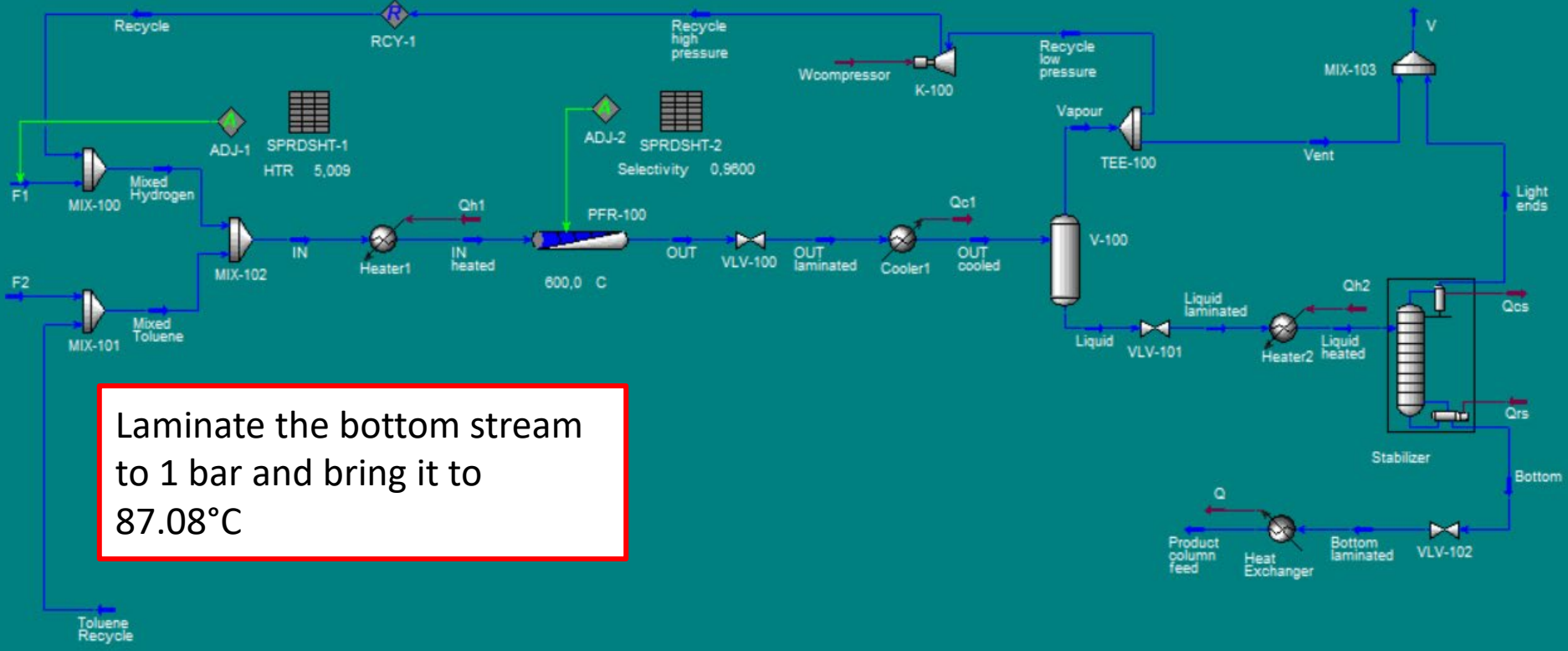
Laminate the bottom stream to 1 bar and bring it to 87.08°C

Add the Product column

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

- purity of the recovered benzene of 99.97%$_{mol}$;
- 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 (FUG) method**.

