Cyclohexane production process: hydrogenation of benzene

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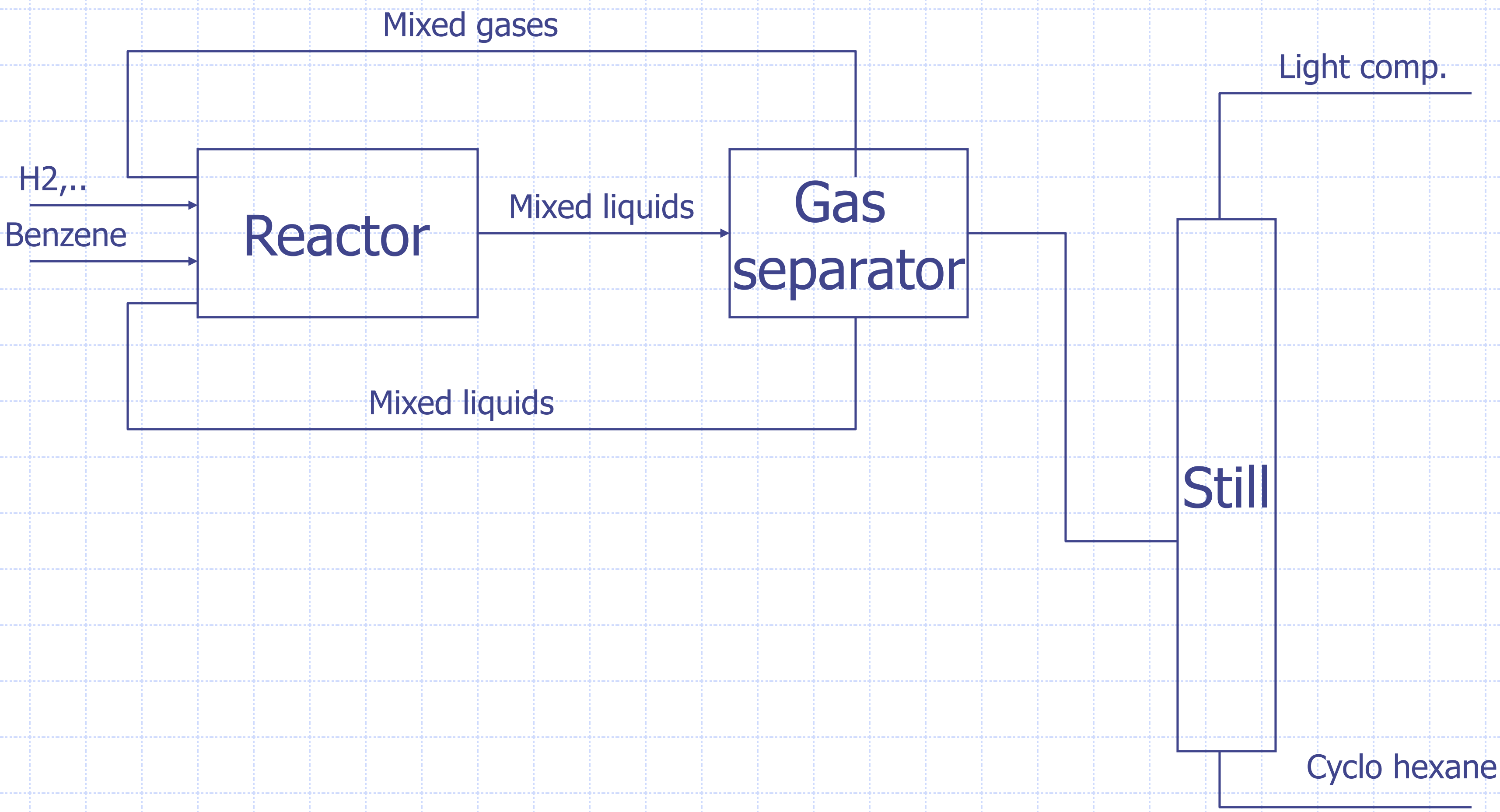
Agenda

- Import Aspen Properties data file
- CyC6 production process
  - without separation section
  - with a SEP block as separator
  - with a FLASH block as separator
  - with a COLUMN (Radfrac) block as separator
  - Entire process with sensitivity and Design specifications

