Getting started with Simulis® Pinch

Water module

Use Case 1: Water integration of an acrylonitrile plant – First steps with Simulis Pinch Water

Release Simulis Pinch 2.0.0

Software & Services In Process Simulation

We guide You to efficiency

ProSim

Introduction

This getting started shows you the basics of Simulis Pinch Water in order to perform a water integration of a process.

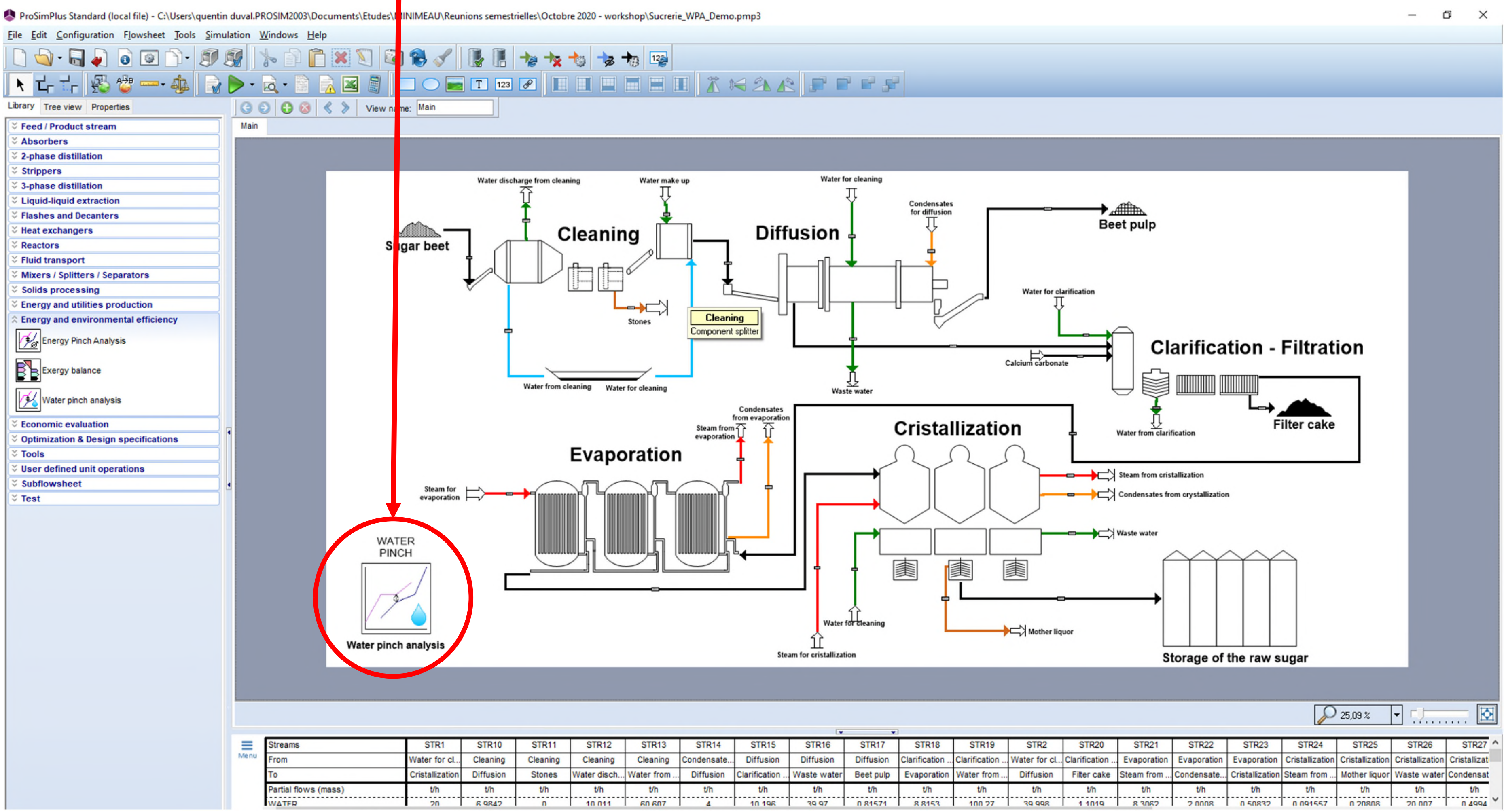
This guide presents the following parts:

- Step 1: Data generation in Microsoft™ Excel
- Step 2: Definition of the theoretical optimum of the process water consumptions
- Step 3: Design of a water network

Step 1: Data generation in Microsoft™ Excel

The data, necessary to perform the analysis, can be generated directly from a ProSimPlus simulation.
In ProsimPlus, open the simulation file you want to study.

