Sensitivity Analysis & Design Specifications

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Agenda

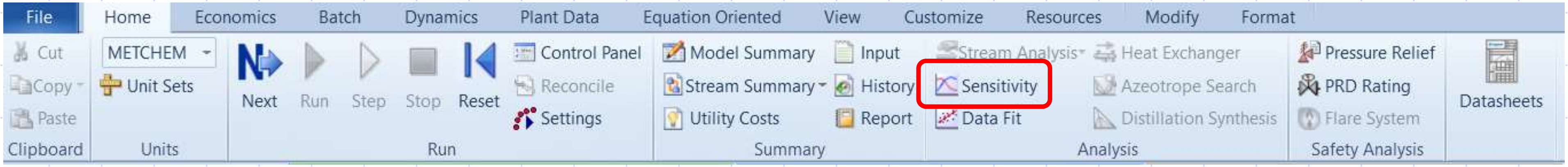
- Sensitivity analysis
  - Procedure
  - Results
  - Plots
- Case studies
- Design specifications
  - Definitions
  - Convergence
- Examples

Objectives

- Use sensitivity analysis to study the relationships between process variables
- Finding and selecting process variables
- Use case studies to run several simulation cases
- Studying and visualize the effect of changes in input variables on process (model) outputs
- Verifying that a solution to a design specification is feasible
- Rudimentary optimization

Sensitivity Analysis in A+

- Located in Navigation Pane | Model Analysis Tools | Sensitivity
- Allows user to study the effect of changes in input variables on process outputs
- Results can be viewed by looking at the Results form in the folder for the Sensitivity block
- Plot results to easily visualize relationships between different variables

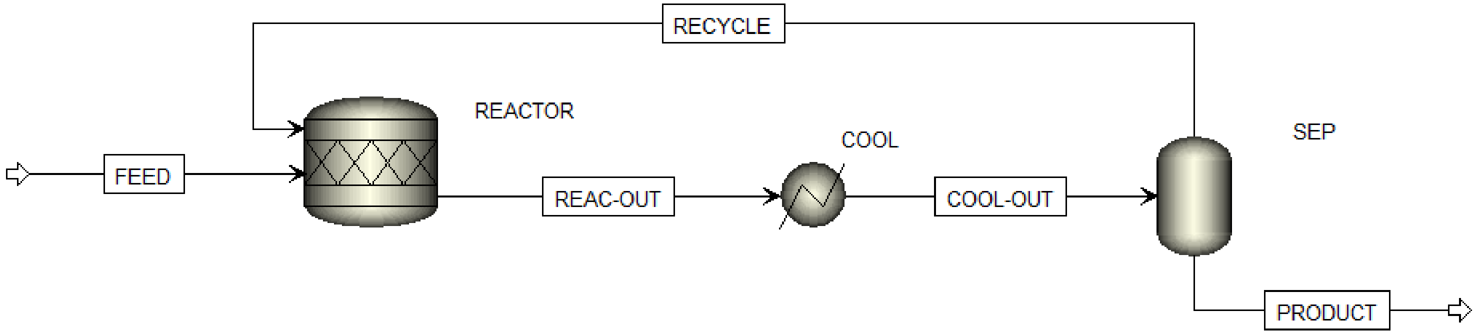


Sensitivity Analysis Procedure

1. Specify manipulated (varied) variable(s)
   - These are the flowsheet variables to be varied (Vary sheet)
2. Specify Range(s) for manipulated variable(s)
   - Variation for manipulated variables can be specified either as equidistant points within an interval or as a list of values for the variable (Vary sheet). It is possible to check the Active checkbox to activate or disable a variable
3. Define measured (samples) variable(s)
   - These are quantities calculated during the simulation to be used in step 4 (Define sheet)
4. Specify quantities to calculate and tabulate
   - Tabulated variables can be any valid Fortran expression containing variables defined in step 1 (Tabulate sheet). “Fill variables” button automatically tabulates all the defined variables