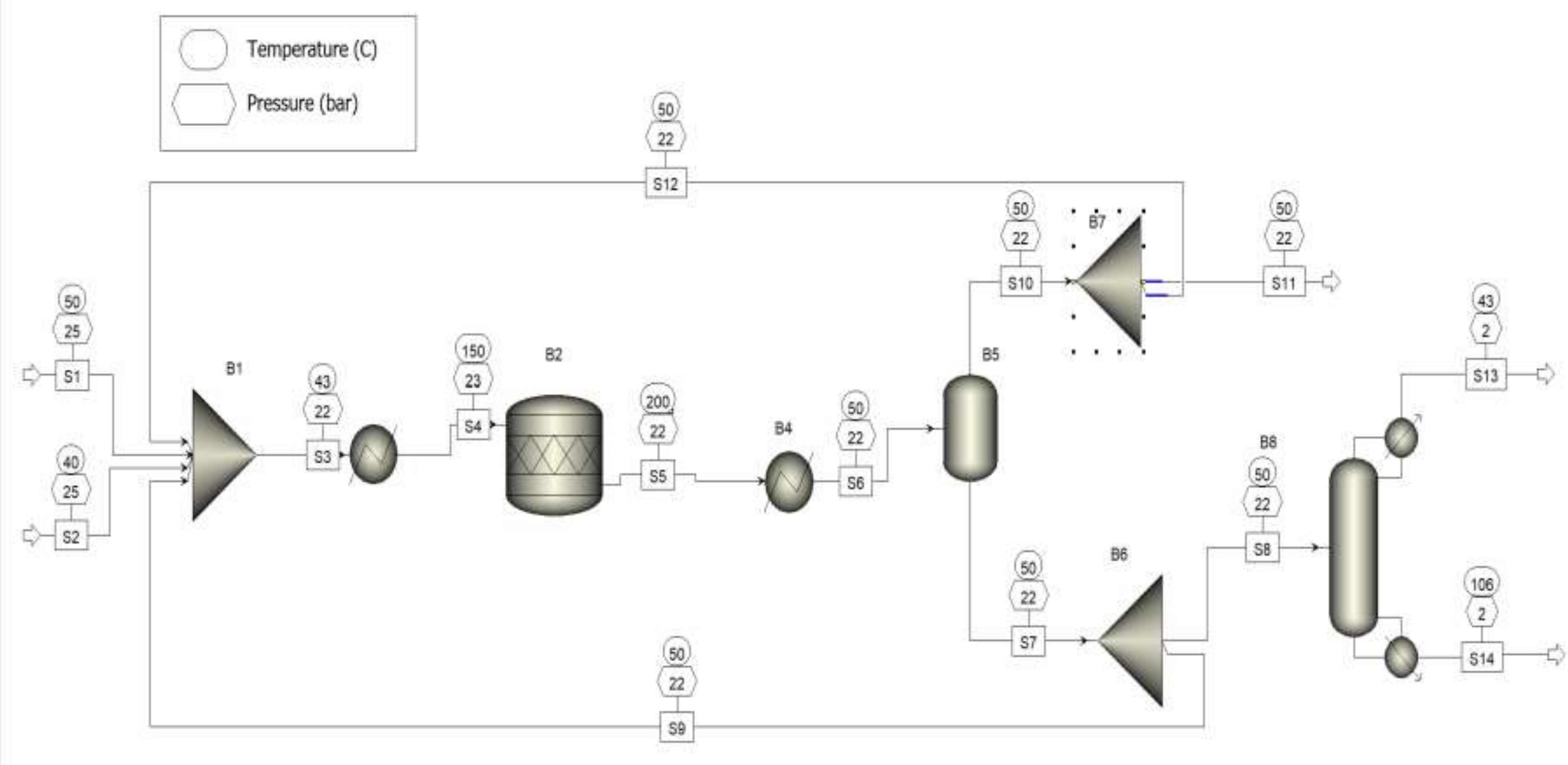
Block flow process diagram (BFD)

- Cyclo hexane production



Cyclohexane production process

- Reaction section $C_6H_6 + 3H_2 \rightarrow C_6H_{12}$
- Separation section



Introduction

- Cyclohexane is produced from catalytic hydrogenation of benzene
  - The conversion is high, but a recycle is necessary of both hydrogen and benzene
- Detailed objectives:
  - It is desired to obtain cyclohexane with high purity (>.998) in the product stream
  - It is desired to keep a maximum operating load of 4.7 Gcal/hr at the reactor (i.e. max duty at the reactor block)
  - It is desired to have a fixed flow rate of gas out from the top of the column (2.3 kmol/hr)
  - It is desired not to loose cyclohexane in the purge (max 0.3 kmol/hr)
  - It is desired to keep the inert concentration input at the reactor at less than 0.08 (mole fraction of CH_4 + N_2)

Simulation steps and prcocedure

- The following steps should be performed:
  - Verification of the thermodynamic data and models
  - Simulate the base case of the reaction section
    - with recycles and without CYC6 purification
  - Simulate the base case of the entire process with a simple model for the separation (SEP)
  - Simulate the base case of the entire process with a simple thermo model for the separation (FLASH)
  - Simulate the base case of the entire process with a rigorous distillation block (Radfrac)
  - Simulate the complete process with a distillation column
  - Add pumps, compressors to the process flowsheet to compensate for pressure drops

