LAB7: Report guidelines and Conclusion

Project recap and final considerations

Process Systems Engineering A – Prof. Davide Manca

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Lab

PROJECT RECAP

Conceptual Design – Hierarchy of decisions

If the potential of the i-level is greater than zero, the process may be economically attractive; vice versa, the process is not economically interesting and the procedure must be interrupted.

- **EP1**: Batch vs Continuous
- **EP2**: Input-Output structure of the flowsheet

$$EP_2 = \sum_{j=1}^{NPRODUCTS} €_{P,j} \cdot \dot{n}_j - \sum_{i=1}^{NREACTANTS} €_{R,i} \cdot \dot{n}_i$$

- **EP3**: Recycle structure of the floowsheet

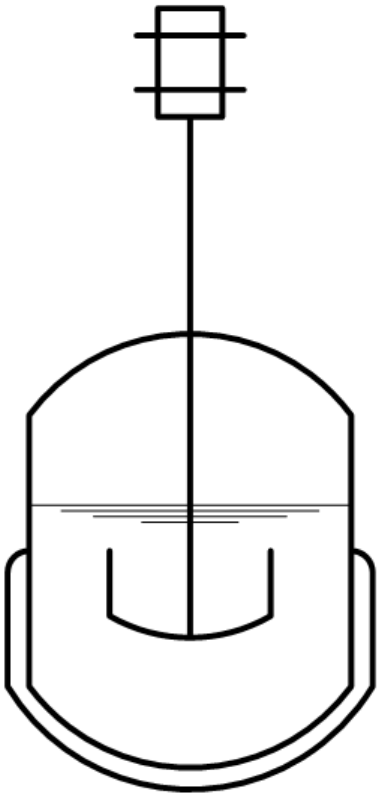
$$EP_3 = EP_2 - €_{reatt} - €_{compr}$$

- **EP4**: General structure of the separation system

$$EP_4 = EP_3 - \left(CAPEX + OPEX\right)_{separation\ section}$$

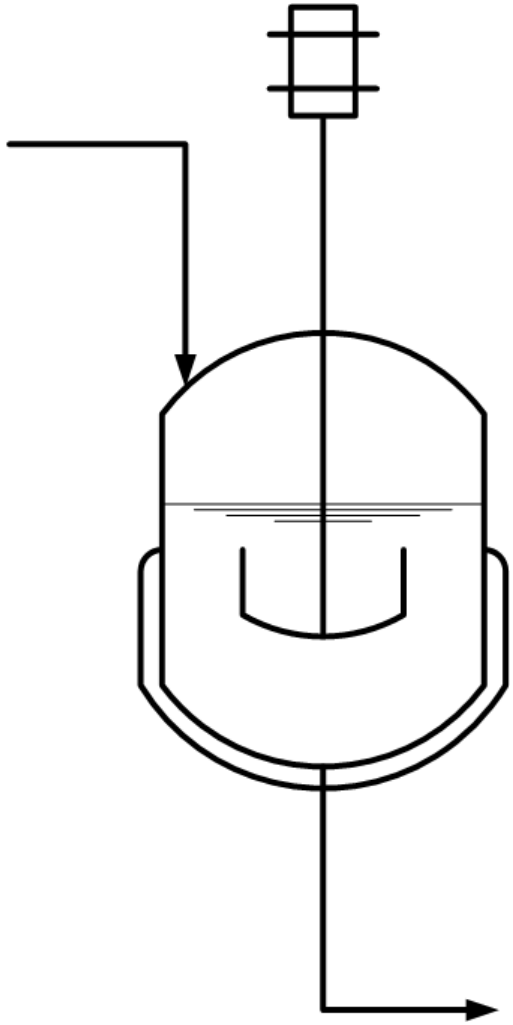
- **EP5**: Heat Exchange Network (not discussed for HDA plant)