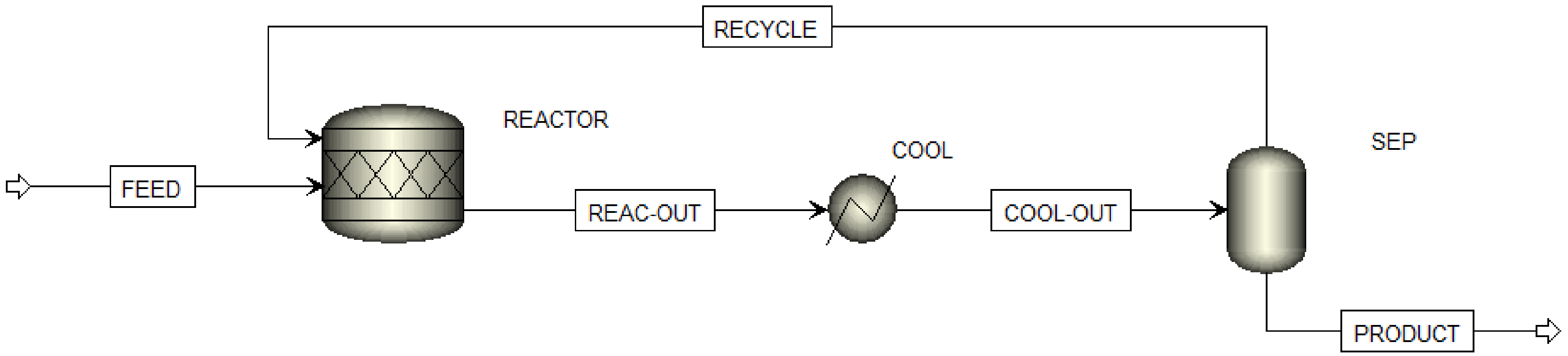
Sensitivity Analysis Demo

- Components:
  - Benzene, Propylene, Cumene
- Thermodynamic model:
  - RK-SOAVE
- Feed
  - Temperature: 100 °C, Pressure: 2.5 bar; Molar flow: Benzene 20 kmol/hr, Propylene 20 kmol/hr
- Cool
  - Temperature: 50 °C; Pressure drop: 0.007 bar
- Reactor
  - Adiabatic, No pressure drop
  - Benzene + Propylene -> Cumene. Conversion of 90% of propylene
- Sep
  - Adiabatic, Pressure: 1 atm

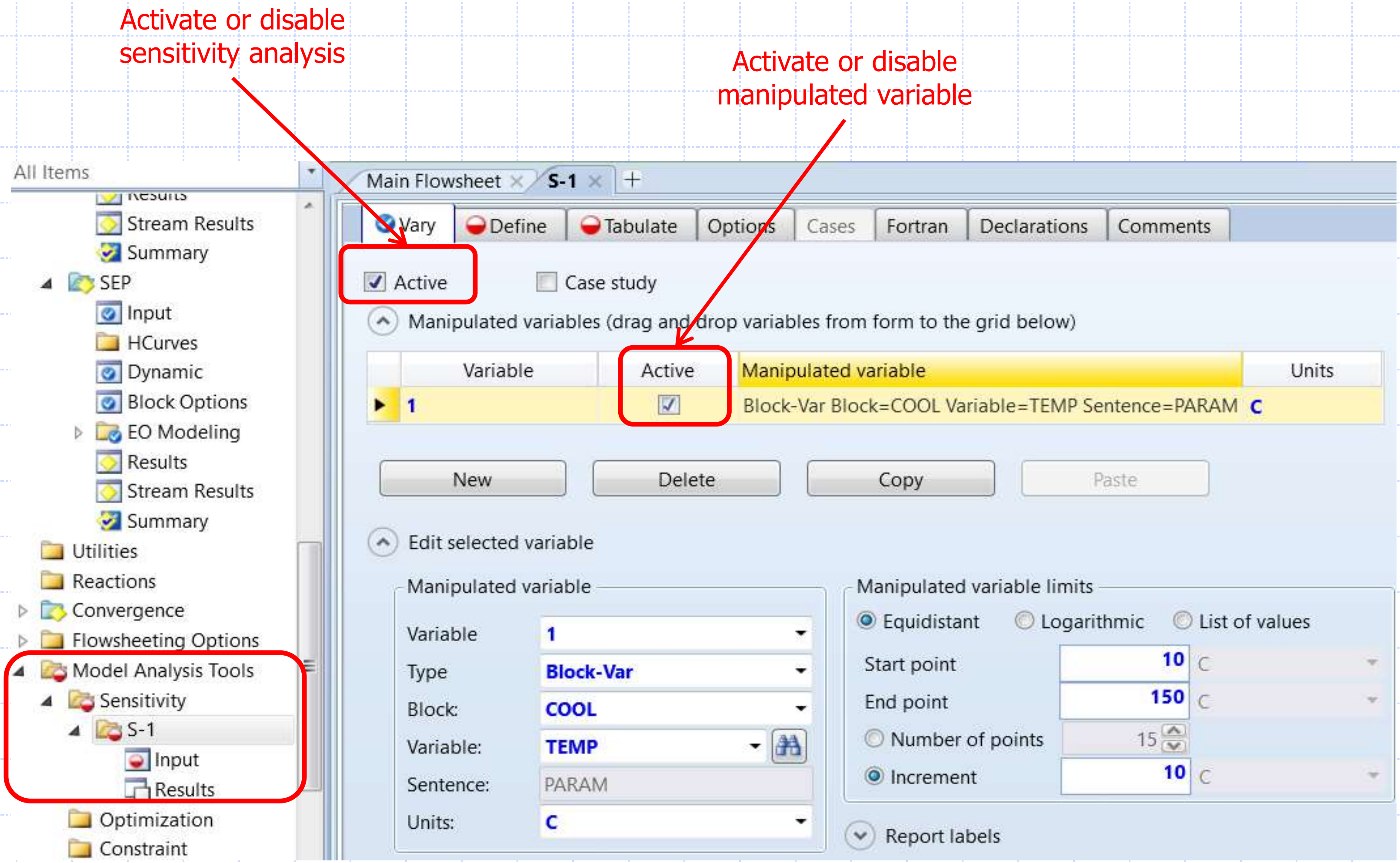


Sensitivity Analysis Demo

- Determine the effect of cooler outlet temperature on the purity of the product stream.
  - What is the manipulated variable?
    - COOL outlet temperature
  - What is the measured variable?
    - Purity (mole fraction) of cumene in PRODUCT stream