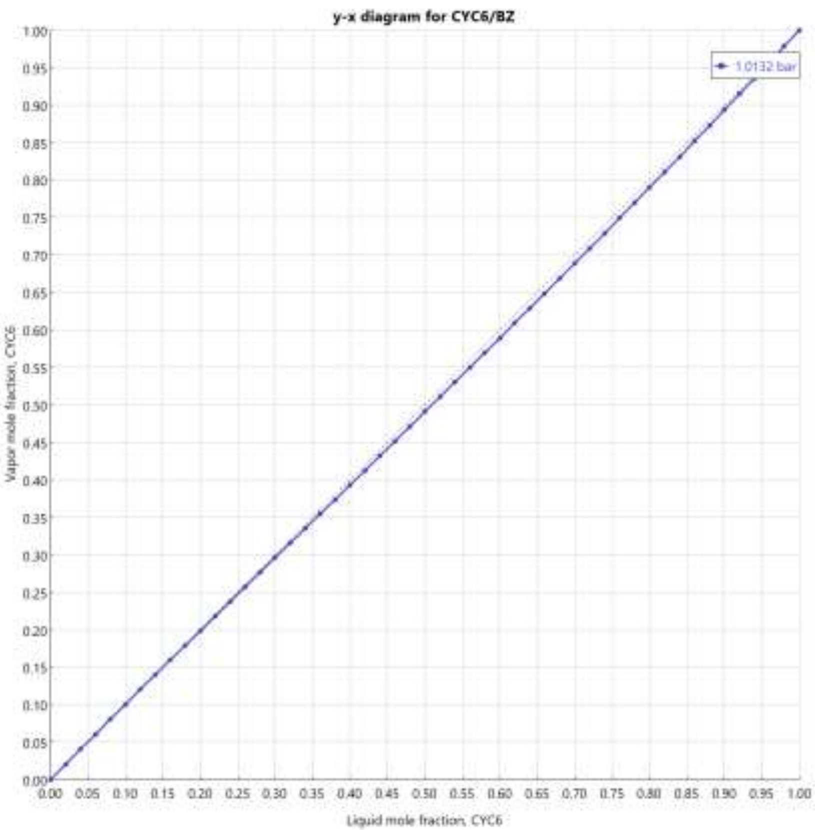
Properties and thermodynamic analysis

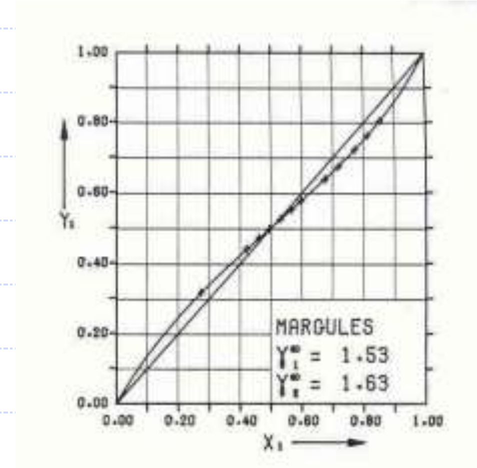
- Components:
  - Hydrogen, Nitrogen, Methane, Benzene, Cyclohexane
- Thermodynamic method:
  - RK-SOAVE
- Use Physical properties to:
  - Check liquid density, critical temperature and normal boiling point
  - Check vapor pressure for benzene and cyclohexane
  - Check VLE for Benzene – Cyclohexane
- Use literature data and data banks

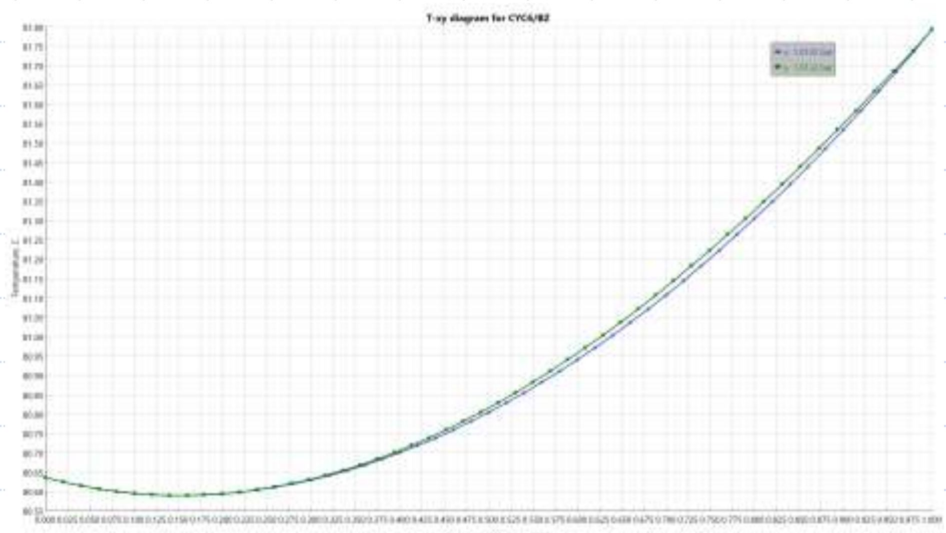
Components	Tc ^{0}F			Pc PSIA			T_{NB} ^{0}F		
	A+	PRO II	Lit.	A+	PRO II	Lit.	A+	PRO II	Lit.
CYCLOHEX	537.17	536.5	536.88	591.75	590.78	591.02	177.29	177.33	177.30
BENZENE	552.02	553.0	552.22	709.96	714.22	710.39	176.16	176.8	176.62
METHANE	-116.7	-116.7	-116.7	667.03	667.19	666.88	-258.68	-258.68	-258.74