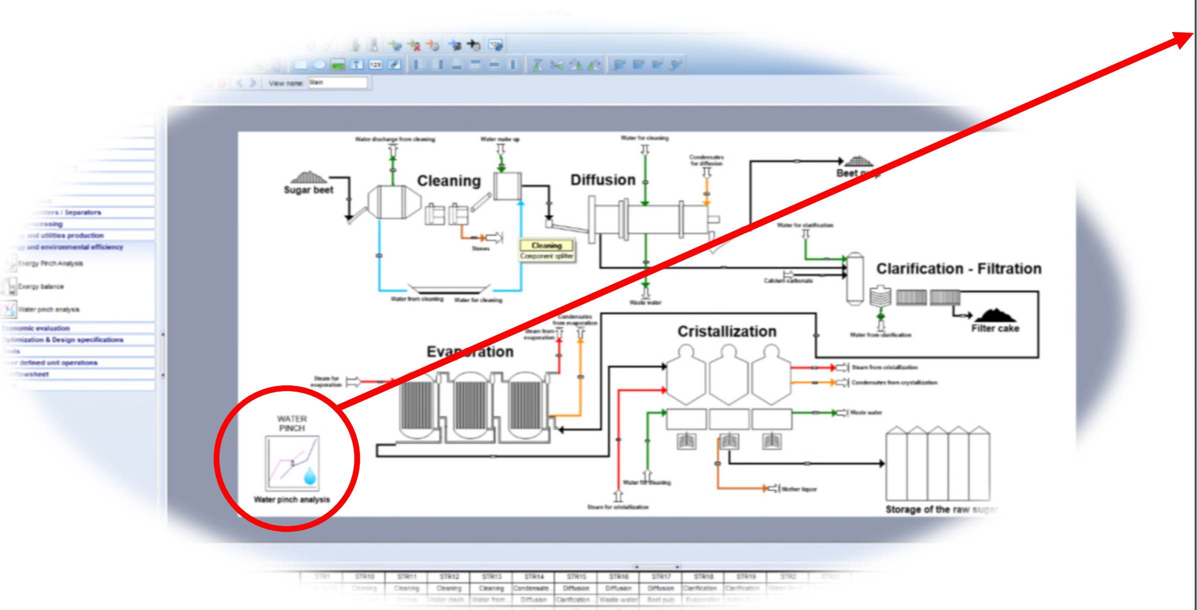
Add a module **Water Pinch Analysis**

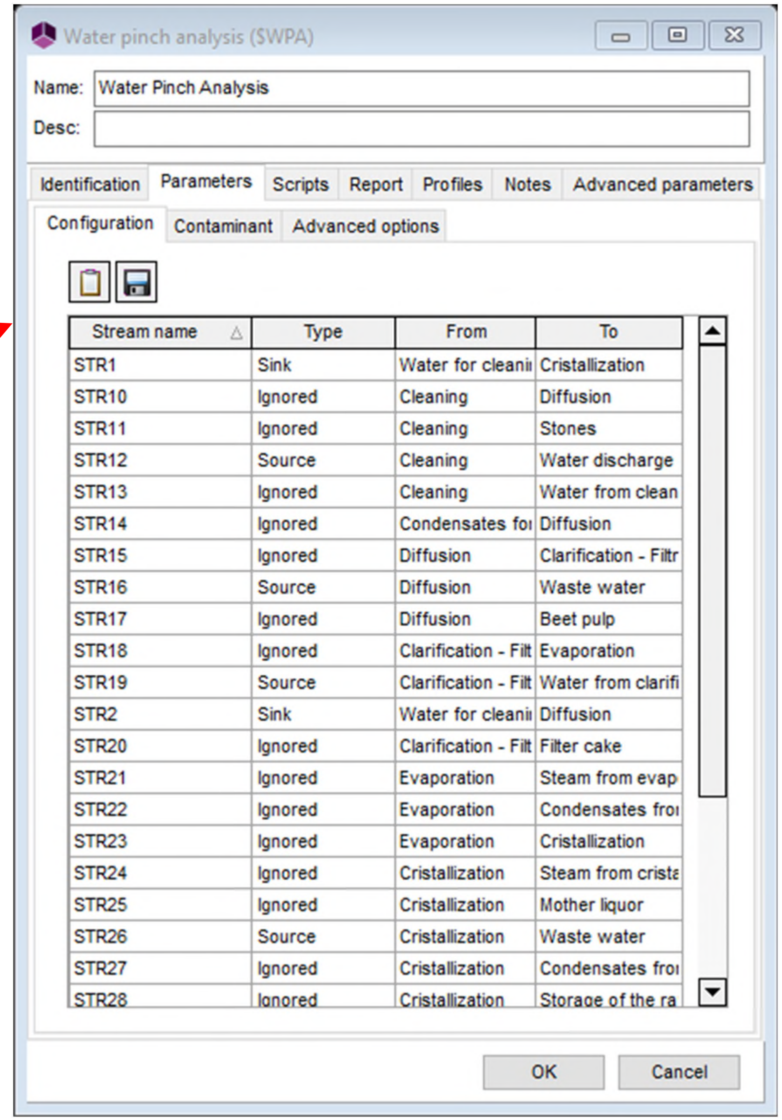


Step 1: Data generation in Microsoft™ Excel

Configure the module **Water Analysis Pinch**

The configuration of the module is based on the definition of the type of each stream. Only the “Sink” and “Source” streams are taken into account for the analysis and the module calculations



