

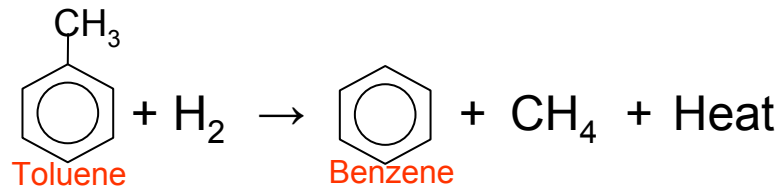
# HDA case study

- S. Skogestad, May 2006
- Thanks to Antonio Araújo

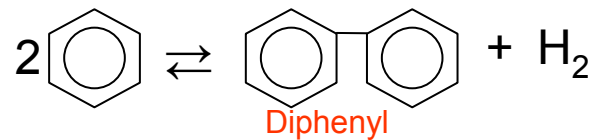
# Process Description

- Benzene production from thermal-dealkalination of toluene (high-temperature, non-catalytic process).

- Main reaction:

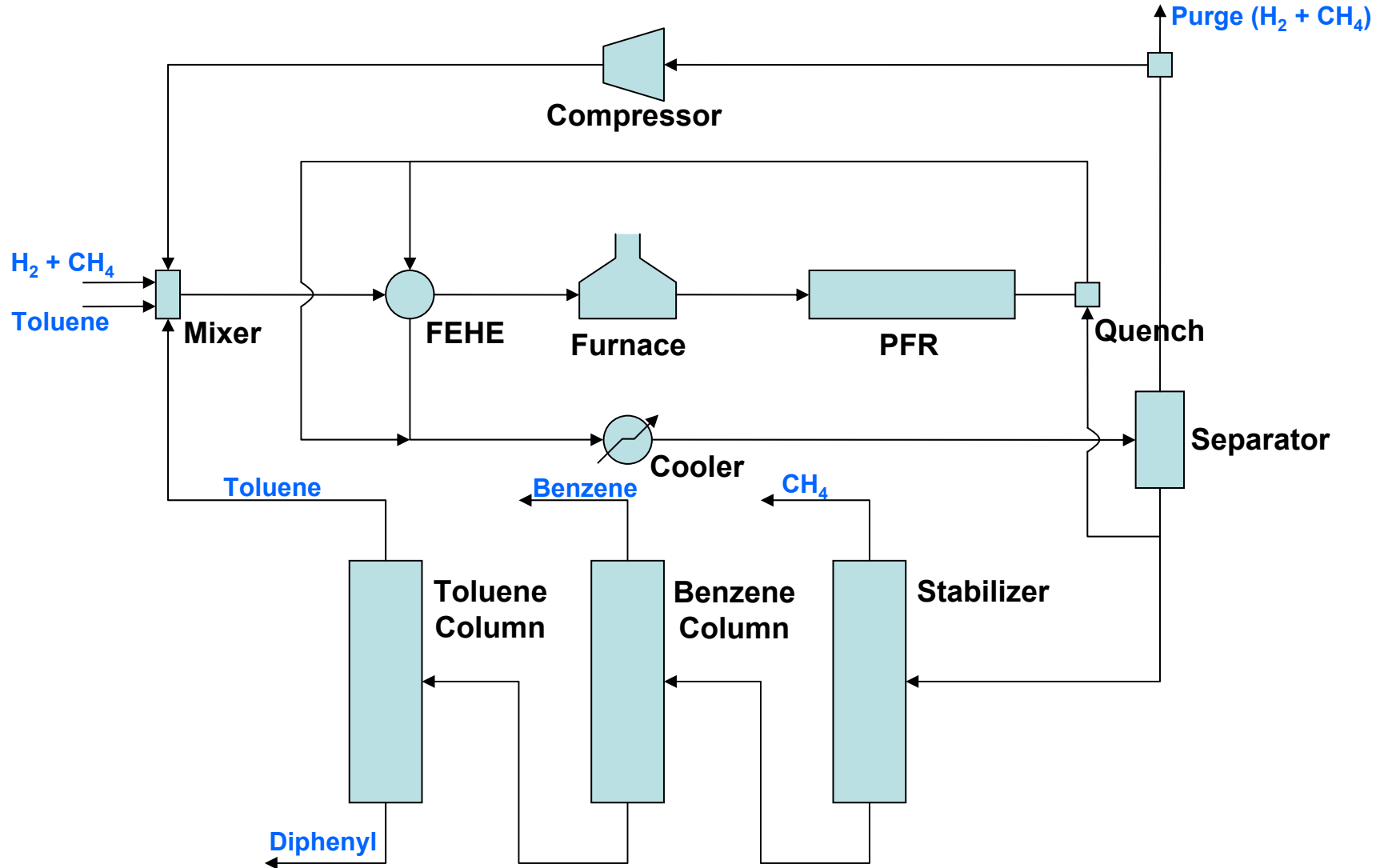


- Side reaction



- Excess of hydrogen is needed to repress the side reaction and coke formation.
- References for HDA process:
  - McKetta (1977) – first reference on the process;
  - Douglas (1988) – design of the process;
  - Wolff (1994) – discuss the operability of the process.
- No references on the optimization of the process for control structure design purposes.