Binary VLE cyclo hexane - benzene

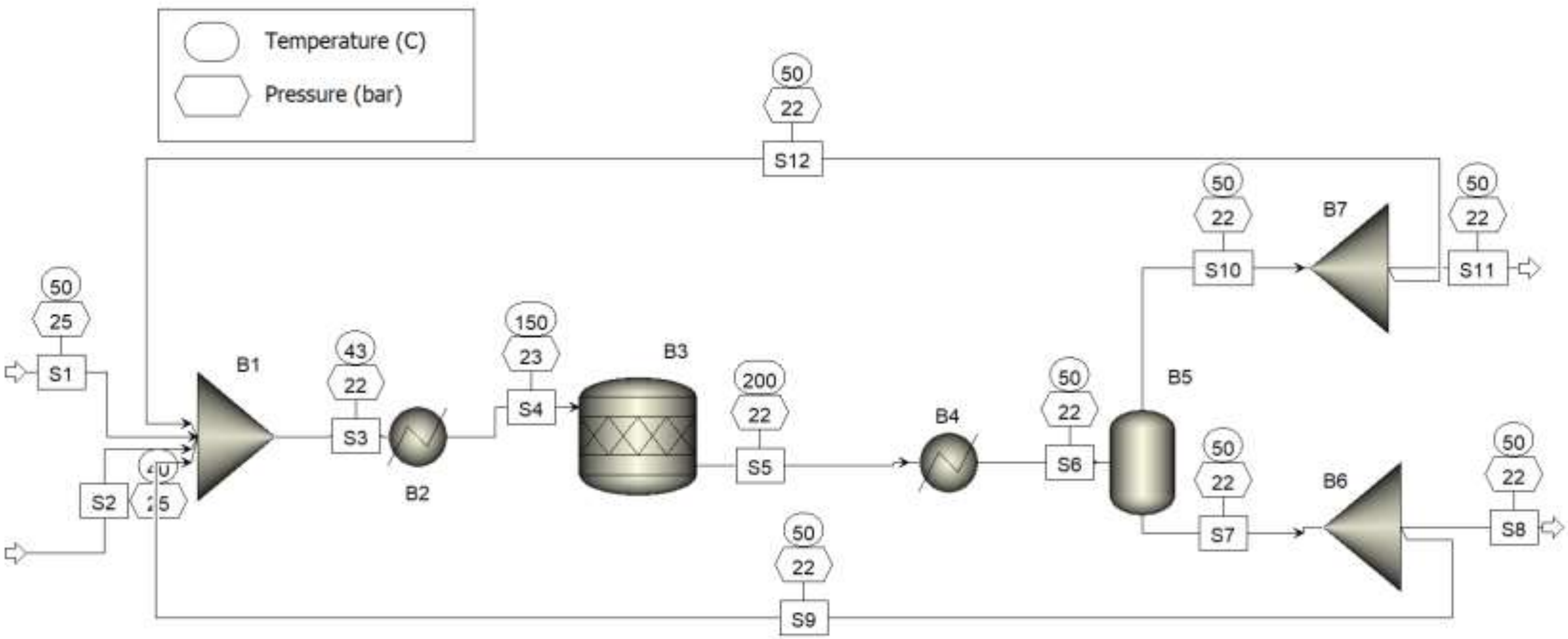
- Thermodynamic model: RKS







Reaction section with recycles



- Units: METCBAR
- Reaction is a catalytic hydrogenation with total conversion = 0.998
- Feeds:
  - H2IN: T=50 °C, P= 25 bar, Moleflow=330 kmol/hr, Mole-Frac: H_2 97.5%, N_2 0.5%, CH_4 2%
  - BZIN: T=40°C, P=25 bar, Benzene Moleflow =100 kmol/hr

Reaction section with recycles

- MIXER:
  - No specifications
- HEATER pre reaction
  - T=150°C, P=23 bar
- REACT:
  - Temperature 200 °C, Pressure drop: -1 bar
  - Conversion of 99.8% of benzene

$$C_6H_6 + 3H_2 \rightarrow C_6H_{12}$$

- RXCOOL:
  - Temperature 50 °C, Pressure drop: -0.5 bar
- HPSEP:
  - T=50°C, No Pressure drop
- VFLOW:
  - 92% of flow to recycle
- LFLOW:
  - 30% of flow to Recycle

