
# LAB1: Material balances

Writing the mass balances of the HDA process

*Process Systems Engineering A* – Prof. Davide Manca

**Andrea Isella** | PSE-Lab

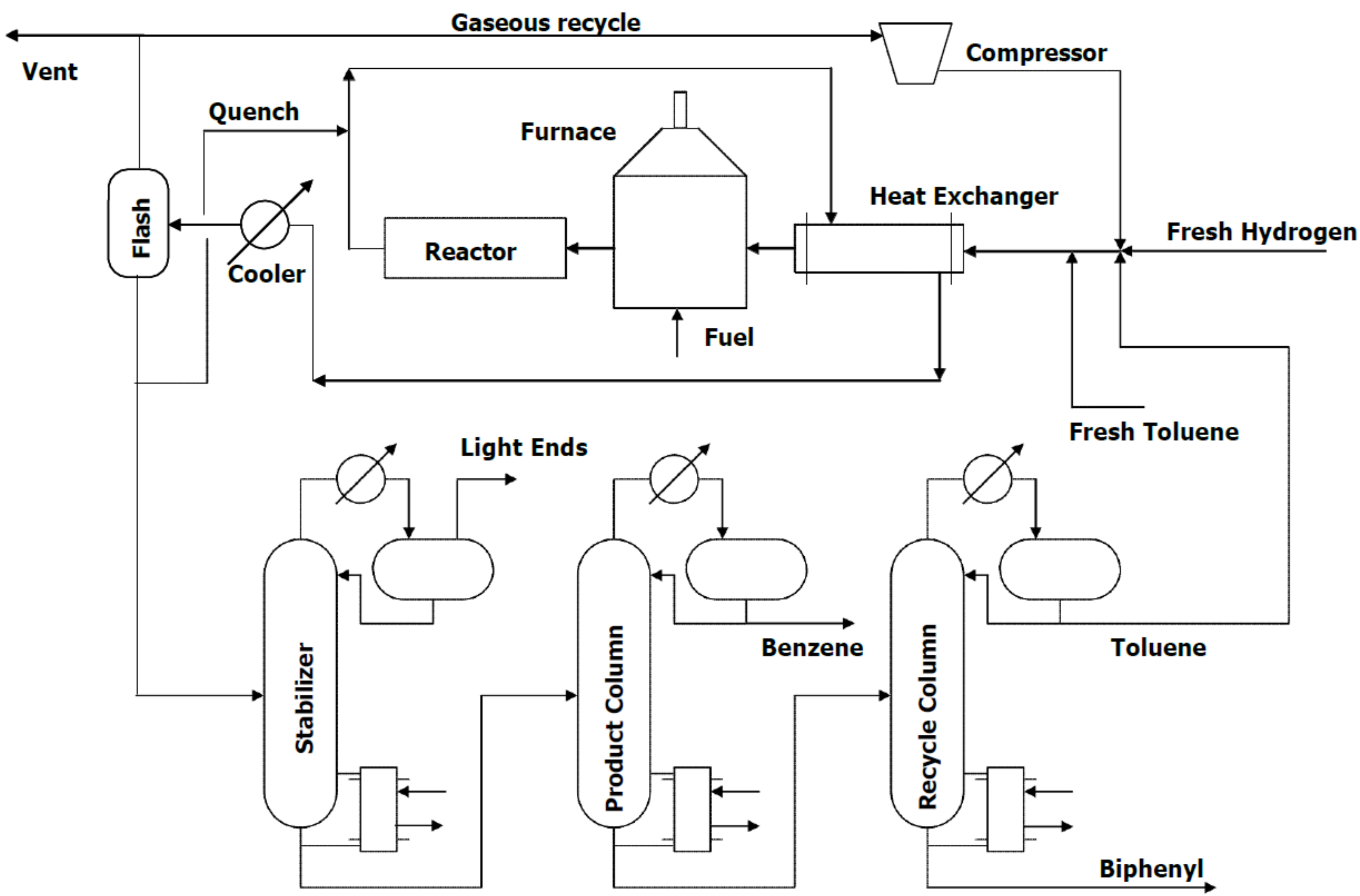
The **conceptual design** is a systematic procedure to evaluate different plant alternatives on an economic basis.