# Process Description

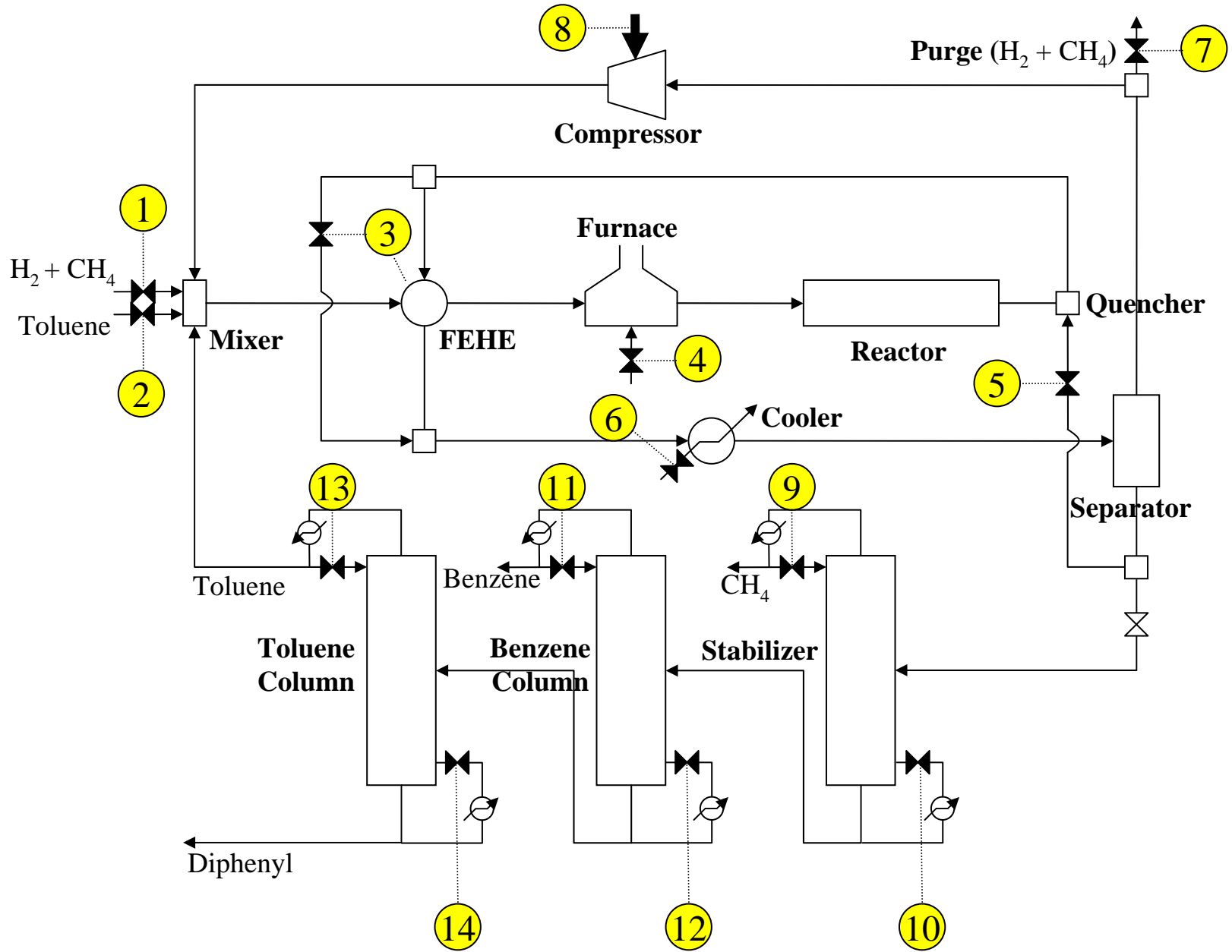


# Steady-state operational degrees of freedom

<b>Process units</b>	<b>DOF</b>
External feed streams (feed rate)	2
Heat exchangers duties (including 1 furnace)	3
Splitters	2
Compressor duty	1
Adiabatic flash <sup>(*)</sup>	0
Gas phase reactor <sup>(*)</sup>	0
Distillation columns	6
	<b>14</b>
<b>Equality constraint</b>	
Quencher outlet temperature	-1
<b>Remaining degrees of freedom at steady state</b>	<b>13</b>

(\*) No adjustable valves (assumed fully open valve before flash)

# Steady-state operational degrees of freedom



# Cost Function and Constraints

- The following profit is maximized (Douglas's EP):

$$-J = p_{\text{ben}} D_{\text{ben}} - p_{\text{tol}} F_{\text{tol}} - p_{\text{gas}} F_{\text{gas}} - p_{\text{fuel}} Q_{\text{fuel}} - p_{\text{cw}} Q_{\text{cw}} - p_{\text{power}} W_{\text{power}} - p_{\text{steam}} Q_{\text{steam}} + \Sigma(p_{v,i} F_{v,i})$$

- Constraints during operation:

- Production rate:  $D_{\text{ben}} \geq 265 \text{ lbmol/h.}$
- Hydrogen excess in reactor inlet:  $F_{\text{Hyd}} / (F_{\text{ben}} + F_{\text{tol}} + F_{\text{diph}}) \geq 5.$
- Bound on toluene feed rate:  $F_{\text{tol}} \leq 300 \text{ lbmol/h.}$
- Reactor pressure:  $P_{\text{reactor}} \leq 500 \text{ psia.}$
- Reactor outlet temperature:  $T_{\text{reactor}} \leq 1300 \text{ }^\circ\text{F.}$
- Quencher outlet temperature:  $T_{\text{quencher}} = 1150 \text{ }^\circ\text{F.}$
- Product purity:  $x_{\text{Dben}} \geq 0.9997.$
- Separator inlet temperature:  $95 \text{ }^\circ\text{F} \leq T_{\text{flash}} \leq 105 \text{ }^\circ\text{F.}$
- + Distillation constraints

- Manipulated variables are bounded.