Reaction section with recycles: sensitivity and design specifications

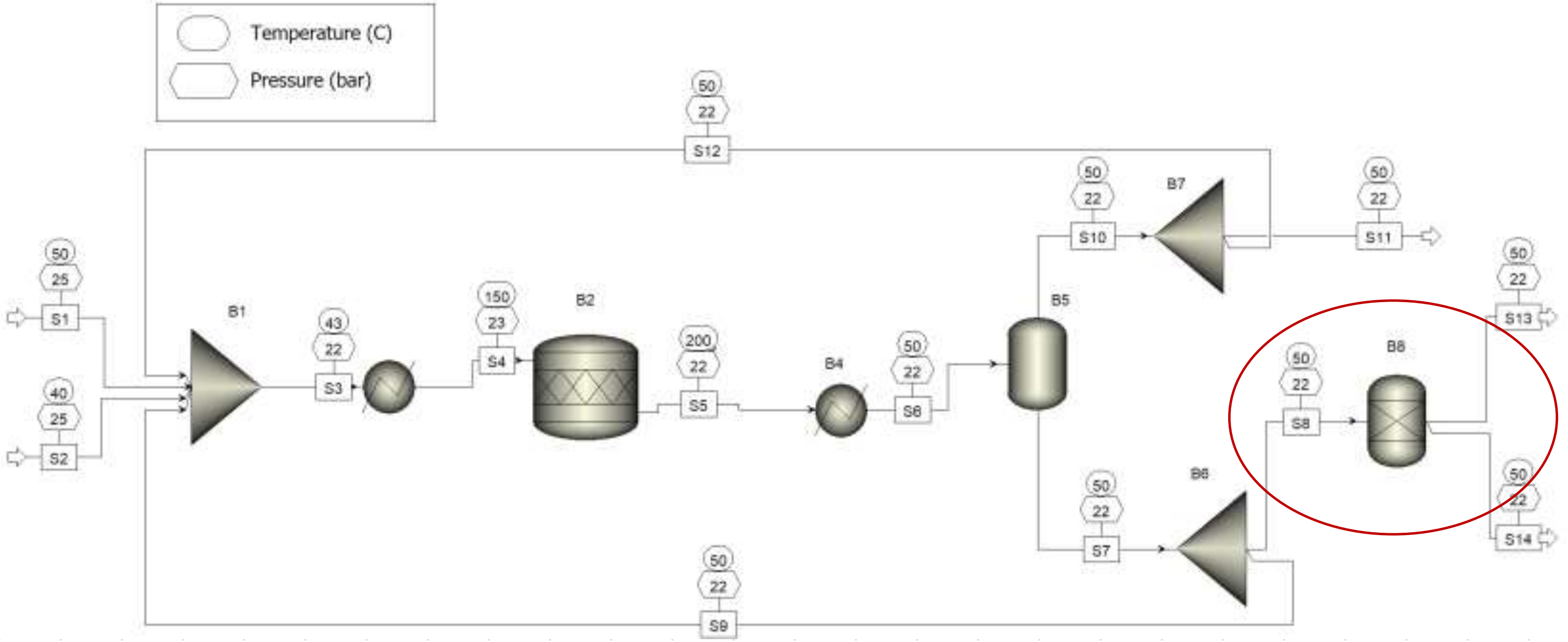
- Sensitivity Analysis
  - analyze the composition of the product stream and the NET-DUTY in the reactor
  - varying the recycle split fraction of LFLOW from 10 to 50%
- Design specification
  - The reactor cooling system can handle a maximum operating load of 4.7 Gcal/hr.
  - Using a design specification, determine the amount of cyclohexane recycle necessary to keep the cooling load on the reactor to this amount
- Results:
  - Sensitivity analysis: range of independent variable 0.1-0.2
  - Design specification output SplitFraction = 0.166678 gives Net-Duty = 4.7073 Gcal/hr

Results | Status

Variable	Initial value	Final value	Units
MANIPULATED	0.166678	0.166678	
COOLING	-4.7073	-4.7073	GCAL/HR