Vary sheet

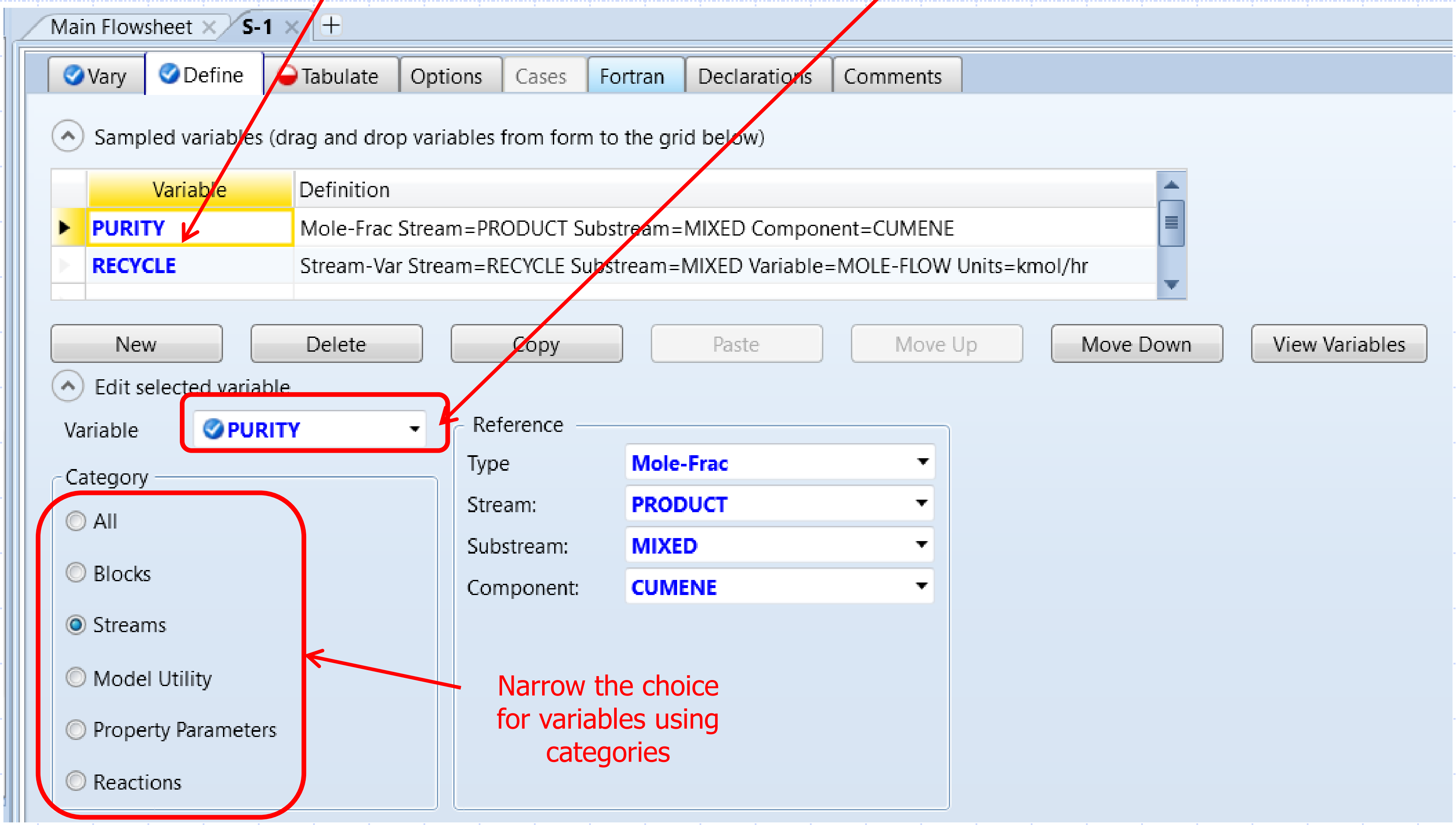


Activate or disable sensitivity analysis
Activate or disable manipulated variable
All Items
Stream Results
Summary
SEP
Input
HCurves
Dynamic
Block Options
EO Modeling
Results
Stream Results
Summary
Utilities
Reactions
Convergence
Flowsheeting Options
Model Analysis Tools
Sensitivity
S-1
Input
Results
Optimization
Constraint
Main Flowsheet
S-1
Vary
Define
Tabulate
Options
Cases
Fortran
Declarations
Comments
Active
Case study
Manipulated variables (drag and drop variables from form to the grid below)
Variable
Active
Manipulated variable
Units
1
Block-Var Block=COOL Variable=TEMP Sentence=PARAM
C
New
Delete
Copy
Paste
Edit selected variable
Manipulated variable
Variable
1
Type
Block-Var
Block:
COOL
Variable:
TEMP
Sentence:
PARAM
Units:
C
Manipulated variable limits
Equidistant
Logarithmic
List of values
Start point
10
End point
150
Number of points
15
Increment
10
Report labels

Define sheet

Add variables by copy and paste or drag and drop from existing input and results forms

