Getting started with ProSimPlus®

Case 8:
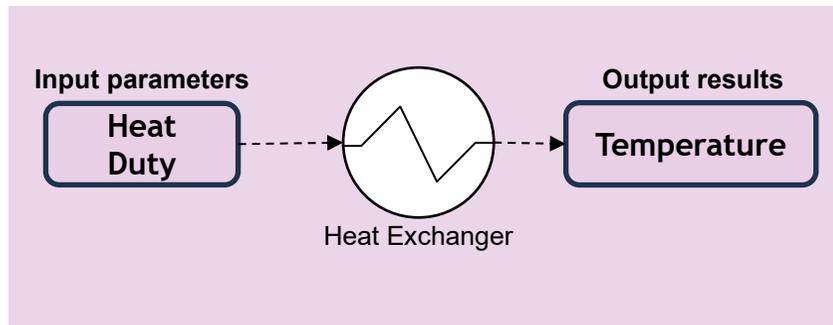## Case studies and Specifications

fives
Industry can do it

Context

This document presents the **case study** tool, which is used to analyze the influence of input parameters on the process output results. In addition, this tool helps identify the right process parameters to adjust in order to meet target **specifications** and optimize the process performance.
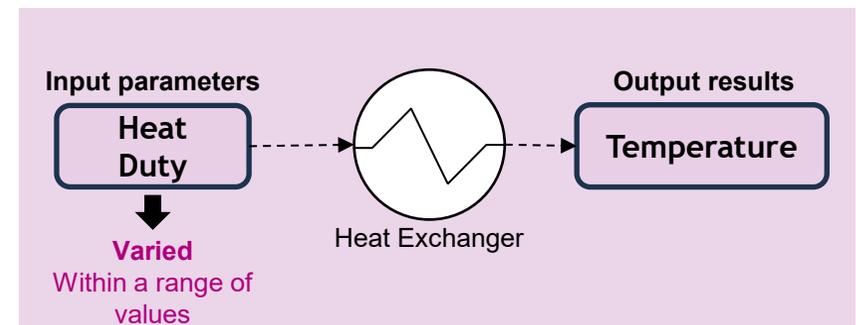
Summary of this Getting Started:

1) Introduction of the concepts and the application example

2) How to create a **Case Study**

3) How to set **Specifications**

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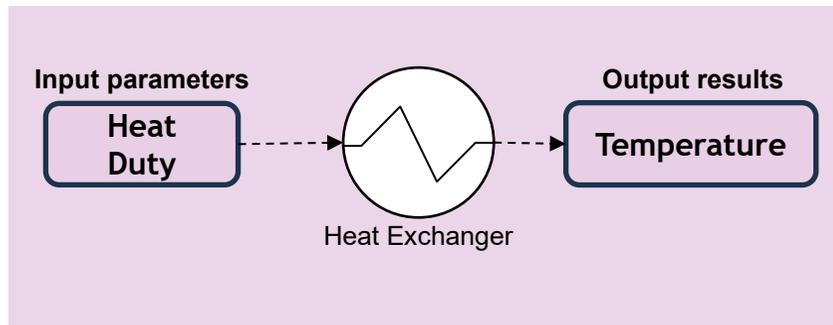
Concept of Case study

Input parameters
Heat Duty → Heat Exchanger → **Output results** Temperature

Nominal simulation

Input parameters
Heat Duty
↓
Varied
Within a range of values
→ Heat Exchanger → **Output results** Temperature

Case Study

Context
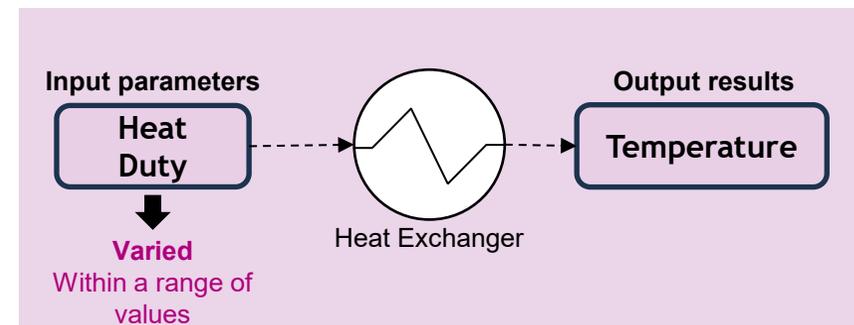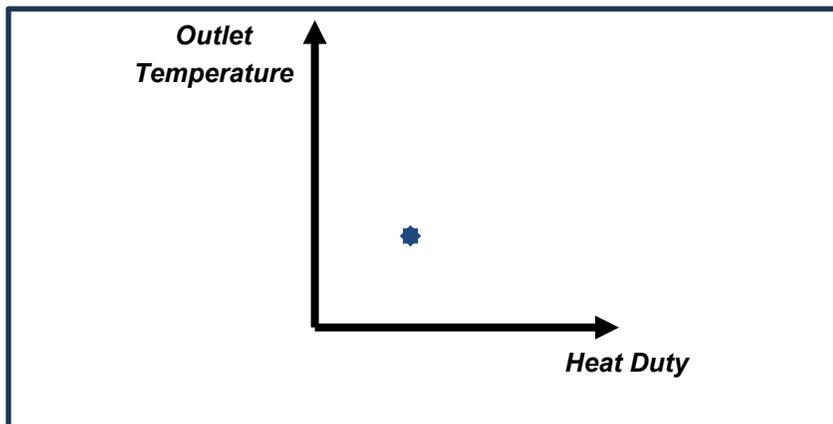
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Concept of Case study

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Case Study

Outlet Temperature

Heat Duty

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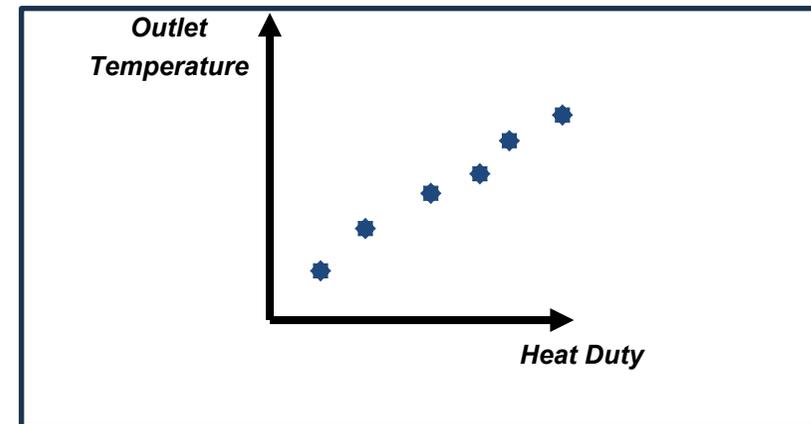
Using the data generated from the **Case study**, users can determine the specific heat duty required to achieve a desired outlet temperature and use it as a specification for the process. This approach enables fine-tuning of the heat duty parameter to meet the target conditions.
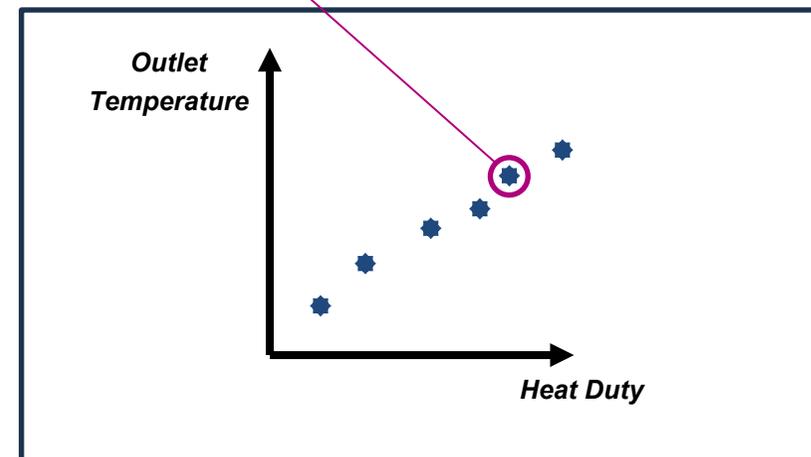
Process specifications

Outlet Temperature

Heat Duty

Note on terminology:
X = Input parameter
Y = Output result = target result

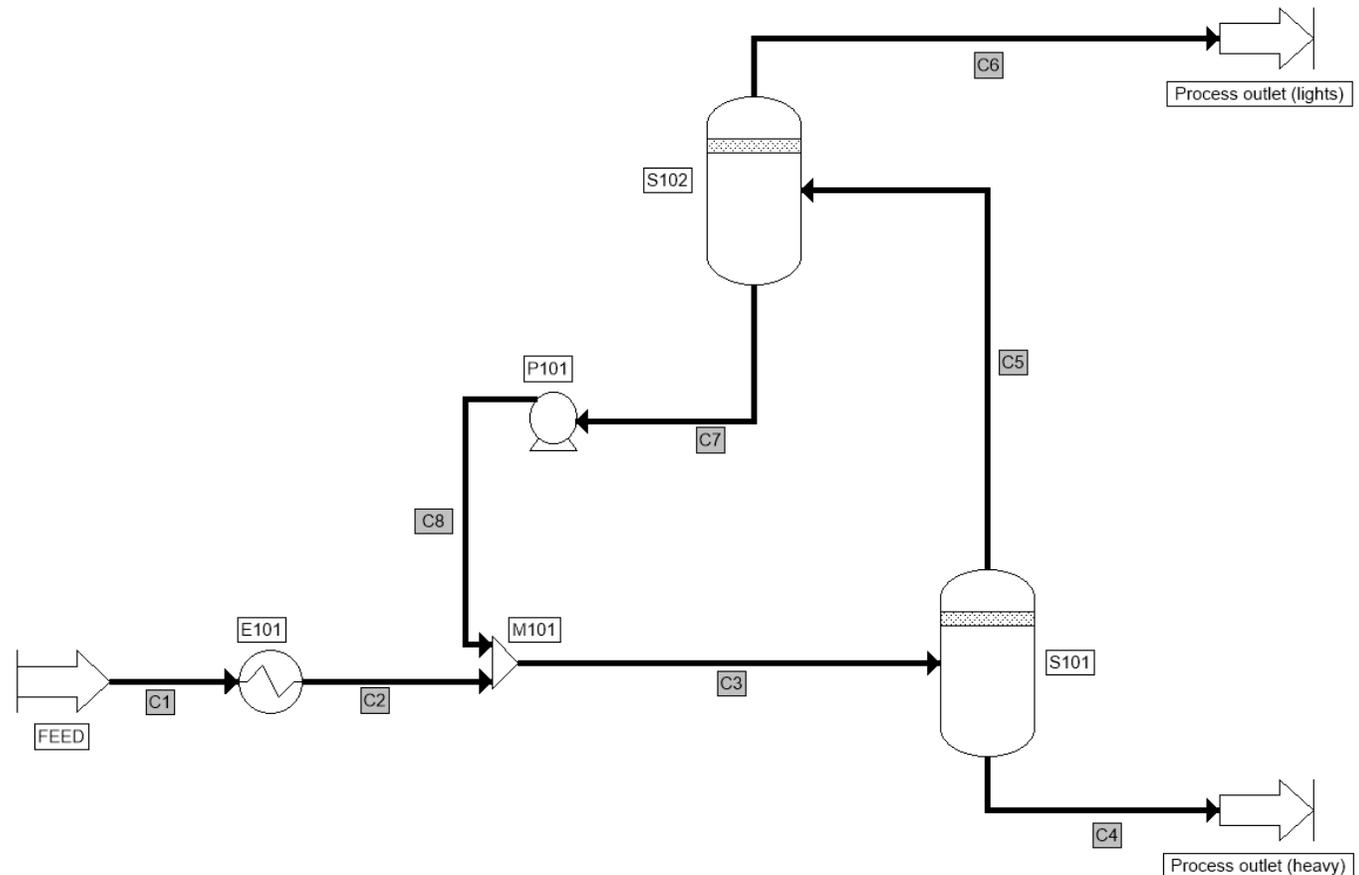# Presentation of example

The example used in this Getting Started to practice with the Case study and Specification features involves separating a hydrocarbon mixture into light and heavy components.

It is located in the ProSimPlus examples directory under the name 'PSPS_EX_EN-Simple-Example'

Presentation of example

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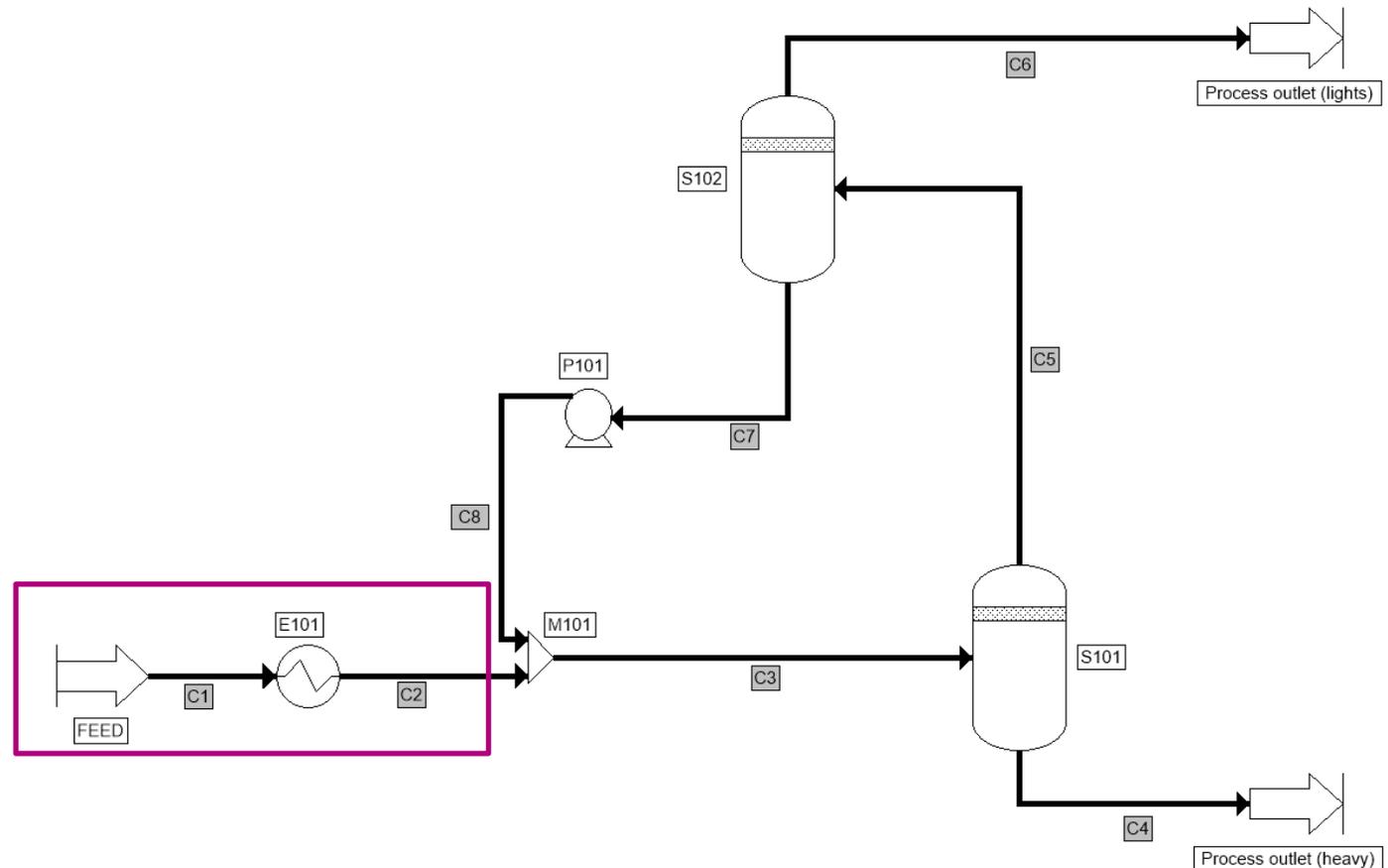

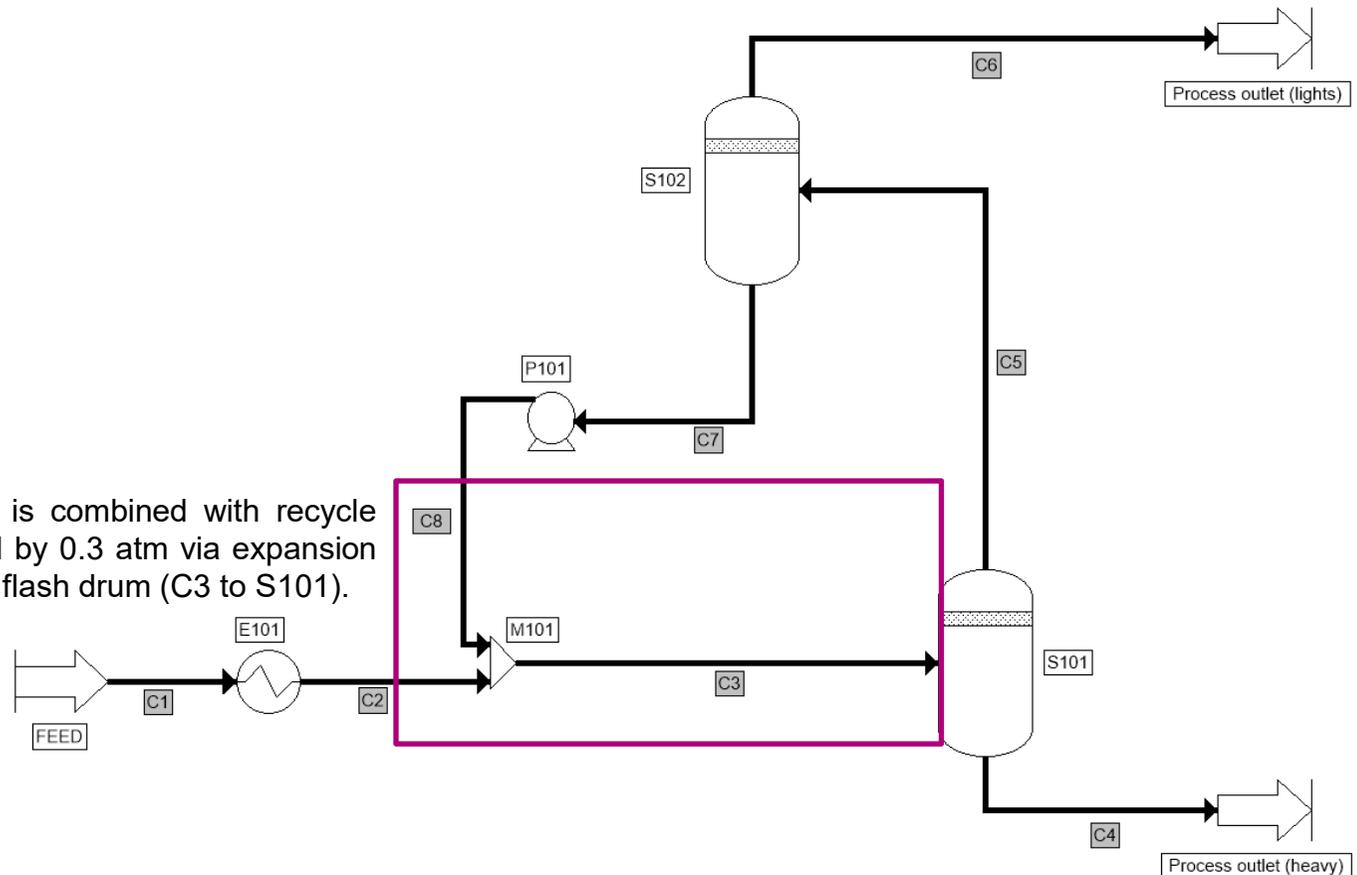**Initial feeding & cooling:** Hydrocarbon mixture (C1) is cooled to 15°C (C2).

Presentation of example

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Mixing & pressure adjustment: C2 is combined with recycle stream (C8), then pressure is dropped by 0.3 atm via expansion valve (not shown here) and sent to the flash drum (C3 to S101).

Presentation of example

The example used in this Getting Started to practice with the Case study and Specification features involves separating a hydrocarbon mixture into light and heavy components.