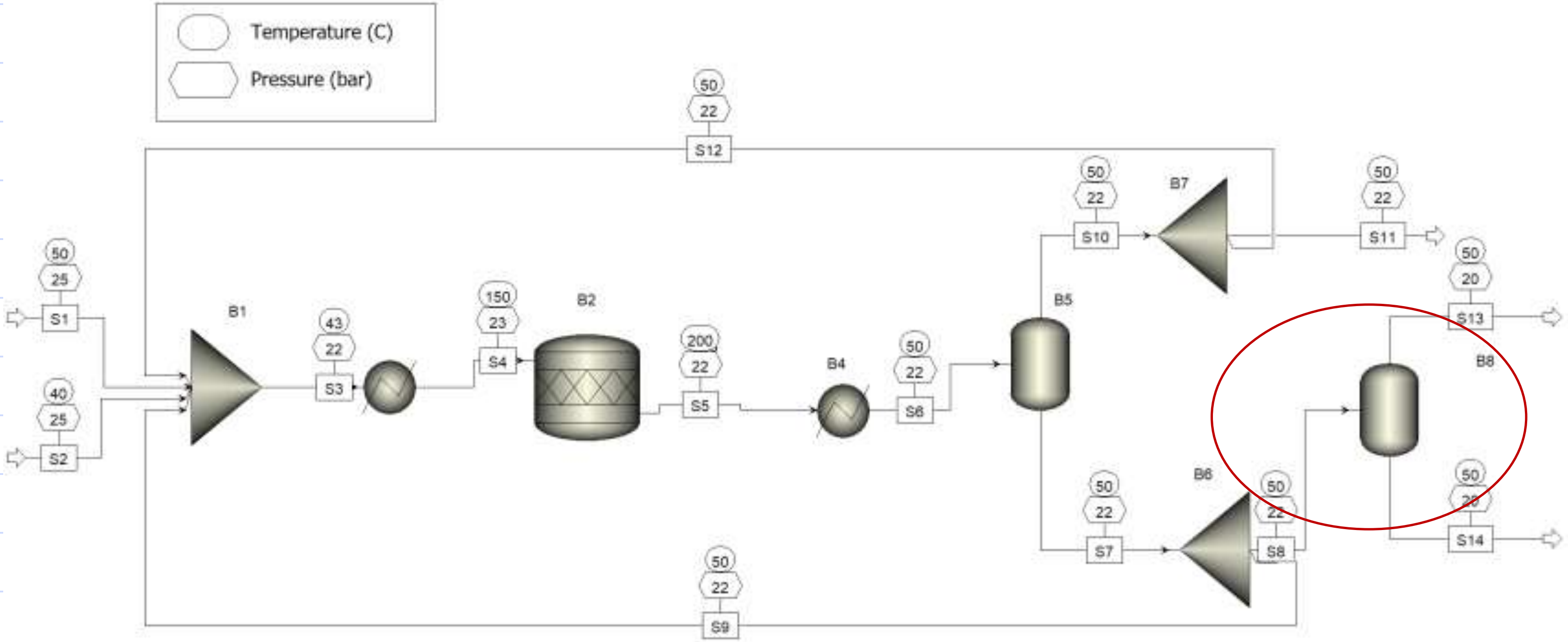
Separation section: SEP block

- Starting from the previous run, add e SEP block after the liquid product from the FLASH
  - fix liquid recycle = .166
- SEP specifications
  - Split Fractions in overhead: H_2=1, N_2=1, CH_4=0.8
  - Split Fractions in bottom: Benzene=1, CyC6=1
- Check X CYC6 at the bottom
  - if > .998 (no, it is .99575) with Heat duty at the reactor = - 4.70 Gcal/hr



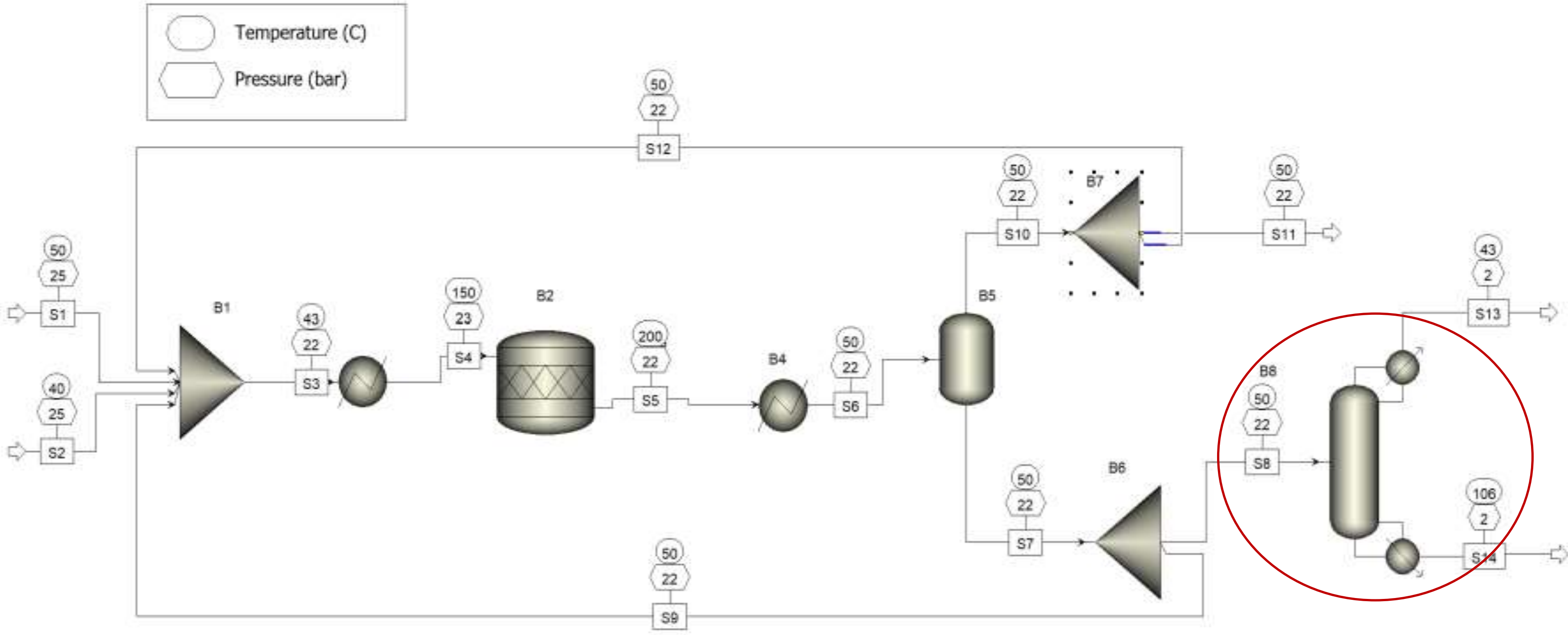
Separation section: FLASH block

- Starting from the previous run, substitute the SEP block with a FLASH
  - Keep liquid recycle = .166
  - FLASH specifications: T=50°C, Pressure drop = 2 bar
- Check X CYC6 at the bottom
  - if > .998 (no, it is .9770)
- Run Sensitivity:
  - Vary Flash T and tabulate X CYC6 in the bottom
  - T should be low (at 30°C X= 0.9776) but it is not sufficient