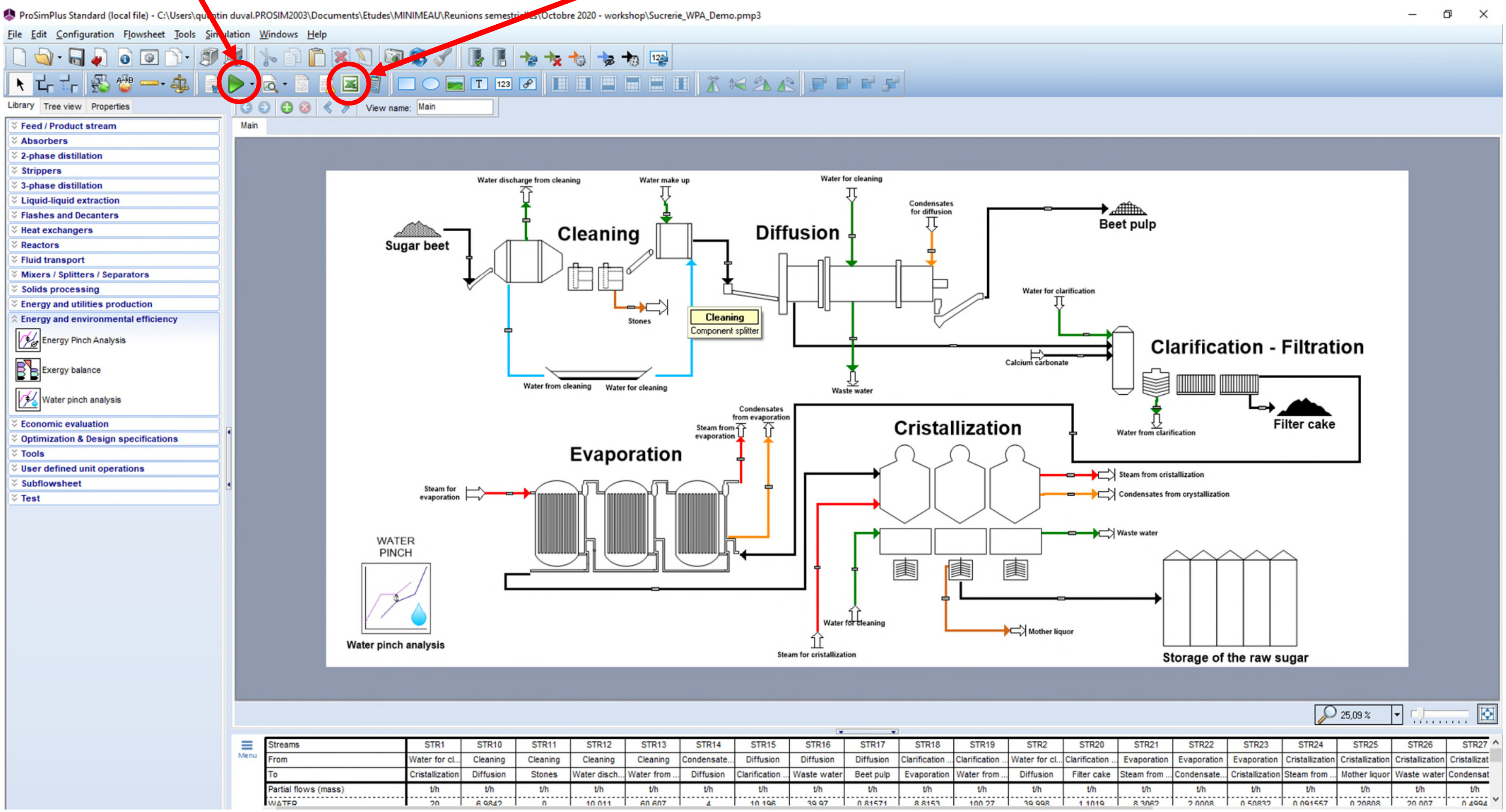


Stream name	Type	From	To
STR1	Sink	Water for cleanii	Cristallization
STR10	Ignored	Cleaning	Diffusion
STR11	Ignored	Cleaning	Stones
STR12	Source	Cleaning	Water discharge
STR13	Ignored	Cleaning	Water from clean
STR14	Ignored	Condensates foi	Diffusion
STR15	Ignored	Diffusion	Clarification - Filtr
STR16	Source	Diffusion	Waste water
STR17	Ignored	Diffusion	Beet pulp
STR18	Ignored	Clarification - Filt	Evaporation
STR19	Source	Clarification - Filt	Water from clarifi
STR2	Sink	Water for cleanii	Diffusion
STR20	Ignored	Clarification - Filt	Filter cake
STR21	Ignored	Evaporation	Steam from evap
STR22	Ignored	Evaporation	Condensates froi
STR23	Ignored	Evaporation	Cristallization
STR24	Ignored	Cristallization	Steam from crista
STR25	Ignored	Cristallization	Mother liquor
STR26	Source	Cristallization	Waste water
STR27	Ignored	Cristallization	Condensates froi
STR28	Ignored	Cristallization	Storage of the ra

Step 1: Data generation in Microsoft™ Excel

Click on the ***Start simulation*** button

At the end of the simulation, click on the ***Excel workbook*** button of the last simulation



Step 1: Data generation in Microsoft™ Excel

The data needed to do the water pinch analysis are automatically generated at the end of the Microsoft™ Excel report.

The column ***Stream*** presents the names of the “Sink” and “Source” streams defined in the “Water Pinch Analysis” module in the simulation.

These streams can be for example:

- A water feed stream (for a “sink” stream)
- A process outlet (for a “source” stream)
- Any stream that can be valued by a water pinch analysis

WPA - Water Pinch Analysis

Stream	F/|M In - M C	Input (M In)	Target (M Out)
SK2	1,20E+06	1,00E-06	0,00E+00
SK1	1,00E-01	5,80E+01	1,00E-06
SR1	8,00E+05	0,00E+00	1,00E-06
SR2	7,14E-02	1,00E-06	7,00E+01
SR3	4,00E-02	7,00E+01	2,18E+02
SR4	2,94E-02	2,18E+02	2,65E+02

These automatically generated data are available in the last Microsoft™ Excel results file

According to the definition of the decimal separator of your computer, it will be or not necessary to replace points “.“ by comma "," so that these values are well interpreted in Microsoft™ Excel.

Step 1: Data generation in Microsoft™ Excel

The column **F/|Min – Mout|** shows the flowrate divided by ΔM (contaminant load difference between the inlet and the outlet).
For each stream, it is possible to express the contaminant load m according to the following formula depending on the flowrate of the stream and the measurement in contaminant C:

$$m = \frac{F\,.\,C}{1000}$$

Generally, the contaminant measurement C is a mass concentration of one or several contaminant(s) (expressed in ppm), the flowrate F is a mass flowrate (t/h) and m is the mass load of contaminant(s) (kg/h).

The **F/|Min – Mout|** represents thus the inverse of the contaminant(s) concentration $(\frac{1}{C})$

In the following documents of Simulis Pinch Water, the contaminant(s) measurement is the mass concentration and m is the mass load of contaminant(s)

WPA - Water Pinch Analysis

Stream	F/|M In - M C	Input (M In)	Target (M Out)
SK2	1,20E+06	1,00E-06	0,00E+00
SK1	1,00E-01	5,80E+01	1,00E-06
SR1	8,00E+05	0,00E+00	1,00E-06
SR2	7,14E-02	1,00E-06	7,00E+01
SR3	4,00E-02	7,00E+01	2,18E+02
SR4	2,94E-02	2,18E+02	2,65E+02

Step 1: Data generation in Microsoft™ Excel

The unit of the mass loads for the input (**Min**) and for the output (**Mout**) are dependent on the type of measurement in contaminant. If the measurement C is a mass concentration so the contaminant loads (m) are expressed in mass flowrate units (kg/h for example).

If the mass load increases (Mout > Min), the stream will be considered as a source stream (waste or outlet of the process).

If the mass load decreases (Mout < Min), the stream will be considered as a sink stream (water need of the process).