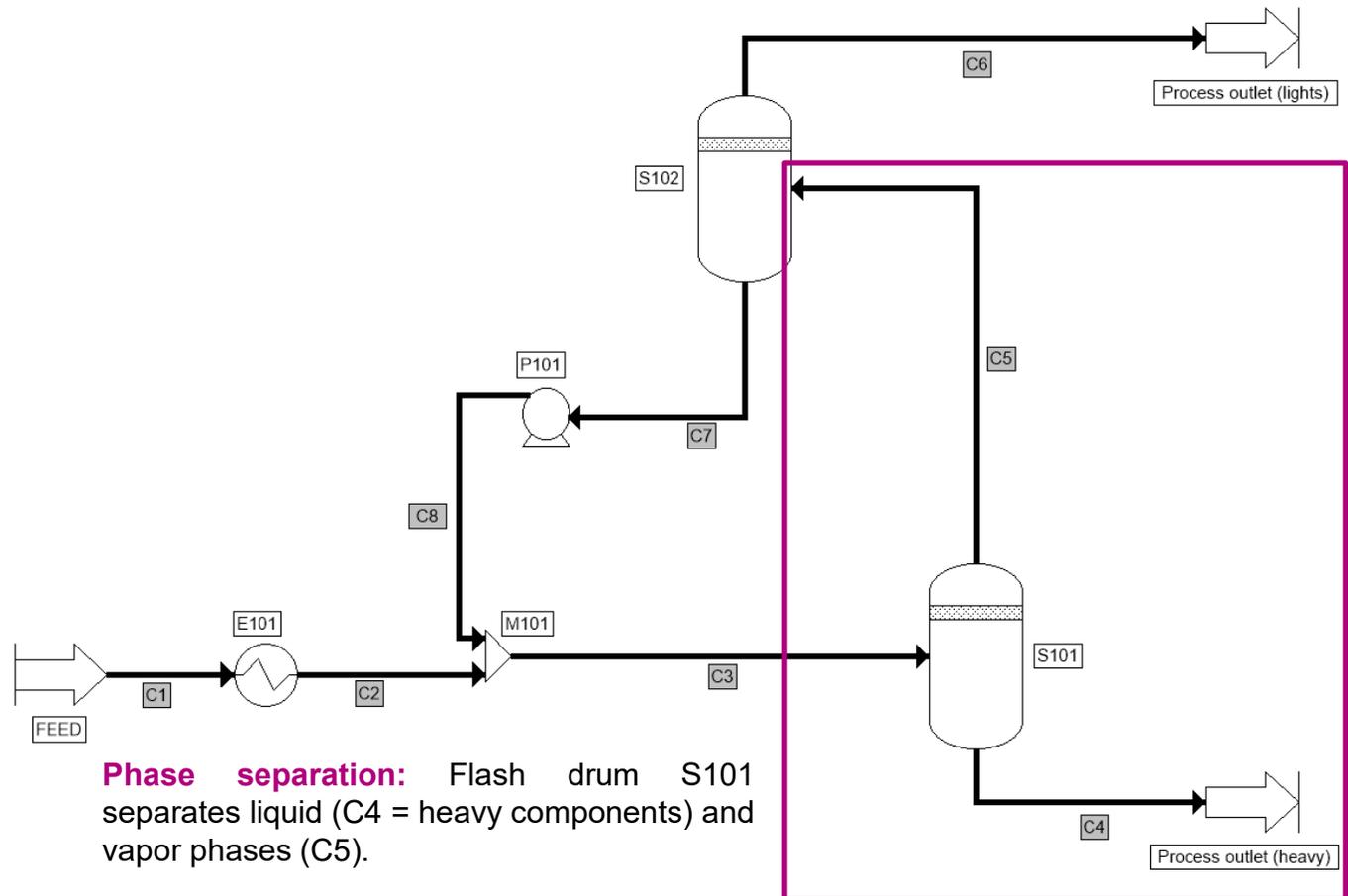*It is located in the ProSimPlus examples directory under the name 'PSPS_EX_EN-Simple-Example'*

Phase separation: Flash drum S101 separates liquid (C4 = heavy components) and vapor phases (C5).
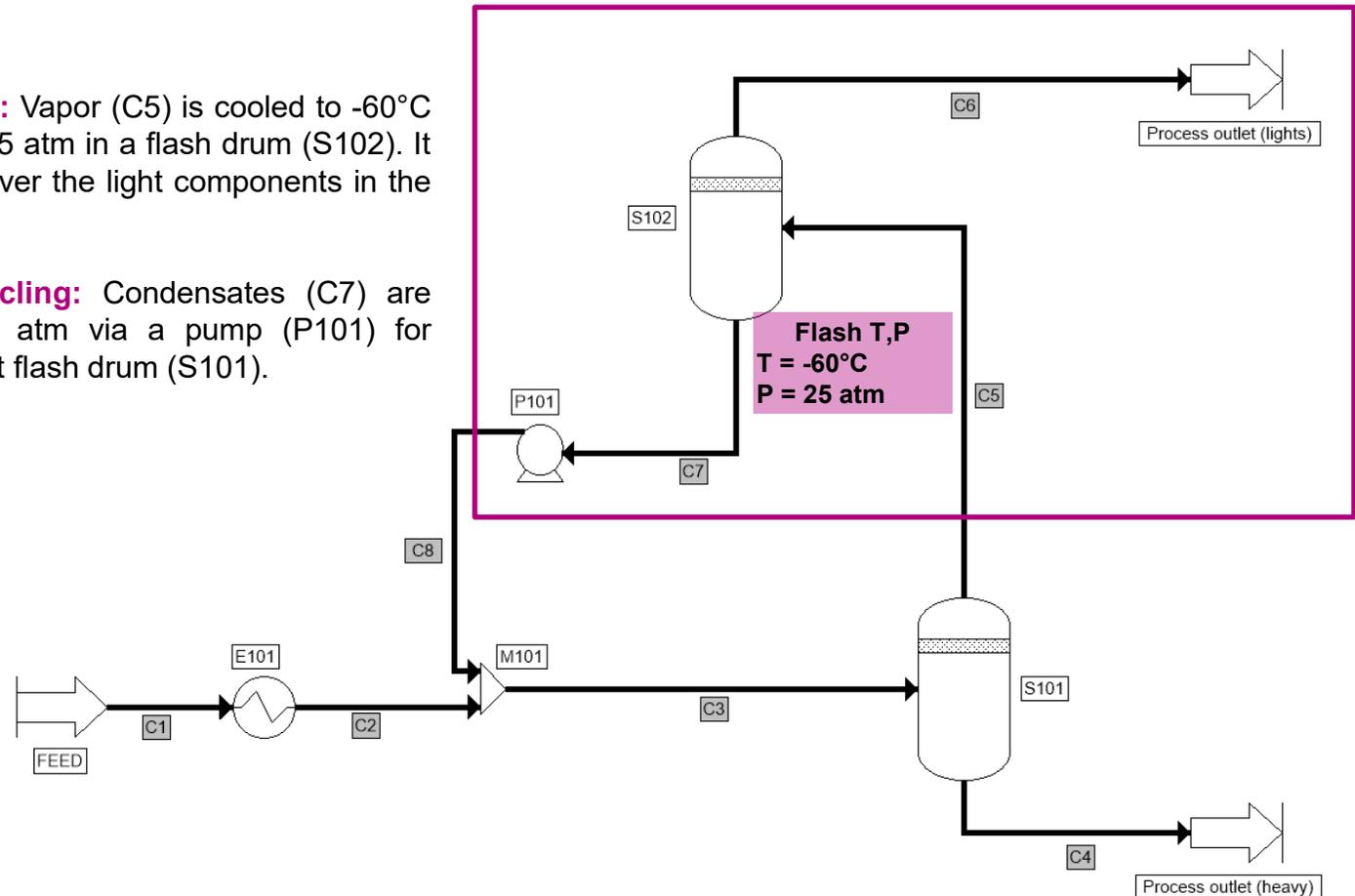
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Vapor processing: Vapor (C5) is cooled to -60°C and expanded to 25 atm in a flash drum (S102). It also allows to recover the light components in the vapor phase.

Condensate recycling: Condensates (C7) are pressurized to 75 atm via a pump (P101) for recycling to the first flash drum (S101).

Flash T,P
T = -60°C
P = 25 atm

C6 — Process outlet (lights)

S102

C5

P101

C7

C8

E101

M101

C3

S101

C1

C2

FEED

C4 — Process outlet (heavy)

Introduction 1	Case Study 2	Specifications 3

Presentation of example

The example used in this Getting Started to practice with the Case study and Specification features involves separating a hydrocarbon mixture into light and heavy components.
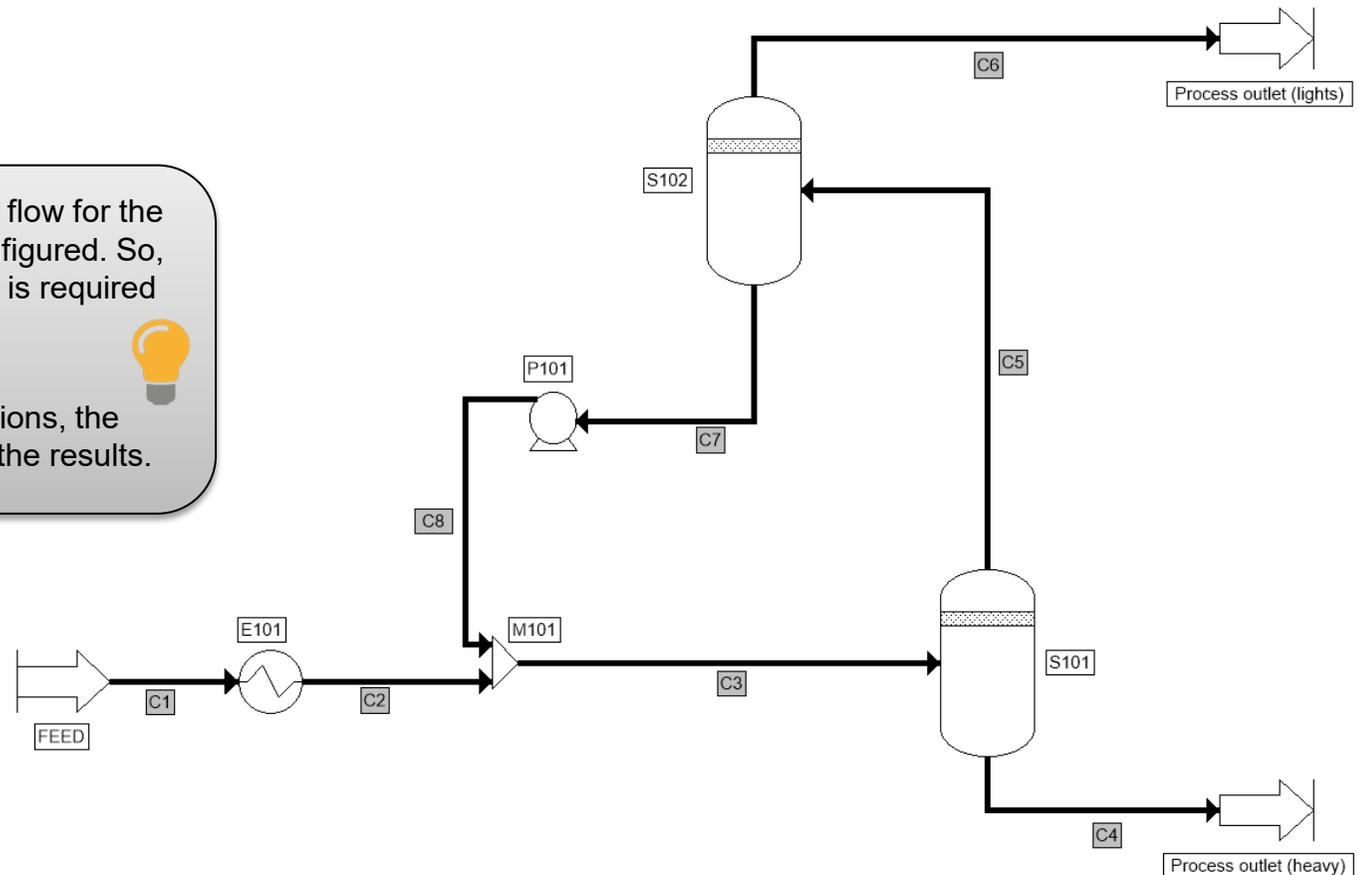
It is located in the ProSimPlus examples directory under the name 'PSPS_EX_EN-Simple-Example'

All the unit operations and input flow for the *Simple-Example* have been configured. So, at this point, no additional input is required from the user

Before making any modifications, the simulation can be run to verify the results.

C6

Process outlet (lights)

S102

P101

C5

C7

C8

E101

M101

S101

C1

C2

C3

FEED

C4

Process outlet (heavy)

Introduction **1**   Case Study **2**   Specifications **3**

Objective

Objective of the case study

Investigate the effect of varying the **temperature** of Flash S102 (input parameter) on the **propane mass fraction** (target result) in the lights stream. Identify the temperature at which a propane concentration of **5000 ppm** is achieved.

Objective
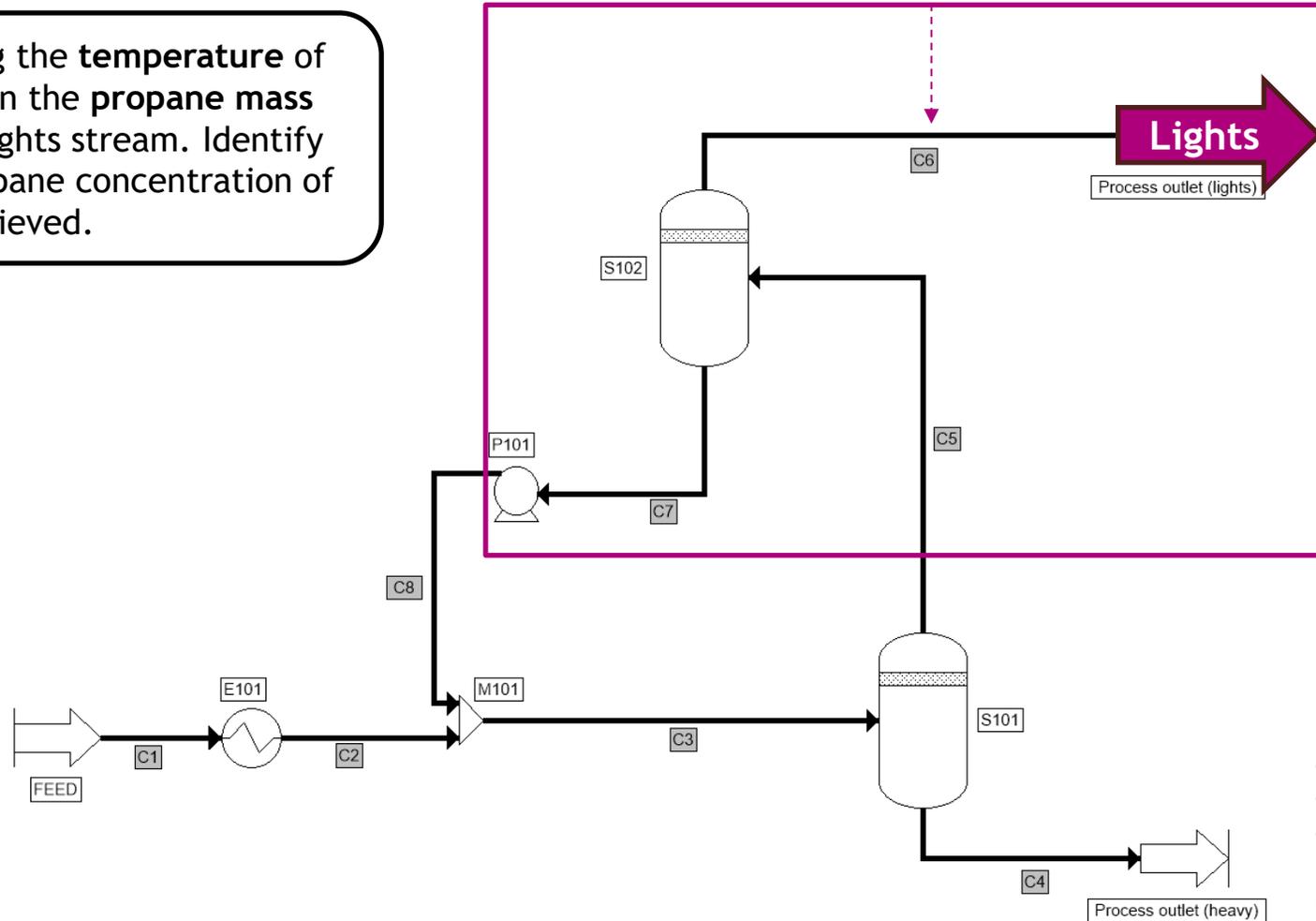
Conditions

Input parameter

o X = Vary the flash S102 **temperature** between -100°C and 0°C (5°C step)
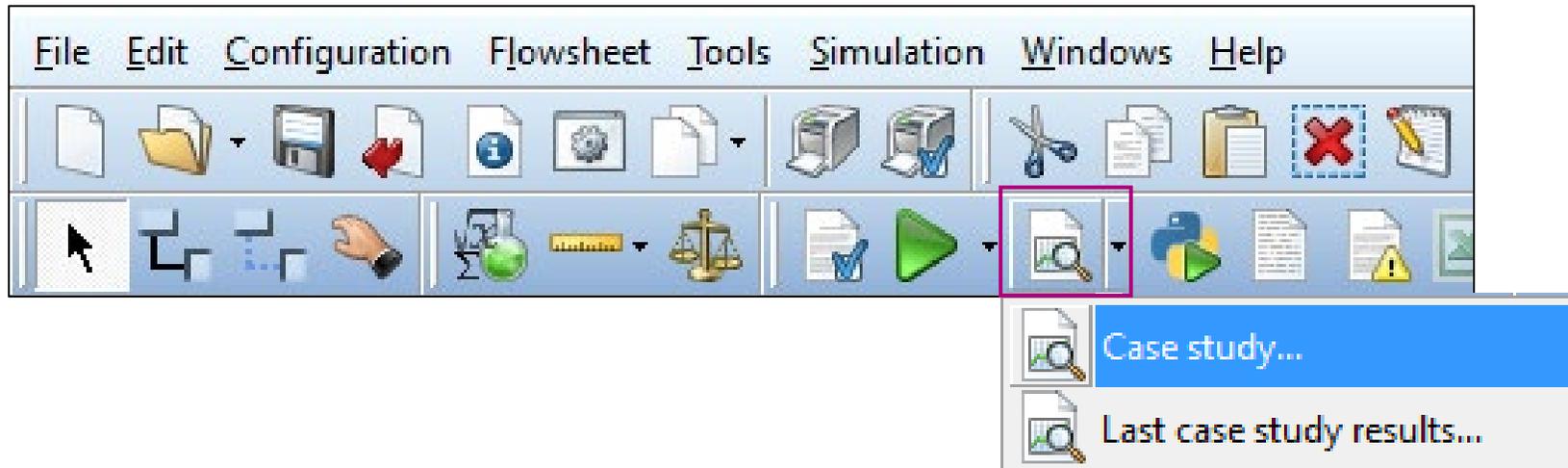
Target result

o Y= **Propane** mass vapor phase composition leaving the flash

Graph plotting

o Evolution of propane composition as a function of the flash drum (S102) temperature

Practical Example

Creation of a Case Study: Let's do it!

1 **Click on the "Case Study" button and select the "Case Study" option**

Practical Example

② **Fill the case study parameters**

Case study

Parameter

Unit operation: S102 (Liquid-vapor separator)

Parameter: Temperature

Unit: °C

Initial value: -100   Step: 5

Final value: 0   Number of points: 21

Monitoring

Filter by

Type: All types   Unit operation: All unit operations

<< Prev. | Next >>   1 variable selected

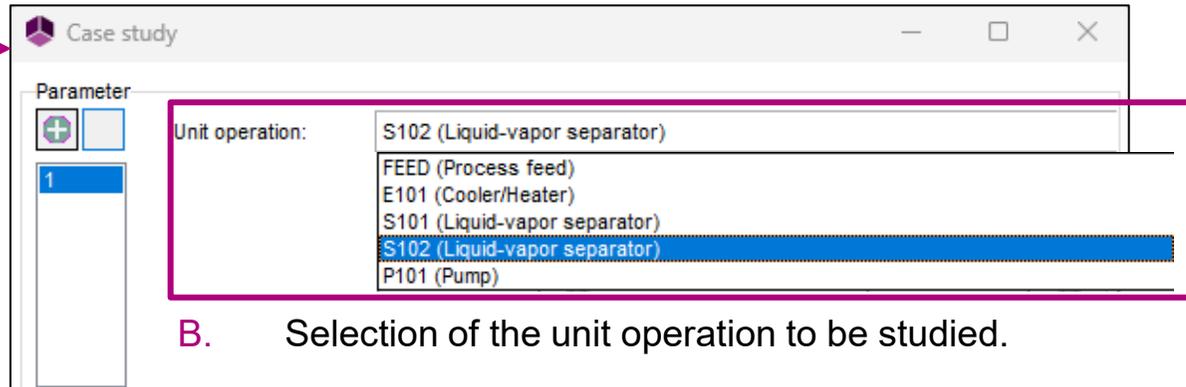| Selected	Variable	Form	Compounds	Stages
☐	Vapor fraction of stream C7			
☐	Duty exchanged			
☐	Vapor fraction (molar)			
☐	Liquid phase compositions	Molar	All	
☑	**Vapor phase compositions**	**Weight**	**A selection**	
⊟ P101				
☐	Flowrate of stream C8	Molar		
☐	Temperature of stream C8			

Ok   Cancel

Practical Example

Case study
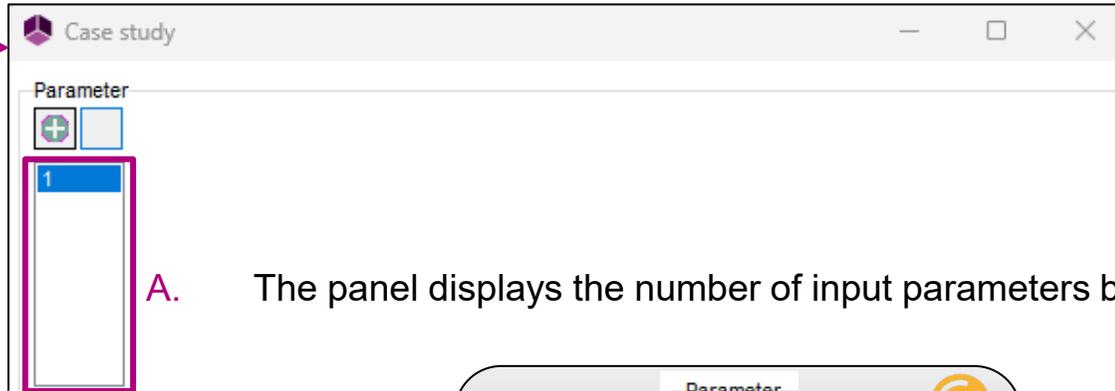
Parameter

A. The panel displays the number of input parameters being varied

Parameter

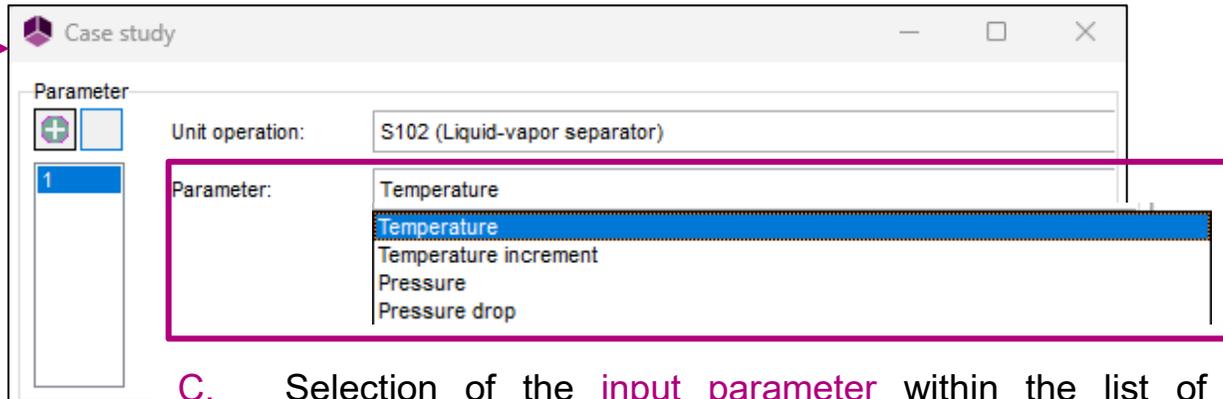If necessary, the green button allows the addition of new input parameters

② **Fill the case study parameters**

Practical Example

Case study

Parameter

| 1 |

Unit operation: S102 (Liquid-vapor separator)

FEED (Process feed)
E101 (Cooler/Heater)
S101 (Liquid-vapor separator)
S102 (Liquid-vapor separator)
P101 (Pump)

B.   Selection of the unit operation to be studied.

② **Fill the case study parameters**

Practical Example

C. Selection of the input parameter within the list of parameters available for the selected unit operation.

2 Fill the case study parameters

Practical Example

D.   Specification of the unit for the input parameter.

2️⃣ **Fill the case study parameters**

Practical Example

Case study

Parameter

Unit operation: S102 (Liquid-vapor separator)

Parameter: Temperature

Unit: °C

Initial value: -100   Step: 5

Final value: 0   Number of points: 21

E.   This section allows to specify the variation range:

- **Initial and final value:** define the range within which the input parameter will vary for the case study.
- **Step and number of points:** specify how the variation is discretized, *i.e.*: the increment between values and the total number of points considered.