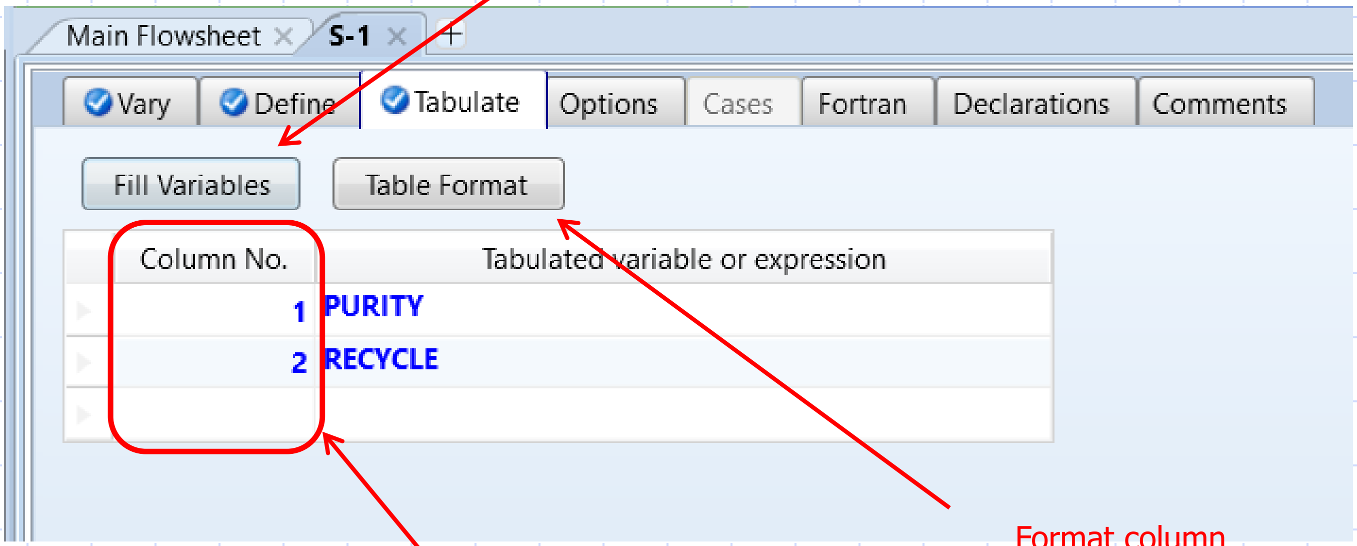
Or use the variable definition form to create variables