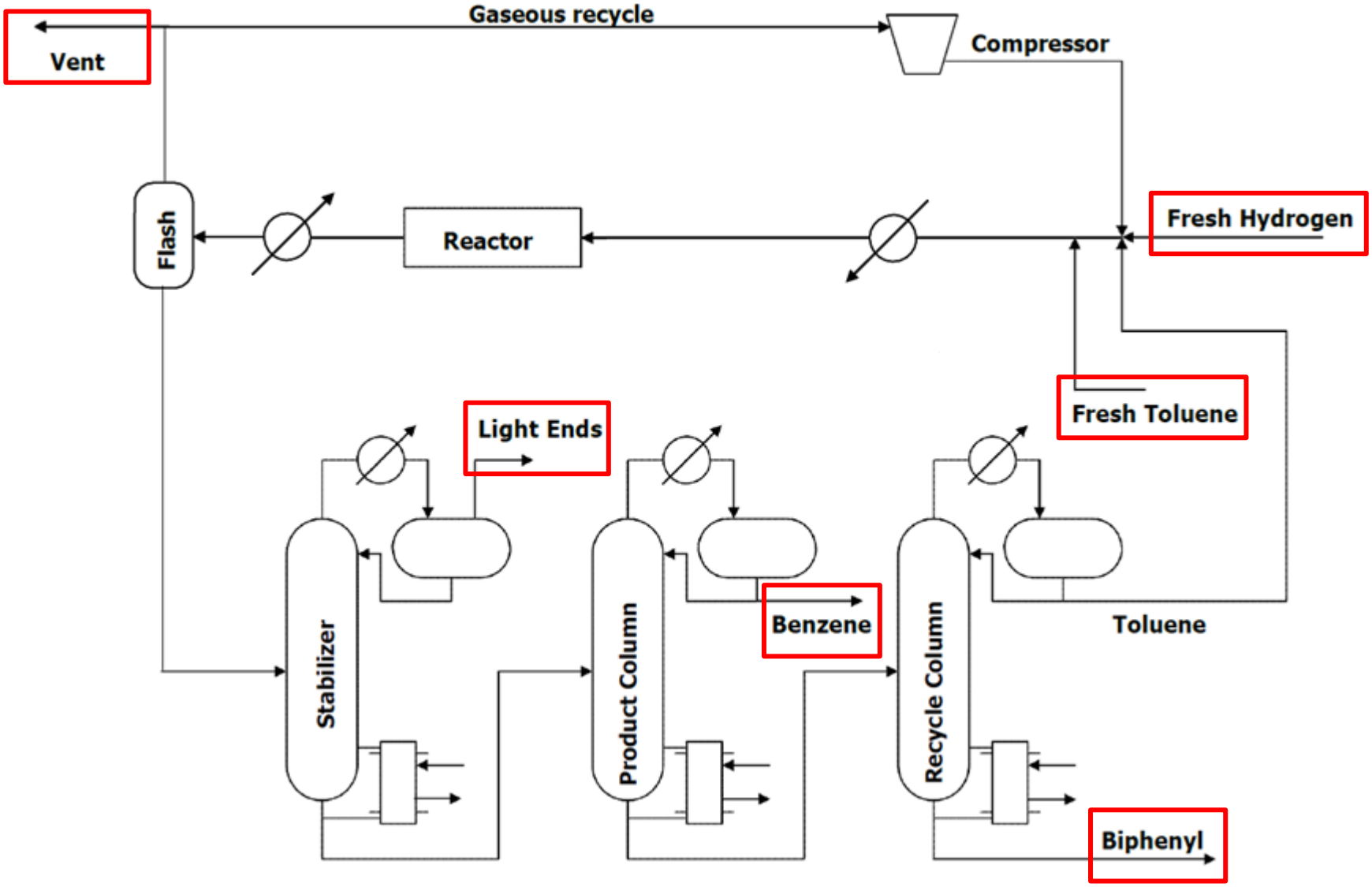
BATCH PROCESS

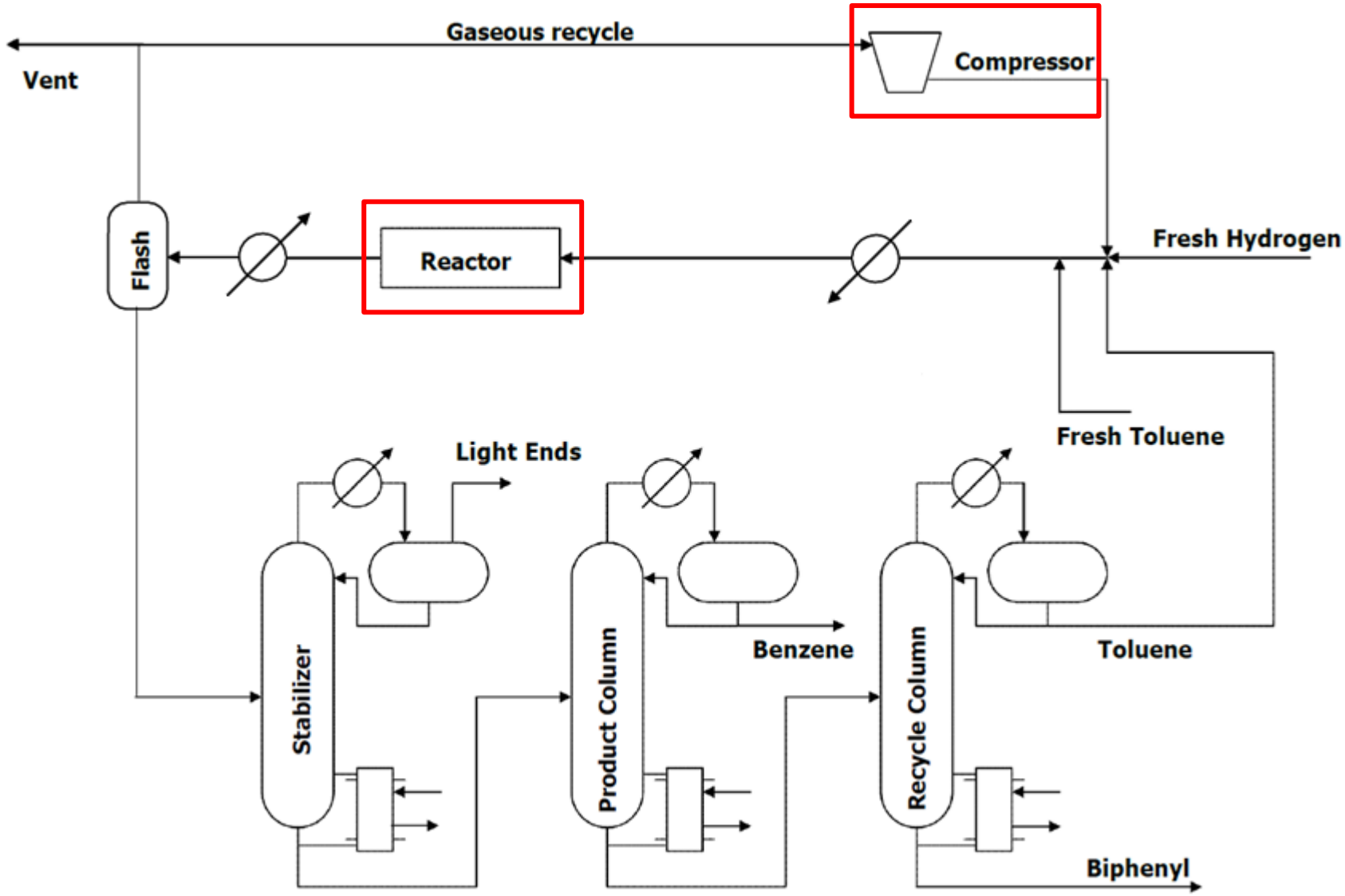