Steps (**E**conomic **P**otentials):

1. Selecting the type of process (EP1)
2. Identification of the input-output structure (EP2)
3. Identification of recycling (EP3)
4. Design of the separation section (EP4)
5. Thermal integration process (EP5)

Each level provides an increased detail compared to the previous one.

The ***Process Systems Engineering A*** practicals will deal with the basic design and economic analysis of a chemical plant dedicated to the hydrodealkylation of toluene to benzene (HDA process).


Gaseous recycle
Vent
Compressor
Quench
Furnace
Flash
Cooler
Reactor
Heat Exchanger
Fresh Hydrogen
Fuel
Fresh Toluene
Light Ends
Stabilizer
Product Column
Benzene
Recycle Column
Toluene
Biphenyl

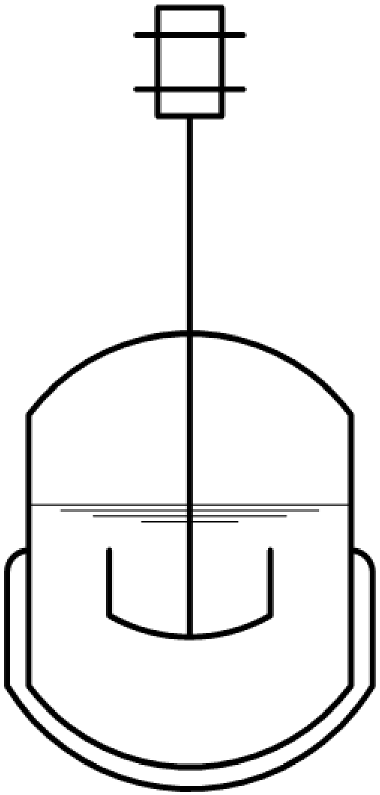
**Desired reaction**

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

**Side reaction**

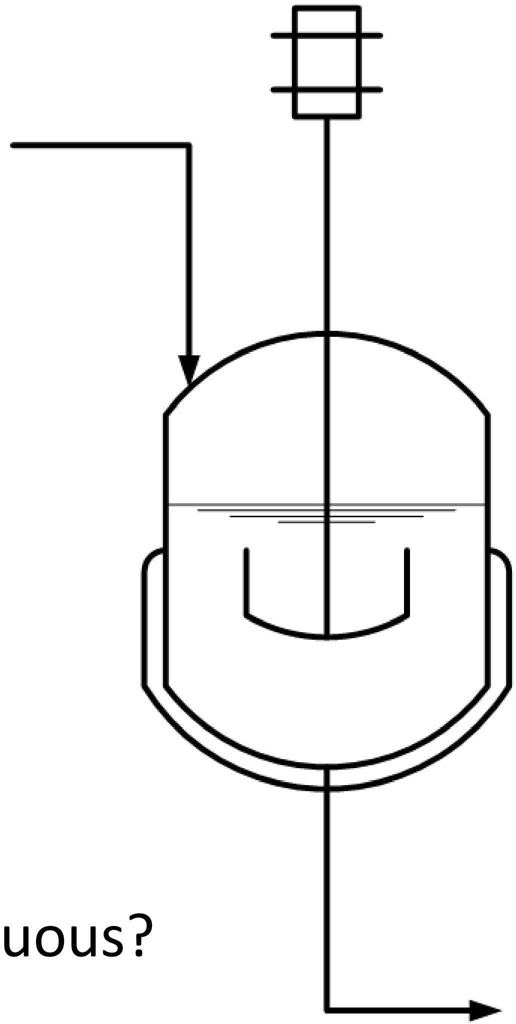
$$2C_6H_6 \rightarrow C_{12}H_{10} + H_2$$