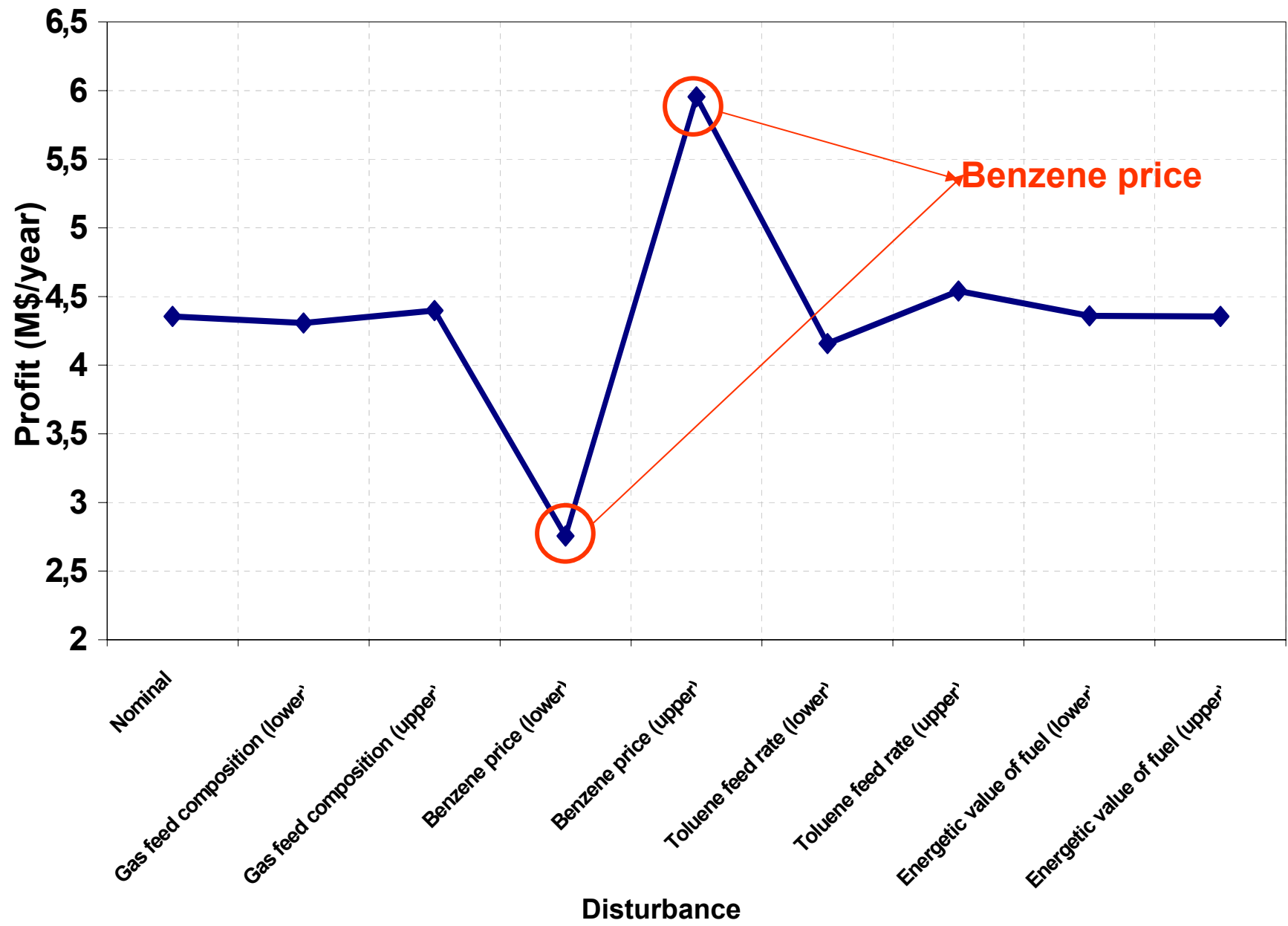
# Disturbances

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<b>Disturbance</b>	<b>Unit</b>	<b>Nominal</b>	<b>Lower</b>	<b>Upper</b>
Toluene feed flow rate	lbmol/h	300	285	315
Gas feed composition	mol% of H <sub>2</sub>	95	90	100
Benzene price	\$/lbmol	9.04	8.34	9.74
Energetic value of fuel to the furnace	MBTU/lbmol	0.1247	0.12	0.13

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# Optimization

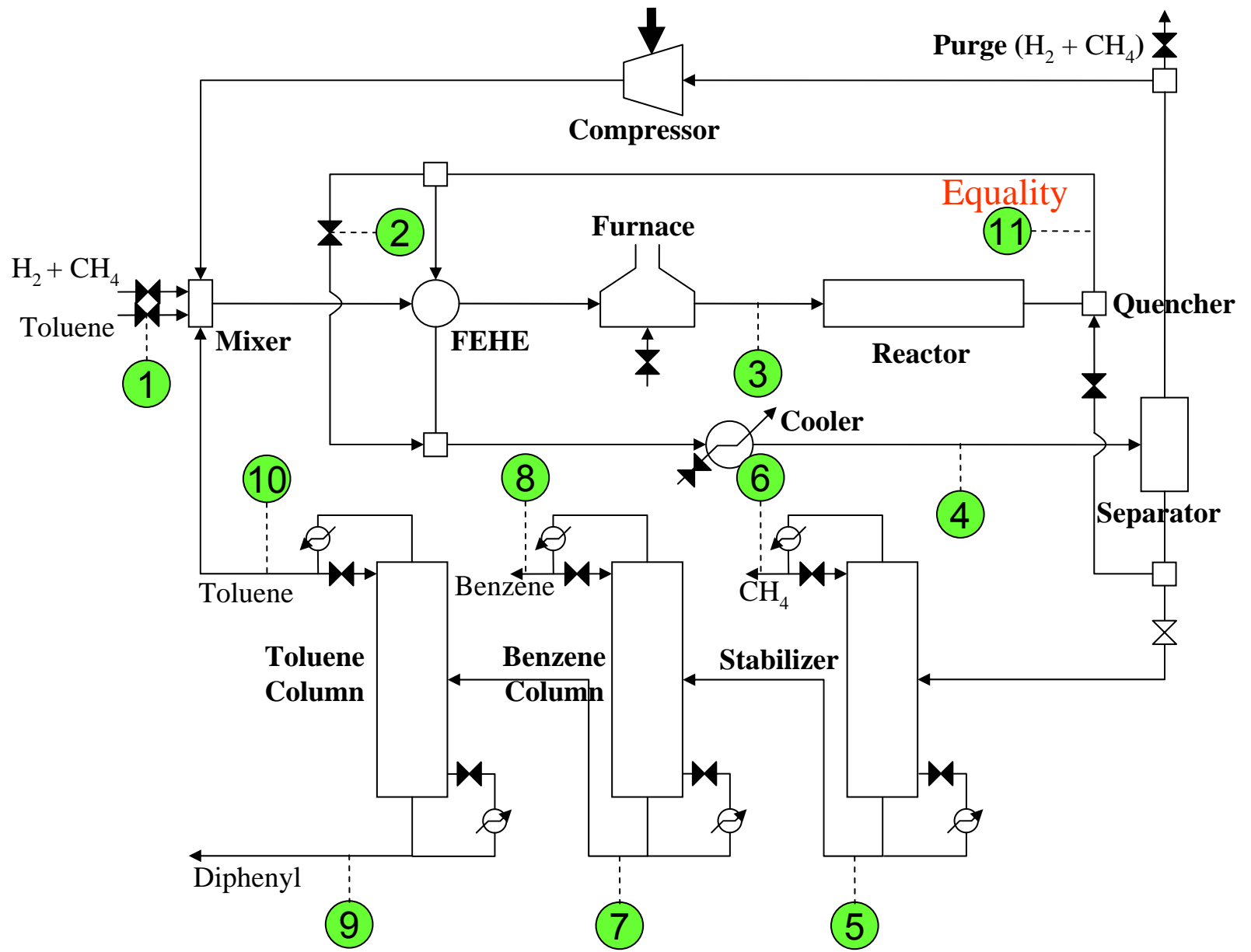




# Optimization

- **14 steady-state degrees of freedom**
- **10 active constraints:**
  1. Pure toluene feed rate (UB)
  2. By-pass valve around FEHE (LB)
  3. Reactor inlet hydrogen-aromatics ratio (LB)
  4. Flash inlet temperature (LB)
  5. Methane mole fraction in stabilizer bottom (UB)
  6. Benzene mole fraction in stabilizer distillate (UB)
  7. Toluene mole fraction in benzene column bottom (LB)
  8. Benzene mole fraction in benzene column distillate (LB)
  9. Diphenyl mole fraction in toluene column bottom (LB)
  10. Toluene mole fraction in toluene column distillate (LB)
- **1 equality constraint:**
  11. Quencher outlet temperature
- **3 remaining unconstrained degrees of freedom.**