It is possible to assume a reflux ratio of 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/UniSim results. Hydrogen and methane traces (whose molar fractions are in the order of 10^{-8} and 10^{-5}, respectively) 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

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

Coefficient for calculation of volatility:

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

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

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

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

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

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

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

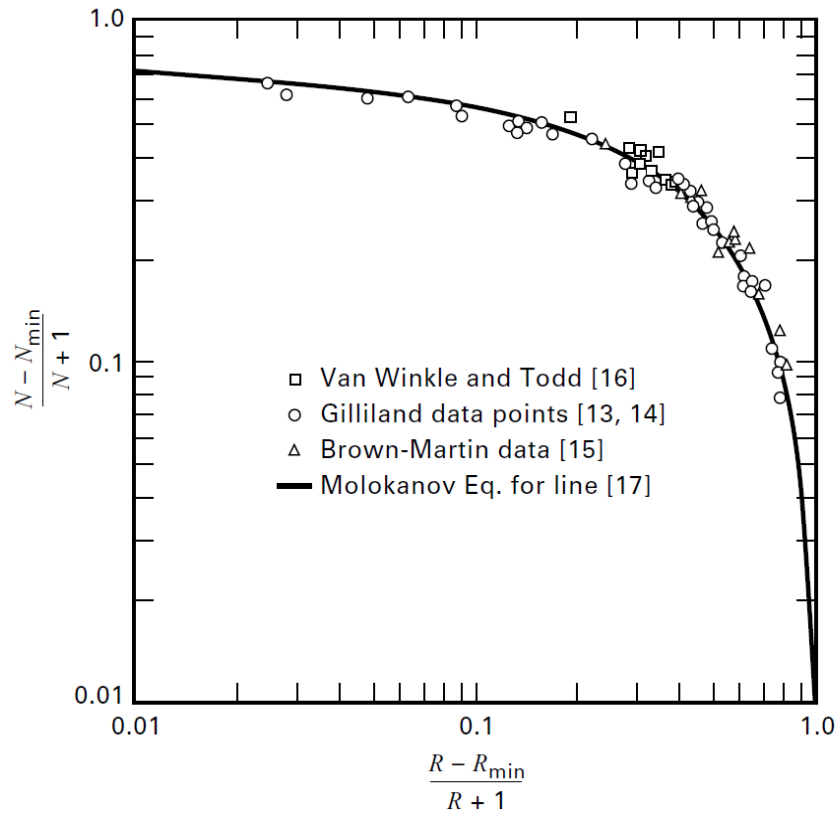**PLEASE NOTE:**

$$\overline{\alpha}=\sqrt{\alpha_{top}\cdot\alpha_{bottom}}$$

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

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

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

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

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

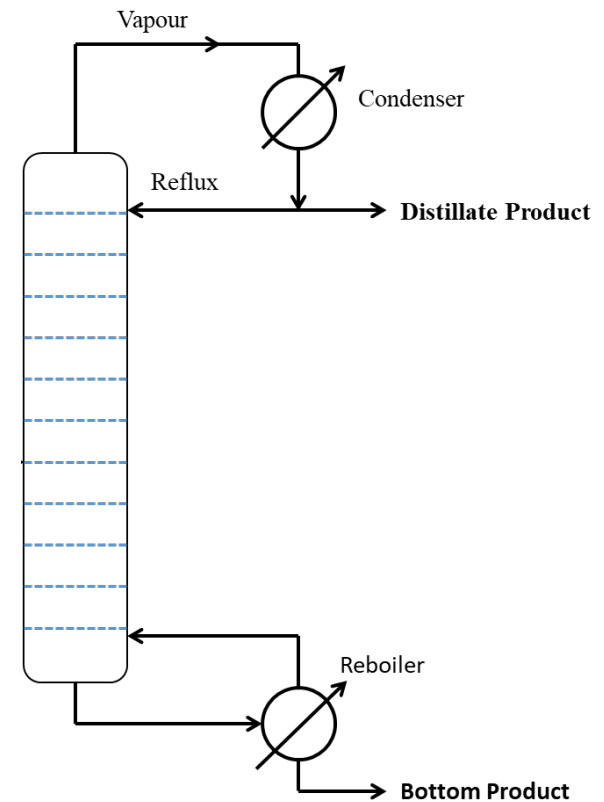$$\phi = 0.75 - 0.75 F^{0.5668} \quad \textit{Eduljee}$$

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

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:

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

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

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: $\eta = \dfrac{N_{ideal}}{N_{real}}$