**BATCH PROCESS**



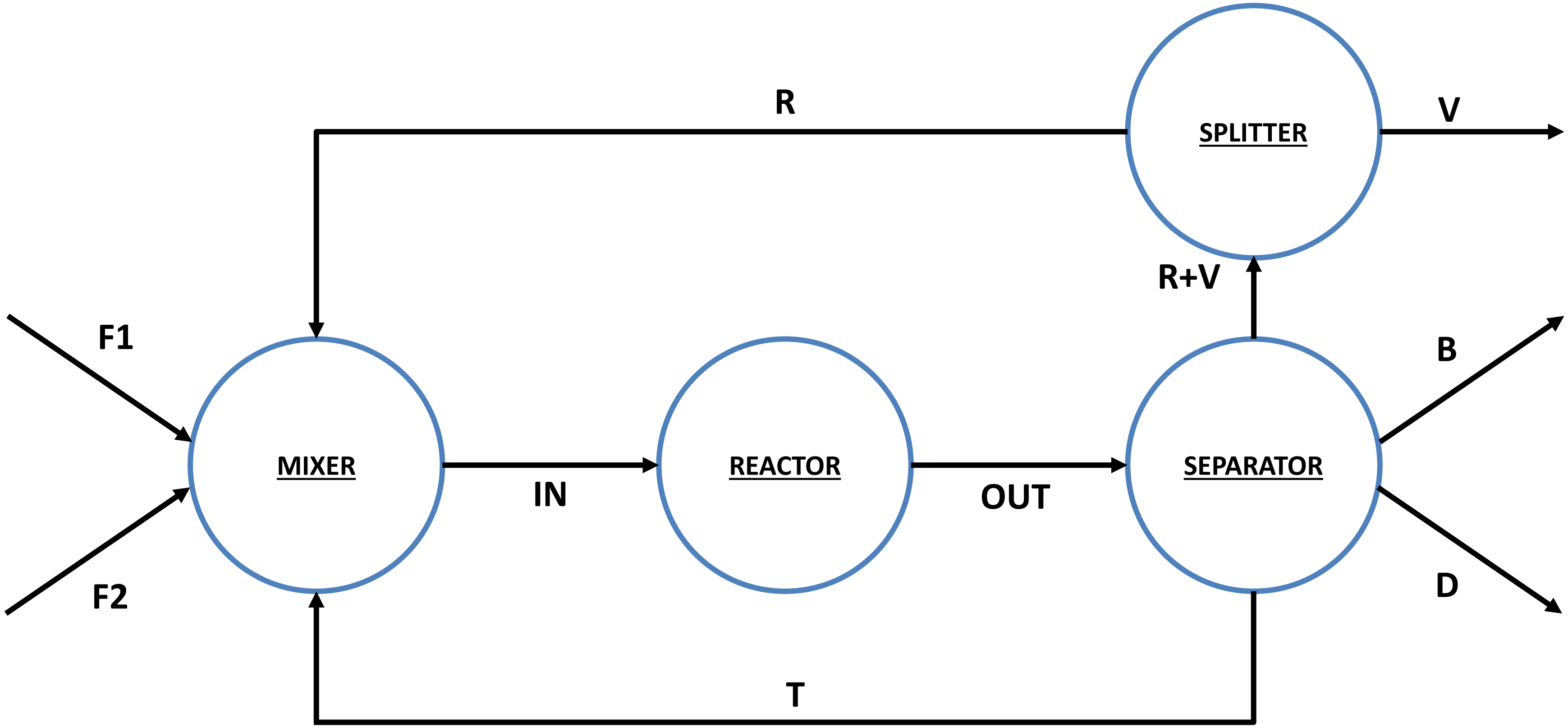
**VS**

**CONTINUOUS PROCESS**



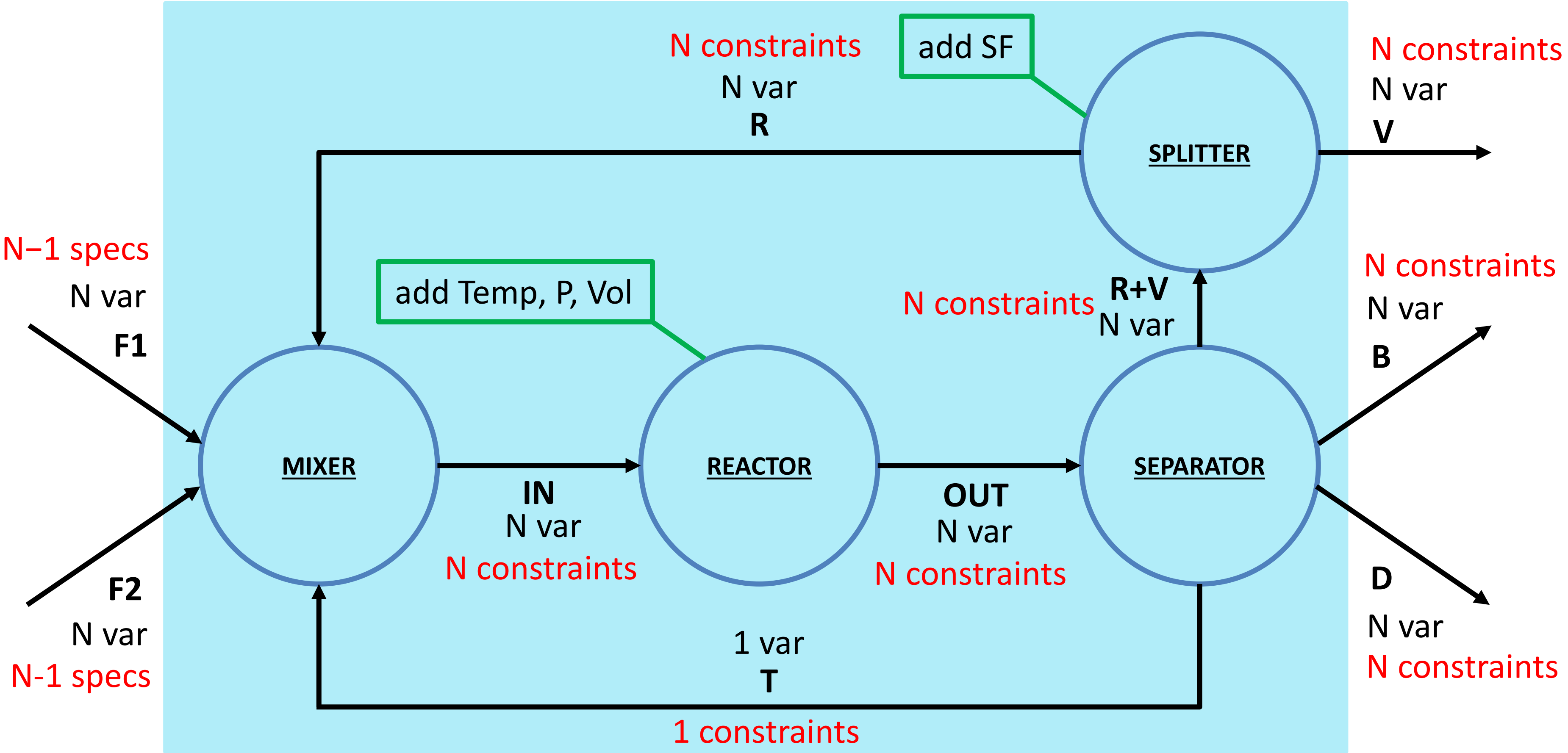
Select the type of process: batch or continuous?

# The model




The HDA plant can be schematized in this simple way

# Process view and material balances (1/2)




10 **flows** each flow: N variables
(N−1 compositions + 1 total flow **OR** N component flows)