Narrow the choice for variables using categories

Tabulate sheet

Creates a column for
each defined variable



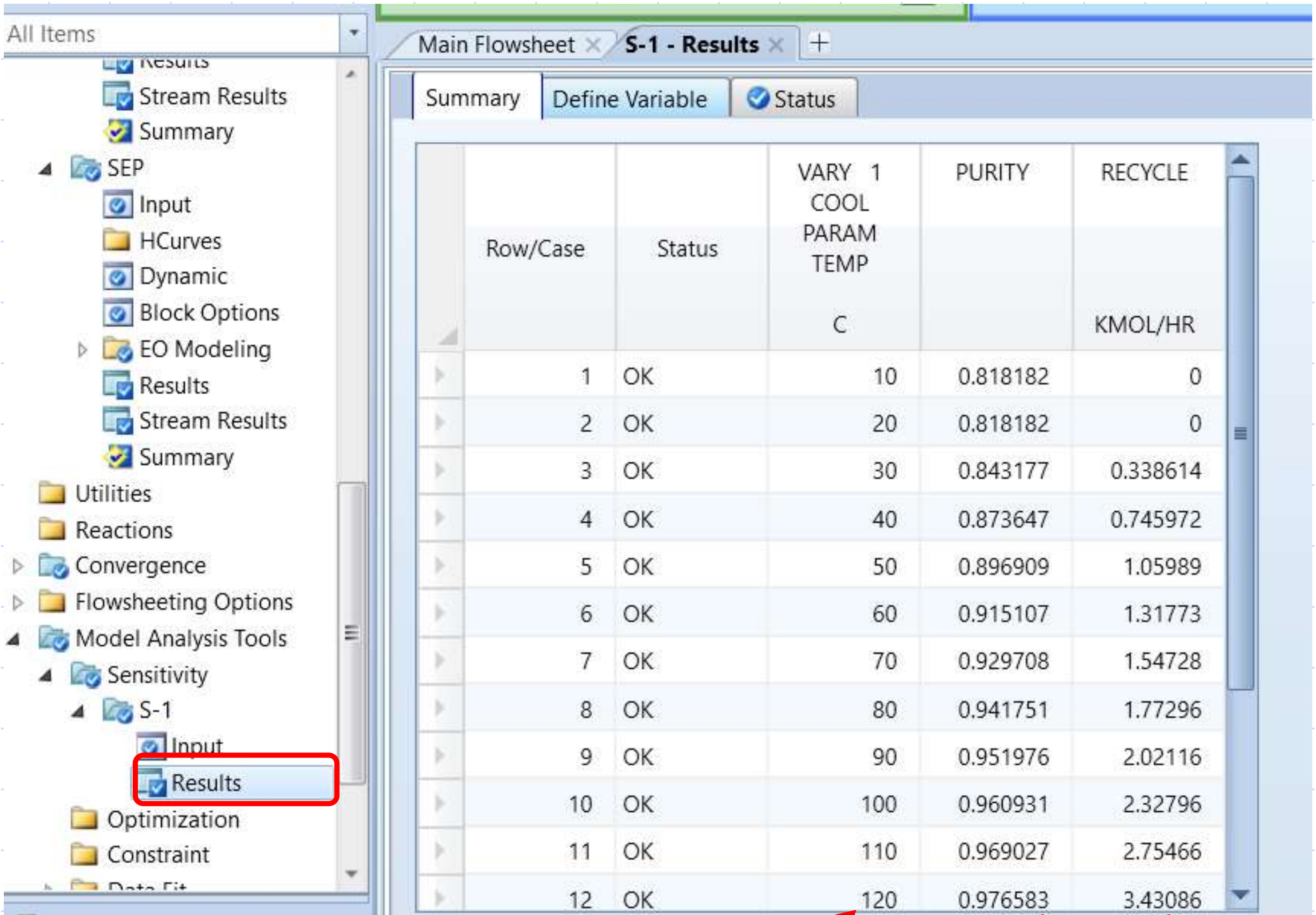
Format column
headings

Column for each
desired result.
Variable or formula

Accessing Variables Notes

- Only streams that are feeds to the flowsheet should be varied or modified directly
- Do NOT vary the Mass-Frac, Mole-Frac or StdVol-Frac of a component in a Feed stream. To change the composition of a Feed stream, vary the Mass-Flow, Mole-Flow or StdVol-Flow of the desired component
- If Duty is specified for a block, that duty can be read and written using the variable DUTY for that block; if the duty is calculated during simulation, it should be read using the variable QCALC
- PRES is the specified pressure or pressure drop, and PDROP is the pressure drop used in calculating pressure profile in heating or cooling curves
- Flowsheet result variables (calculated quantities) should not be overwritten or varied

Sensitivity Analysis Results

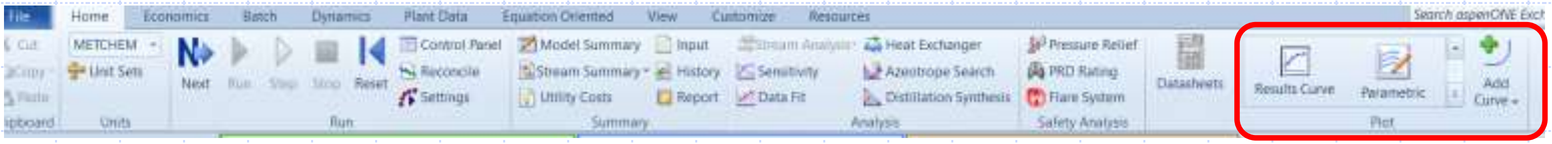


Row/Case	Status	VARY 1 COOL PARAM TEMP C	PURITY	RECYCLE KMOL/HR
1	OK	10	0.818182	0
2	OK	20	0.818182	0
3	OK	30	0.843177	0.338614
4	OK	40	0.873647	0.745972
5	OK	50	0.896909	1.05989
6	OK	60	0.915107	1.31773
7	OK	70	0.929708	1.54728
8	OK	80	0.941751	1.77296
9	OK	90	0.951976	2.02116
10	OK	100	0.960931	2.32796
11	OK	110	0.969027	2.75466
12	OK	120	0.976583	3.43086