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

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

Where μ_F is the viscosity of liquid feed at bubble point (*measured in centipoise, cP*) and α is the relative volatility of the two species to be separated.
The viscosity of the inlet stream is **0.3 cP**.
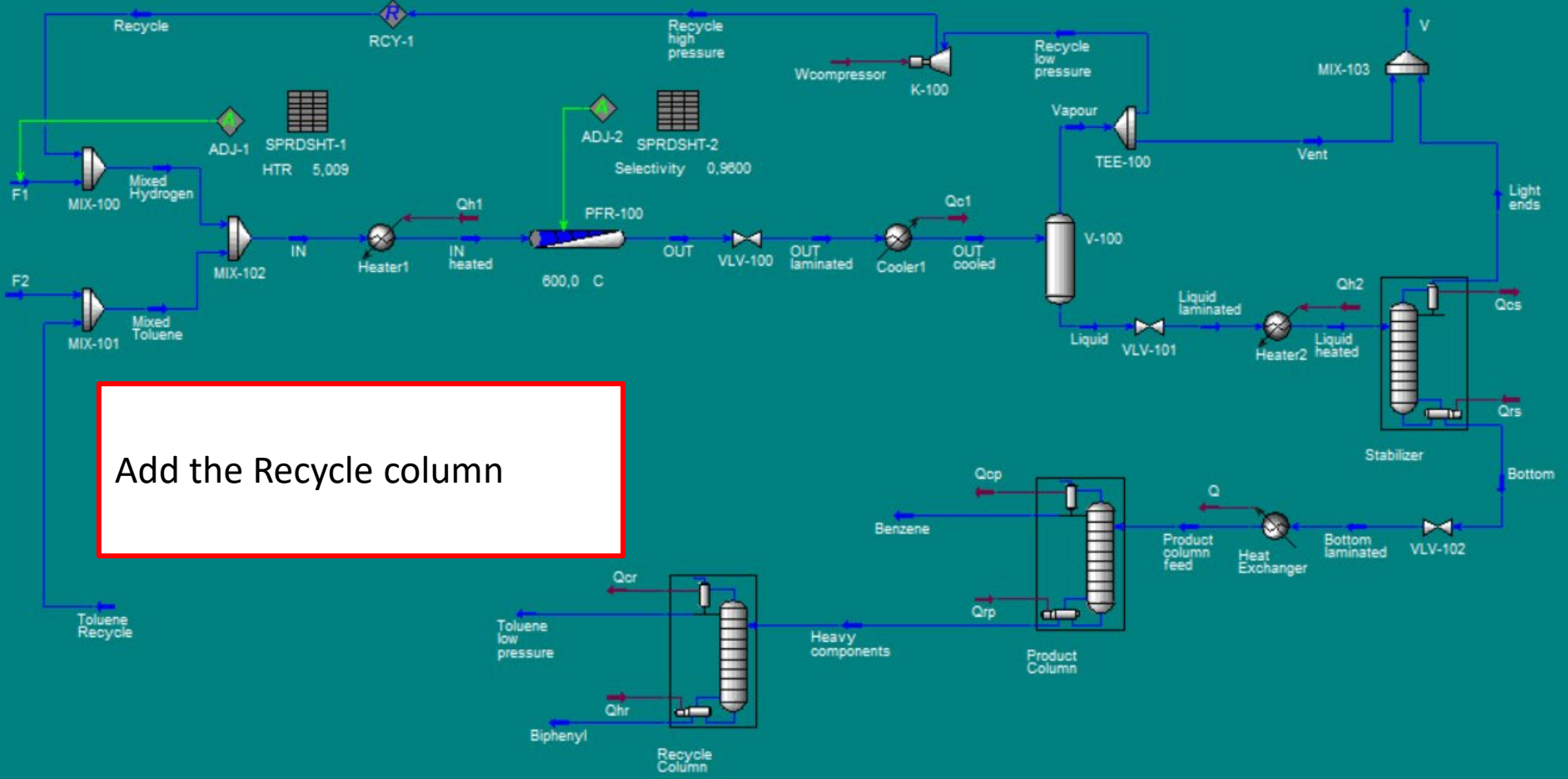
Add the Recycle column

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.