2 **Fill the case study parameters**

Clicking on the blue button: Calculation of the respective value according to the 3 other given parameters

The 4 values are **consistent**

Practical Example

2   **Fill the case study parameters**

F.   Next, the results to monitor can be selected, with filtering options available (filter by unit operation type or unit operation name).

Practical Example

(2) **Fill the case study parameters**

G. This table displays each unit operation with its corresponding target results. By checking the box, the target result (vapor phase composition) is activated.

The propane component is selected

Practical Example

Case study

Parameter

Unit operation: S102 (Liquid-vapor separator)

Parameter: Temperature

Unit: °C

Initial value:	-100	Step:	5
Final value:	0	Number of points:	21

Monitoring

Filter by

Type: Liquid-vapor separator   Unit operation: S102

<< Prev.   Next >>   1 variable selected

Selected	Variable	Form	Compounds	Stages
☐	Vapor fraction of stream C7			
☐	Duty exchanged			
☐	Vapor fraction (molar)			
☐	Liquid phase compositions	Molar	All	
☑	**Vapor phase compositions**	**Weight**	**A selection**	
⊟	P101			
☐	Flowrate of stream C8	Molar		
☐	Temperature of stream C8			

Ok   Cancel

③ Click on "OK" to run the simulation

Practical Example

Simulation run

Simulation progress

Time: 00:00:02,937   ☐ Display simulation times

☑ Visual update   Opacity:

Complete simulation

Case number: 12

-45 °C

✔ ☐ FEED

✔ ☐ E101

✔ ☐ $_01

Iteration: 1

Runs in the MCN: 2

Convergence criterion: 1.09723

Damping factor: 1.00000

✔ ☐ M101

✔ ☐ S101

✔ ☐ S102

✔ ☐ P101

> Case #9: -60 °C
> Case #10: -55 °C
> Case #11: -50 °C
> Case #12: -45 °C

Status: **Print unit operations**
Preparing the report

Case index for each iteration of the input parameter during the case study

Each case corresponds to a different value

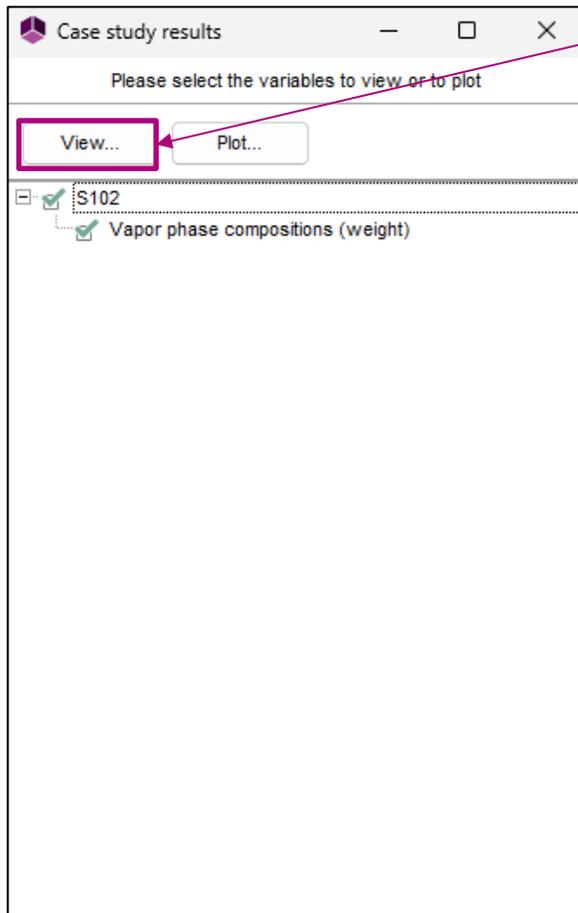within the range of the studied parameter

Practical Example

Simulation run

(4) When the simulation ends, close the simulation window to open the results window, for table and graphical analysis
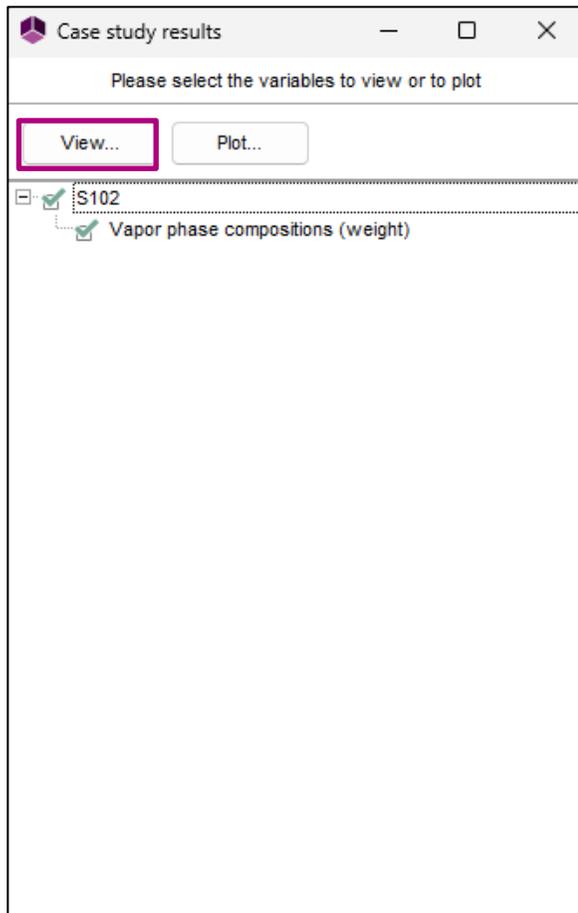
Practical Example

5 Analyze the case study results: TABLE RESULTS

Table View: Displays results as **raw data** and as **table** format for easy comparison and analysis

Case study results

Please select the variables to view or to plot

View... | Plot...

☑ S102
  ☑ Vapor phase compositions (weight)

Case study results

Raw data | Table

Drag a column header here to group by that column

#	S102 Temperature (°C)	Unit	Compound	Variable	Value	Unit
1	-100	°C	PROPANE	Vapor phase compositions (weight)	0,000719047	
2	-95	°C	PROPANE	Vapor phase compositions (weight)	0,00121279	
3	-90	°C	PROPANE	Vapor phase compositions (weight)	0,00194108	
4	-85	°C	PROPANE	Vapor phase compositions (weight)	0,00301789	
5	-80	°C	PROPANE	Vapor phase compositions (weight)	0,0045987	
6	-75	°C	PROPANE	Vapor phase compositions (weight)	0,00686972	

Practical Example

⑤ Analyze the case study results: TABLE RESULTS

Ⓐ

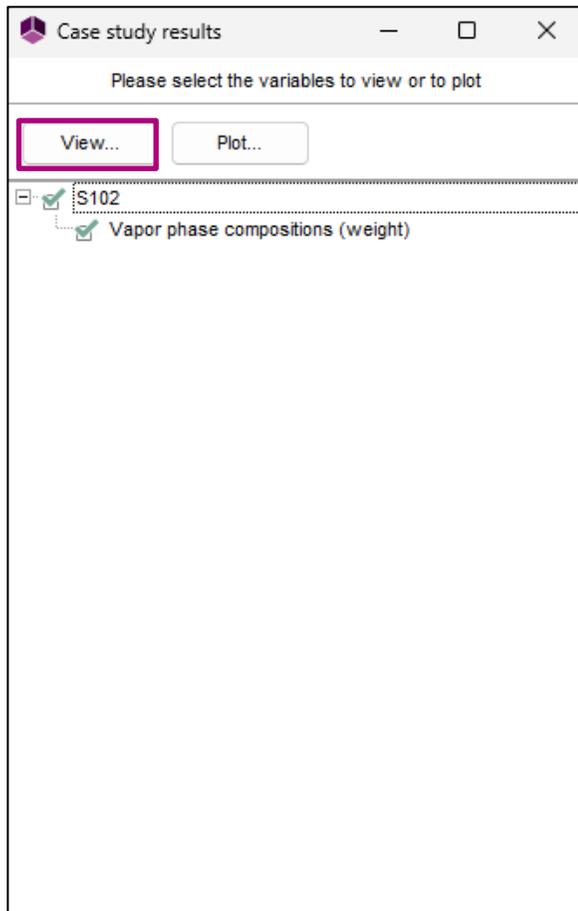> **Raw Data allows to group, filter and sort:** by studied variable value, compound, impacted variable, units, etc… 💡

#	S102 Temperature (°C)	Unit	Compound	Variable	Value	Unit
1	-100	°C	PROPANE	Vapor phase compositions (weight)	0,000719047	
2	-95	°C	PROPANE	Vapor phase compositions (weight)	0,00121279	
3	-90	°C	PROPANE	Vapor phase compositions (weight)	0,00194108	
4	-85	°C	PROPANE	Vapor phase compositions (weight)	0,00301789	
5	-80	°C	PROPANE	Vapor phase compositions (weight)	0,0045987	
6	-75	°C	PROPANE	Vapor phase compositions (weight)	0,00686972	

Practical Example

(5) Analyze the case study results: TABLE RESULTS

B

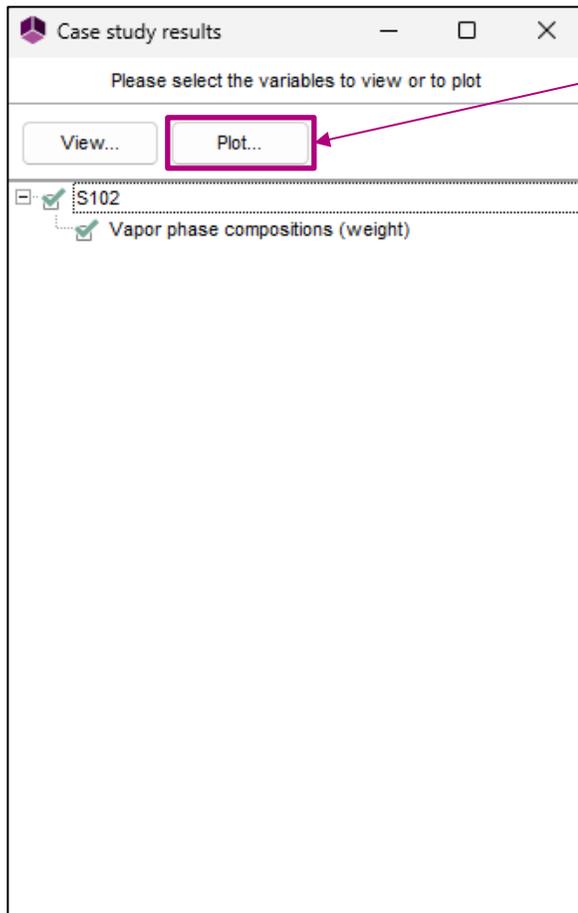> **Table** format allows for direct use of the data due to its structured organization, unlike the raw data 💡

Practical Example

6 Analyze the case study results: GRAPH PLOTTING

Plot view: Displays results in a graph
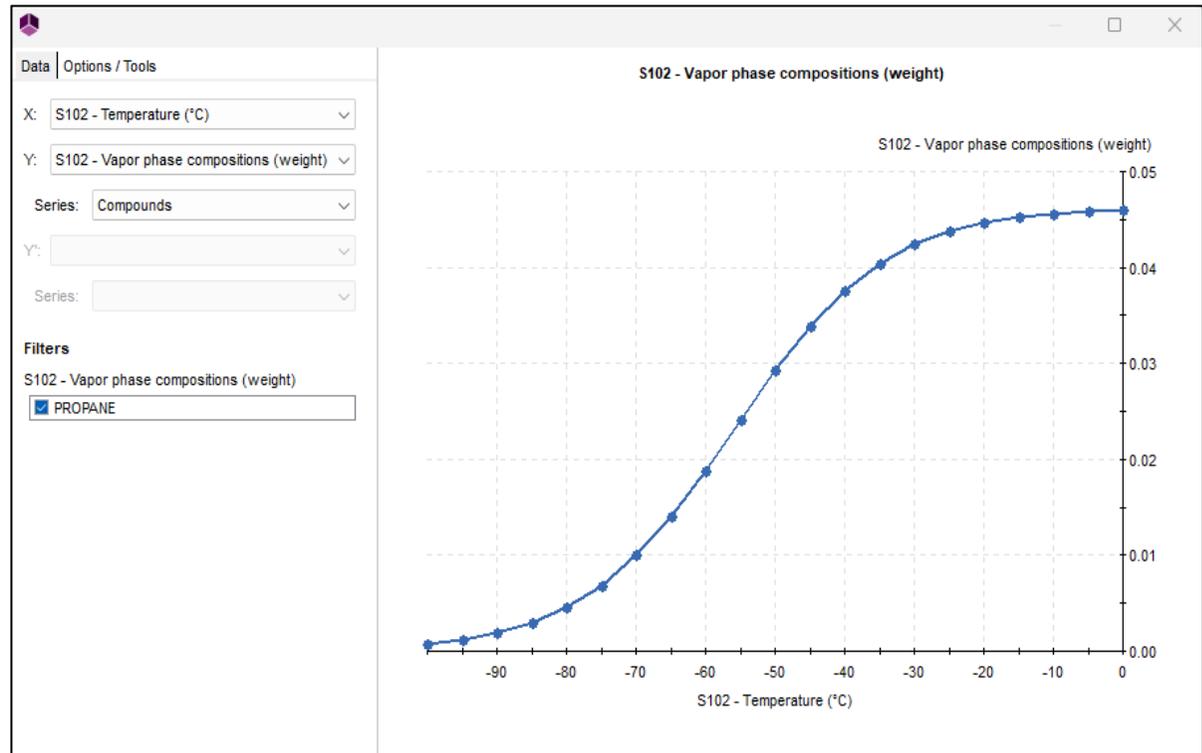
Practical Example

6 Analyze the case study results: GRAPH PLOTTING

A **Select input parameter (X):** Temperature of S102

Practical Example

6 Analyze the case study results: GRAPH PLOTTING

Case study results

Please select the variables to view or to plot

[View...] [Plot...]
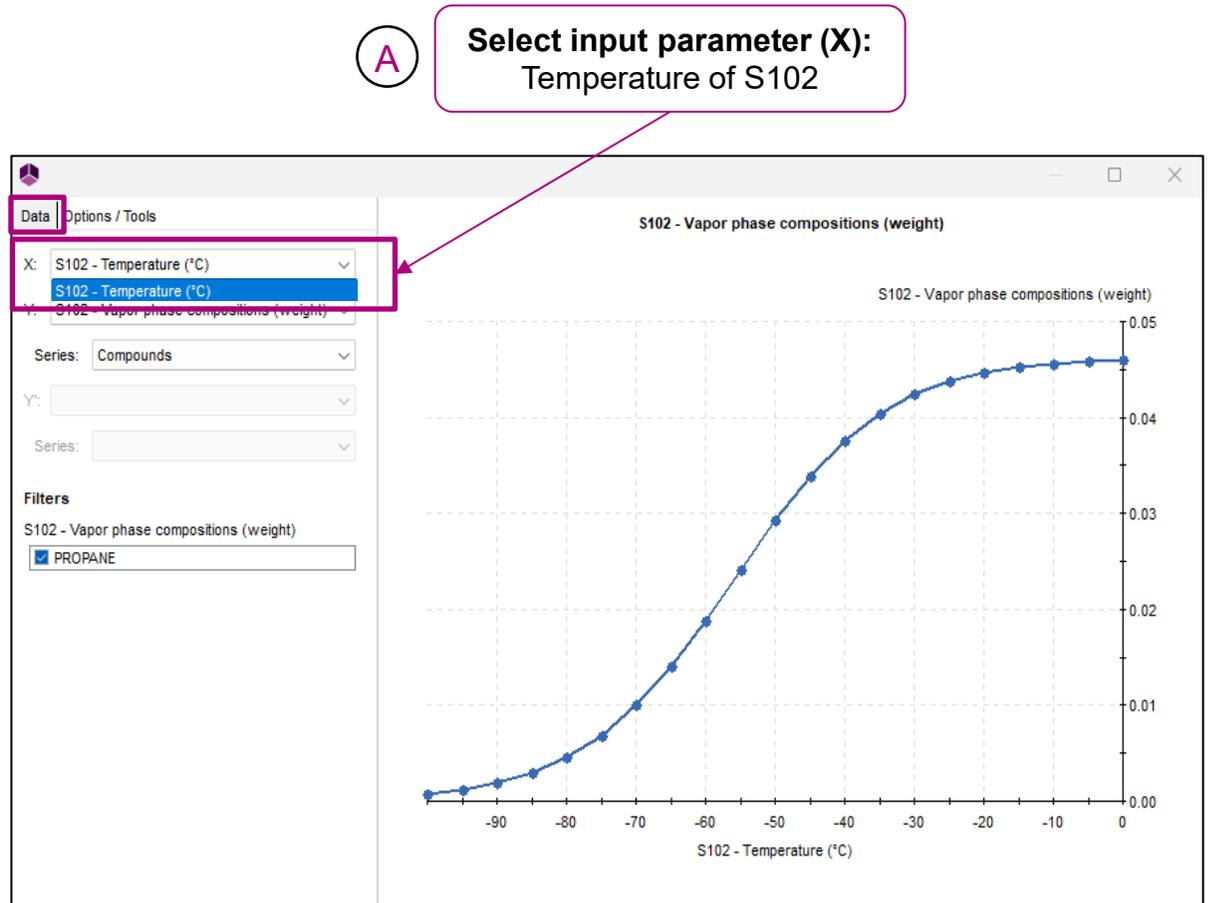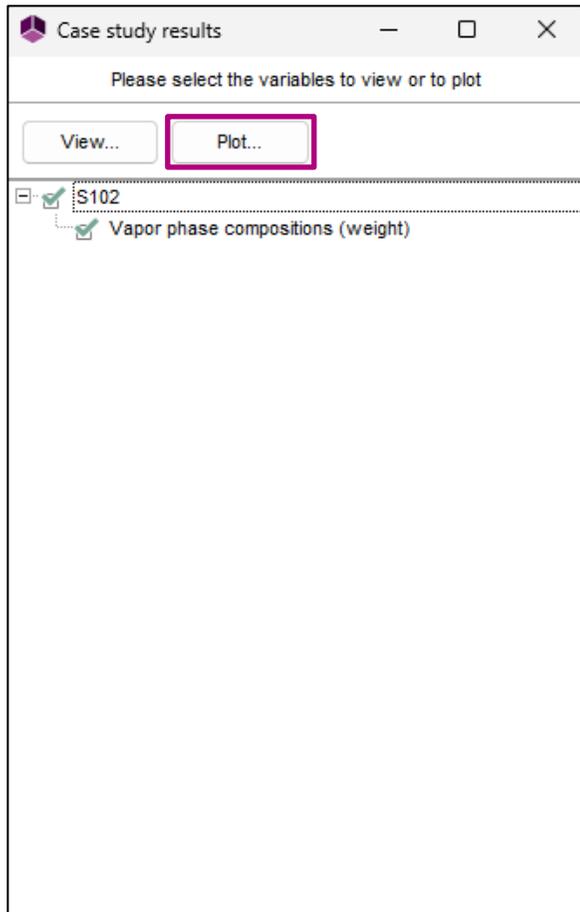
☑ S102
　☑ Vapor phase compositions (weight)
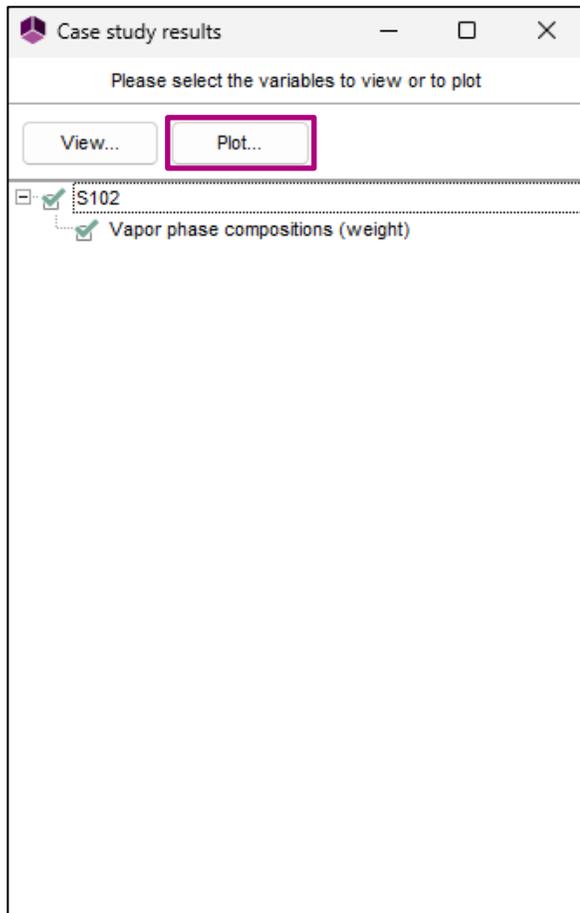
B **Select target result (Y):**
Vapor phase composition of
S102