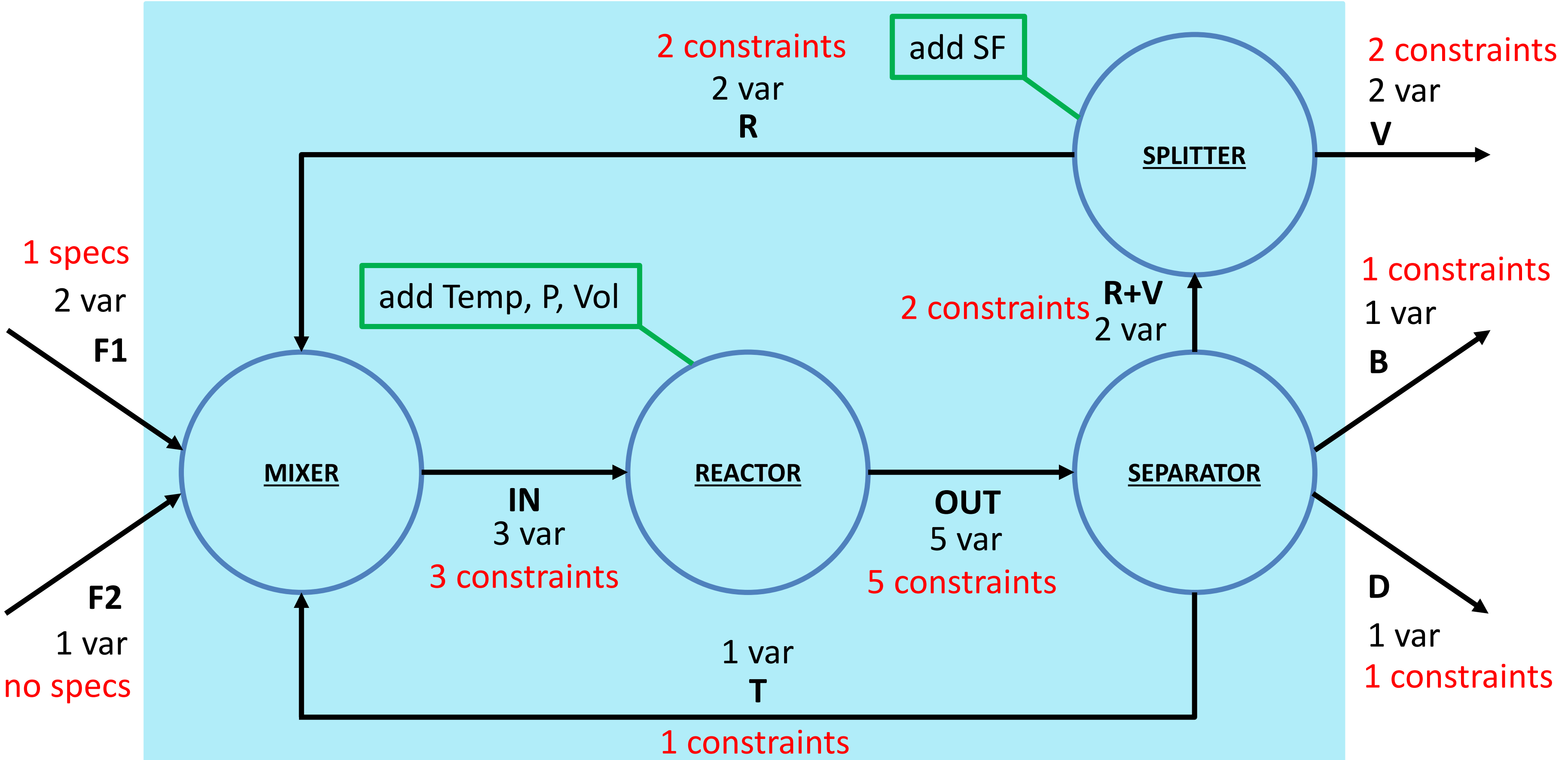
4 **nodes** each node represents a constraint

VAR: **10N** **+4** (SF, Temp, P, Vol)

EQS: **8N**
and specifications: **2N−2**

**(10N+4)−(10N−2) = 6**

# Process view and material balances (2/2)




10 **flows** each flow requires from 1 to 5 variables

4 **nodes** each node represents a constraint

VAR: **20** **+4** (SF, Temp, P, Vol)