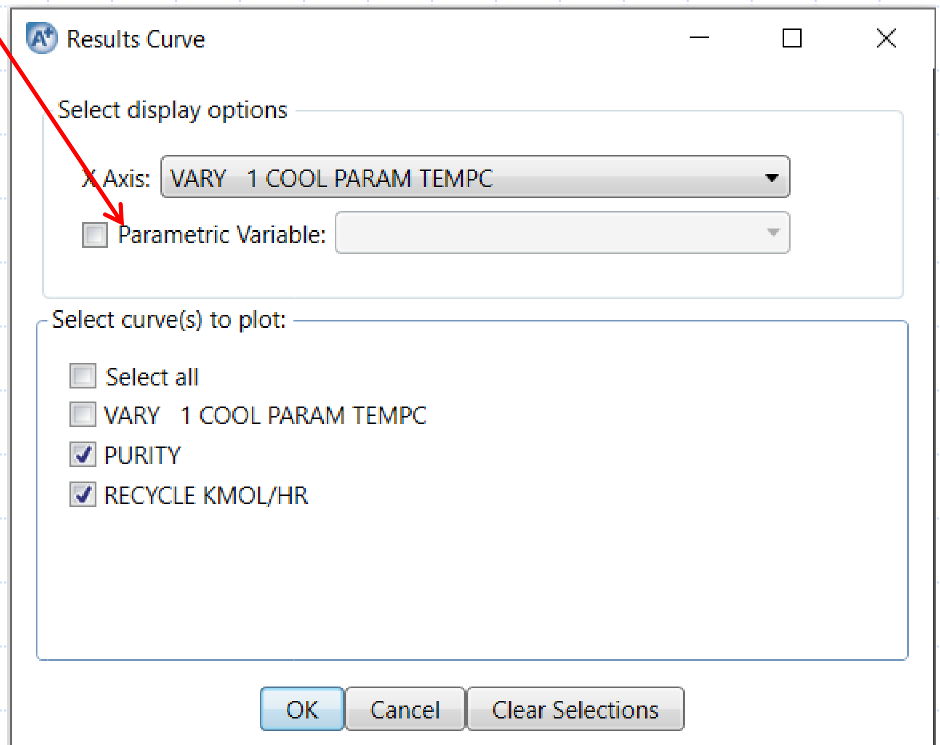
Manipulated variable

Calculated variables

Sensitivity Analysis Plot



- Use the plotting tool from the Home Ribbon when the table of results is open. It is possible to generate plots of Sensitivity
- For a second Vary select parametric variable

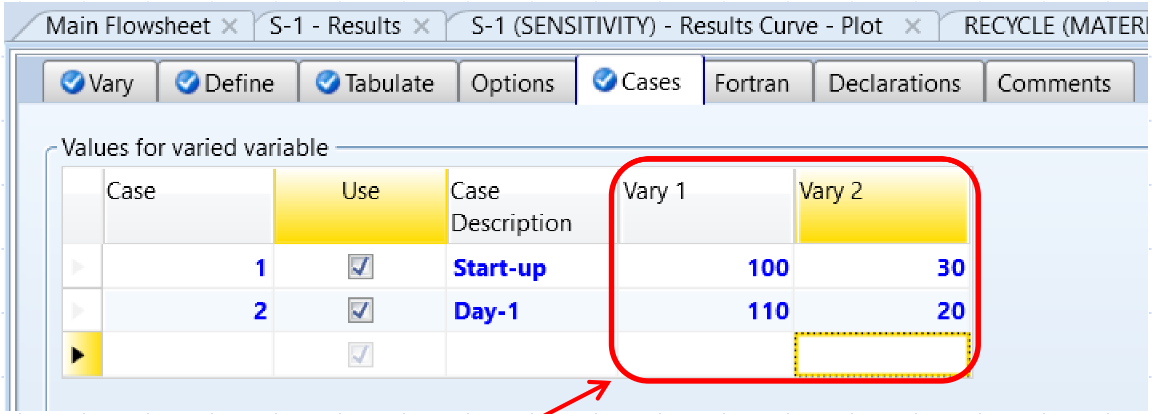


Sensitivity Analysis Plot

- Use Custom Plot when no built-in plotting option exists
- Use “Add Curve” to ass a variable to an existing plot
  - Select column of data to add to plot
  - Choose the Add Curve option from the Home Ribbon Plot group
  - Select the plot to add curve
- Use the “Merge Plot” option to combine two existing plots
  - Highlight one of the plots to merge
  - Choose the Merge Plots option from the Plot | Design Ribbon | Data group
  - Select the second plot

Case Studies

- Use Case Studies to set up a case study with any number of manipulated variables
- Use Case studies sheet to enter the input data for each case
- This makes much easier to run multiple sets of data through a single model



Combination of variables to be modified

Sensitivity Analysis Notes

- Only quantities that have been input to the flowsheet should be varied or manipulated
- Multiple inputs can be varied
- The simulation is run for every combination of manipulated variables unless using Cases
- Check the Cases box to specify the variable values for a list of individual cases
- You can control on the Optional tab when the based case should be executed (default is to execute base case last)
- Remember you can deactivate a Sensitivity study to save it for future analysis

Design Specification

- Similar to a feedback controller
- Allows user to set the value of a calculated flowsheet quantity to a particular value
- Objective is achieved by manipulating a specified input variable
- Located in the Navigation Pane | Flowsheeting Options | Design Specs or the Manipulators tab of the Model Palette
- Design Specifications change the simulation results, sensitivity analysis does not!

Design Specification Procedure

1. Specify measured (sampled) variable(s)
   - These are flowsheet quantities, usually calculated during the simulation, to be included in the objective function (Define sheet)
   - Like Sensitivity, it is possible to copy and past or drag and drop the variables from the appropriate input or result
2. Specify objective function (Spec) and goal (Target)
   - This is the equation that the specification attempts to satisfy (Spec sheet)
3. Set tolerance for objective function
   - The specification is converged when the objective function equation is satisfied within this tolerance (Spec sheet)
4. Specify manipulated (varied) variable
   - This is the flowsheet variable whose value changes in order to satisfy the objective function equation (Vary sheet)
5. Specify range for manipulated variable
   - These are the lower and upper bounds of the interval within which A+ will vary the manipulated variable (Vary sheet)

Design Specification Notes

- Only quantities that have been input to the flowsheet should be varied or manipulated
- The calculation performed by a design specification are iterative; providing a good estimate for the manipulated variable will help the design specification converge in fewer iterations; this is particularly important for large flowsheets with several interrelated design specifications
- Viewing results of a design specification:
  - Design-Spec Results form
  - Results Summary | Convergence | DesignSpec Summary
  - Convergence | Convergence and by choosing the Results form in the appropriate solver block
  - The final values of the manipulated and/or sampled variables can be viewed directly on the appropriate Stream or Block Results forms