Data | Options / Tools

X: S102 - Temperature (°C)
Y: S102 - Vapor phase compositions (weight)
　　S102 - Vapor phase compositions (weight)
Series: Compounds
Y':
Series:

Filters
S102 - Vapor phase compositions (weight)
☑ PROPANE

S102 - Vapor phase compositions (weight)
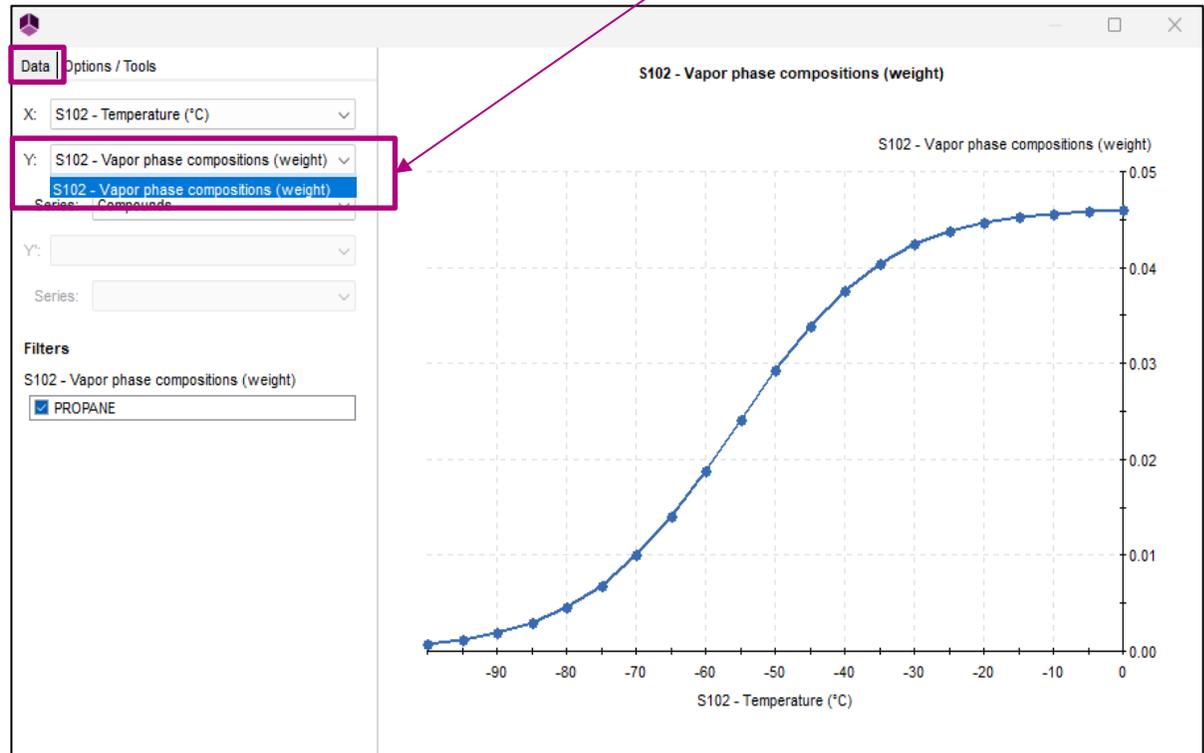
6 Analyze the case study results: GRAPH PLOTTING
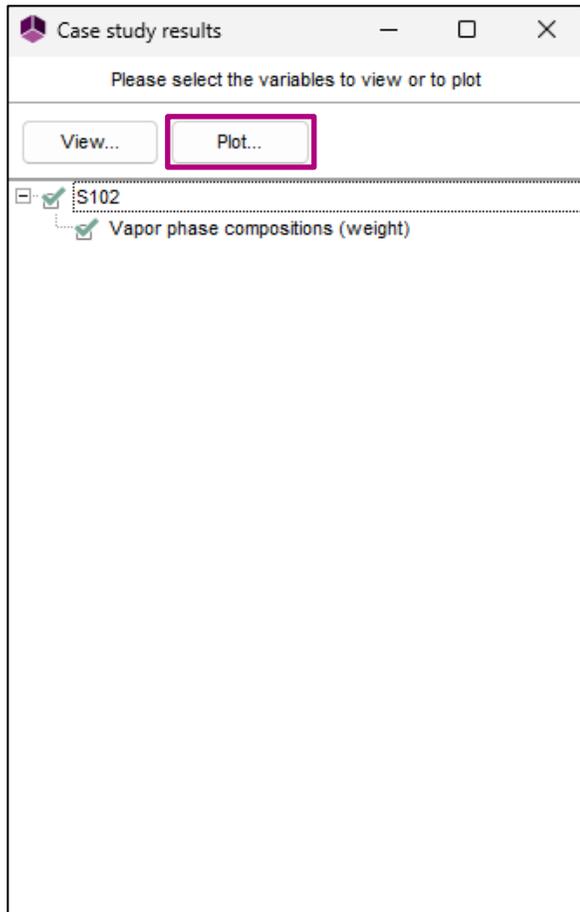
C **Filter by data series:** to plot only the propane composition

Practical Example
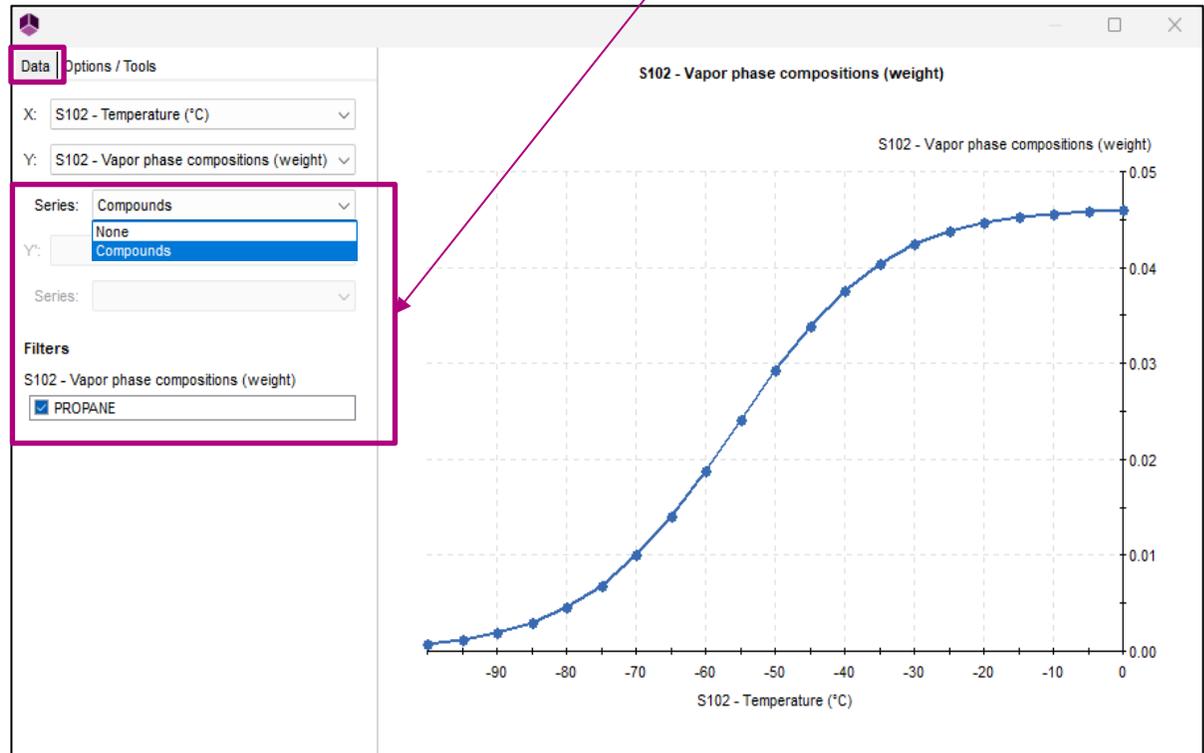
6 Analyze the case study results: GRAPH PLOTTING
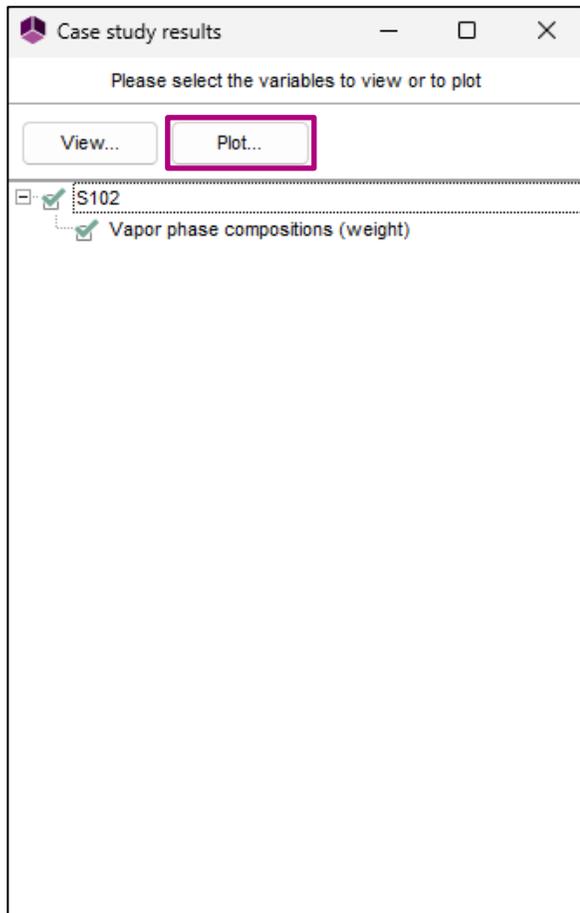
To change graph formatting
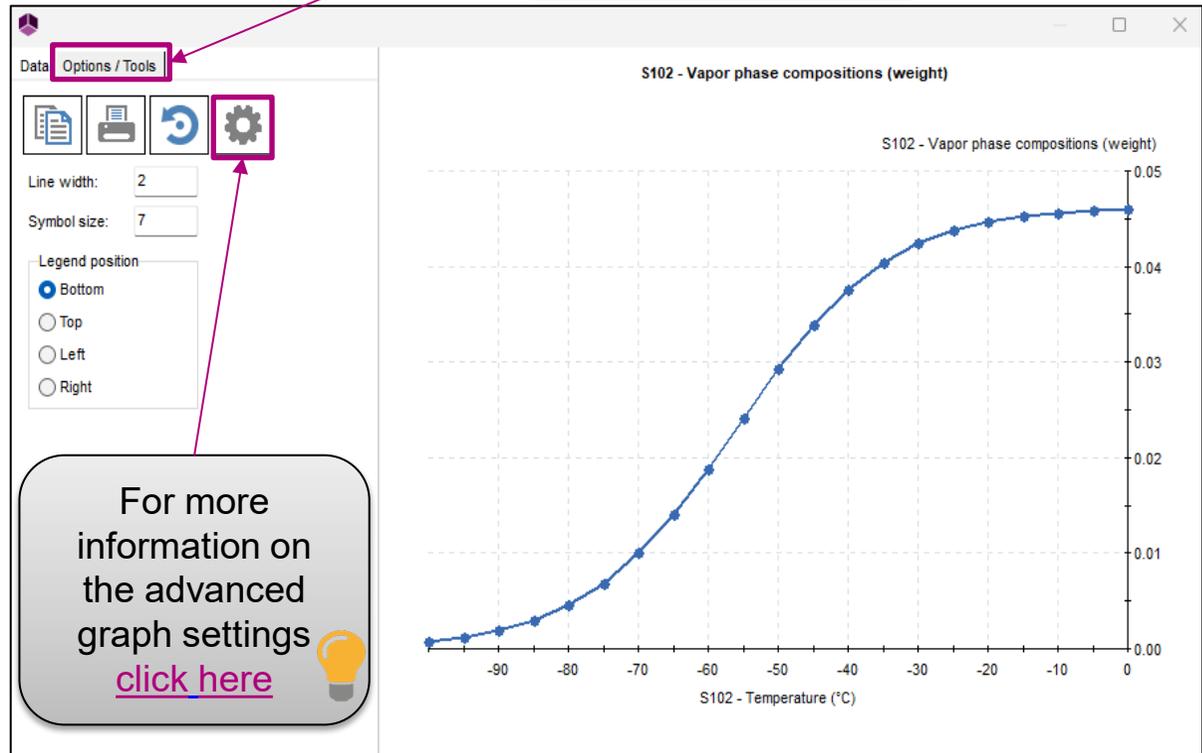
For more information on the advanced graph settings click here

Results analysis
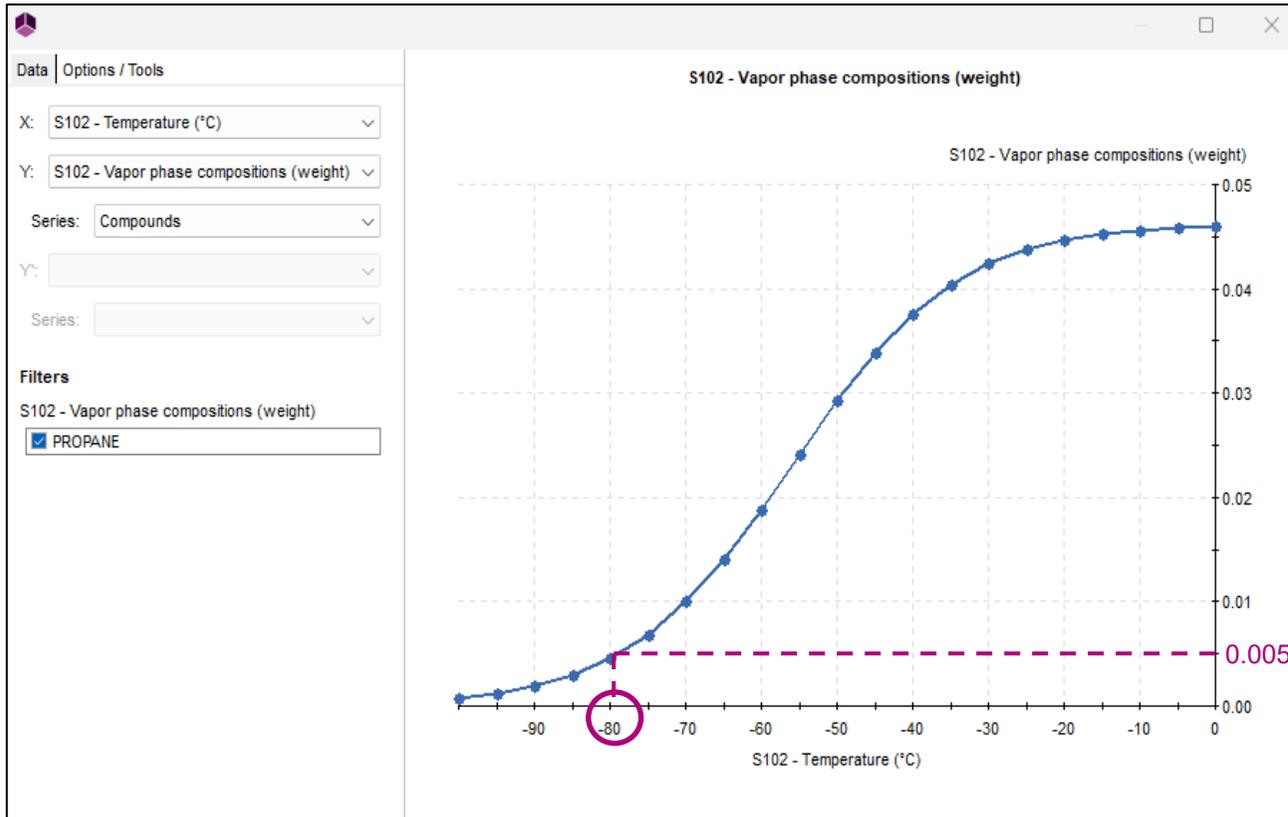
- The graph shows that the propane mass fraction in the vapor phase (lights stream) increases with temperature, reaching the target value of 0.005 at approximately -79°C.

- The temperature could then be manually adjusted in order to reach the required propane composition.

The **next step** describes how to configure the software to automatically adjust the temperature in order to meet the specified target

For more case study features click here

Context

Now that the **case study** has analyzed the impact of **action variables** on **target results**, we can set the **specifications** to let the software automatically adjust the action variable.

| **1** case study | → | **Identification of suitable variable values** | → | **2** **Specifications** |

Note on terminology:
X= Input parameter = action variable
Y= Output result = target result

Context

Now that the **case study** has analyzed the impact of **action variables** on **target results**, we can set the **specifications** to let the software automatically adjust the action variable.

Generic example

1 case study → Identification of suitable variable values → 2 Specifications

Reactor → Heat Exchanger → Flash

Modification of the action variable to meet the objective ← Deviation between the objective value and the measured value

Context

Now that the **case study** has analyzed the impact of **action variables** on **target results**, we can set the **specifications** to let the software automatically adjust the action variable.

1 case study → **Identification of suitable variable values** → **2** **Specifications**

Generic example

Reactor → *Heat Exchanger* → *Flash*

Modification of the action variable to meet the objective

HOW?

Deviation between the objective value and the measured value

Context

Now that the **case study** has analyzed the impact of **action variables** on **target results**, we can set the **specifications** to let the software automatically adjust the action variable.
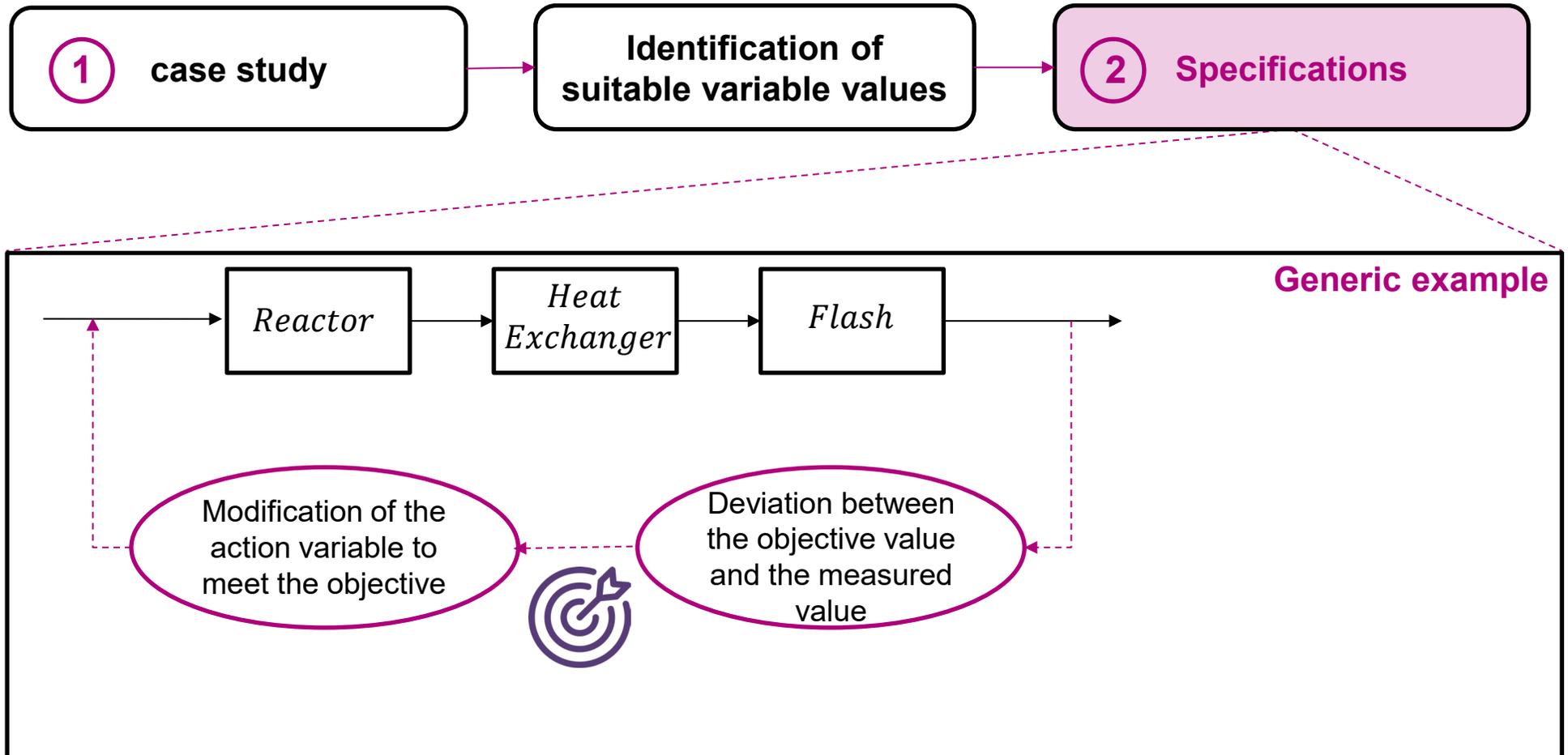