Preliminarly, use a **short-cut distillation column** in the process simulator to estimate the number of ideal trays and the optimal feed tray, assuming R_{eff} = 1.3 R_{min}.
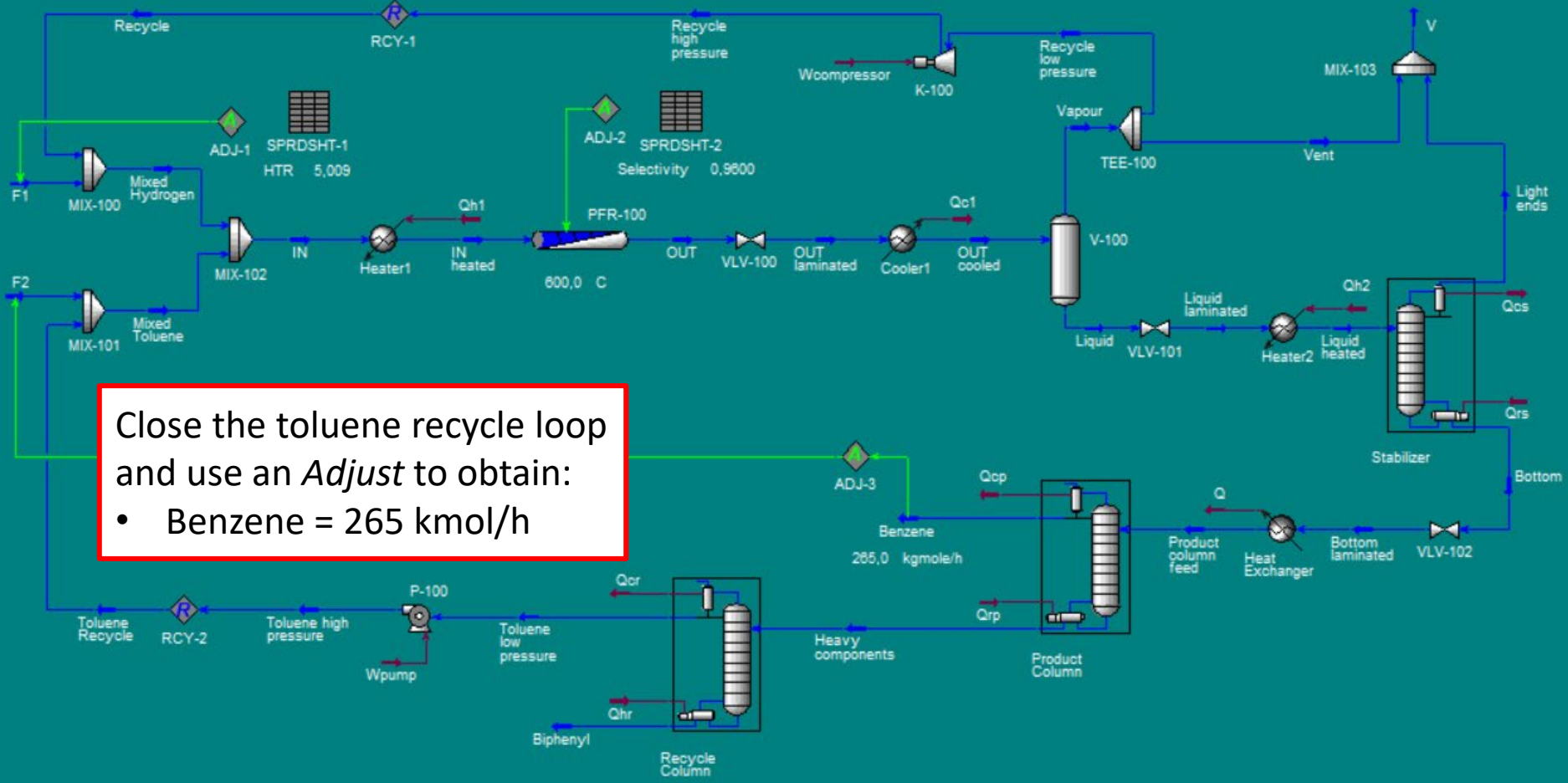
Then, using the results of the short-cut design tool, **simulate** the distillation by means of a **standard distillation column**, using the "*Modified (HYSIM) Inside-Out*" solver.