WPA - Water Pinch Analysis

Stream	F/|M In - M O	Input (M In)	Target (M Out)
SK2	1,20E+06	1,00E-06	0,00E+00
SK1	1,00E-01	5,80E+01	1,00E-06
SR1	8,00E+05	0,00E+00	1,00E-06
SR2	7,14E-02	1,00E-06	7,00E+01
SR3	4,00E-02	7,00E+01	2,18E+02
SR4	2,94E-02	2,18E+02	2,65E+02

Step 1: Data generation in Microsoft™ Excel

The input data for the water pinch analysis can come from external sources (i.e. different from the Microsoft™ Excel file generated by ProSimPlus). For instance, the user can perform contaminant(s) measurements and flowrates measurements on site in order to fill directly these data in Microsoft™ Excel.

If the user wants to provide the raw data directly in a Microsoft™ Excel sheet, the sheet layout has to be:

- 1st column: Streams names
- 2nd column: F
- 3rd column: C

Process	Stream	F (kg/s)	C (ppm)
Scrubber	SK1	5,8	10
Boiler	SK2	1,2	0
Distillation bottoms	SR1	-0,8	0
Off-gas condensate	SR2	-5	14
Aqueous layer	SR3	-5,9	25
Ejector condensate	SR4	-1,4	34

The user can generate the missing measurements (C) for one or more streams by using the thermodynamic properties calculation server provided by ProSim, **Simulis Thermodynamics** directly in Microsoft™ Excel environment.

If the user provides **raw data**, the **flowrate** has to be **positive for « sink » streams** (process input) and **negative for the sources** (process outlet)

Step 1: Data generation in Microsoft™ Excel

The data used in this document are based on an acrylonitrile production plant. This example is studied in: *Klemes J.J., « Process Integration Intensification (saving energy, water and resources) », De Gruyter, 2014.*

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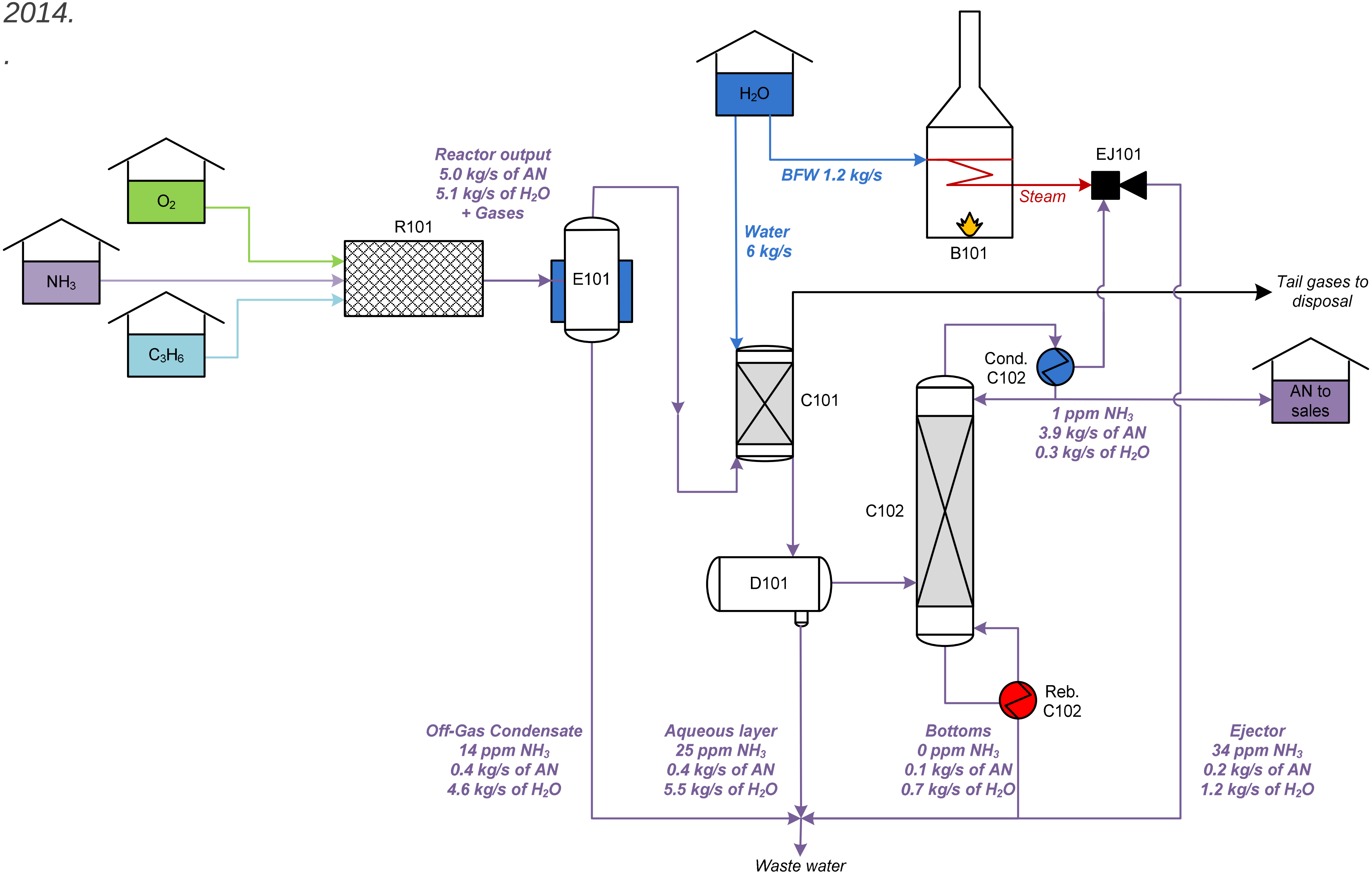


Step 1: Data generation in Microsoft™ Excel

The input data for Simulis Pinch Water can be obtained by two methods:

1. Data extracted from a process simulation of an acrylonitrile production plant in ProSimPlus
2. Raw data (flowrates and contaminant(s) measurements on site)

These two types of datasets are equivalent:

WPA - Water Pinch Analysis

Stream	F/|M In - M C	Input (M In)	Target (M Out)
SK2	1,20E+06	1,00E-06	0,00E+00
SK1	1,00E-01	5,80E+01	1,00E-06
SR1	8,00E+05	0,00E+00	1,00E-06
SR2	7,14E-02	1,00E-06	7,00E+01
SR3	4,00E-02	7,00E+01	2,18E+02
SR4	2,94E-02	2,18E+02	2,65E+02