Generic example
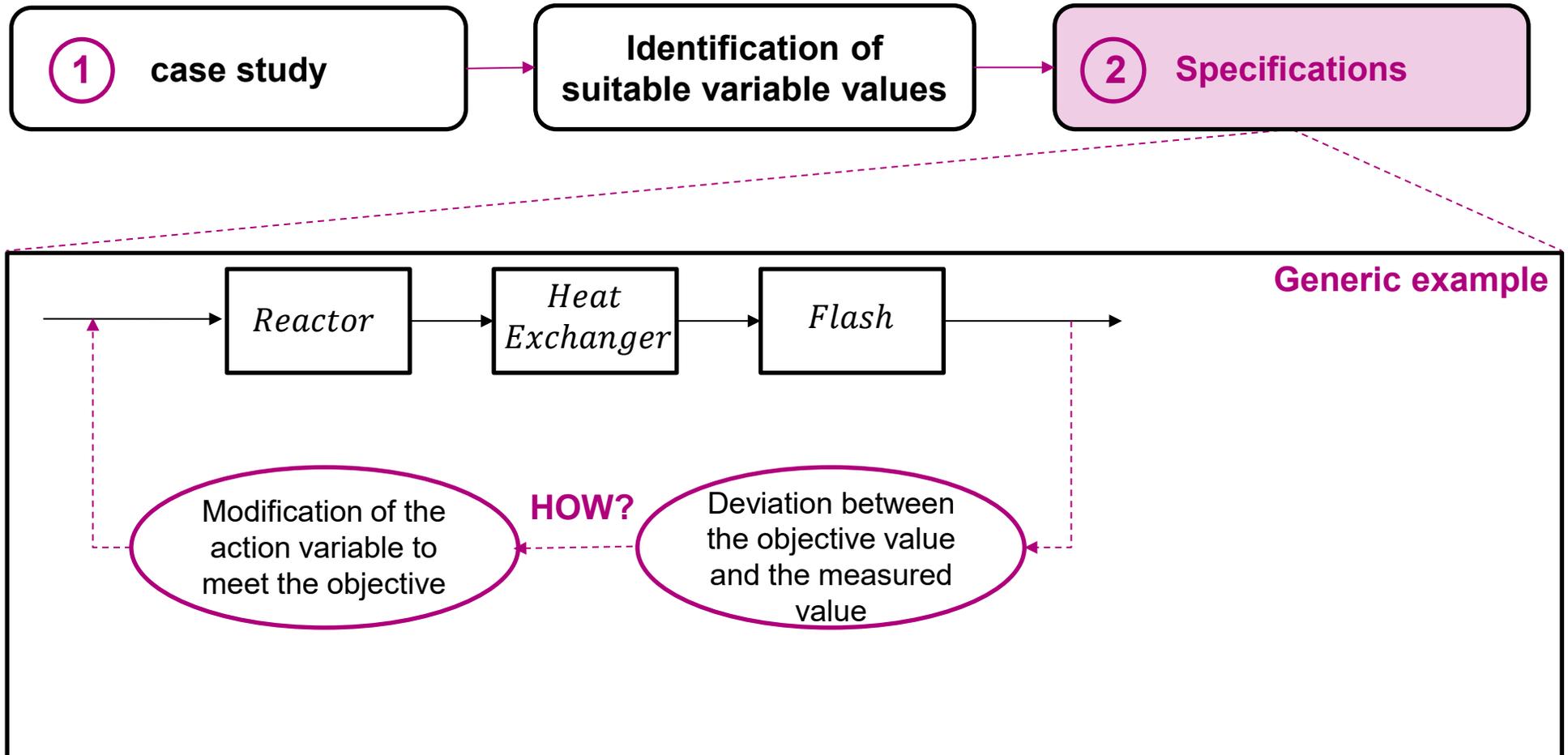
Reactor → Heat Exchanger → Flash

Modification of the action variable to meet the objective

Deviation between the objective value and the measured value

Controller

SPEC
Constraints and recycles

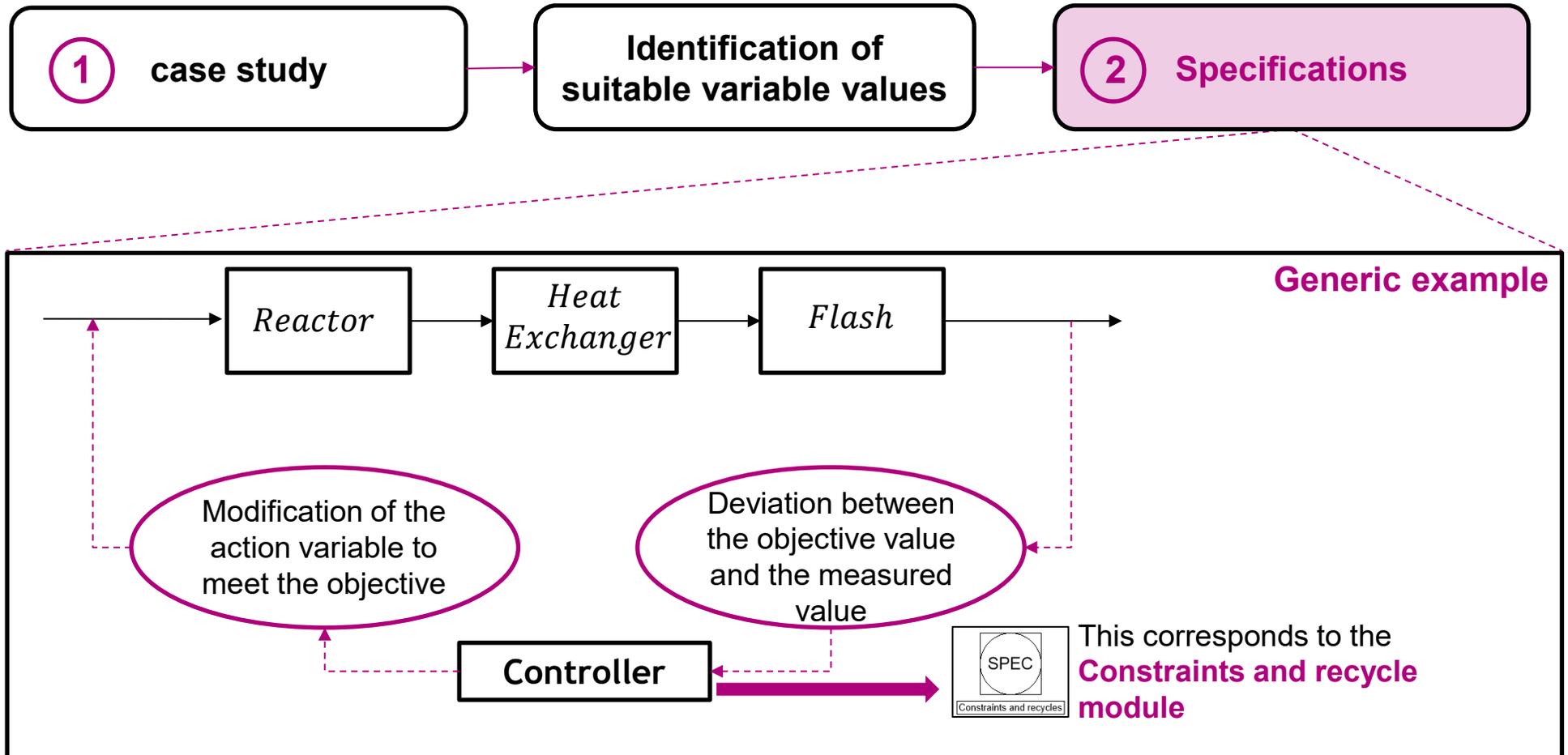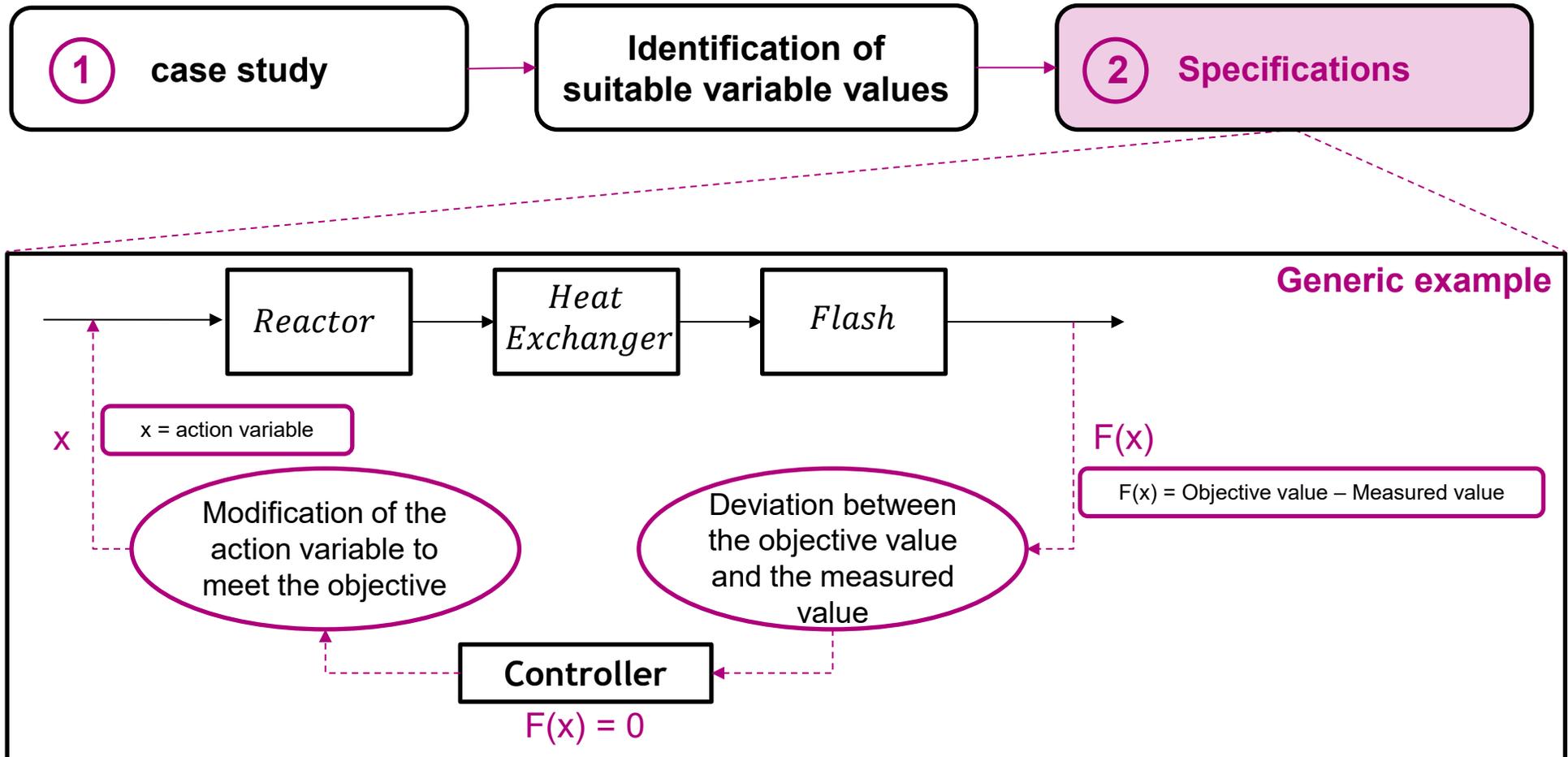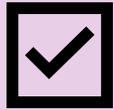This corresponds to the **Constraints and recycle module**

Now that the **case study** has analyzed the impact of **action variables** on **target results**, we can set the **specifications** to let the software automatically adjust the action variable.

1 **case study** → **Identification of suitable variable values** → 2 **Specifications**

Generic example

$Reactor$ → $Heat\ Exchanger$ → $Flash$

x   x = action variable   F(x)

F(x) = Objective value – Measured value

Modification of the action variable to meet the objective

Deviation between the objective value and the measured value

Controller

F(x) = 0

Why do we need specifications ?

☑ To ensure efficient process operation and meet operational targets

This involves controlling certain action variables to satisfy constraints:

(objective value – measured value (x)) = 0

or

F(x) = 0

HOW?

By transferring relevant information, including **action variables** and **target result** values, from one unit operation to another.

Each available **process variable** = a **degree of freedom**

Objective

Objective of the specification

In the simple example, adjust the Flash S102 temperature to reach 5000 ppm of propane in the "Light" stream (C6)
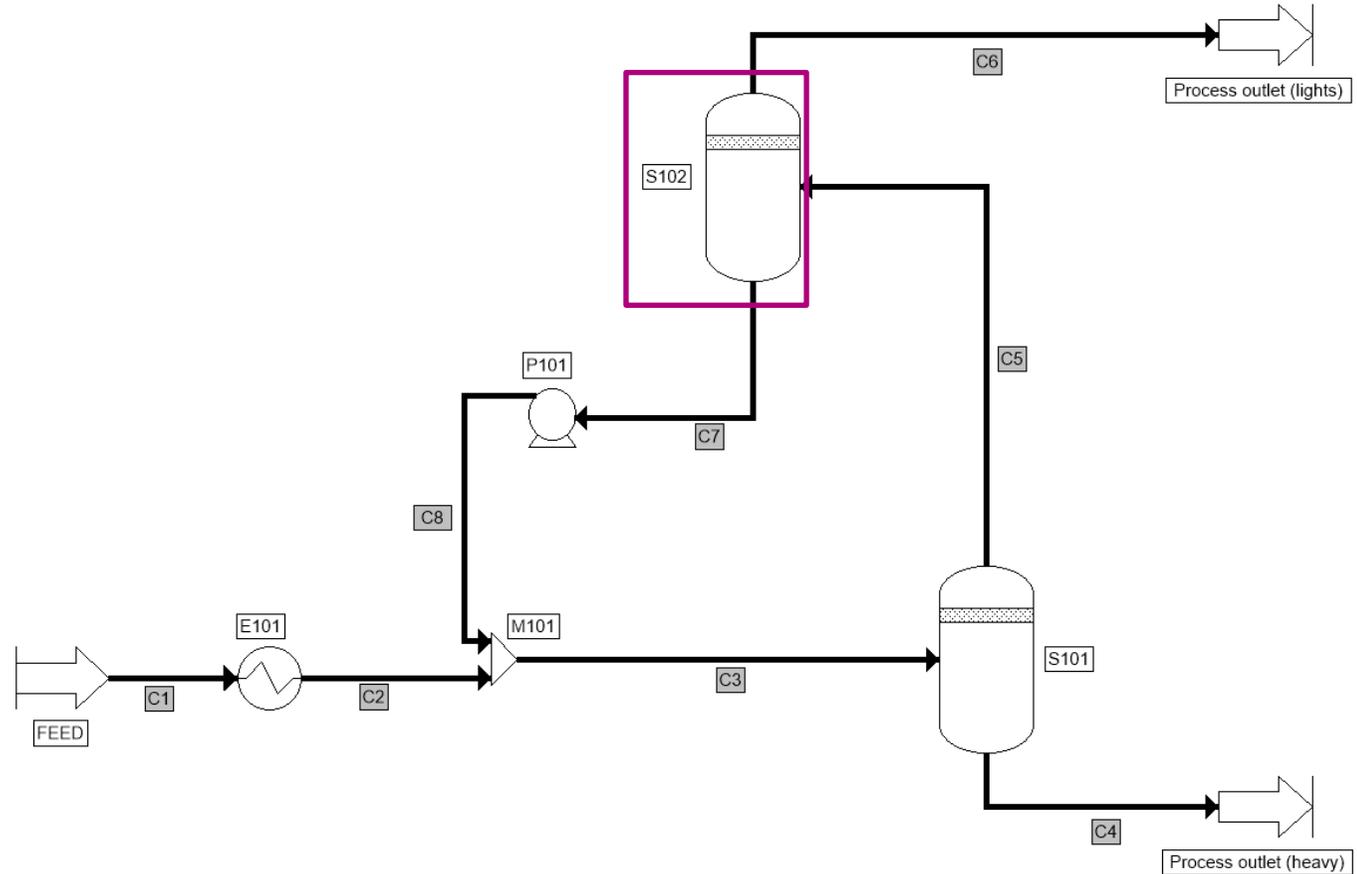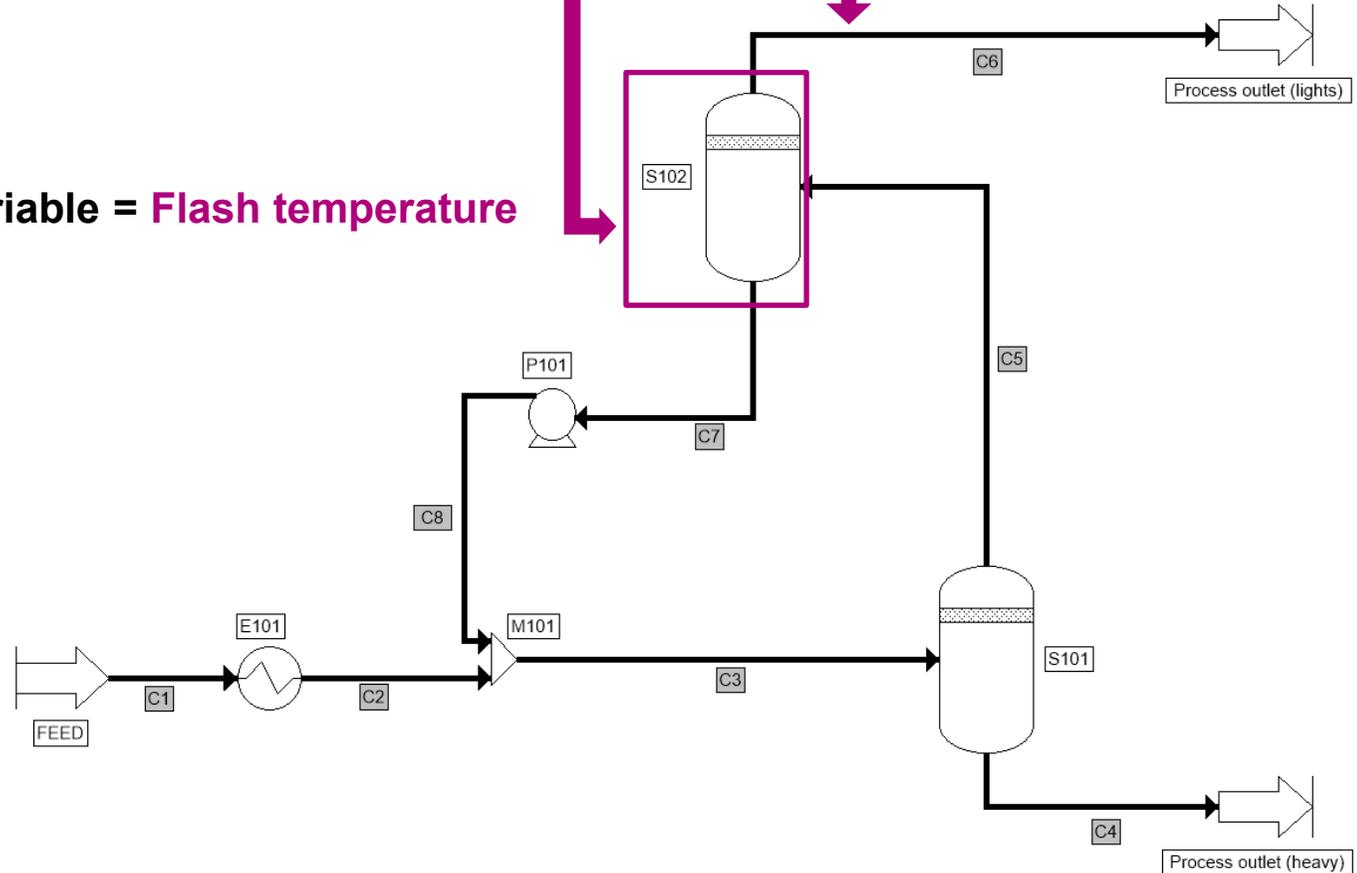
Objective