Design Specification Convergence

- If Design Specification does not converge:
  1. Double-check if the manipulated variable is not at its lower or upper bound
  2. Verify that a solution exists within the bounds specified for the manipulated variable, perhaps by performing a sensitivity analysis
  3. Ensure that the manipulated variable does indeed affect the value of the sampled variables
  4. Provide a better estimate for the value of the manipulated variable
  5. Narrow the bounds of the manipulated variable or loosening the tolerance on the objective function to help convergence
  6. Make sure that the objective function does not have a flat region within the range of the manipulated variable
  7. Change the characteristics of the convergence block associated with the design-spec (Step size, number of iterations, algorithm, etc…)

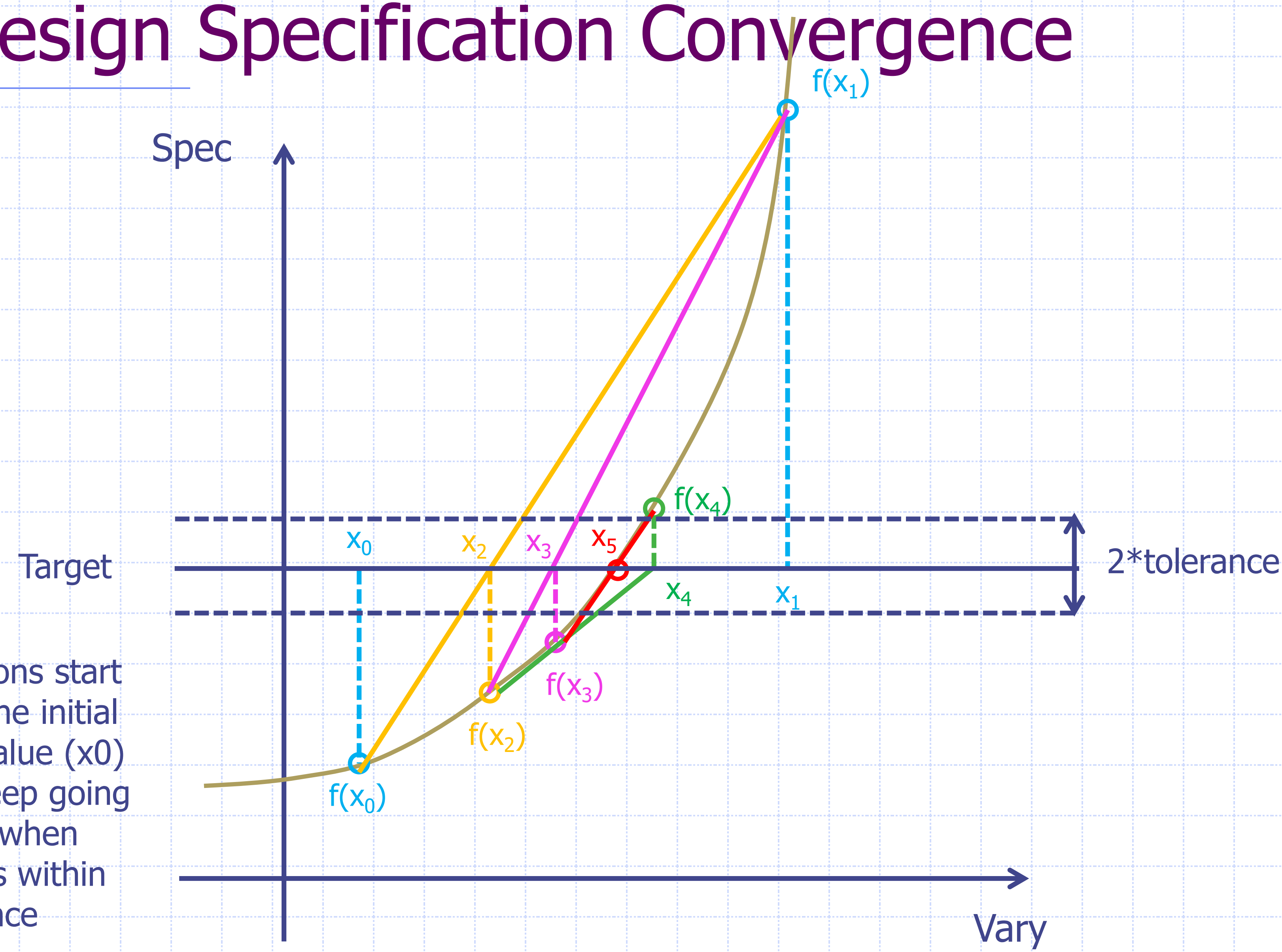
Design Specification Convergence

- Convergence of single design specifications involves the use of Secant Method
- Uses three points quadratic polynomial

$$x_{n+1} = x_n - \frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})} f(x_n)$$

