



LAB7 - Summary, Report Guidelines, Additional Steps and Conclusion

Process Systems Engineering – Master Degree Course

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PROJECT RECAP



HDA Process – Inlet and outlet flows

Toluene

Hydrogen



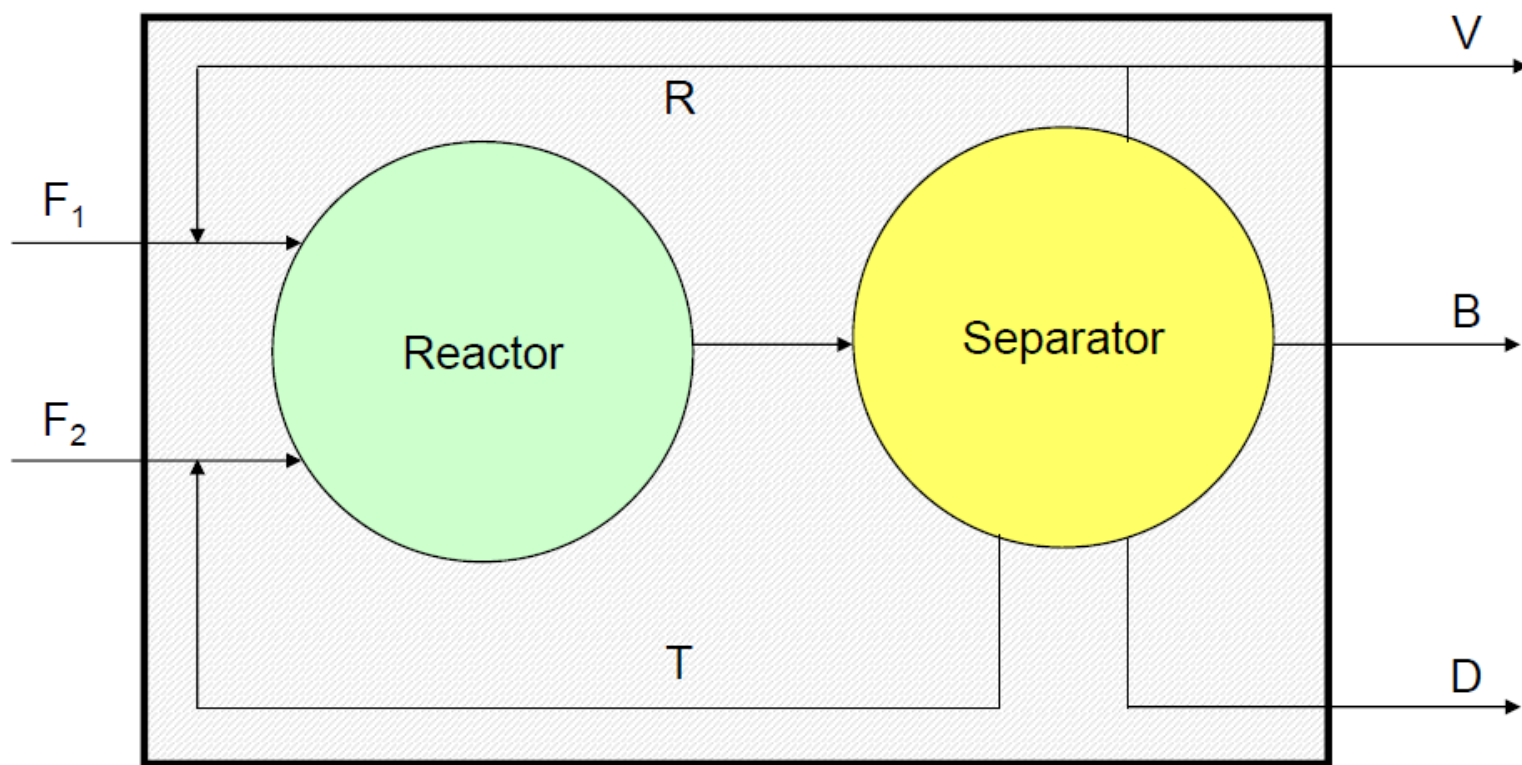
Benzene

Light Products

Heavy Products



HDA Process – Inlet and outlet flows, recycles





Conceptual Design – Hierarchy of decisions

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

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

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

$$EP_3 = EP_2 - \epsilon_{reatt} - \epsilon_{compr}$$



Conceptual Design – Hierarchy of decisions

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

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

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

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.



REPORT GUIDELINES

Report Guidelines – Include the following (1/5):

- 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 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 (2/5):

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

LAB2

- EP2 results and diagrams:
 - Split factor vs xv, at changing T
 - EP2 vs split factor, at changing T
 - EP2 vs xv, at changing T
 - EP2 vs T, at changing xv
 - EP2 vs conversion, at changing xv
evaluating EP2 if we burn or sell biphenyl

LAB3

Report Guidelines – Include the following (3/5):

- EP3 results and diagrams:
 - R flowrate vs xv, at changing T
 - Reactor volume vs xv, at changing T
 - Reactor diameter vs xv, at changing T
 - Reactor CAPEX vs xv, at changing T
 - Compressor CAPEX vs xv, at changing T
 - Compressor OPEX vs xv, at changing T
 - EP3 vs xv, at changing T
suggestion: also show the EP2 line(s) on the same diagram
 - optimum EP3 vs T, according to the optimum xv for each T
suggestion: also show the corresponding EP2 line on the same diagram



Report Guidelines – Include the following (4/5):

- 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

Report Guidelines – Include the following (5/5):

- Separation section results:

For each distillation column, show the main results at the investigated temperatures (e.g. in table form):

- *Number of separation stages, height*
- *Tray sizing and diameter, 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*

Report Guidelines – Recommendations:

For every result in the report:

- don't forget the units of measurement
- use a reasonable format and number of digits
- remember **how** you obtained it, the **assumptions** made and their **limits**

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

- add the x/y axes labels (*xlabel*, *ylabel*) and units of measurement
- show ranges which are meaningful and can be discussed
- make sure it's understandable
 - *if needed, add the title of the plot (title), e.g. to specify the temperature*
 - *if needed, add 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**

DON'T FORGET



ADDITIONAL STEPS



Possible additional steps, improvements and results:

- **Improve the MATLAB initial calculations:** consider methane in the kinetics study
This changes the starting values for the process simulator, and sets the split factor used, changing the final results
- **Improve the HYSYS/UNISIM calculations**
e.g. check the consistency of split factor definition, or re-design the separation section until convergence
- **Update the EP2-EP3 calculations** using 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**?
estimate the furnace costs, describe the heat exchanger network, apply the Pinch technology...



FEEDBACK



THANK YOU