Objective of the Specification

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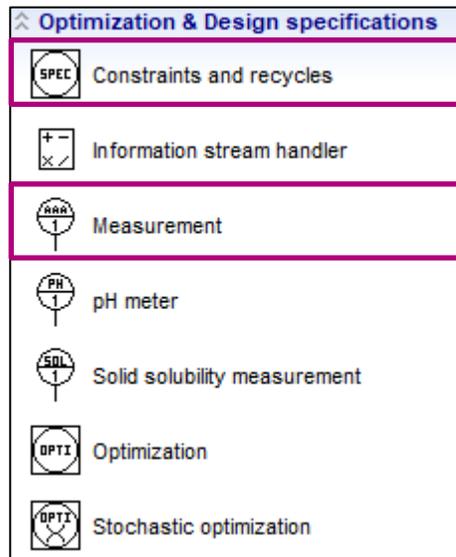
Propane composition (ppm) in Lights (C6) - 5000 ppm = 0 ← **Target result = 5000 ppm (propane)**

action variable = Flash temperature

Creation of a process specification

Optimization & Design specifications
- (SPEC) Constraints and recycles
- Information stream handler
- Measurement
- (PH) pH meter
- (SOL) Solid solubility measurement
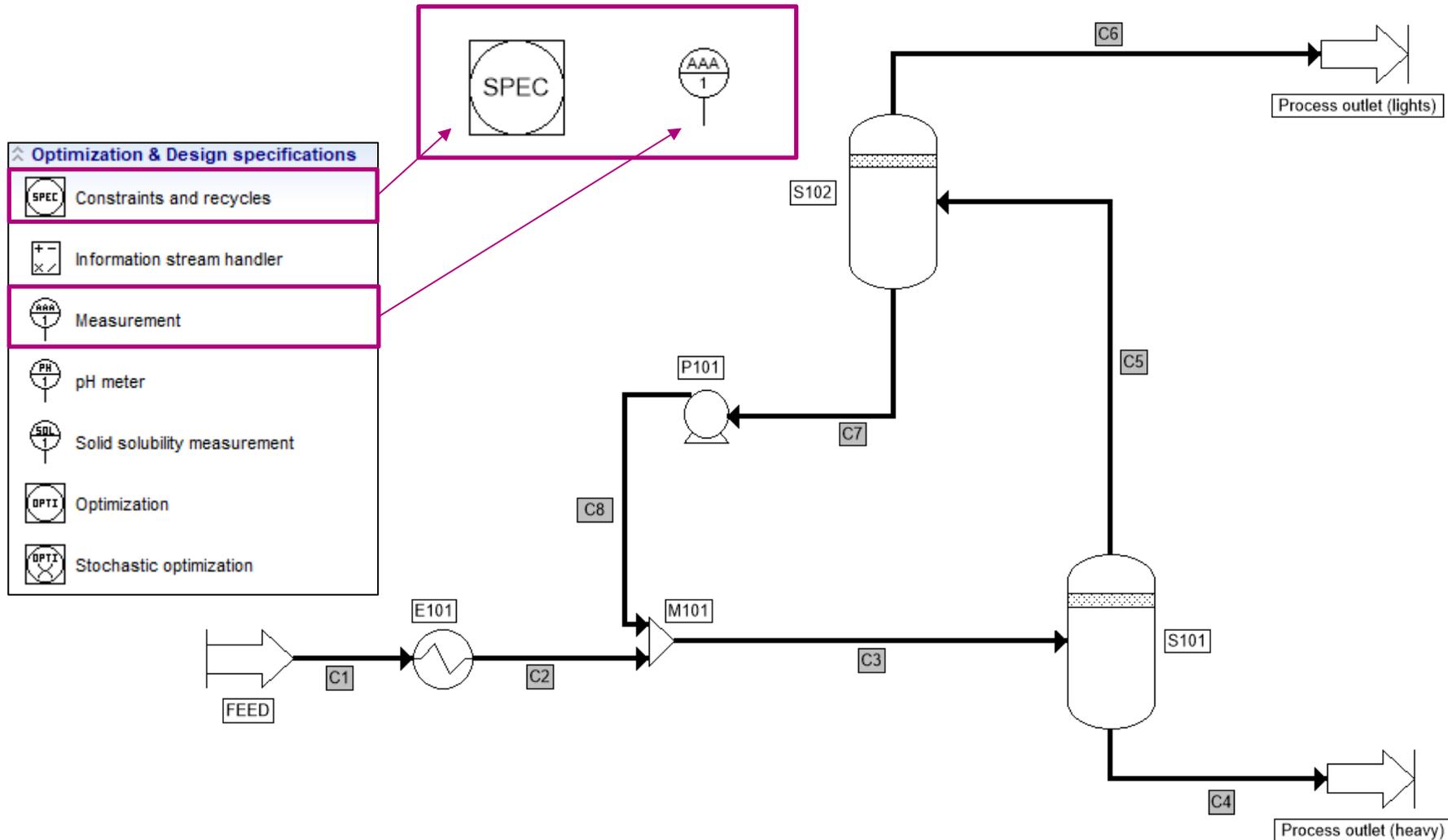- (OPTI) Optimization
- (OPTI) Stochastic optimization

Management of constraints and recycles, known as "SPEC" module

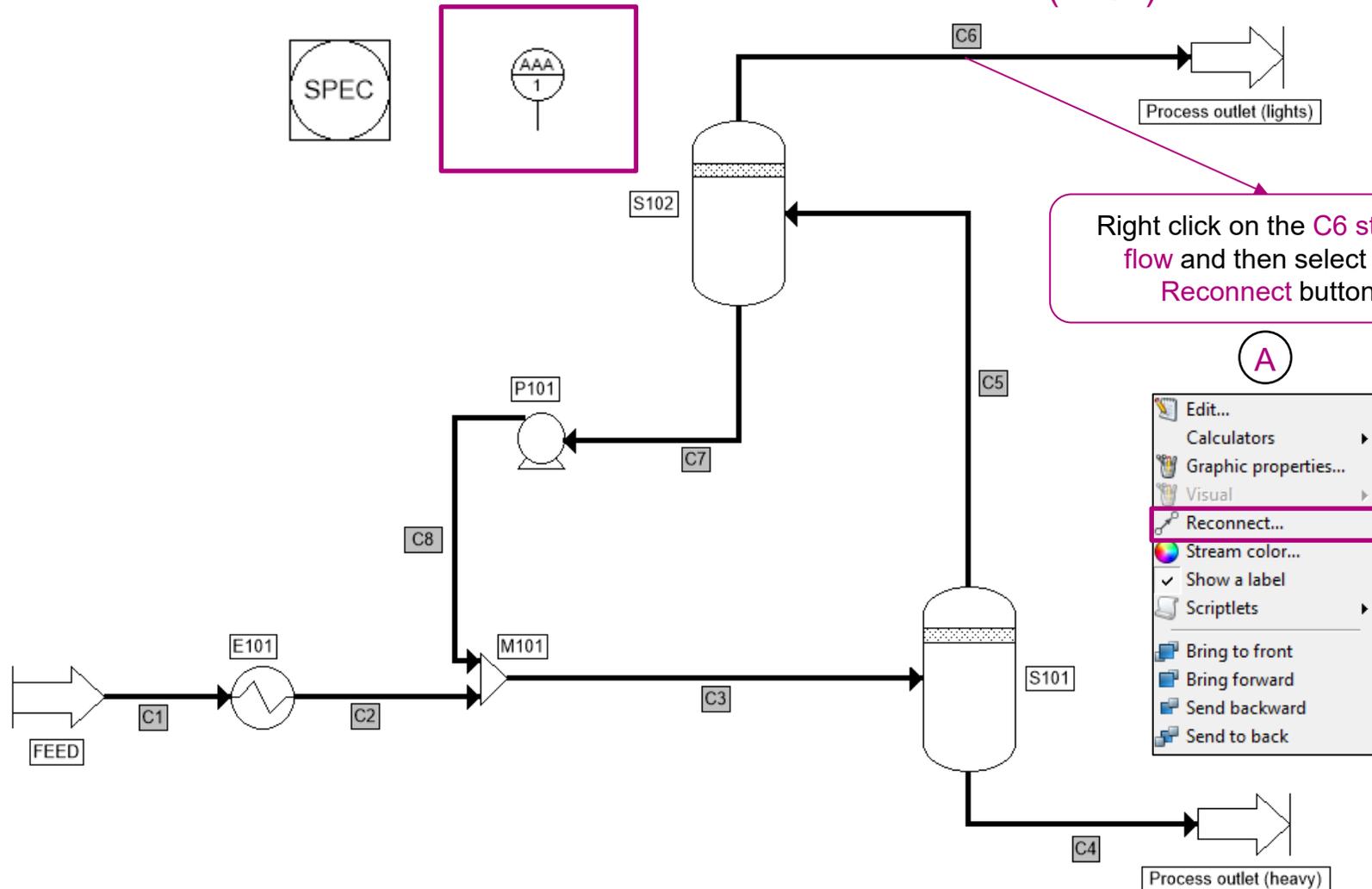**Measure of different process variables**

Practical Example

1 Insertion of "SPEC" and Measurement modules in the flowsheet

Practical Example

2 Reconnect the Measurement module to the vapor stream of the Flash unit (S102)

SPEC

AAA
1

C6

Process outlet (lights)

S102

Right click on the C6 stream flow and then select the Reconnect button

A

P101

C5

C7

C8

Edit...
Calculators
Graphic properties...
Visual
Reconnect...
Stream color...
Show a label
Scriptlets

Bring to front
Bring forward
Send backward
Send to back

E101

M101

S101

FEED

C1

C2

C3

C4

Process outlet (heavy)

Practical Example

2 Reconnect the Measurement module to the vapor stream of the Flash unit (S102)

Select the outlet connection port **B**

Select the inlet connection port **C**

Reconnect...

Click "OK" to save the data **D**

Practical Example

SPEC

C6

AAA 1

Measurement

Process outlet (lights)

S102

P101

C7

C5

C8

E101

M101

C3

S101

C1

C2

FEED

C4

Process outlet (heavy)

3
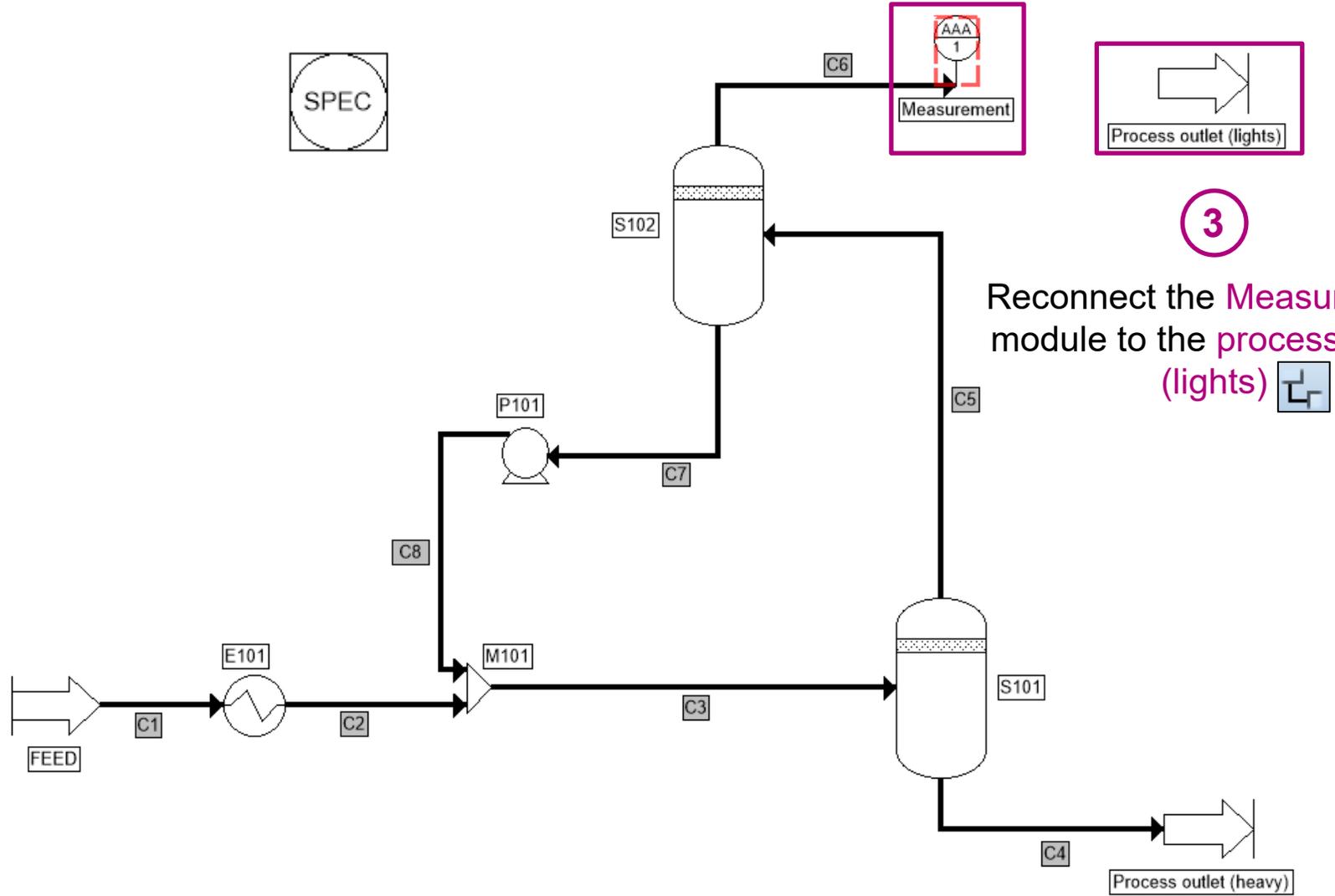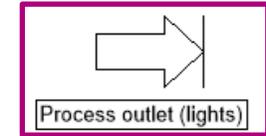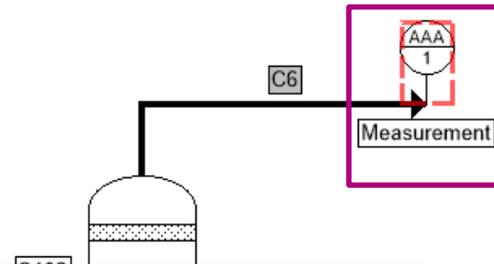
Reconnect the Measurement module to the process outlet (lights)

Practical Example

SPEC

C6

AAA 1

Measurement

Process outlet (lights)

3

Reconnect the Measurement module to the process outlet (lights)

Change the connections

Outlet connection port:

- Measurement
  - ⦿ Controlled stream 02

Process streams:
1
C1
C2
C3
C4
C5
C6
C7
C8

Inlet connection port:

- M101
- Process outlet (lights)
  - ⦿ Process outlet
- S101
- S102

Select the outlet connection port **A**

Select of the inlet connection port **B**

AAA 1

☑ Show only available connections

Click "OK" to save the data **C**

OK   Cancel

Practical Example

④ Connect the Measurement module to the "SPEC" module

SPEC

C6

AAA 1

Measurement

1

Process outlet (lights)

Change the connections

Outlet connection port: | New stream | Inlet connection port:

Measurement
- ⦿ Information outlet 01
- ◯ Information outlet 02

A

Constraints and recycles
- ⦿ Measured deviation 01
- ◯ Measured deviation 02
- ◯ Measured deviation 03
- ◯ Measured deviation 04
- ◯ Measured deviation 05
- ◯ Measured deviation 06
- ◯ Measured deviation 07
- ◯ Measured deviation 08
- ◯ Measured deviation 09
- ◯ Measured deviation 10
- ◯ Measured deviation 11
- ◯ Measured deviation 12
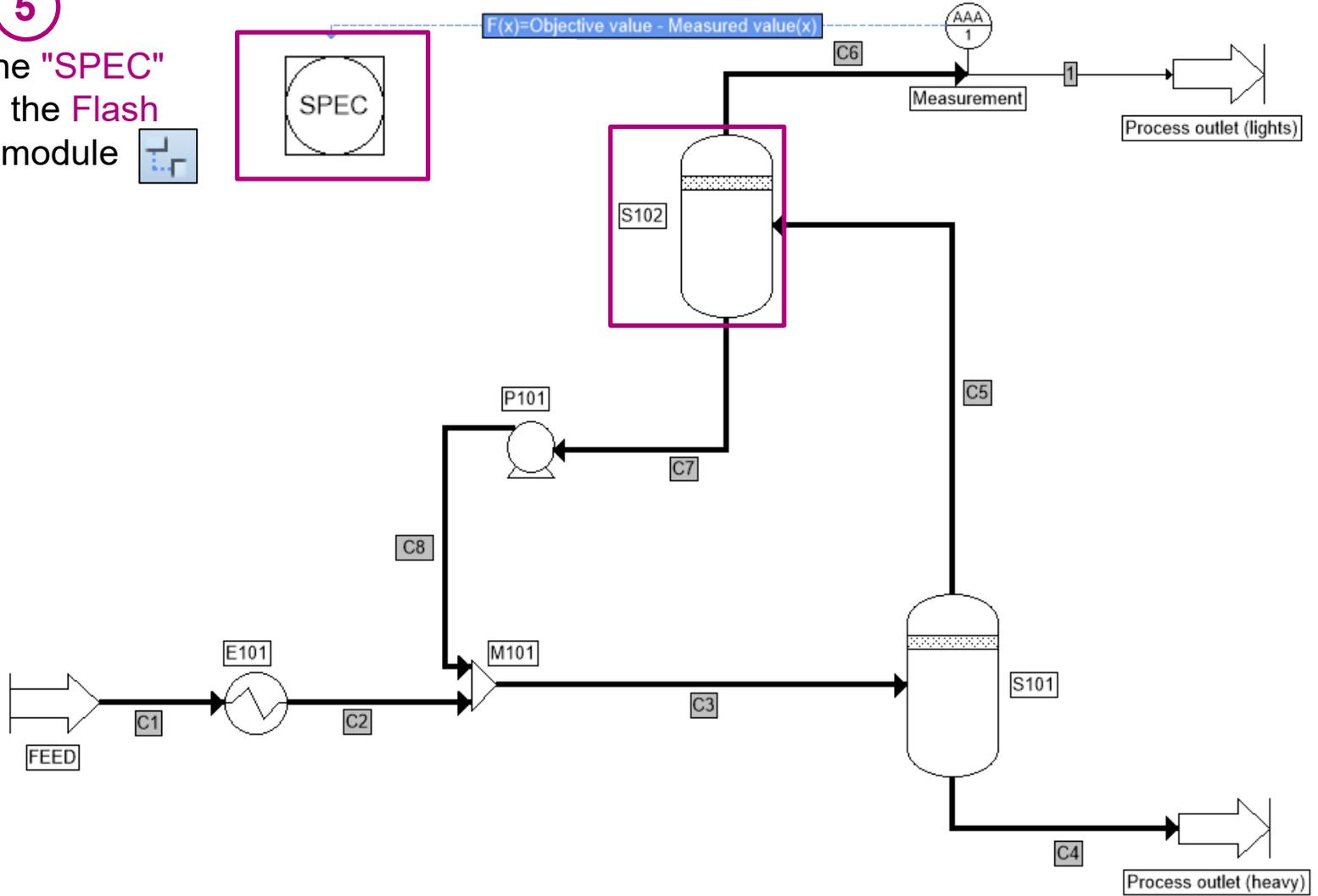
B

AAA 1

SPEC

☑ Show only available connections

OK   Cancel

Click "OK" to save the data

C

Practical Example

5

Connect the "SPEC" module to the Flash (S102) module

$F(x) = \text{Objective value} - \text{Measured value}(x)$

SPEC

AAA 1

C6

Measurement

1

Process outlet (lights)

S102

C5

P101

C7

C8

P101

E101

FEED

C1

C2

M101

C3

S101

C4

Process outlet (heavy)

5

Connect the "SPEC" module to the Flash (S102) module

F(x)=Objective value - Measured value(x)

SPEC

Constraints and recycles

AAA 1

C6

Measurement

1

Process outlet (lights)

S102

Change the connections
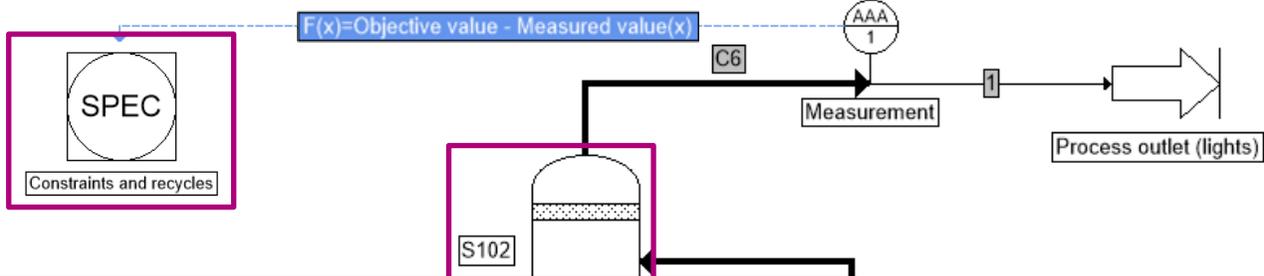
Outlet connection port: New stream   Inlet connection port:

Constraints and recycles
- ○ Action 01
- ○ Action 02
- ○ Action 03
- ○ Action 04
- ○ Action 05
- ○ Action 06
- ○ Action 07
- ◉ Action 08
- ○ Action 09
- ○ Action 10
- ○ Action 11
- ○ Action 12

S102
- ○ Information input/output 01
- ◉ Information input/output 02
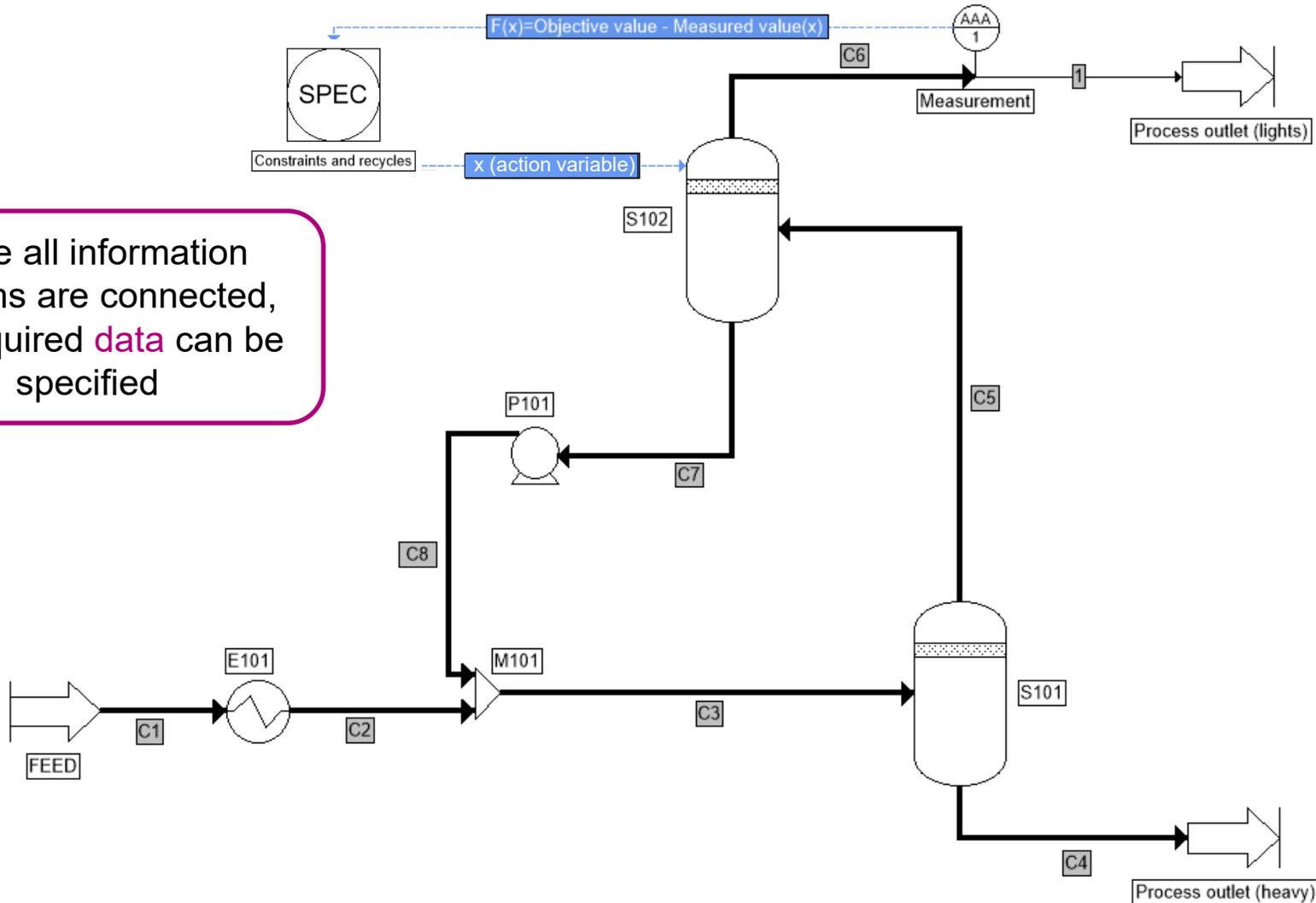- ○ Information input/output 03
- ○ Information input/output 04