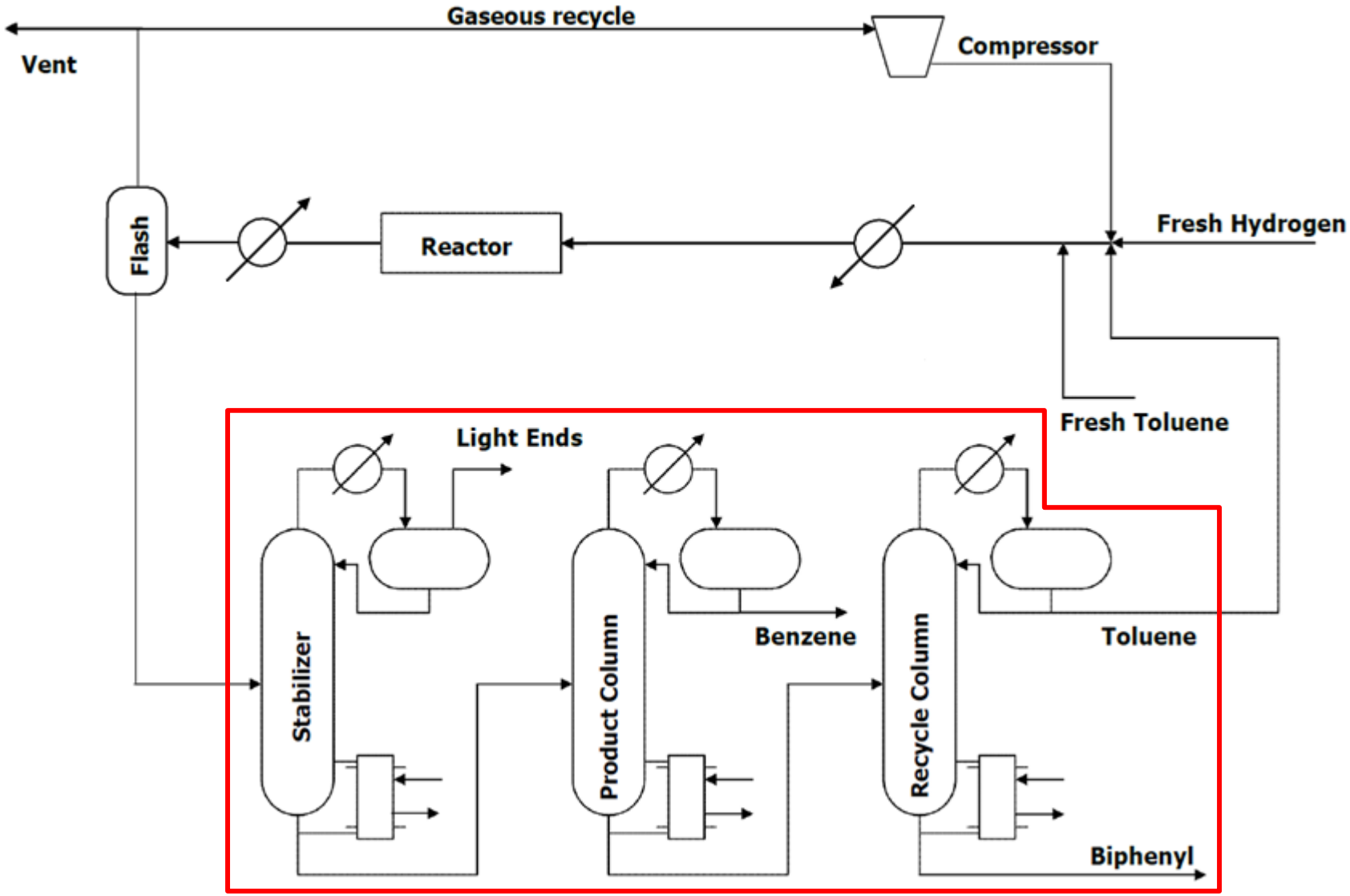
VS

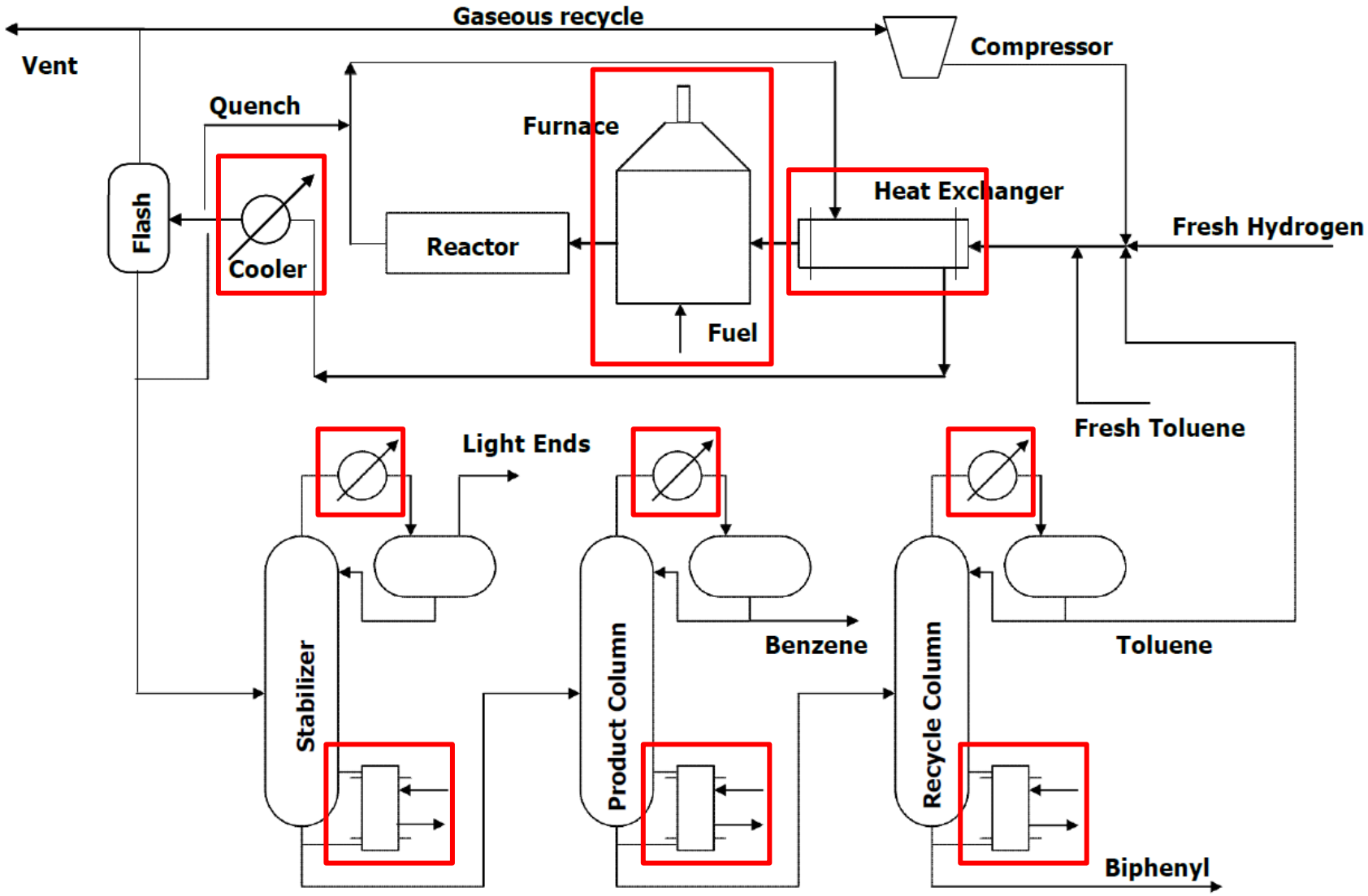
CONTINUOUS PROCESS




Gaseous recycle
Vent
Compressor
Flash
Reactor
Fresh Hydrogen
Fresh Toluene
Light Ends
Stabilizer
Product Column
Benzene
Recycle Column
Toluene
Biphenyl