# Optimization – Active Constraints



# Candidate Controlled Variables

- Candidate controlled variables:
  - Pressure differences;
  - Temperatures;
  - Compositions;
  - Heat duties;
  - Flow rates;
  - Combinations thereof.
- 138 candidate controlled variables might be selected.
- 14 degrees of freedom.
- Number of different sets of controlled variables:

$$\frac{138}{14} \quad \frac{138!}{124!14!} \quad 5.3 \cdot 10^{18}$$

- 10 active constraints + 1 equality constraint leaving 3 DOF:

$$\frac{127}{3} \quad \frac{127!}{124!3!} \quad 333,375$$

- What should we do with the remaining 3 DOF?
  - **Self-optimizing control!!!**

# Analysis of the linear model

a. All measurements ( $\underline{\sigma}(G_{\text{full}}) = 1.58$ ):

Branch-and-bound:  $\underline{\sigma}(G_{3 \times 3}) = 0.864$

- I Quencher outlet benzene mole fraction
- II Compressor power
- III Liquid (cooling) flow to quencher

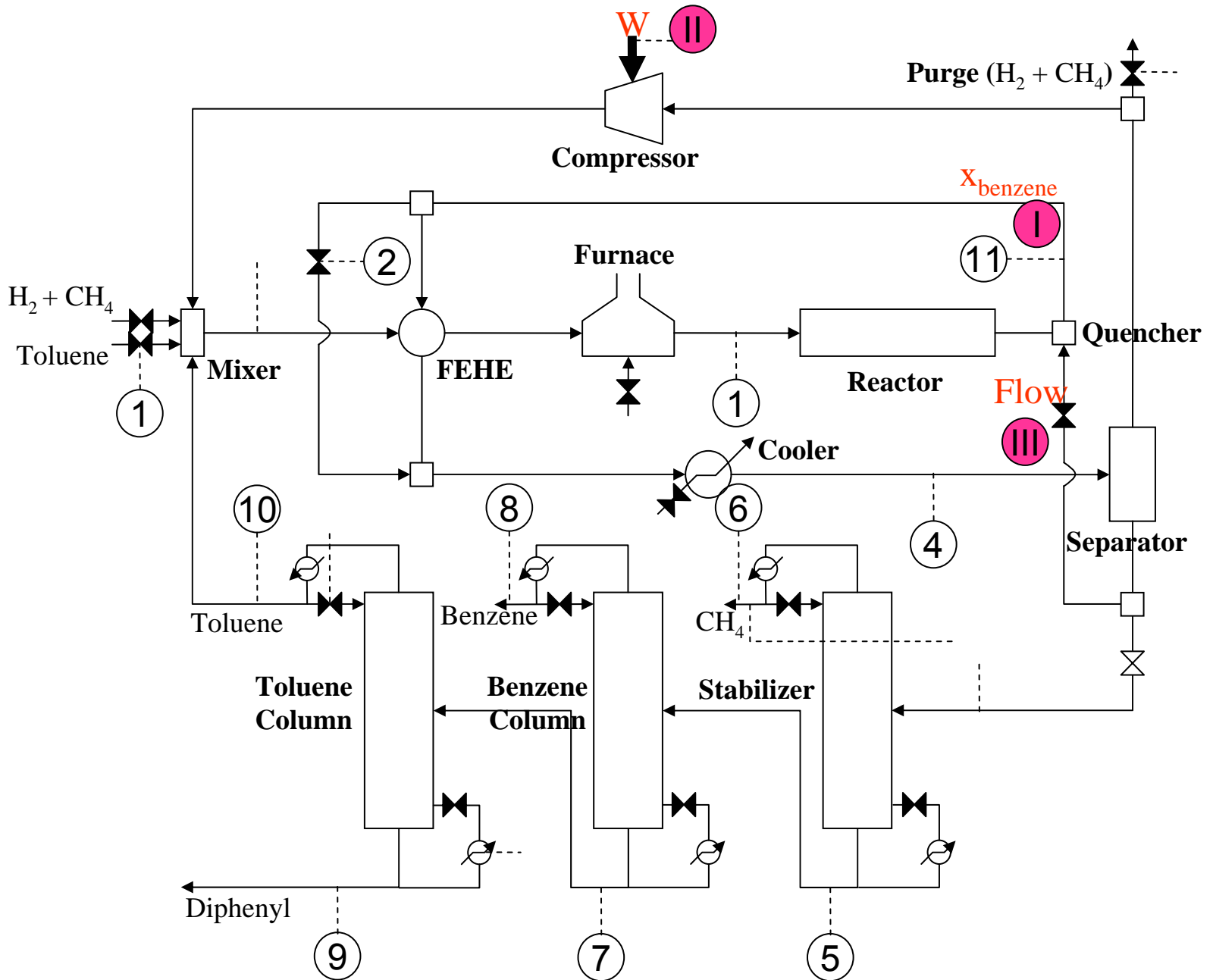
Branch-and-bound:  $\underline{\sigma}(G_{3 \times 3}) = 0.853$

- Separator liquid outlet benzene mole fraction
- II Compressor power
- III Liquid (cooling) flow to quencher

Branch-and-bound:  $\underline{\sigma}(G_{3 \times 3}) = 0.852$

- Benzene mole fraction in stabilizer bottom
- II Compressor power
- III Liquid (cooling) flow to quencher