Assume an overall O'Connell efficiency equal to 0.24.
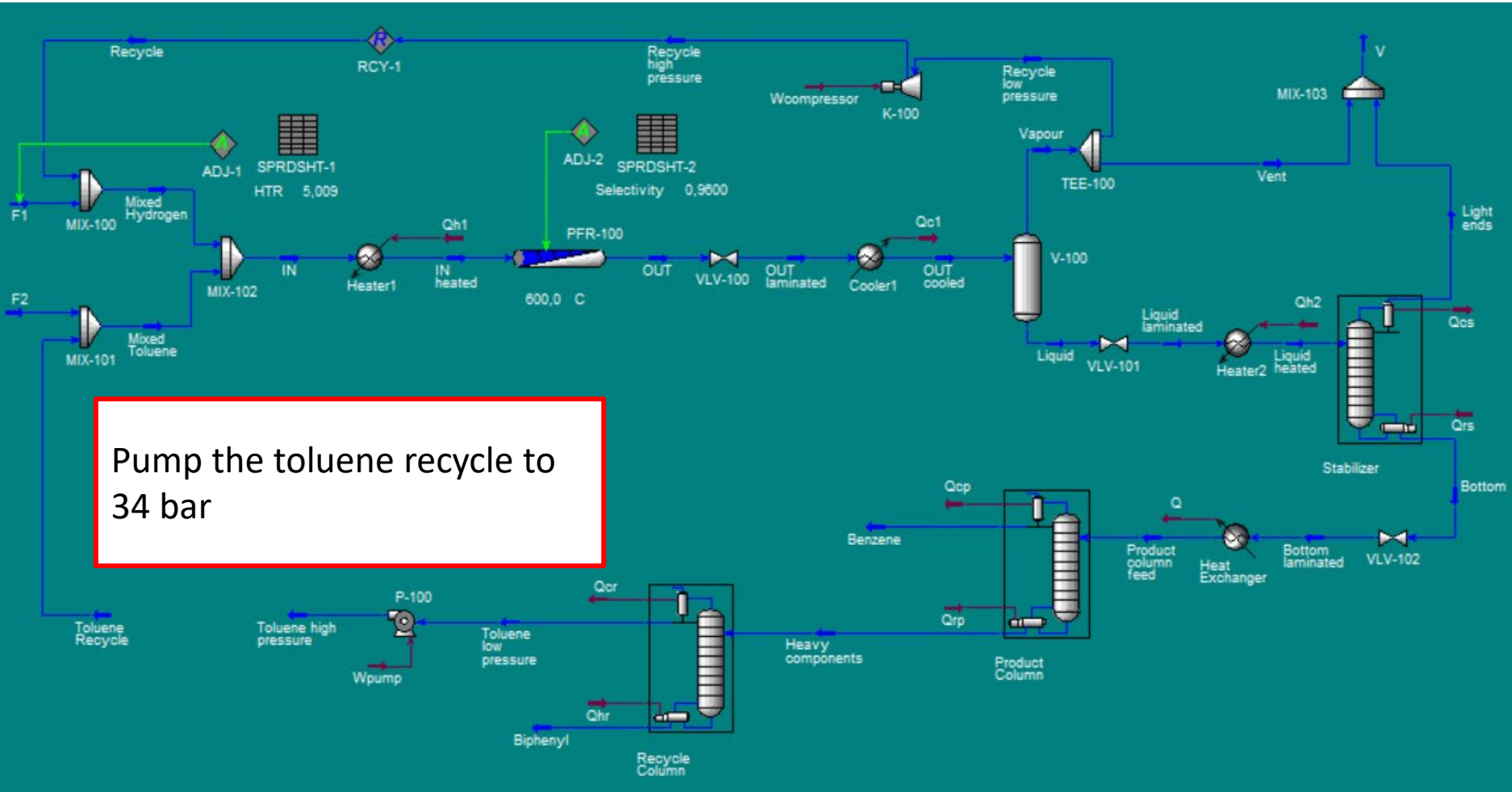
Pump the toluene recycle to 34 bar

Close the toluene recycle loop and use an *Adjust* to obtain:
- Benzene = 265 kmol/h

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

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

Define a tray section that 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', 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 to a Theoretical Plate).