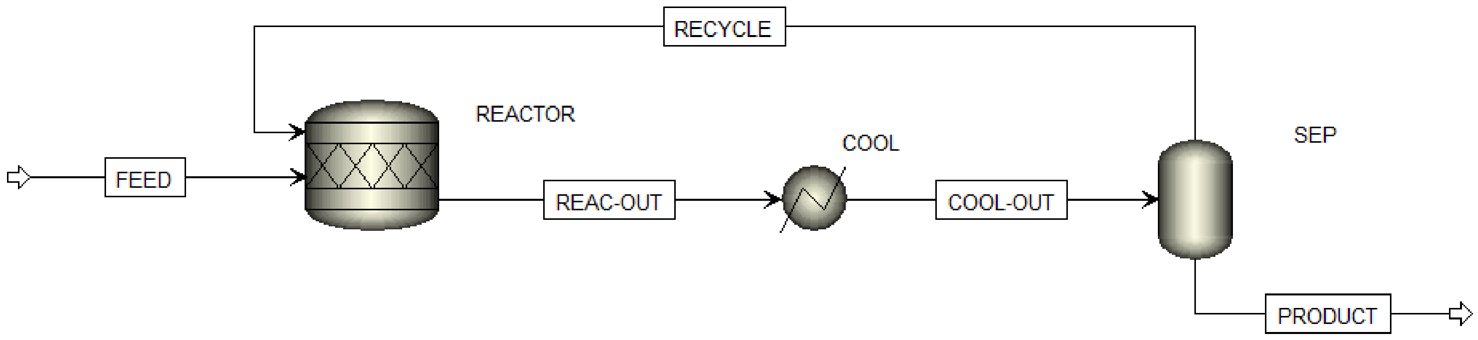
- Support brackets strategy:
  - Bracket=Yes or Bracket=Check Bounds
  - Good for non-monotonic functions, i.e. phase changes
  - Eliminates flat region and switches back to secant method if possible
  - Aid convergence
- Can limit maximum step size as a function of range
- Best method when Design Spec contains discontinuity

Design Specification Convergence



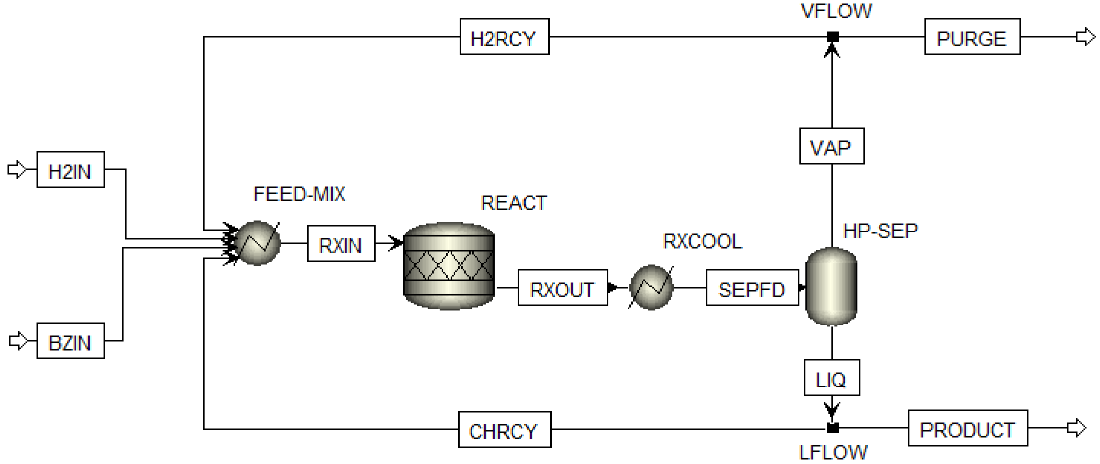
Iterations start from the initial vary value (x0) and keep going to x5, when f(x5) is within tolerance

Design specification Demo



- Determine the effect of cooler outlet temperature to achieve a Cumene product purity of 98% mol.
- What is the manipulated variable?
  - COOL outlet temperature
- What is the measured variable?
  - Purity (mole fraction) of cumene in PRODUCT stream
- What is the specification?
    - Purity (mole fraction) of cumene in PRODUCT stream=0.98

Exercise: Hydrogenation of benzene



- Components:
  - Hydrogen, Nitrogen, Methane, Benzene, Cyclohexane
- Thermodynamic method:
  - RK-SOAVE
- Feed:
  - H2IN: T=50 °C, P= 25 bar, Moleflow=330 kmol/hr, Mole-Frac: H2 97.5%, N2 0.5%, CH4 2%
  - BZIN: T=40°C, P=1 bar, Benzene Moleflow =100 kmol/hr

Exercise: Data

- FEED-MIX:
  - Temperature 150 °C, Pressure 23 bar
- REACT:
  - Temperature 200 °C, Pressure drop: 1 bar
  - Benzene+3 Hydrogen -> Cyclohexane. Conversion of 99.8% of benzene
- RXCOOL:
  - Temperature 50 °C, Pressure drop: 0.5 bar
- HPSEP:
  - Adiabatic, No Pressure drop
- VFLOW:
  - 92% of flow to stream H2RCY
- LFLOW:
  - 30% of flow to CHRCY

Exercise: Objective

- Set up a Sensitivity Analysis to analyze the composition of the product stream varying the separation of LFLOW from 10 to 50% to CHRCY
- 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.
  - First, add the calculated variable of my interest to sensitivity analysis, in order to select the best range for Design Specification objective!!!