# Optimal self-optimizing variables



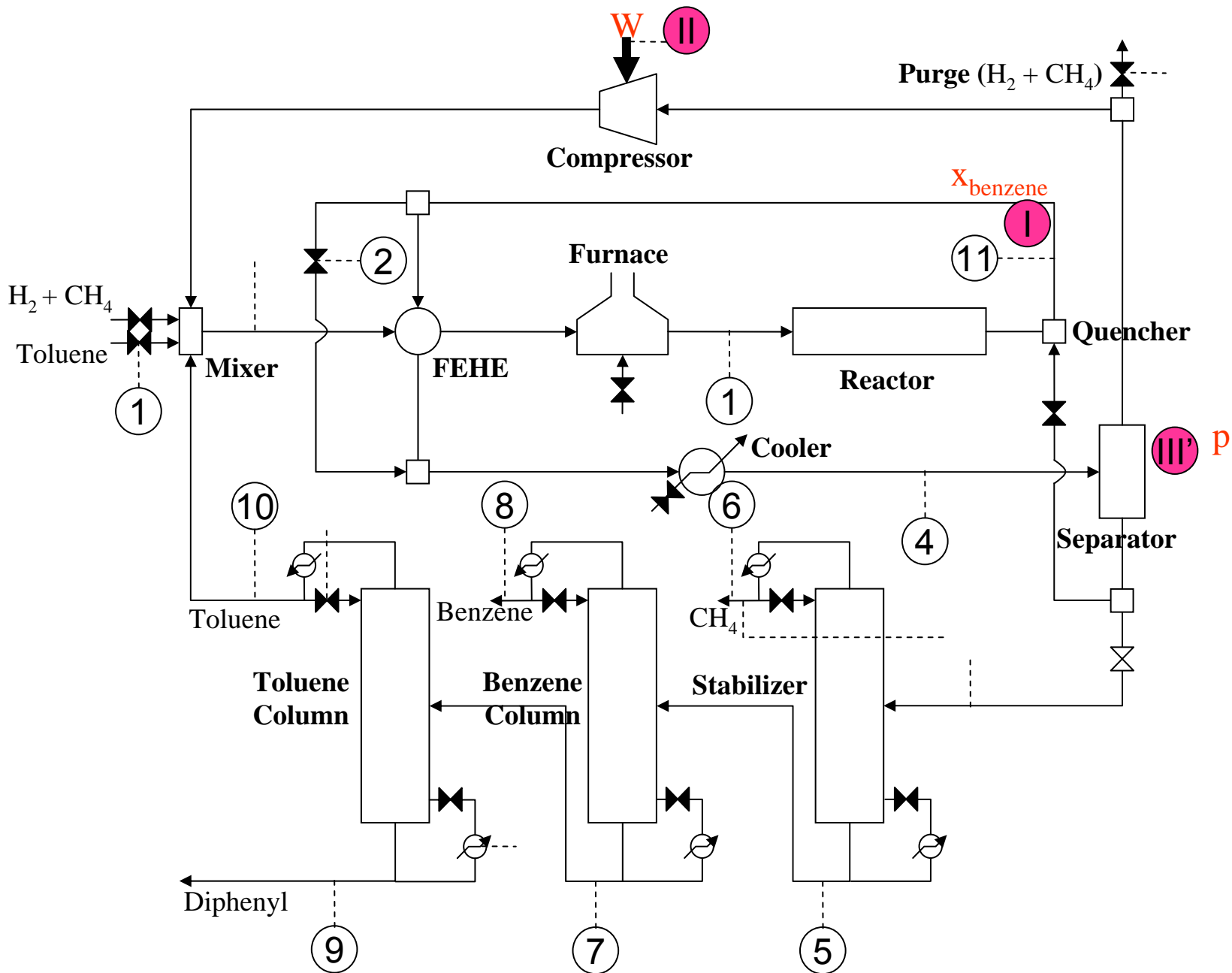
# Analysis of the linear model

b. Separator pressure constant ( $\underline{\sigma}(G_{\text{full}}) = 1.50$ ):

Branch-and-bound:  $\underline{\sigma}(G_{3 \times 3}) = 0.835$

- I Quencher outlet benzene mole fraction
- II Compressor power
- III Separator pressure

# Alternative self-optimizing variables



# Conclusion steady-state analysis

- Many similar alternatives in terms of loss
- Need to consider dynamics (Input-output controllability analysis):
  - RHP-zeros
  - RHP-poles
  - Input saturation
  - Easy of implementation (decentralized control of final 3x3 supervisory control problem)!
- Now: Consider “bottom-up” design of control system