Gaseous recycle
Vent
Compressor
Flash
Reactor
Fresh Hydrogen
Fresh Toluene
Light Ends
Stabilizer
Product Column
Benzene
Recycle Column
Toluene
Biphenyl


Gaseous recycle
Vent
Compressor
Flash
Reactor
Fresh Hydrogen
Fresh Toluene
Light Ends
Stabilizer
Product Column
Benzene
Recycle Column
Toluene
Biphenyl


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

REPORT GUIDELINES

Report guidelines – Include the following (1/6):

- General overview of the HDA process/plant and the reactions involved
- EP1 decision: batch or continuous?
- Material balances and plant specifications, degrees of freedom analysis

LAB1

- Kinetic study results and diagrams:
  - Toluene flow rate (or concentration) vs. Residence time, at changing Temperature (T)
  - Benzene flow rate (or concentration) vs. Residence time, at changing T
  - Biphenyl flow rate (or concentration) vs. Residence time, at changing T
  - Conversion vs. Residence time, at changing T
  - Selectivity vs. Residence time, at changing T
  - Selectivity vs. Conversion, at changing T
  - Conversion vs. T, according to the specified selectivity
  - Residence time vs. T, according to the specified selectivity

LAB2

Report guidelines – Include the following (2/6):

- Adiabatic ΔT evaluation
  Discuss the isothermal assumption for the reactor
  Compare with the results from HYSYS/UniSim

LAB2

- <u>EP2 results and diagrams</u>:
  - Molar fraction of H_2 in the vent (x_V) vs. Split factor (SF), at changing T
  - EP2 vs. SF, at changing T
  - EP2 vs. x_V, at changing T

  evaluating EP2 for both burn/sell biphenyl scenarios

  - EP2 vs. T, at changing SF
  - EP2 vs. Conversion, at changing SF

  according to the best EP2 choice (burn OR sell)

LAB3

Report guidelines – Include the following (3/6):

- EP3 results and diagrams:
  - R molar flow vs. SF, at changing T
  - Reactor volume vs. SF, at changing T
  - Reactor diameter vs. SF, at changing T
  - Reactor CapEx vs. SF, at changing T
  - Compressor CapEx vs. SF, at changing T
  - Compressor OpEx vs. SF, at changing T
  - EP3 vs. SF, at changing T
    suggestion: also show the EP2 line(s) on the same diagram
  - optimum EP3 vs. T, according to the optimum SF for each T
    suggestion: also show the corresponding EP2 line on the same diagram

LAB4

Report guidelines – Include the following (4/6):

- HYSYS/UniSim process simulator results:
  - show the plant layout at one of the four investigated temperatures
  - in the layout, display (*show Table*) the reaction temperature and the split factor
  - in the layout, display (*show Table*) the values of the Adjust targets (HTR, selectivity, B)
    expected precision: approximately within 0.1% error
  - make sure the layout image in the report is readable and can be zoomed

LAB5

Report guidelines – Include the following (5/6):

- Separation section results:
  For each distillation column, show the main results at the investigated temperatures (e.g. in table form):
  - *Number of separation stages*
  - *Tray sizing: tray spacing, diameter, height*
  - *CapEx of vessel and internals*
  - *Reboiler and condenser duties and OpEx*
  - *Reboiler and condenser exchange areas and CapEx*
  - *Overall CapEx+OpEx*

- EP4 results and diagrams:
  - Separation section cost vs. T
  - EP4 vs. T
    ***requirement**: also show the corresponding EP2 and EP3 lines on the same diagram*

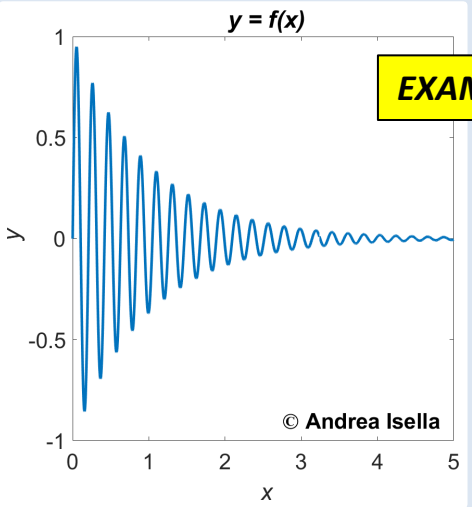
LAB6

Report guidelines – Include the following (6/6):