Data from ProSimPlus

Process	Stream	F (kg/s)	C (ppm)
Scrubber	SK1	5,8	10
Boiler	SK2	1,2	0
Distillation bottoms	SR1	-0,8	0
Off-gas condensate	SR2	-5	14
Aqueous layer	SR3	-5,9	25
Ejector condensate	SR4	-1,4	34

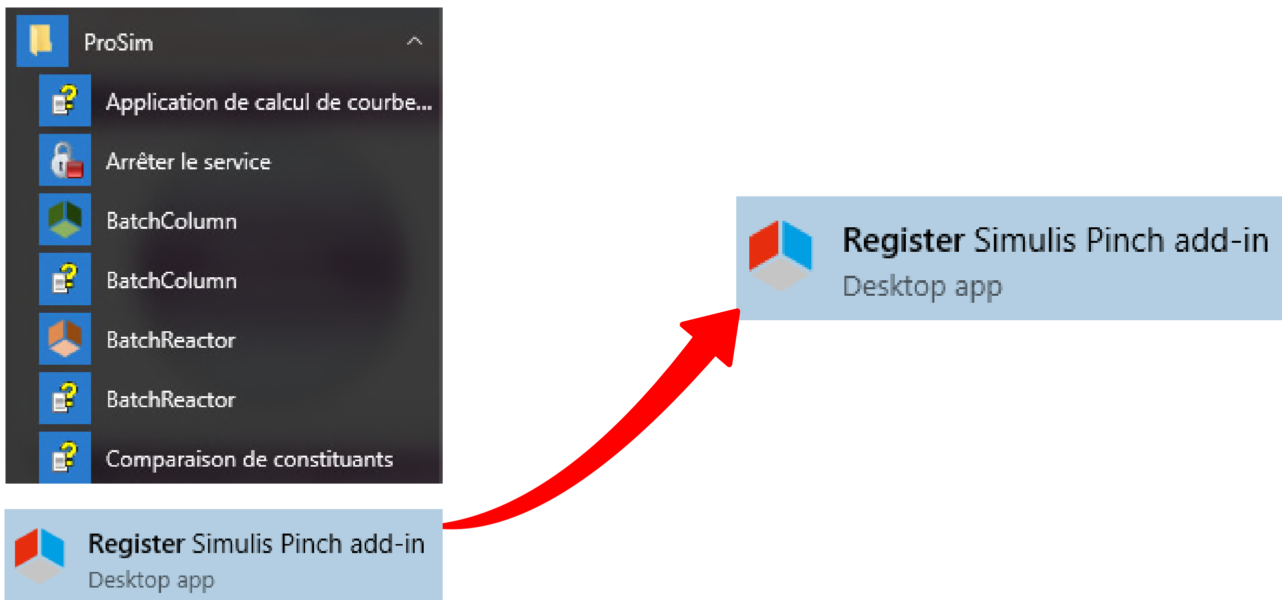
Raw data

Step 2: Definition of the theoretical optimum of the process water consumptions

After installing Simulis Pinch, the tool has to be registered in Microsoft™ Excel using the dedicated ProSim tool with one of the two following methods:

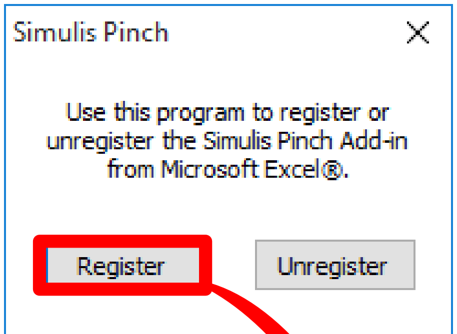
1. In the "ProSim" application folder, click on "Register Simulis Pinch add-in"

2. Find directly the tool "Register Simulis Pinch add-in" on your computer (using the search bar)

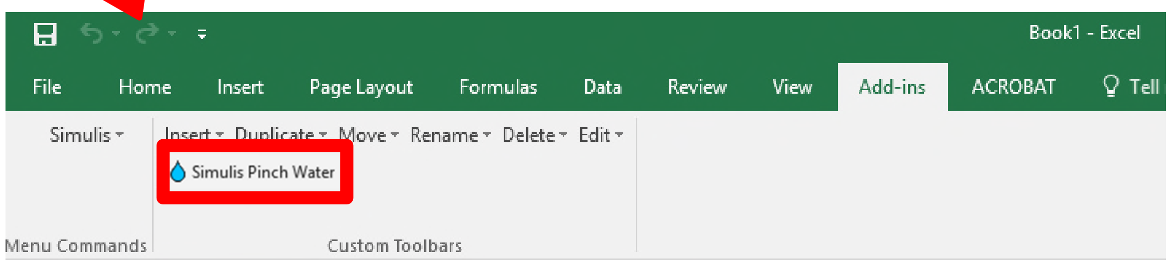


Step 2: Definition of the theoretical optimum of the process water consumptions

Register Simulis Pinch by clicking on “Register”:

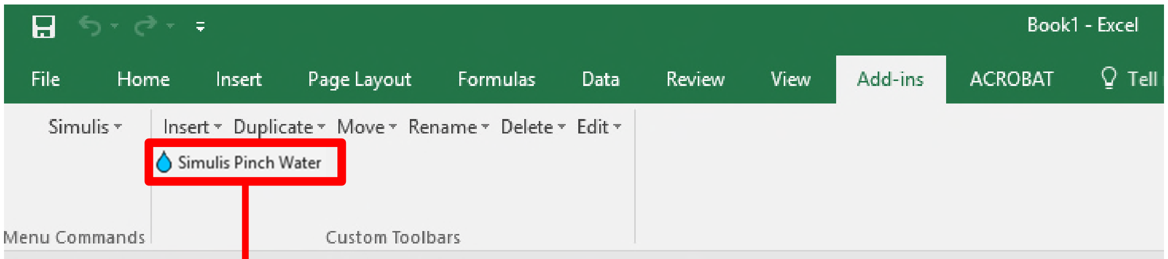


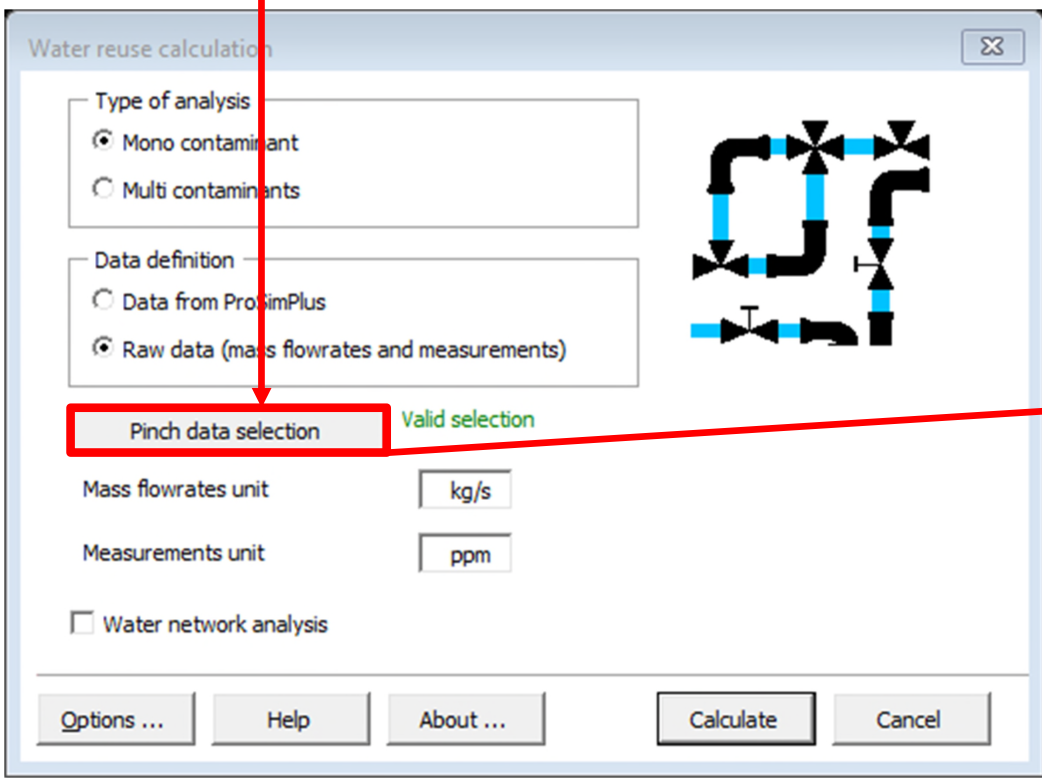
When Simulis Pinch is registered, it’s available in Microsoft™ Excel in the “Add-Ins” tab



Step 2: Definition of the theoretical optimum of the process water consumptions

1. Run Simulis Pinch
2. Select the columns of the flowrates F, and of the measurements C (only numerical values, not the column headings, as shown in the screenshots below)





Process	Stream	F (kg/s)	C (ppm)
Scrubber	SK1	5,8	10
Boiler	SK2	1,2	0
Distillation bottoms	SR1	-0,8	0
Off-gas condensate	SR2	-5	14
Aqueous layer	SR3	-5,9	25
Ejector condensate	SR4	-1,4	34

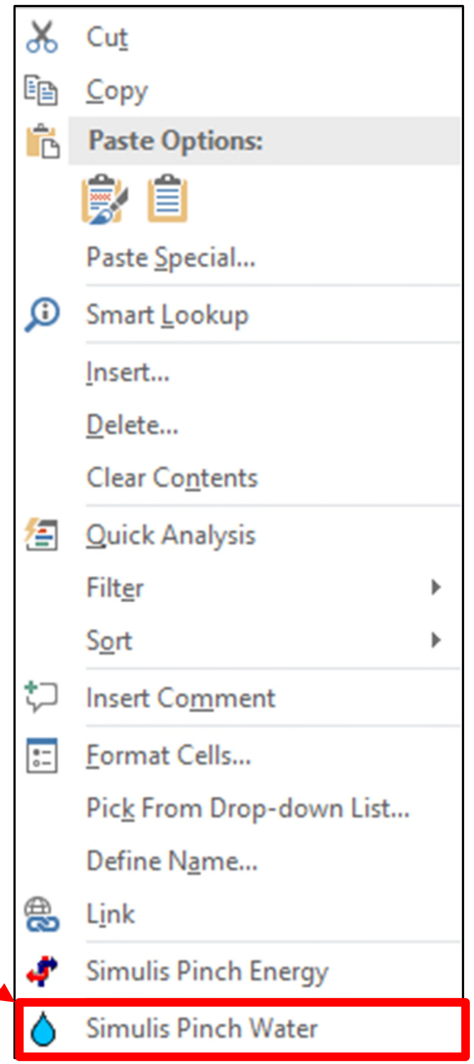
Raw data

Step 2: Definition of the theoretical optimum of the process water consumptions

Simulis Pinch Water can also be run from the context menu (right click) after you select the input data:

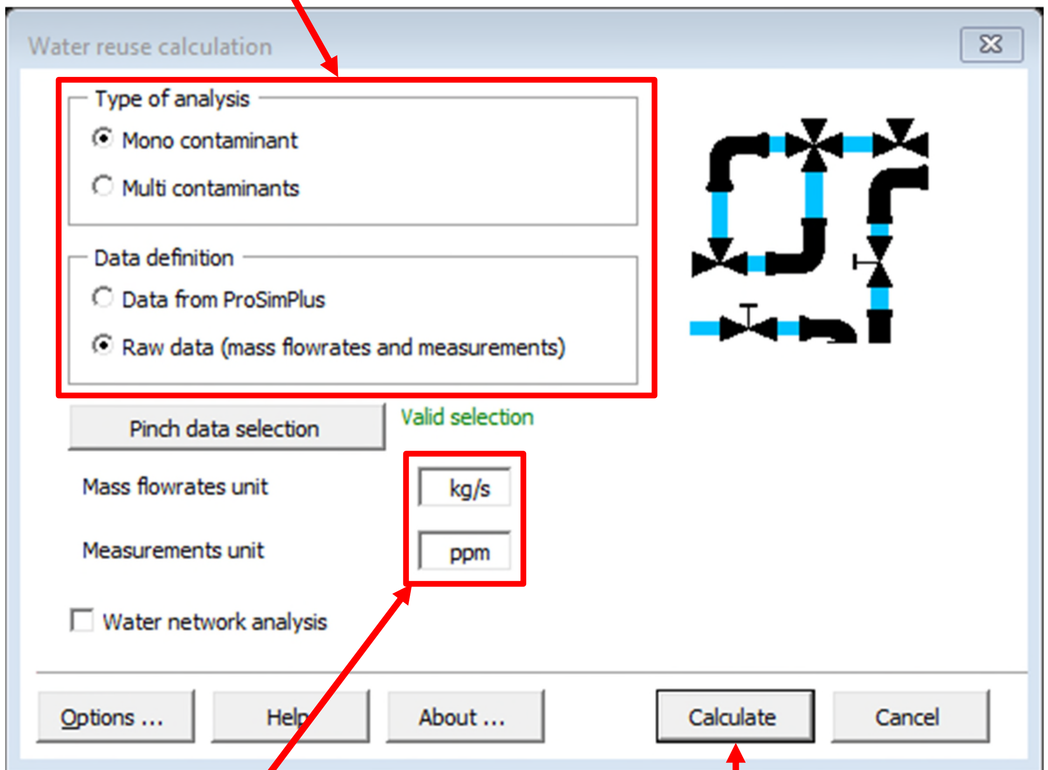
1. Select the columns of the flowrates F and the concentration C (only numerical values, not the column headings, as shown in the screenshots below)
2. Right-click to access the context menu

Process	Stream	F (kg/s)	C (ppm)
Scrubber	SK1	5,8	10
Boiler	SK2	1,2	0
Distillation bottoms	SR1	-0,8	0
Off-gas condensate	SR2	-5	14
Aqueous layer	SR3	-5,9	25
Ejector condensate	SR4	-1,4	34



Step 2: Definition of the theoretical optimum of the process water consumptions

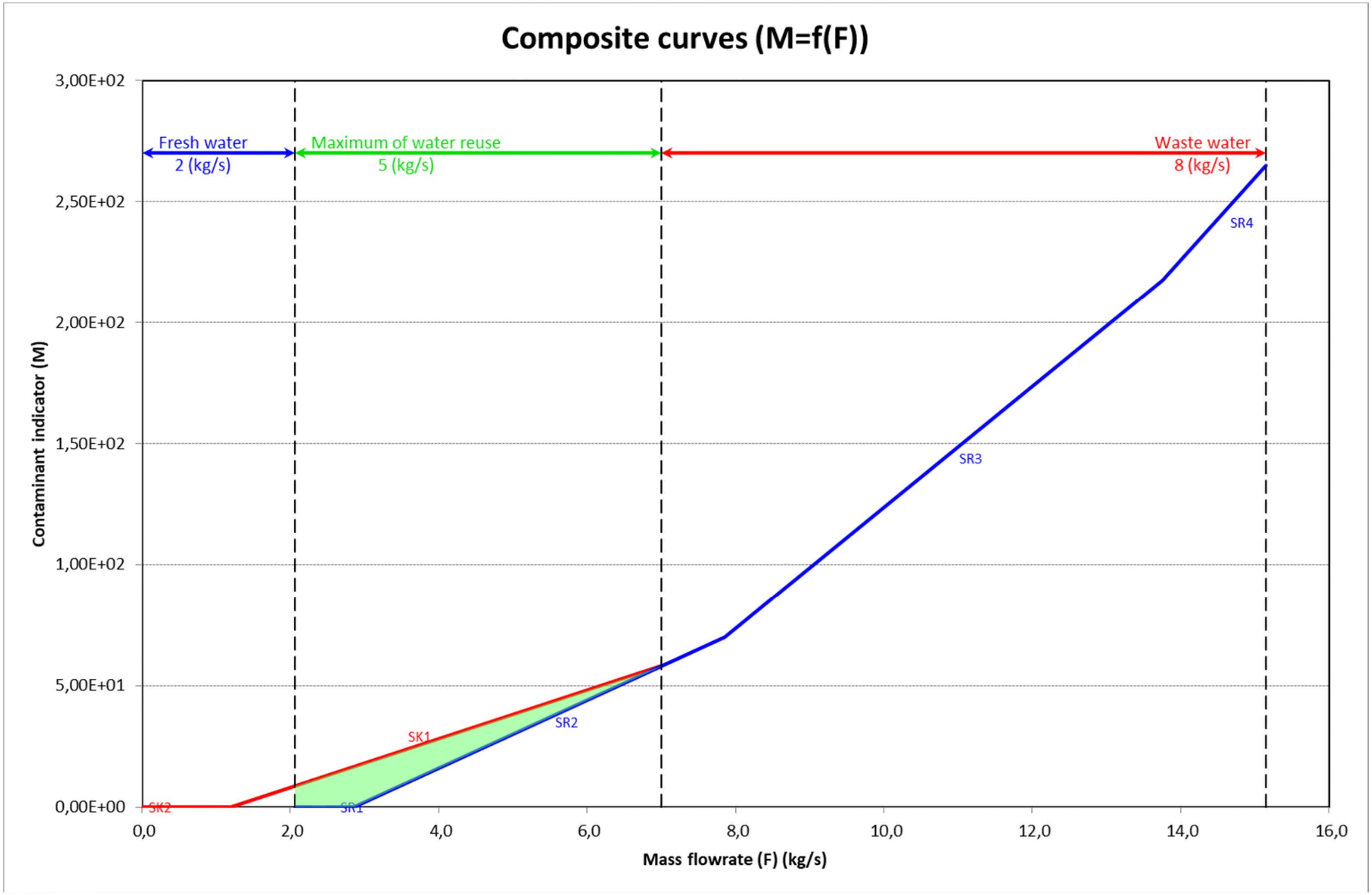
1. Define the type of analysis and the data definition (mono contaminant analysis from raw data for this example)