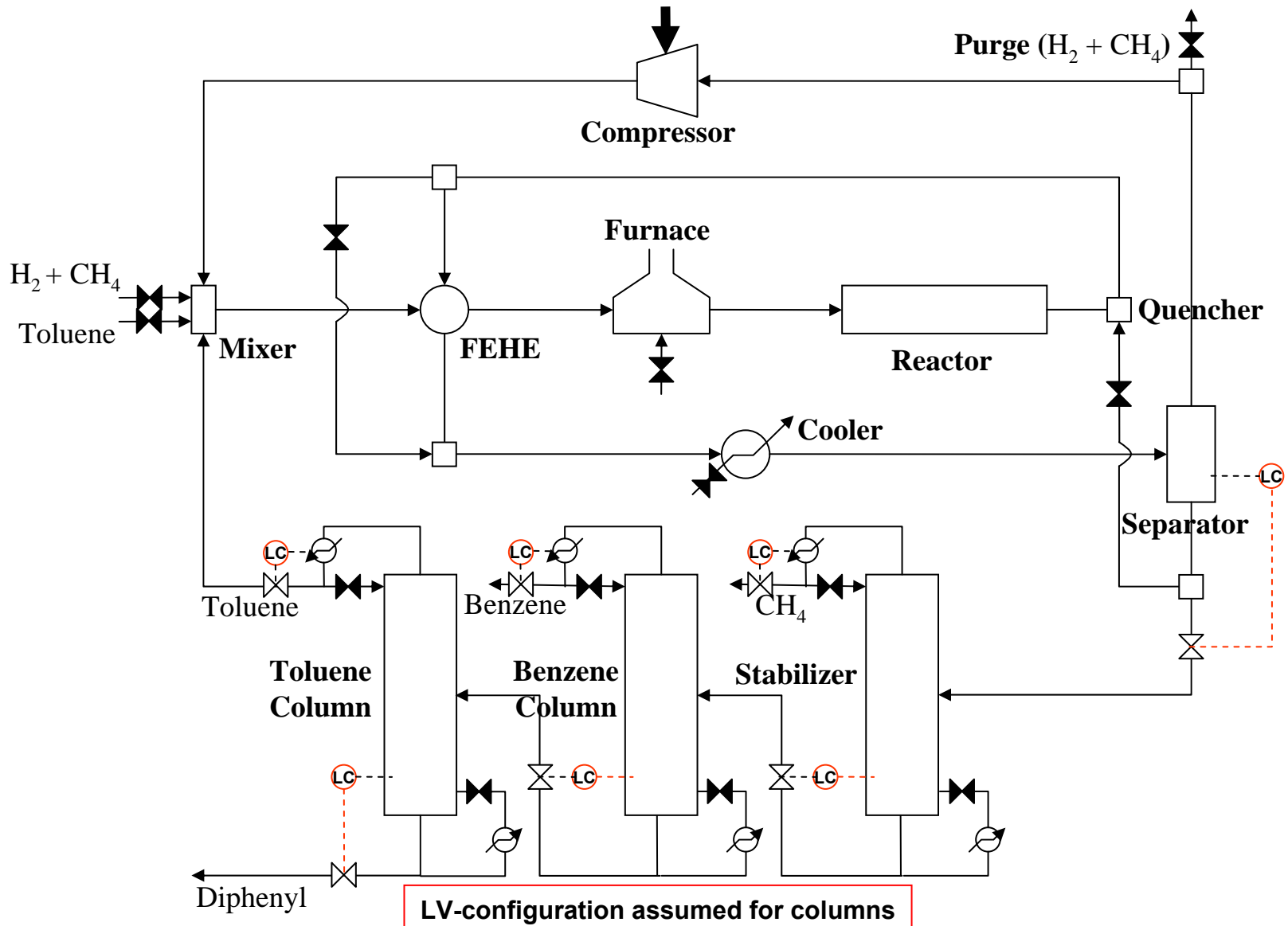


# Bottom-up design of control system

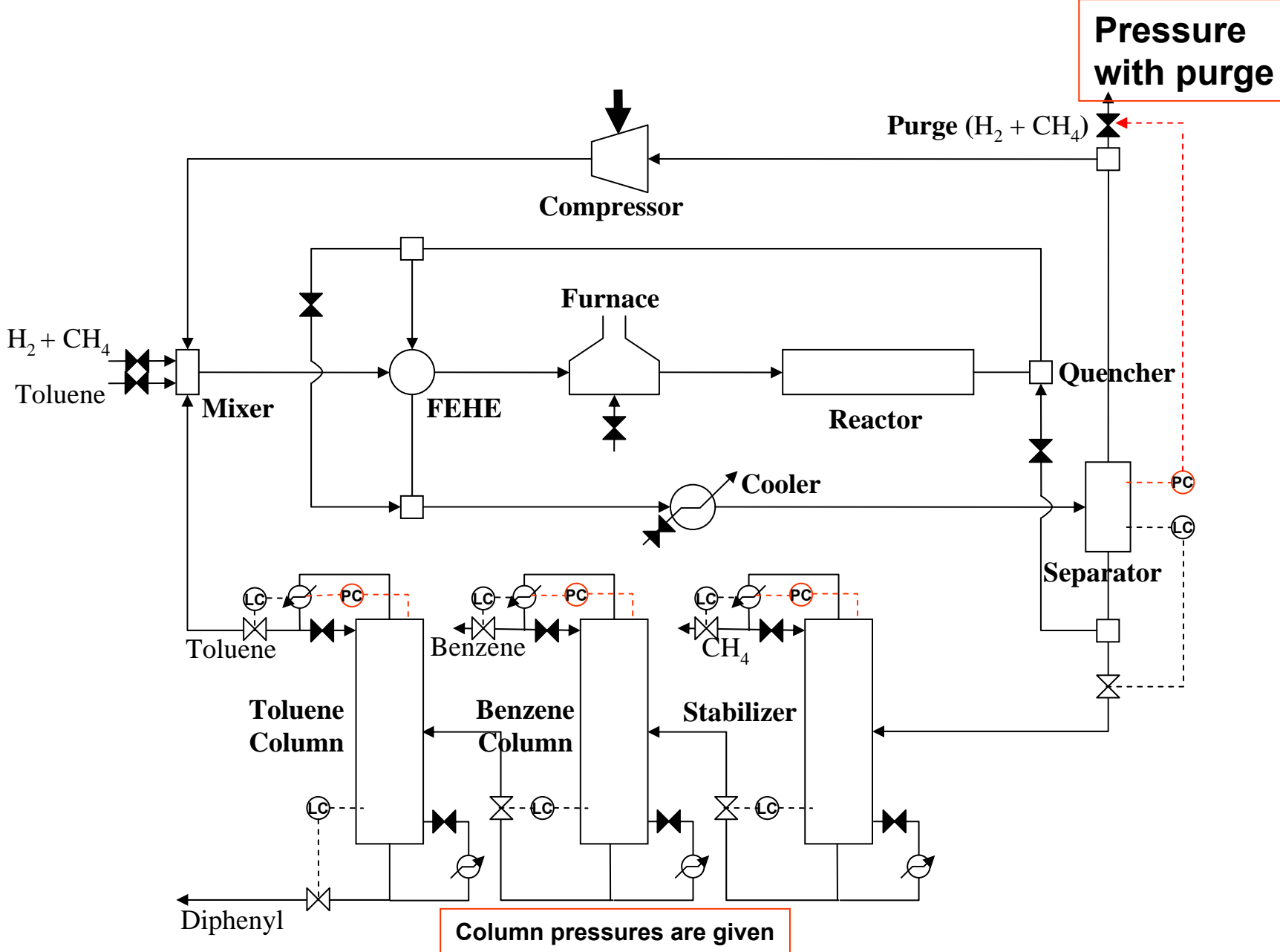
- Start with stabilizing control
  - Levels
  - Pressure
  - Temperatures
- Normally start with fastest loops (often pressure)
  - but let is start with levels

# “Bottom-up”: Proposed Control Structure

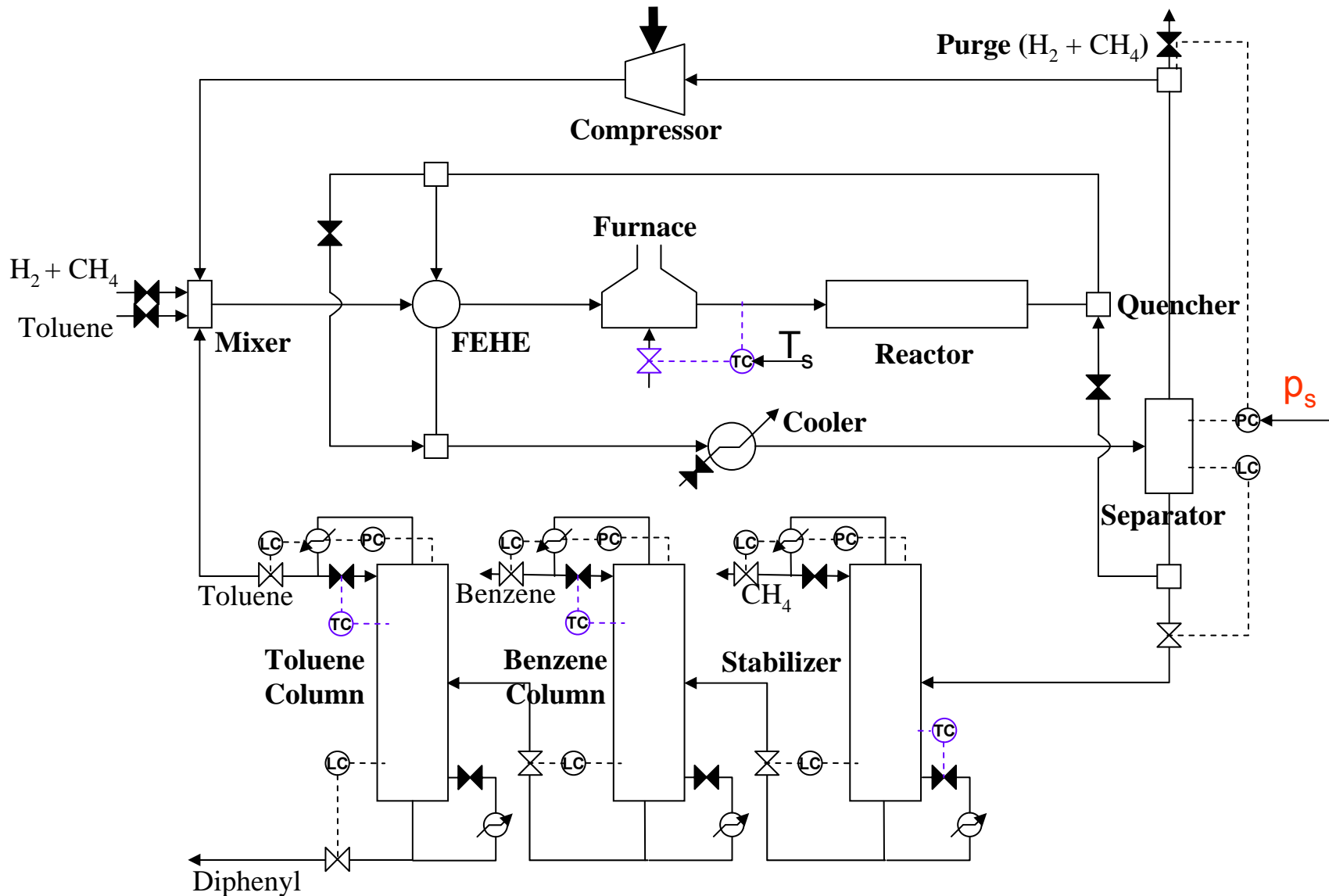
## Stabilizing Control: Control 7 liquid levels