A

B

SPEC

☑ Show only available connections

OK   Cancel

Click "OK" to save the data

C

Practical Example

F(x)=Objective value - Measured value(x)

AAA 1

C6

Measurement

1

Process outlet (lights)

SPEC

Constraints and recycles

x (action variable)

S102

Once all information streams are connected, the required data can be specified

P101

C7

C5

C8

E101

M101

S101

FEED

C1

C2

C3

C4

Process outlet (heavy)

Practical Example

Measurement ($MESU)

Name: Measurement
Desc:

Identification | **Parameters** | Scripts | Report | Streams | Notes | Ac

Measurement

Fraction

Temperature
Pressure
Total flowrate
Partial flowrate
Fraction
Partial flowrate ratio
Fraction ratio
NOx content
NO oxidation degree
Humidity
Concentration
pH

n-BUTANE

OK | Cancel

F(x)=Objective value - Measured value(x)

x (action variable)

Process outlet (lights)

6 Configuration of Measurement module

A Double click on the Measurement module

B Select the parameter to measure

💡 The measurement variable is the target result (mass fraction)

Practical Example

Measurement ($MESU)

Name: Measurement
Desc:

Identification | **Parameters** | Scripts | Report | Streams | Notes | Ac

Measurement

Fraction

Set point for a fraction
○ Mole fraction
● Mass fraction

Mass fraction   0.005

NITROGEN	☐	All
METHANE	☐	None
ETHANE	☐	
PROPANE	☑	
n-BUTANE	☐	

OK   Cancel

F(x)=Objective value - Measured value(x)

C6

AAA 1

Measurement

1

Process outlet (lights)

x (action variable)

S102

6 Configuration of Measurement module

Enter the desired value of mass fraction of propane, which is the specification
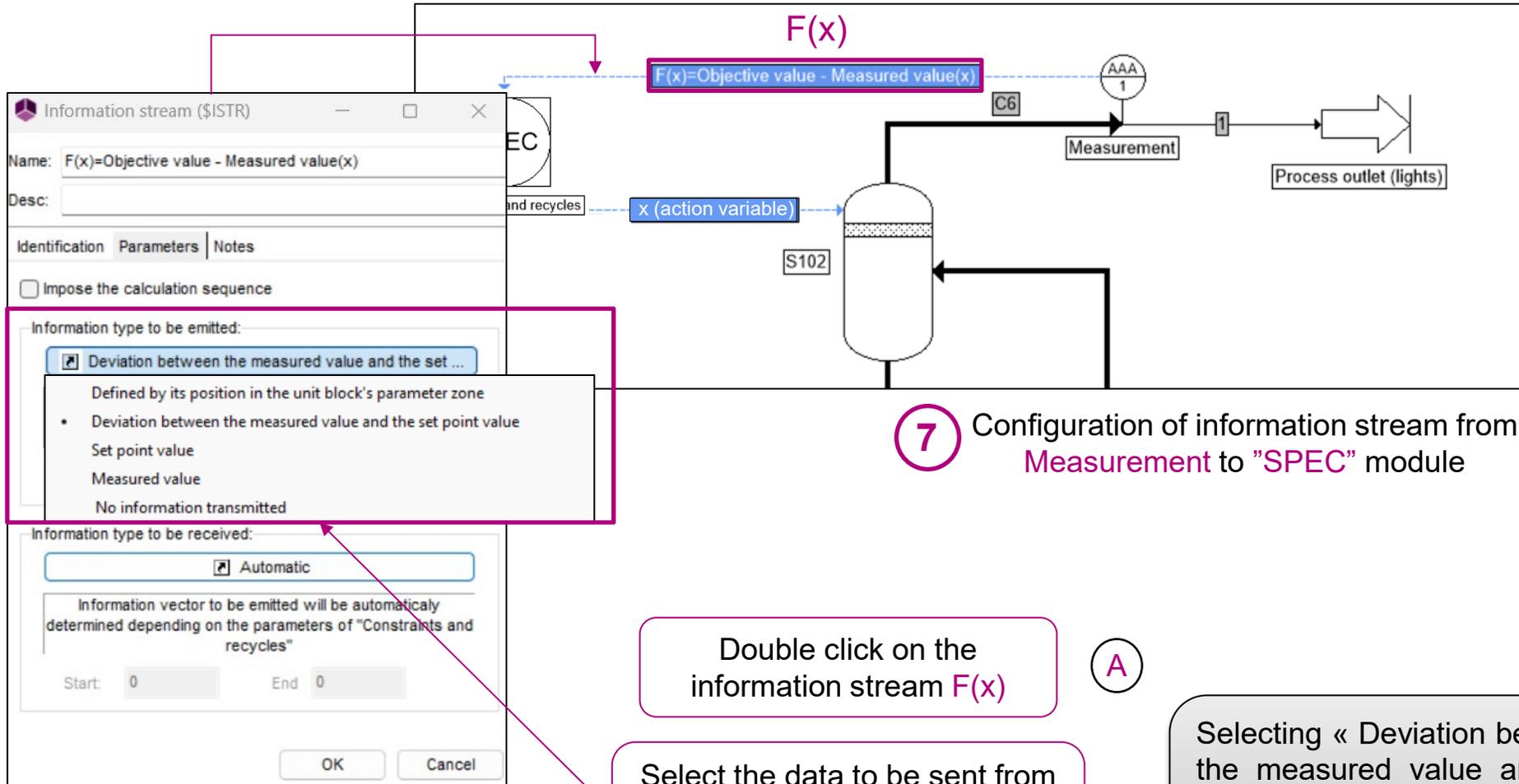
C

Practical Example

Measurement ($MESU)

Name: Measurement
Desc:

Identification | **Parameters** | Scripts | Report | Streams | Notes | Ac ◀ ▶

Measurement

Fraction

Set point for a fraction
○ Mole fraction
● Mass fraction

Mass fraction   0.005

NITROGEN   ☐   All
METHANE   ☐
ETHANE   ☐   None
PROPANE   ☑
n-BUTANE   ☐

OK   Cancel

$F(x)=Objective\ value - Measured\ value(x)$

C6

AAA
1

Measurement

1

Process outlet (lights)

x (action variable)

S102

6 Configuration of Measurement module

Select propane as compound of interest   **D**

Click "OK" to save the data   **E**

$F(x)$

F(x)=Objective value - Measured value(x)

AAA 1

C6

Measurement

1

Process outlet (lights)

x (action variable)

S102

Information stream ($ISTR) — ☐ ✕

Name: F(x)=Objective value - Measured value(x)

Desc:

Identification | Parameters | Notes

☐ Impose the calculation sequence

Information type to be emitted:

↗ Deviation between the measured value and the set ...

- Defined by its position in the unit block's parameter zone
- • Deviation between the measured value and the set point value
- Set point value
- Measured value
- No information transmitted

Information type to be received:

↗ Automatic

Information vector to be emitted will be automaticaly determined depending on the parameters of "Constraints and recycles"

Start: 0   End: 0

OK   Cancel

(7) Configuration of information stream from Measurement to "SPEC" module

Double click on the information stream F(x)   (A)

Select the data to be sent from the Measurement module to the "SPEC" module   (B)

Selecting « Deviation between the measured value and the set point value » aims to satisfy the condition $F(x) = 0$

Introduction 1	Case Study 2	Specifications 3	**Practical Example**

F(x)

F(x)=Objective value - Measured value(x)

AAA 1

C6

Measurement

1

Process outlet (lights)

EC

and recycles — — x (action variable)

S102

Information stream ($ISTR) — □ ✕

Name: F(x)=Objective value - Measured value(x)

Desc:

Identification | Parameters | Notes

☐ Impose the calculation sequence

Information type to be emitted:

▣ Deviation between the measured value and the set ...

Information vector to be emitted will be automaticaly determined depending on the parameters of "Measurement"

Start: 0   End: 0

Information type to be received:

▣ Automatic

Defined by its position in the unit block's parameter zone
• Automatic
No information transmitted

Start: 0   End: 0

OK   Cancel

7 Configuration of information stream from Measurement to "SPEC" module

Selection of the type of information to be received by the constraints and recycle module   ⓒ

💡 Information type toward or from a "SPEC" module is always "automatic"

Practical Example

F(x)

F(x)=Objective value - Measured value(x)

AAA
1

EC

C6

Measurement

and recycles

x (action variable)

S102

1

Process outlet (lights)

Information stream ($ISTR) — □ ✕

Name: F(x)=Objective value - Measured value(x)

Desc:

Identification | Parameters | Notes

☐ Impose the calculation sequence

Information type to be emitted:

↗ Deviation between the measured value and the set ...

Information vector to be emitted will be automaticaly determined depending on the parameters of "Measurement"

Start: 0   End: 0

Information type to be received:

↗ Automatic

Information vector to be emitted will be automaticaly determined depending on the parameters of "Constraints and recycles"

Start: 0   End: 0

OK   Cancel

⑦ Configuration of information stream from Measurement to "SPEC" module

Click "OK" to save the data Ⓓ

Introduction 1	Case Study 2	Specifications 3

Practical Example

$$F(x) = 0$$

F(x)=Objective value - Measured value(x)

SPEC

Constraints and recycles

x (action variable)

C6

AAA 1

Measurement

1

Process outlet (lights)

Constraints and recycles ($SPEC)

Name: Constraints and recycles

Desc:

Identification | **Parameters** | Scripts | Report | Streams | Notes | Advanced parameters

☑ Module enabled

Numerical methods: Default

Stop tests

Convergence criterion	1E-8
Non evolution of criterion	1E-7
Non evolution of variables	1E-6
Maximum number of passages in the MCN	100
Maximum number of iterations	20

Print

Print every [10] iterations

Tear streams iterative variables

☑ Temperatures

☐ Pressures

Resume

☑ Use of values obtained at convergence of the previous problem

Damping strategy

Initial damping factor: [1]

Sensitivity analysis

Step size on the tear streams variables proportional to... : the difference between 2 itera

Proportionality factor: [0,1]

Step size of the adjusted variables proportial to... : the difference between 2 itera

Proportionality factor: [0,1]

Constraints Parameters...

Tear streams Parameters...

OK | Cancel

8 Configuration of the "SPEC" module

A Double click on the SPEC module

The "SPEC" module parameters are set to default values and do not require modification, but users can adjust them if needed.

For more information on the "SPEC" module module parameters click here.

Practical Example

F(x)=Objective value - Measured value(x)

AAA 1

C6

Measurement

Process outlet (lights)

1

SPEC

x

Constraints and recycles

x (action variable)

S102

Information stream ($ISTR1)

Name: x (acting parameter)

Desc:

Identification | **Parameters** | Notes

☐ Impose the calculation sequence

Information type to be emitted:

↗ Automatic

Defined by its position in the unit block's parameter zone
- Automatic
No information transmitted

Start: 0   End: 0

Information type to be received:

↗ Operating temperature

Information vector to be emitted will be automaticaly determined depending on the parameters of "S102"

Start: 0   End: 0

OK   Cancel

9 Configuration of the information stream from the "SPEC" to Flash S102 module

Double click on the x information stream **A**

Select the type of information to be sent by the "SPEC" module **B**

Information type toward or from a "SPEC" module is always "automatic" 💡
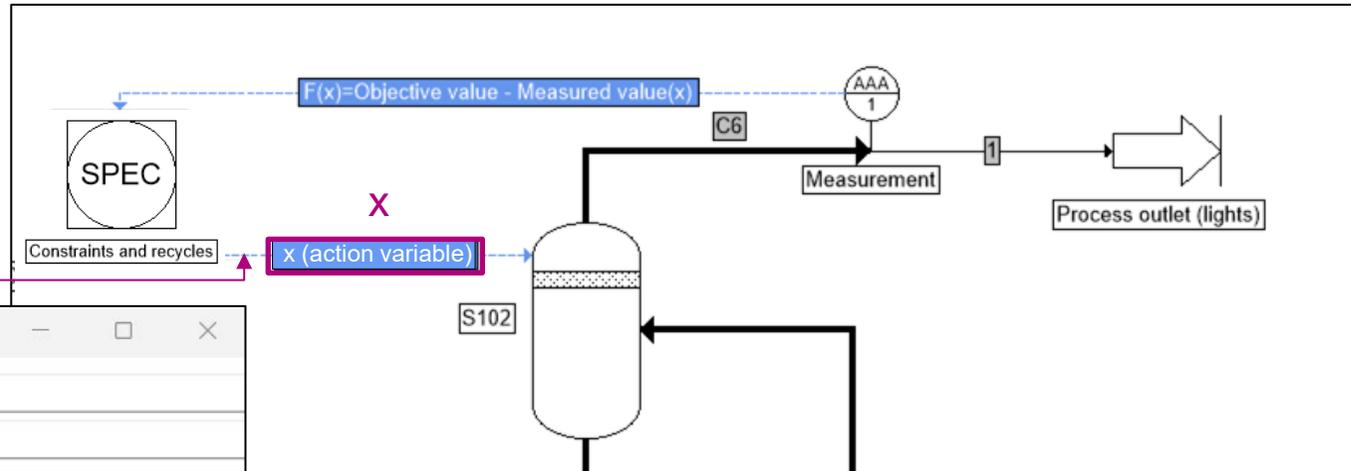
Practical Example

F(x)=Objective value - Measured value(x)

AAA 1

C6

Measurement

Process outlet (lights)

SPEC

Constraints and recycles

x

x (action variable)

S102

Information stream ($ISTR1) — □ ✕

Name: x (acting parameter)

Desc:

Identification | **Parameters** | Notes

☐ Impose the calculation sequence

Information type to be emitted:

⬈ Automatic

Information vector to be emitted will be automatically determined depending on the parameters of "Constraints and recycles"

Start: 0   End: 0

Information type to be received:

⬈ Operating temperature

Information vector to be emitted will be automaticaly determined depending on the parameters of "S102"

Start: 0   End: 0

OK   Cancel

⑨ Configuration of the information stream from the "SPEC" to Flash S102 module

Defined by its position in the unit block's parameter zone
- Operating temperature
  Operating pressure
  Temperature increment
  Pressure drop
  Vapor fraction
  Heat duty to be supplied
  Heat duty to be removed
  Efficiency (utility)
  Utility saturation temperature
  Utility inlet temperature
  Utility outlet temperature
  Utility pressure
  Utility saturation pressure
  No information transmitted

! **IMPORTANT STEP**
Select the action variable within the list of parameters

Ⓒ

Practical Example

F(x)=Objective value - Measured value(x)

SPEC

Constraints and recycles

X

x (action variable)

AAA 1

C6

Measurement

Process outlet (lights)

S102

Information stream ($ISTR1)

Name: x (acting parameter)

Desc:

Identification | **Parameters** | Notes

☐ Impose the calculation sequence

Information type to be emitted:

⬀ Automatic

Information vector to be emitted will be automaticaly determined depending on the parameters of "Constraints and recycles"

Start: 0   End: 0

Information type to be received:

⬀ Operating temperature

Information vector to be emitted will be automaticaly determined depending on the parameters of "S102"

Start: 0   End: 0

OK   Cancel

9 Configuration of the information stream from the "SPEC" to Flash S102 module

Click "OK" to save the data

D

Practical Example

! IMPORTANT

The **action variable** must be a **modifiable input** in the unit operation (*i.e.*, a value the user can supply in the unit operation window). If it comes from another unit operation or isn't initialized, the specification won't work. 💡
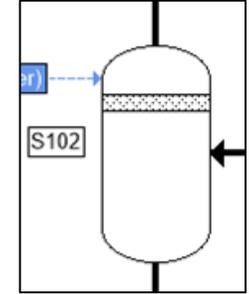
For this example:
Module: Flash S102
Specification: propane composition in the lights stream achieved by temperature adjustment (action variable)
Action variable to be selected in the module: supplied temperature
Initialize variable: Indicate a temperature value, *e.g.*: -60°C

Practical Example
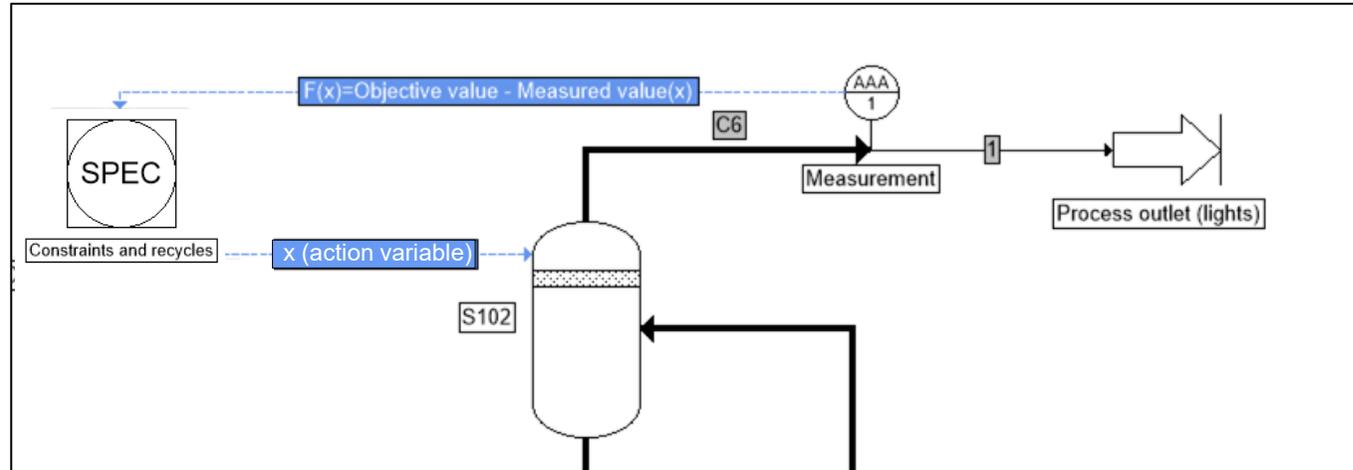
10 Once all parameters have been provided, the simulation can be run

Introduction 1	Case Study 2	Specifications 3

Practical Example

(11) Simulation results
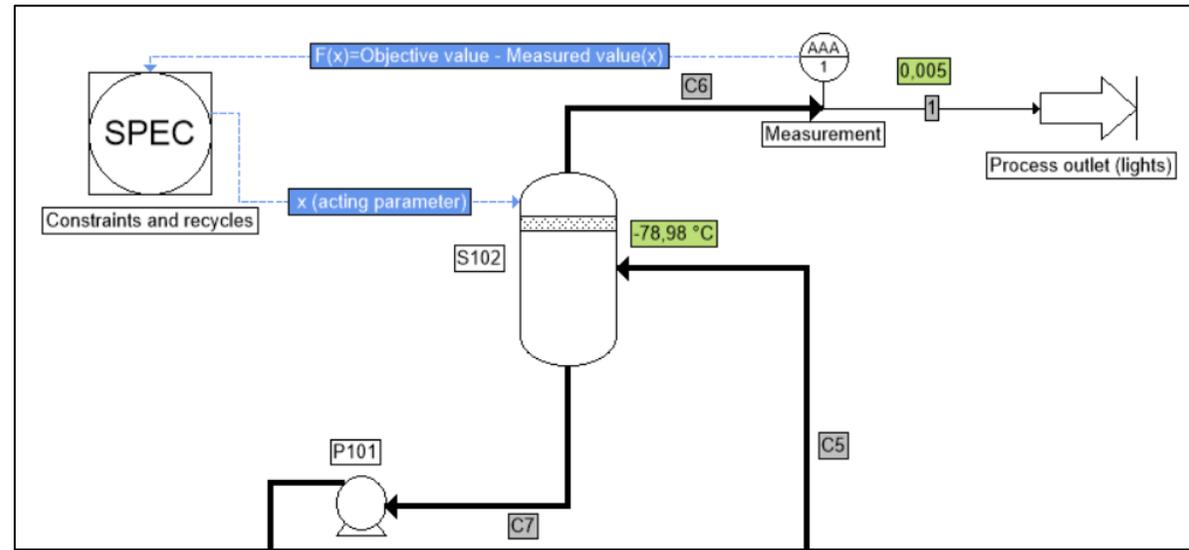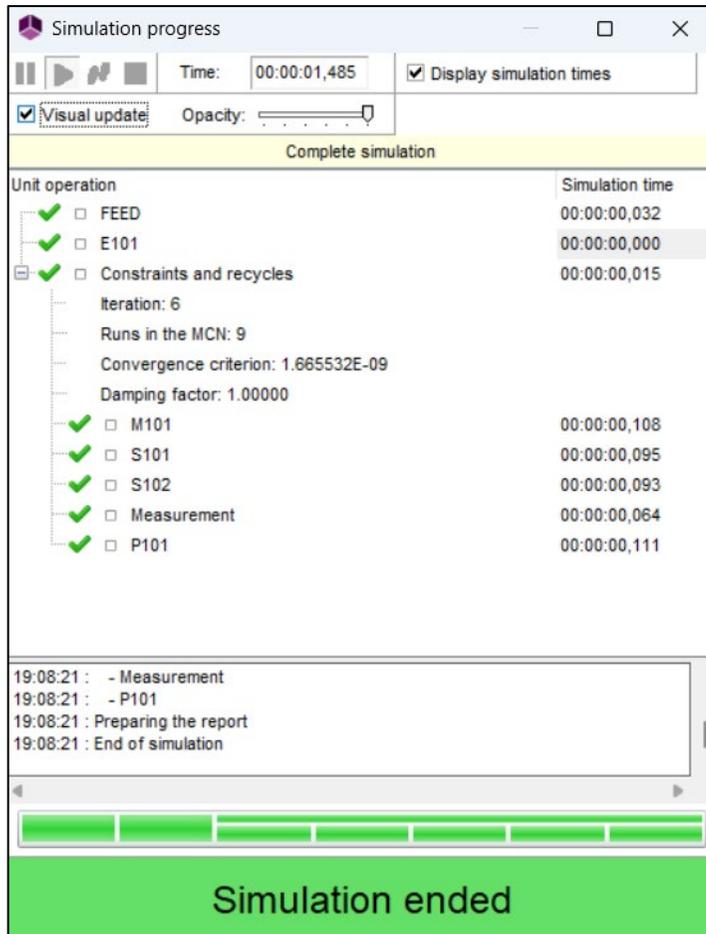
The information of interest:

1. Stream 1 – Propane mass fraction
2. Flash S102 Unit operation – Flash Temperature

Can be displayed by using the tag feature **123** and selecting respectively:

1. MassFraction – Compound (Propane)
2. TemperatureSpecValue

(For more information on the tag feature please consult PSPS_GS01_EN-Main-features-overview documentation)

Introduction 1	Case Study 2	Specifications 3

Practical Example

11 **Simulation results**
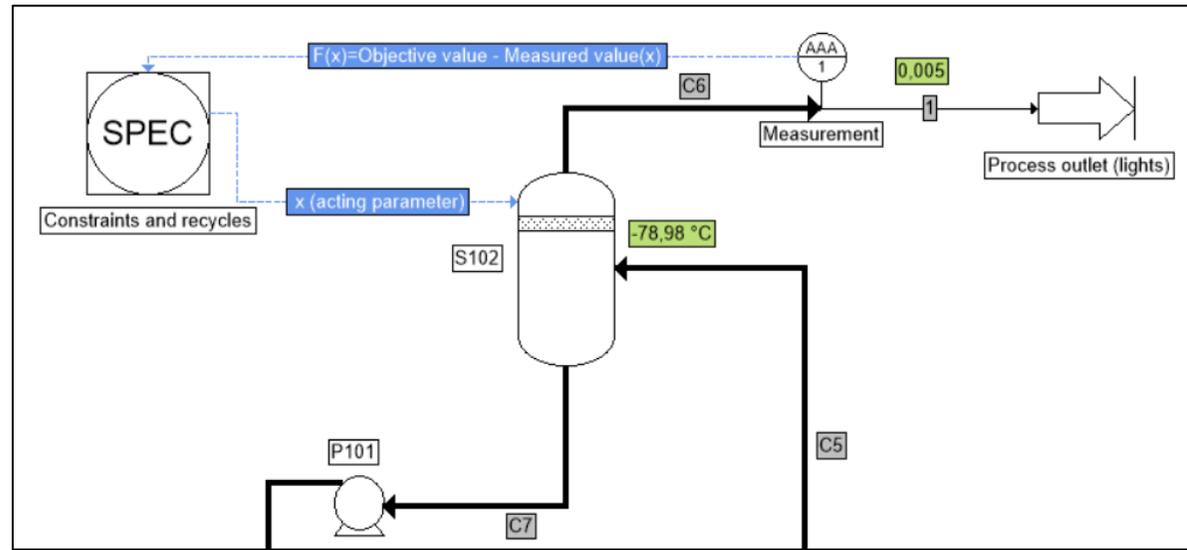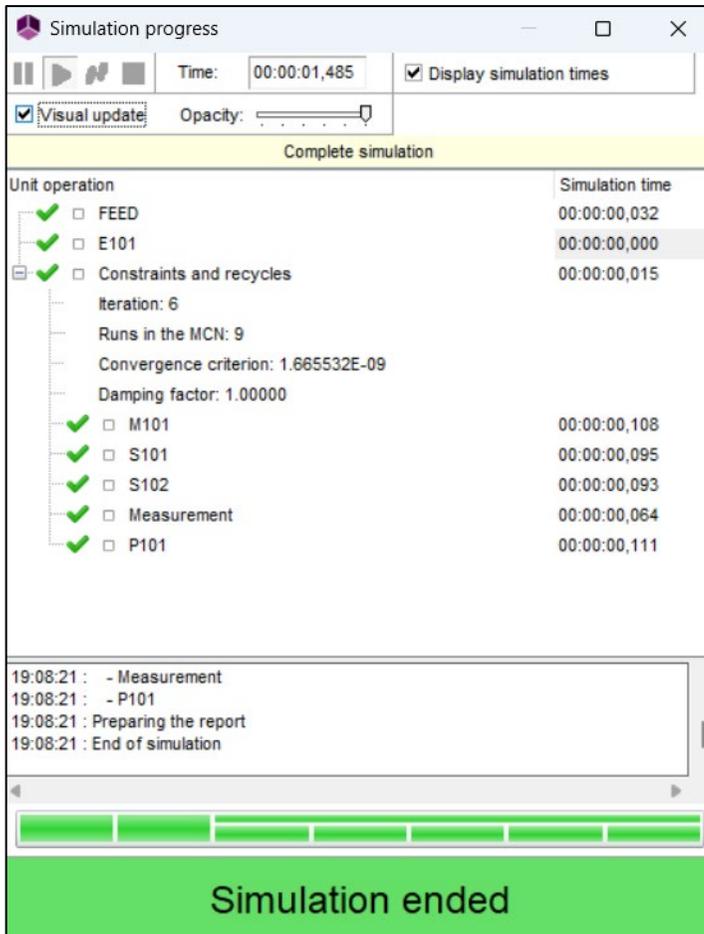
The « SPEC » module automatically adjusted the **temperature** value (-78.98 °C) at which the flash unit S102 will have an output **mass fraction** of 0.005 (5000 ppm) for **propane**

Practical Example

11 **Simulation results**
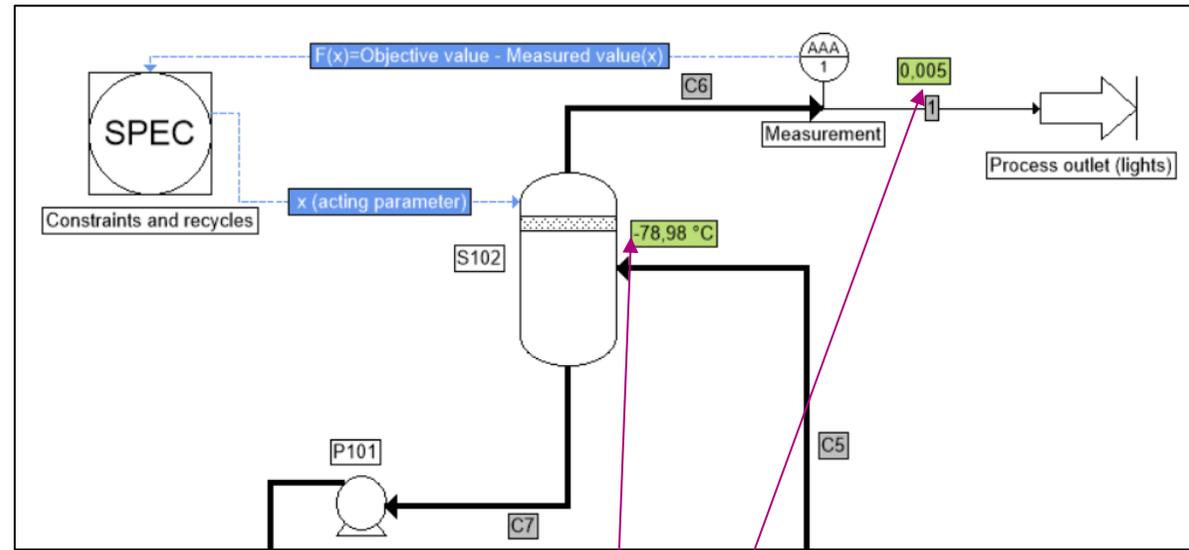
This temperature matches the value observed in the **case study** (approximately -79 °C) where the propane mass fraction is 0.005.

Conclusion
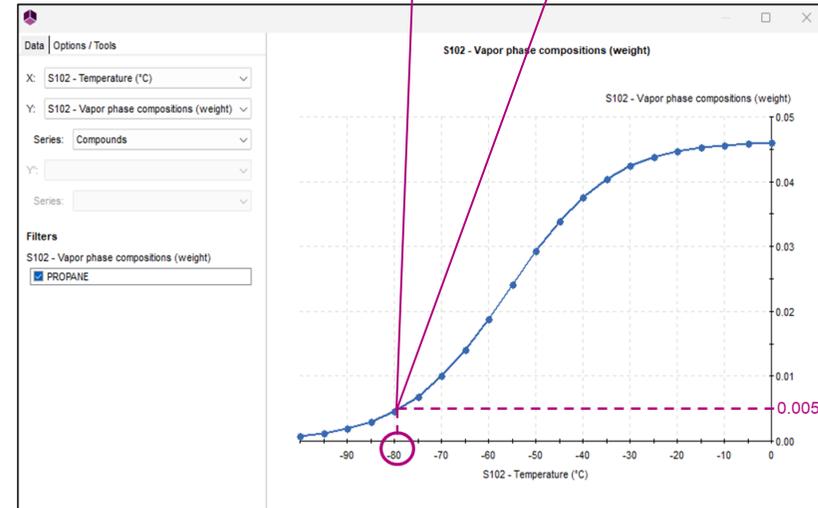
Once your standard simulation is complete, case studies and specifications become powerful tools to deepen your understanding of the process.

Case studies allow you to explore how the system responds to varying conditions.

Specifications enable the software to automatically adjust input variables to meet defined process targets.

fives

Industry can do it

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Getting started
with ProSimPlus®

Case 8:
APPENDICES

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Industry can do it

Graph plotting features

Back to Case study

Copy data to clipboard

APPENDICES

Graph plotting features

Print graph

Graph plotting features

Back to Case study

Case study results

Please select the variables to view or to plot

View...   Plot...

☐ ☑ S102
  ☑ Vapor phase compositions (weight)

Reset graph zoom setting

Data   Options / Tools

Line width: 2

Symbol size: 7

Legend position
- ● Bottom
- ○ Top
- ○ Left
- ○ Right

S102 - Vapor phase compositions (weight)

S102 - Vapor phase compositions (weight)

S102 - Temperature (°C)

Graph plotting features

Back to Case study

Basic graph settings

Graph plotting features

Back to Case study

Advanced graph settings

Additional calculation #1: We can also observe the effect of the action variable (temperature in this case) on other target results:

Target results

- Stream C6 flowrate
- Stream C7 flowrate
- Heat duty exchanged within the process
- Vapor fraction (molar)

! IMPORTANT

To perform this simulation, the "SPEC" module must be deactivated. This can be done by double-clicking the "SPEC" module and unchecking the **'Module enabled'** option.

Constraints and recycles ($SPEC)

Name: Constraints and recycles
Desc:

Identification | Parameters | Scripts | Report | Streams | Notes | Advan

☐ Module enabled

Numerical methods: Default

Back to Case study

Monitoring

Filter by

Type: All types   Unit operation: All unit operations

<< Prev.   Next >>   No variable selected

Selected	Variable	Form	Compounds	Stages
⊞ E101				
⊞ S101				
⊟ S102				
☐	Flowrate of stream C6	Molar		
☐	Temperature of stream C6			
☐	Pressure of stream C6			
☐	Vapor fraction of stream C6			
☐	Flowrate of stream C7	Molar		
☐	Temperature of stream C7			
☐	Pressure of stream C7			
☐	Vapor fraction of stream C7			
☐	Temperature			
☐	Duty exchanged			
☐	Vapor fraction (molar)			
☐	Liquid phase compositions	Molar	All	
☐	Vapor phase compositions	Weight	A selection	
⊞ P101				
⊞ M101				
⊞ Measurement				

Additional calculation #1

Additional calculation #1: We can also observe the effect of the action variable (temperature in this case) on other target results:
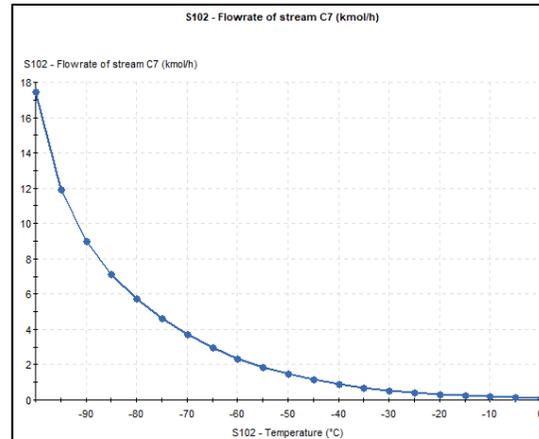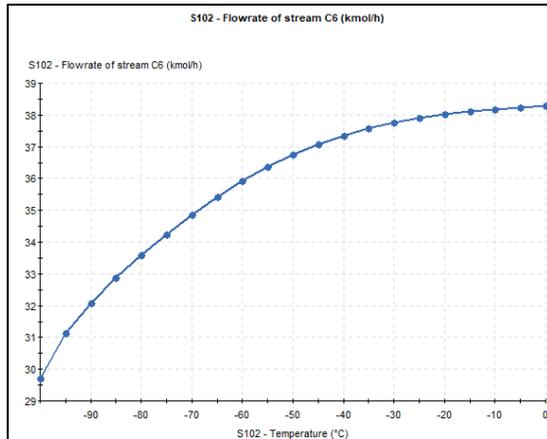
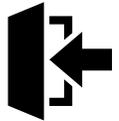**Plotting two variables on the same graph allows for a more comprehensive analysis of process behavior**

Back to Case study

APPENDICES
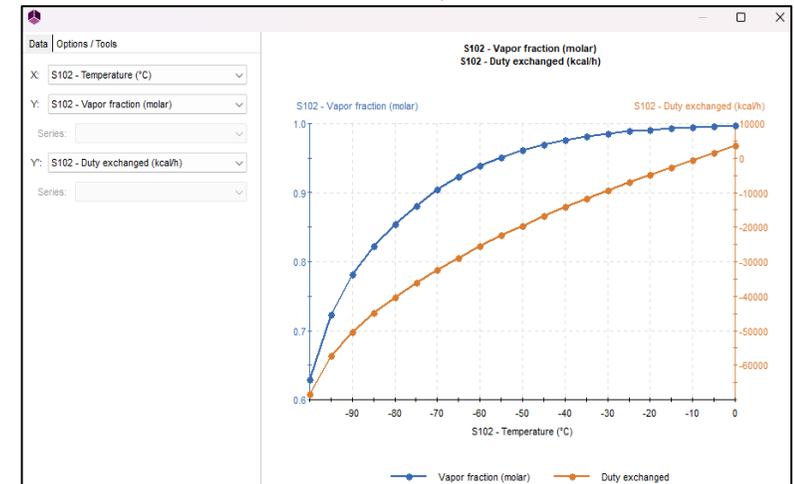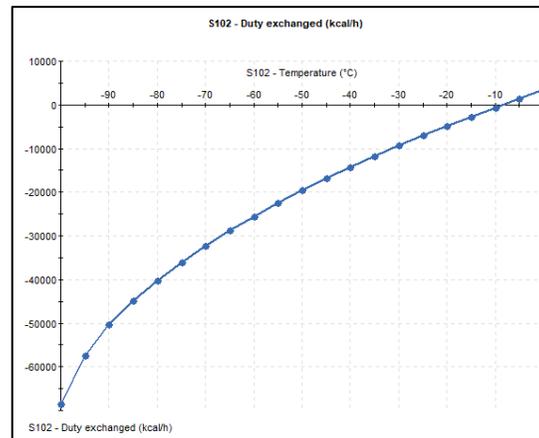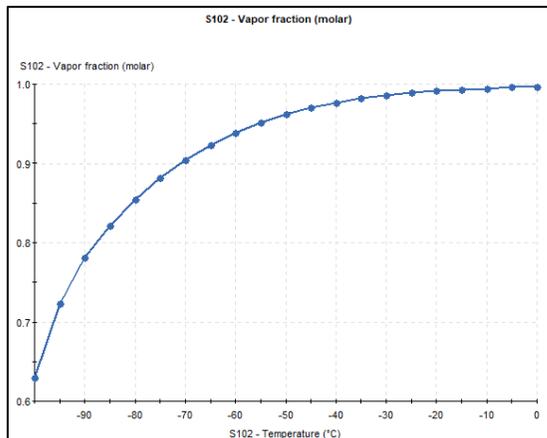
Additional calculation #2

Additional calculation #2: Multivariable sensitivity analysis
- It allows observation of the impact of multiple action variables on the target variables.

Conditions

action variables:
X_1 = Vary the flash S102 temperature between -100°C and 0°C (5°C step)
X_2 = Vary the flash S102 pressure between 20 atm and 30 atm (1 atm step)

Target variables:
Y = Duty exchanged, mass vapor phase composition of propane

Graph plotting
Varying temperature and pressure
X_1 = -100°C to 0°C, X_2 = 20 to 30 atm

Increasing the number of variables in the case study will extend the simulation time. This is due to the added complexity and the greater number of calculations required.

Back to Case study

Additional calculation #2

- **Multivariable sensitivity analysis**
  - It allows observation of the impact of multiple action variables on the target variables.

First action variable (temperature)
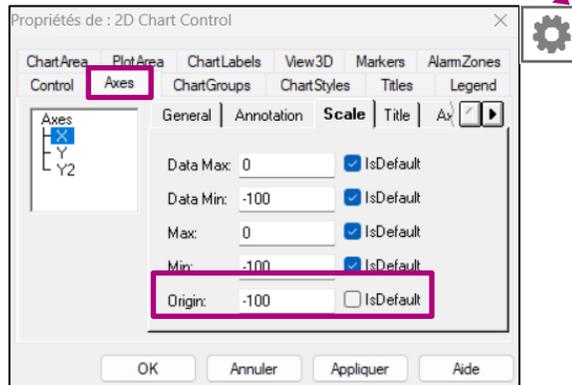
Second action variable (pressure)
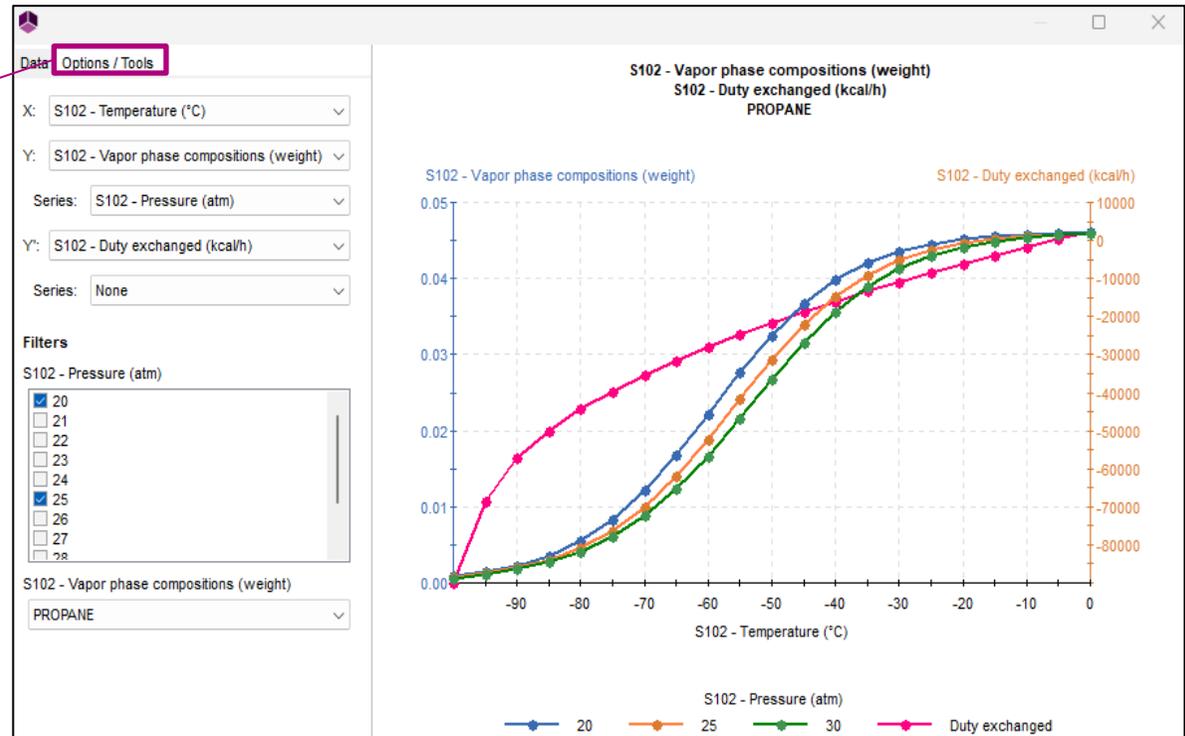
Back to Case study

APPENDICES

Additional calculation #2

Effect of the variation of temperature and pressure on the heat duty exchanged and the vapor phase composition of the flash drum S102

Through the **properties editor** the origin of the graph can be edited to correctly display the Y and Y ' axis

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Practical Example - Specifications

Press **F1** to quickly access information about the module you're working on

Number	Function
❶	Selection of the numerical method.
❷	Parameters of the method previously selected.
❸	Parameters for the sensitivity analysis.
❹	Convergence and stop criteria.
❺	Allows to specify that the temperatures/pressures of the tear streams have to be variables of the problem.
❻	Allows to specify bounds for the search interval for each action variable.
❼	Enables to specify the list of tear streams to impose to the constraints and recycles management block unit, as well as bounds on the tear streams temperatures.

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