EQS: **17**

and specifications: **1**

**24−18 = 6**

**F1**: 2 variables

$F_{h,F1}$ $F_{m,F1}$

**F2**: 1 variable

$F_{t,F2}$

**IN**: 3 variables

$F_{h,IN}$ $F_{m,IN}$ $F_{t,IN}$

**OUT**: 5 variables

$F_{h,OUT}$ $F_{m,OUT}$ $F_{b,OUT}$ $F_{t,OUT}$ $F_{d,OUT}$

**R+V**: 2 variables

$F_{h,R+V}$ $F_{m,R+V}$

**B**: 1 variable

$F_{b,B}$

**T**: 1 variable

$F_{t,T}$

**D**: 1 variable

$F_{d,D}$

**R**: 2 variables

$F_{h,R}$ $F_{m,R}$

**V**: 2 variables

$F_{h,V}$ $F_{m,V}$

**Splitter**

$SF$

**Reactor**

$Temp$ $P$ $Vol$

# Equations: 17

**MIXER**: 3 constraints

$$F_{h,IN} = F_{h,F1} + F_{h,R}$$
$$F_{m,IN} = F_{m,F1} + F_{m,R}$$
$$F_{t,IN} = F_{t,F2} + F_{t,T}$$

**SEPARATOR**: 5 constraints

$$F_{h,R+V} = F_{h,OUT}$$
$$F_{m,R+V} = F_{m,OUT}$$
$$F_{b,B} = F_{b,OUT}$$
$$F_{t,T} = F_{t,OUT}$$
$$F_{d,D} = F_{d,OUT}$$

**SPLITTER**: 4 constraints

$$F_{h,V} = SF \cdot F_{h,R+V}$$
$$F_{m,V} = SF \cdot F_{m,R+V}$$
$$F_{h,R} = (1-SF) \cdot F_{h,R+V}$$
$$F_{m,R} = (1-SF) \cdot F_{m,R+V}$$

add SF

**REACTOR**: 5 constraints

$$F_{i,OUT} = F_{i,IN} + \int_V \sum_{j=1:NR} \nu_{i,j} R_j(T,P,\boldsymbol{x})\, dV$$

add Temp, P, Vol

$$\begin{cases} \dfrac{dF_h}{dV} = \nu_{h,1}R_1(T,P,\boldsymbol{x}) + \nu_{h,2}R_2(T,P,\boldsymbol{x}) \\ \dfrac{dF_m}{dV} = \nu_{m,1}R_1(T,P,\boldsymbol{x}) \\ \dfrac{dF_b}{dV} = \nu_{b,1}R_1(T,P,\boldsymbol{x}) + \nu_{b,2}R_2(T,P,\boldsymbol{x}) \\ \dfrac{dF_t}{dV} = \nu_{t,1}R_1(T,P,\boldsymbol{x}) \\ \dfrac{dF_d}{dV} = \nu_{d,2}R_2(T,P,\boldsymbol{x}) \end{cases}$$

$$\begin{cases} F_h(V=0) = F_{h,IN} \\ F_m(V=0) = F_{m,IN} \\ F_b(V=0) = 0 \\ F_t(V=0) = F_{t,IN} \\ F_d(V=0) = 0 \end{cases}$$

$$\begin{cases} F_h(V=V_{tot}) = F_{h,OUT} \\ F_m(V=V_{tot}) = F_{m,OUT} \\ F_b(V=V_{tot}) = F_{b,OUT} \\ F_t(V=V_{tot}) = F_{t,OUT} \\ F_d(V=V_{tot}) = F_{d,OUT} \end{cases}$$

# Specifications

VAR: **24**

EQS: **17**

**Feed F1** $$\frac{F_{h,F1}}{F_{h,F1}+F_{m,F1}}=0.95$$ → and specifications: **1**

**remaining: 6**

*What can we specify/assign to saturate the remaining degrees of freedom?*

**Benzene productivity** $$F_{b,B}=265\ kmol\ /\ h$$

**Inlet hydrogen-toluene ratio** $$5=\frac{F_{h,IN}}{F_{t,IN}}$$

**Benzene selectivity** $$0.96=\frac{F_{b,OUT}}{F_{t,IN}-F_{t,OUT}}$$

**Reactor pressure** $$P=34\ bar$$

**Reactor temperature** $$Temp$$

**Split factor** $$SF=\frac{F_{h,V}+F_{m,V}}{F_{h,R}+F_{m,R}+F_{h,V}+F_{m,V}}$$ ← related to $x_{h,V}$