Separation section: RADFRAC block

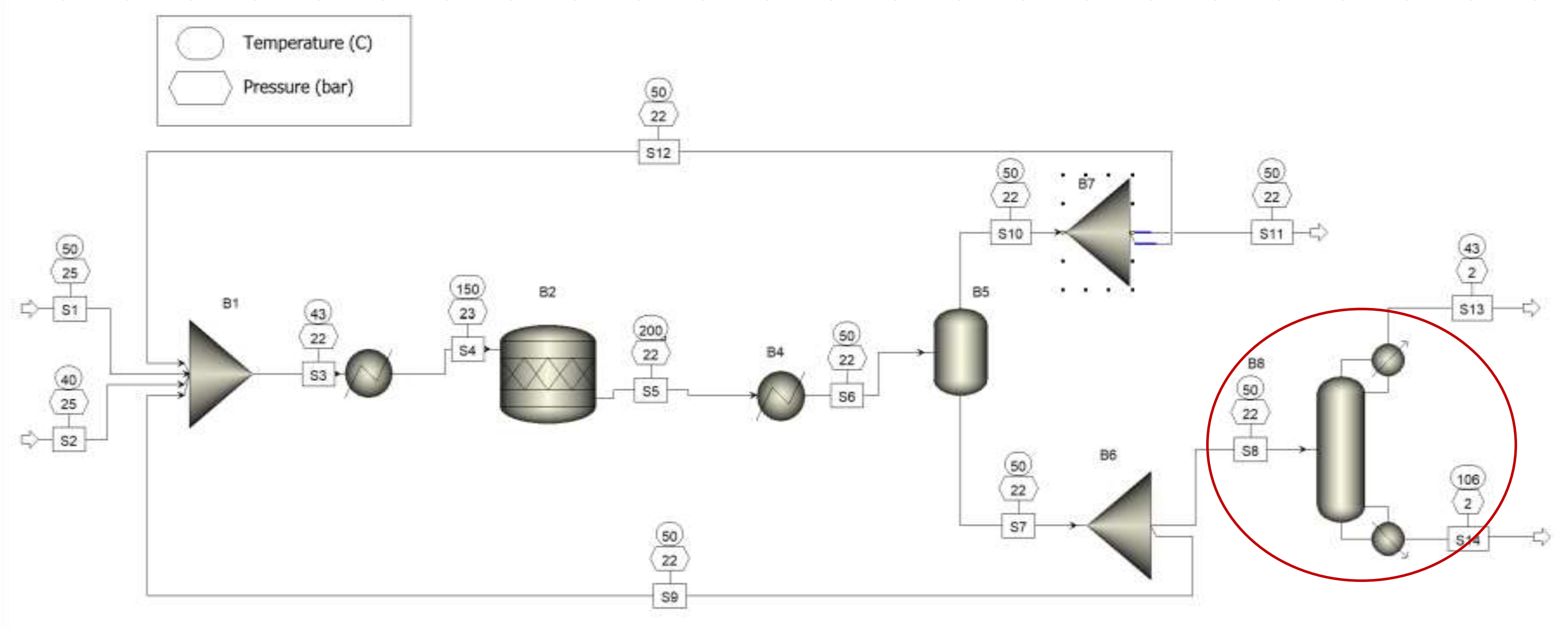
- Starting from the previous run, substitute the FLASH block with a RADFRAC block
  - Keep liquid recycle = .166



Separation section: RADFRAC block

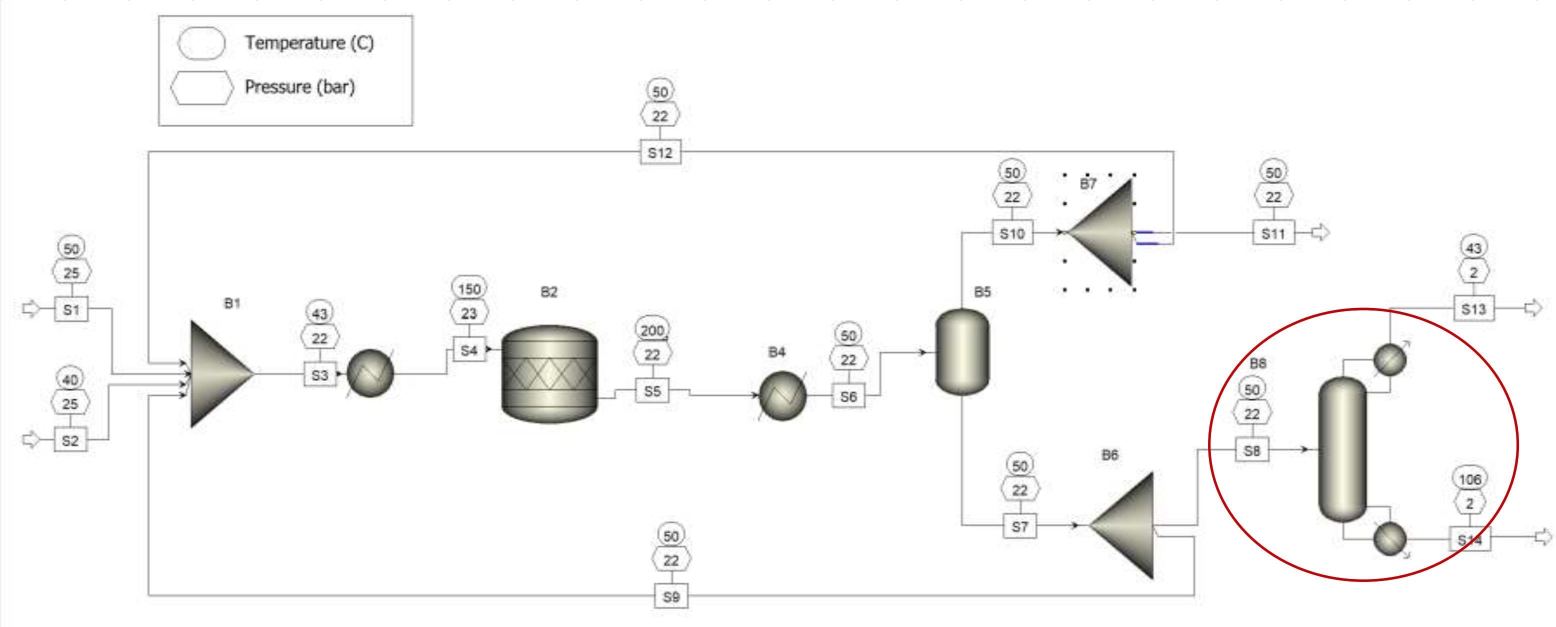
- Column specification:
  - Number of stages: 20
  - Feed at stage 10
  - Top tray pressure: 2 bar, no pressure drop
  - Reboiler: kettle
  - Condenser: partial (vapor phase top product)
  - Reflux ratio: 1.5
  - Distillate rate (vapor): 2.3 kmol/hr