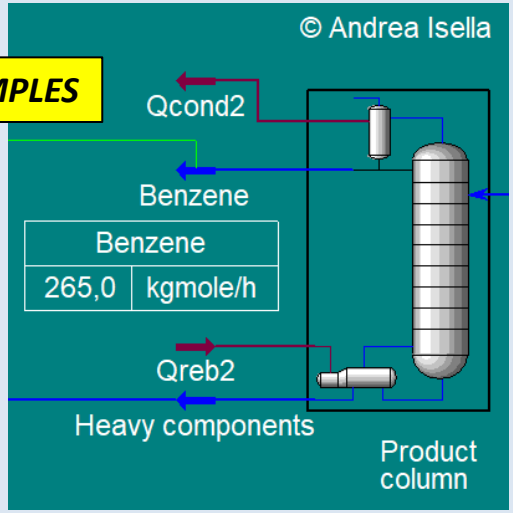
- MATLAB scripts and functions:
  All your MATLAB codes must be included in the report (at the end, as an *Appendix*)

- MATLAB/Excel figures and HYSYS/UniSim screenshots:
  All figures from MATLAB/Excel and screenshots from HYSYS/UniSim must include the last names of both groupmates.

  Add them directly in MATLAB (e.g. by *title* or *text*), Excel, and HYSYS/UniSim (e.g. by *Add text*), respectively: no post-processing additions are allowed.



EXAMPLES



FINAL REQUIREMENTS

Report guidelines – Recommendations:

For every result in the report:

- do not forget the units of measurement
- use a reasonable format and number of digits
- remember **how** you obtained it (e.g. the **assumptions** made and their **ranges of validity**)

For every plot in the report, don't forget to:

- add the x/y axes labels (*xlabel, ylabel*) and units of measurement
- show ranges that are meaningful and can be discussed
- make sure it is understandable
  - *if needed, add the title of the plot (title), e.g. to specify the temperature*
  - *if needed, add a legend of the curves (legend), e.g. to distinguish different lines*
  - *you can also use captions for figures and tables*
- reason about **how** you obtained it, **what** it shows/means, and **why**

DO NOT FORGET

ADDITIONAL STEPS

Additional steps

Possible additional steps, improvements, and results:

- **Improve** the **MATLAB calculations**
  e.g. consider recycles in the kinetics study (if you did not yet), or remove the isothermal reactor hypothesis (to evaluate how the reaction temperature evolves along the reactor length)
- **Improve** the **HYSYS/UniSim calculations**
  e.g. check the consistency of the split factor definition, or re-design the separation section until convergence
- **Update the EP2-EP3** calculations using the results from **HYSYS/UniSim**

  then in principle, we could also…
  - Perform the EP3 (or EP4) optimization vs. Split factor using HYSYS/UniSim

You might also think about…
- how to study the **dynamic EP** employing econometric models?
  e.g. for the EP4 optimum, studying different scenarios
- how to estimate the **EP5**?
  evaluate the furnace costs, describe the heat exchanger network, apply the Pinch technology...

EXAM RULES

Exam rules – Essential information:

The PSE-A final evaluation consists of an **oral exam** that comprises:

- *Practical part*: questions related to the HDA project (i.e. LAB1, LAB2, LAB3, etc.)
- *Theoretical part*: questions related to the theoretical lectures (i.e. L1, L2, L3, etc.)

To achieve the final mark, the candidate should pass **both parts**.

Remember to:

- **enroll** in the exam through **Online Services → Exams → Exams registration**
- bring with you a **printed copy** of the report on the day of the exam

It is **highly** recommended to take the exam together with your groupmate

FINAL SURVEY

THANK YOU