# Avoiding "Drift" I – 4 Pressure loops

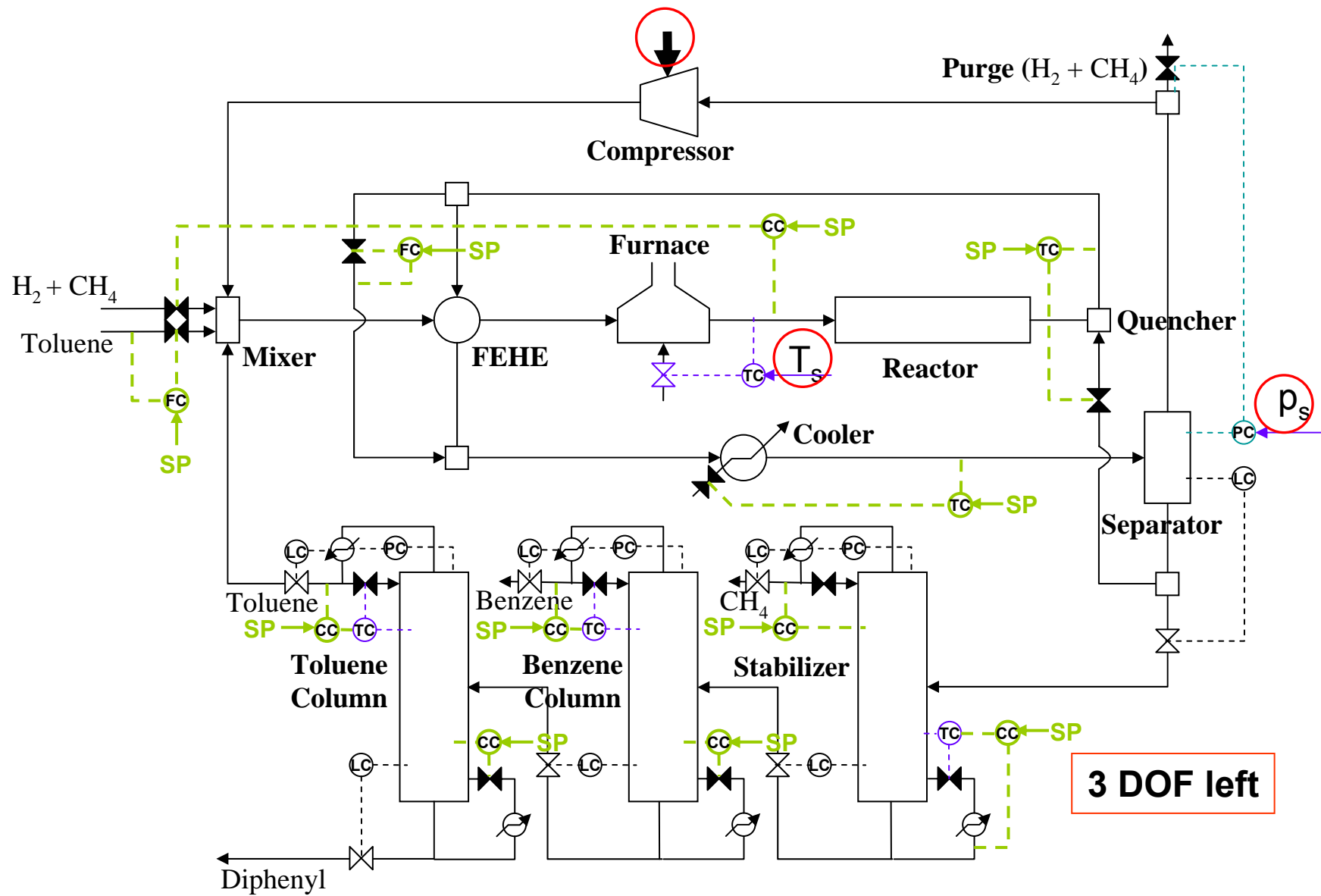


# Avoiding "Drift" II – 4 Temperature loops



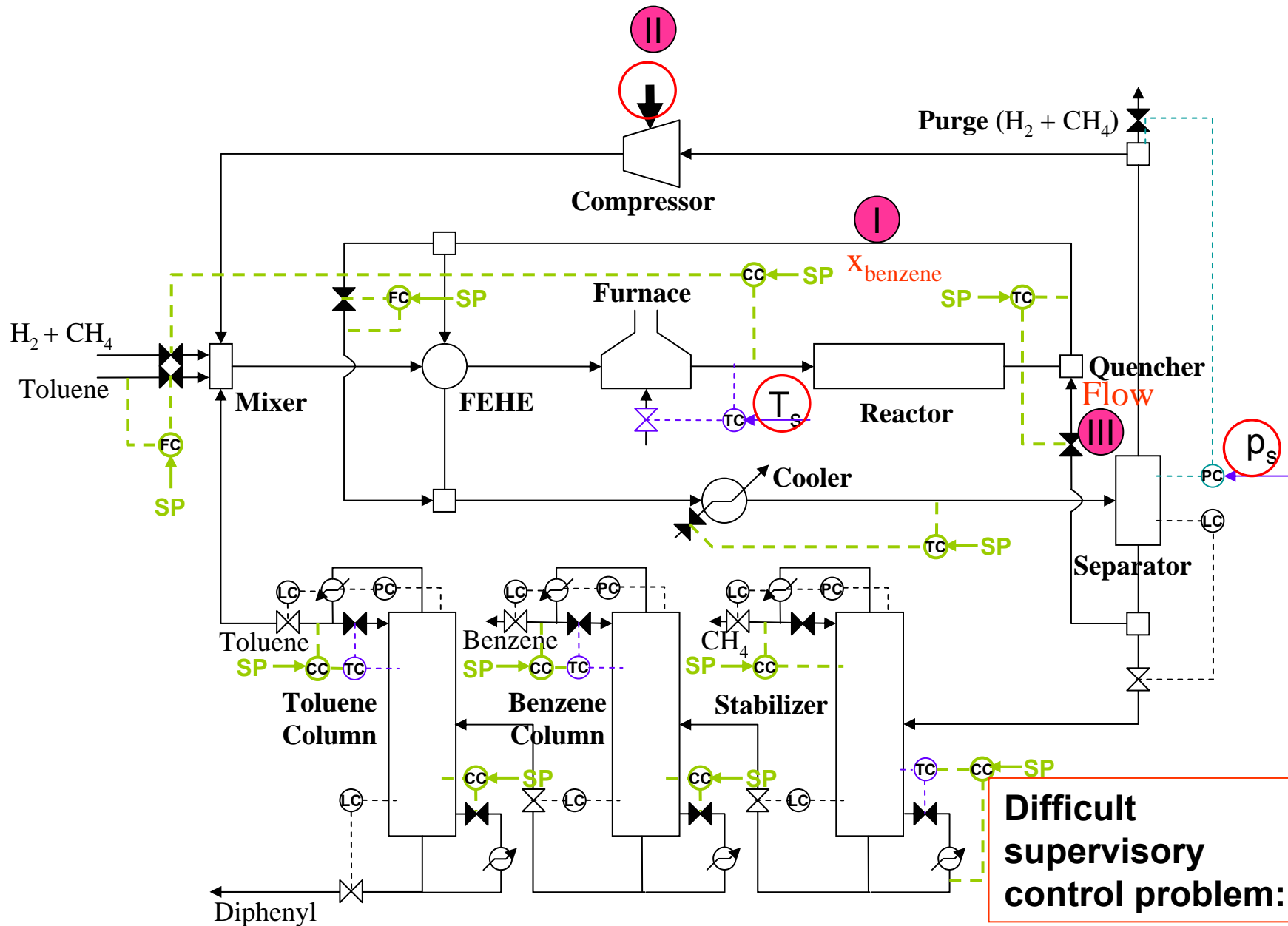
Now suggest pairings for  
supervisory control

# Control of 11 active constraints.

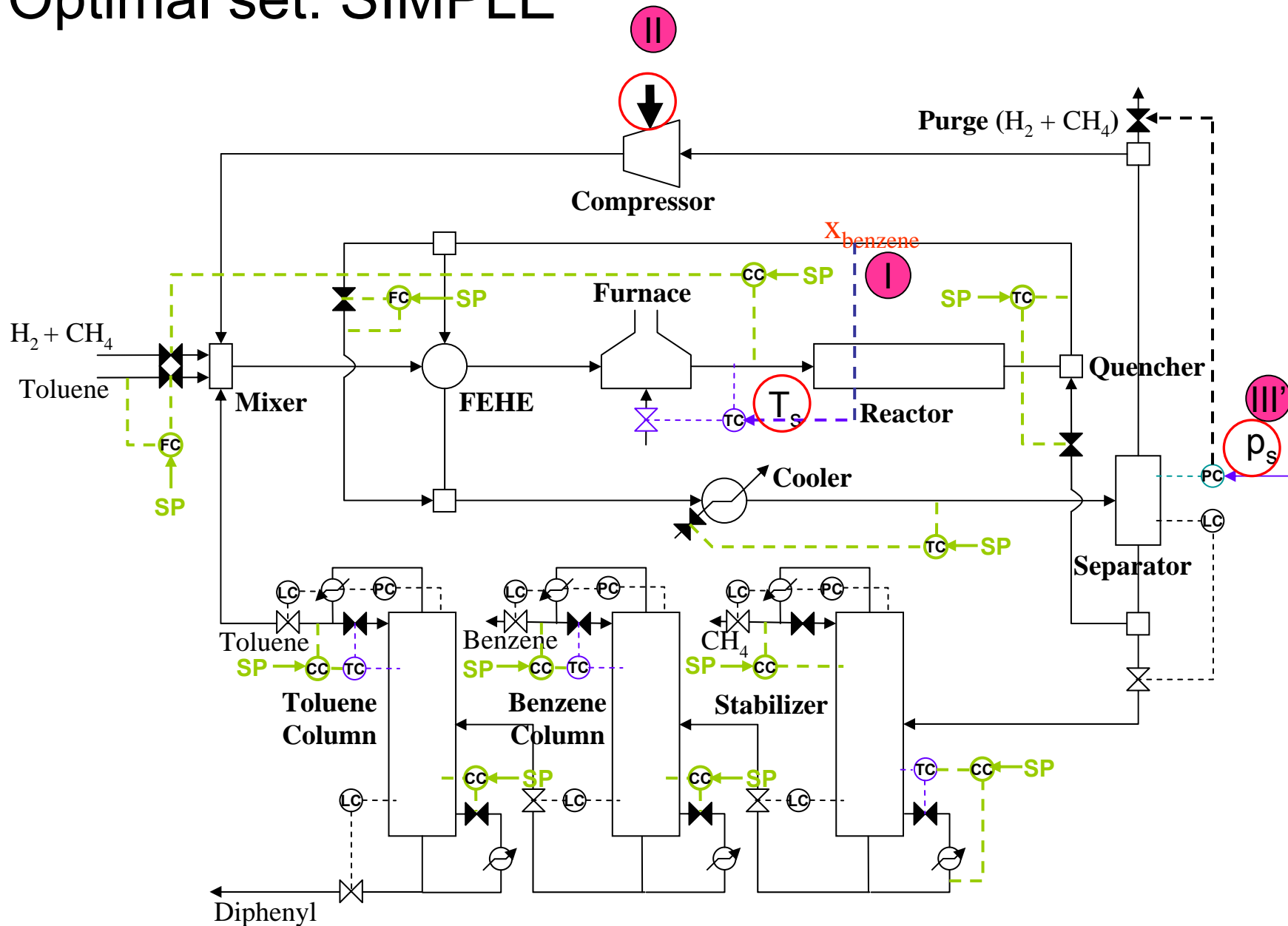


3 DOF left

# Control of 3 self-optimizing variables: Optimal set



# Control of 3 self-optimizing variables: Near-Optimal set: SIMPLE





# Conclusion HDA

- Follow systematic procedure
- May want to keep several candidate sets of “almost” self-optimizing variables
- Final evaluation: Non-linear steady-state simulations + Dynamic simulations