- Check X CYC6
  - X cyc6 at feed and bottom of column
  - if cyc6 bottom > .998 (ok, it is .99846)
  - Liquid recycle split (0.166)
  - Cooling spec. at reactor (-4.7 Gcal/hr)



Separation section: RADFRAC block

- Relevant results:
  - Flash Temperature = 50°C
  - Purge split fraction = 0.8%
  - Purge emission: 29 kmol/hr with 1.8% mole CYC6
  - Molar flow rate of CYC6 in the bottom = 98.9987 kmol/hr
  - CYC6 purity in the bottom = 0.99846 mole fraction
  - Cyclohexane recovery (S14/(S14+S13+S11))
  - Cyclohexane recovery = 98.99 /(98.99+0.31+0.53) = 0.9916 %



Entire process analysis

- Starting from the previous run with RADFRAC
  - fix liquid recycle =.166
  - Keep specifications of the column as obtained in previous run
- Objectives for the entire process
  - Purity of cyC6 bottom of the distillation column of > 0.998 mole fraction
  - Study the sensitivity of the process to
    - Flash temperature
    - Vapor phase purge
  - And identify the parameters
    - not to loose cyclohexane in the purge (max 0.3 kmol/hr)
    - to keep the inert concentration at the reactor < 0.08 (mole fraction of $CH_4 + N_2$)
- Sensitivity on FLASH temperature
  - VARY Flash T
  - TABULATE: x and F cyC6 in product and F cyC6 in purge
  - TABULATE: inert concentration at the reactor (mole fraction of $CH_4 + N_2$)
- Sensitivity on split fraction
  - VARY Vapor phase purge (split fraction)
  - TABULATE: inert concentration at the reactor (mole fraction of $CH_4 + N_2$)

Entire process analysis

- Objectives for the entire process
  - Purity of cyC6 bottom of the distillation column of > 0.998 mole fraction
  - Reduce cyclohexane in the purge
  - keep inert concentration at the reactor < 0.08 (x CH_4 + x N_2)
- Design specification on FLASH temperature
  - VARY: Flash T
  - SPEC: mol fraction of CYC6 in purge =0.01
- Design specification on vapor purge
  - VARY: Vapor phase purge (split fraction)
  - SPEC: inert concentration at the reactor (x CH_4 + x N_2) = 0.08

Final results of the simulation

- Objectives
  - Reactor cooling capacity maximum 4.7 Gcal/hr
  - Purity of cyC6 bottom of the distillation column of > 0.998 mole fraction
  - Flow rate of distillate = 2.3 kmol/hr
  - Maximum amount of CYC5 in purge = 0.3 kmol/hr
  - Maximum inert concentration input to reactor = 0.08 mole fraction of CH_4 + N_2
- Final parameters
  - Liquid recycle split fraction =0.166
  - Flash Temperature= 34°C
  - Purge split fraction = 0.14
  - Purge emission: 28.77 kmol/hr with less than 0.01 mole fraction of CYC6
    - Corresponding to less than 0.3 kmol/hr of CYC6 lost in purge
  - Molar flow rate of CYC6 in the bottom = 99.26 kmol/hr
  - CYC6 purity in the bottom = 0.99836 mole fraction
  - Cyclohexane recovery (S14/(S14+S13+S11))
  - Cyclohexane recovery =99.27 /(99.27+0.29+0.28) = 0.994

Cyclohexane production process

- Complete the scheme by adding pumps, compressors and tanks.
  - Pumps and compressor to compensate for pressure drops
  - Valve to perform pressure reductions