2. Provide the units of the flowrates (F) and of the measurements (C)

3. Click on ***Calculate***

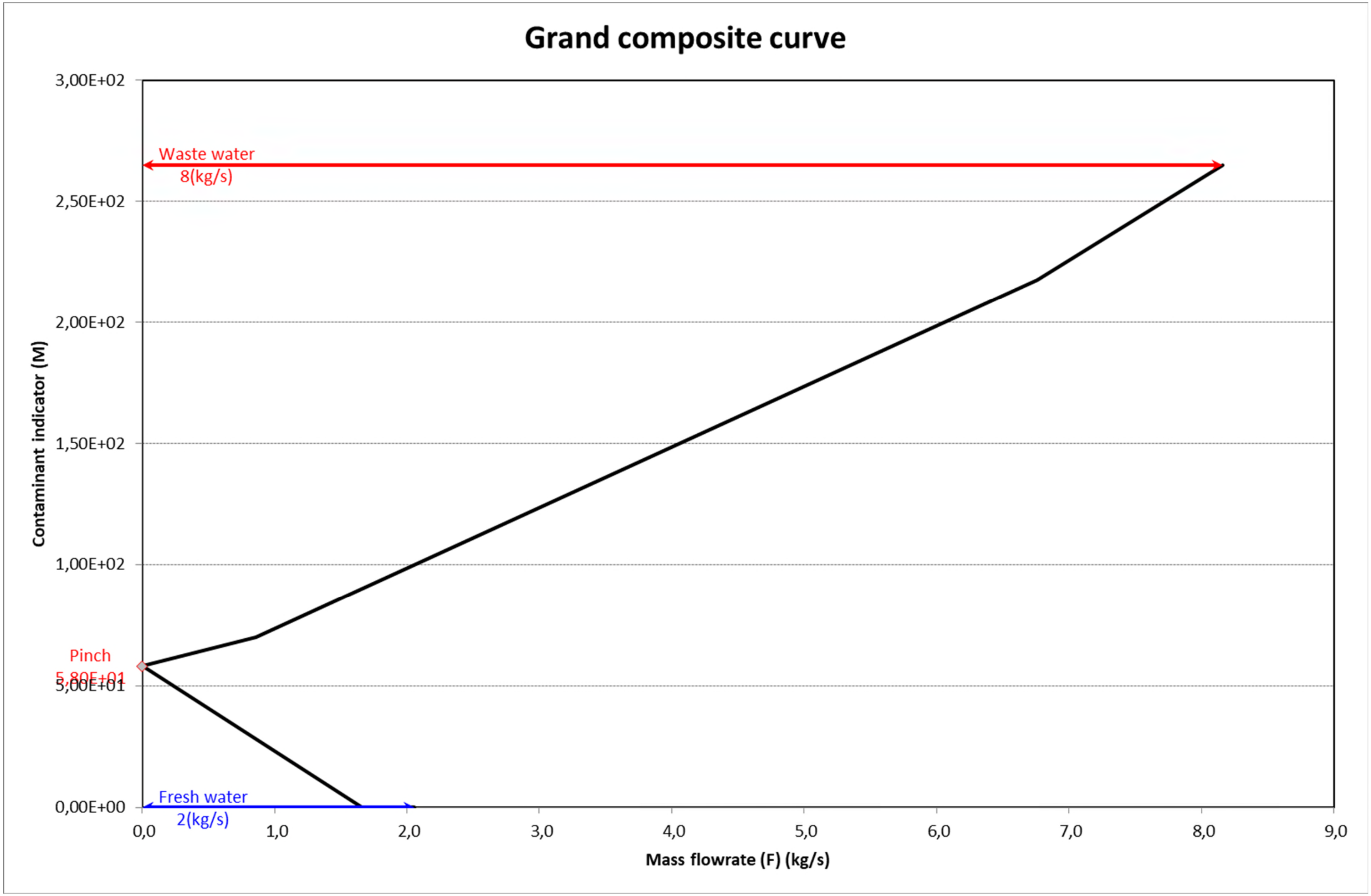
Step 2: Definition of the theoretical optimum of the process water consumptions



4 sheets are generated for the water pinch analysis:

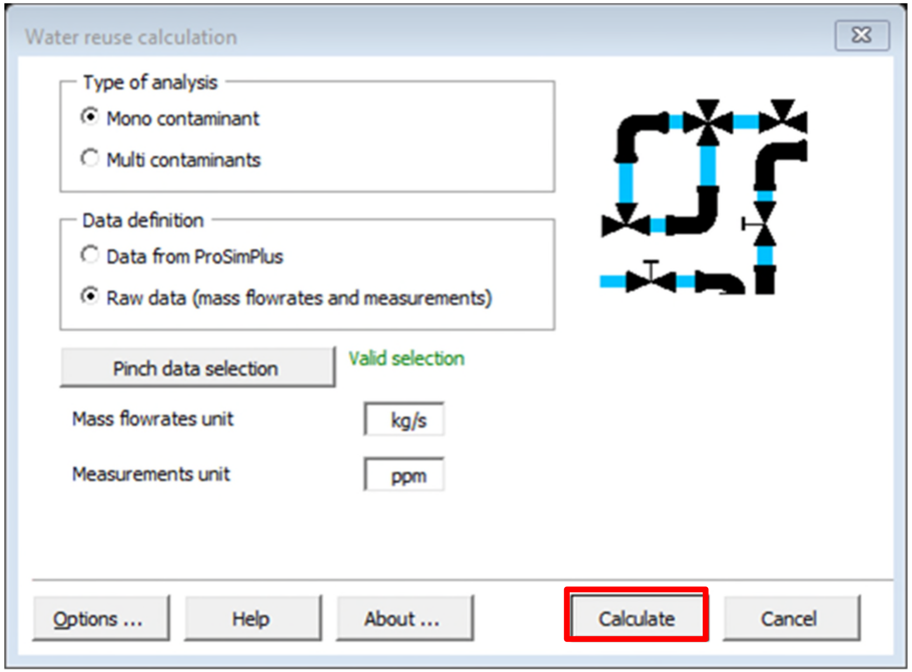
1. The grand composite curve
2. The sinks and sources composite curves
3. The streams (sources streams and sinks streams)
4. The results of the pinch analysis (data and summary of results)

Step 2: Definition of the theoretical optimum of the process water consumptions

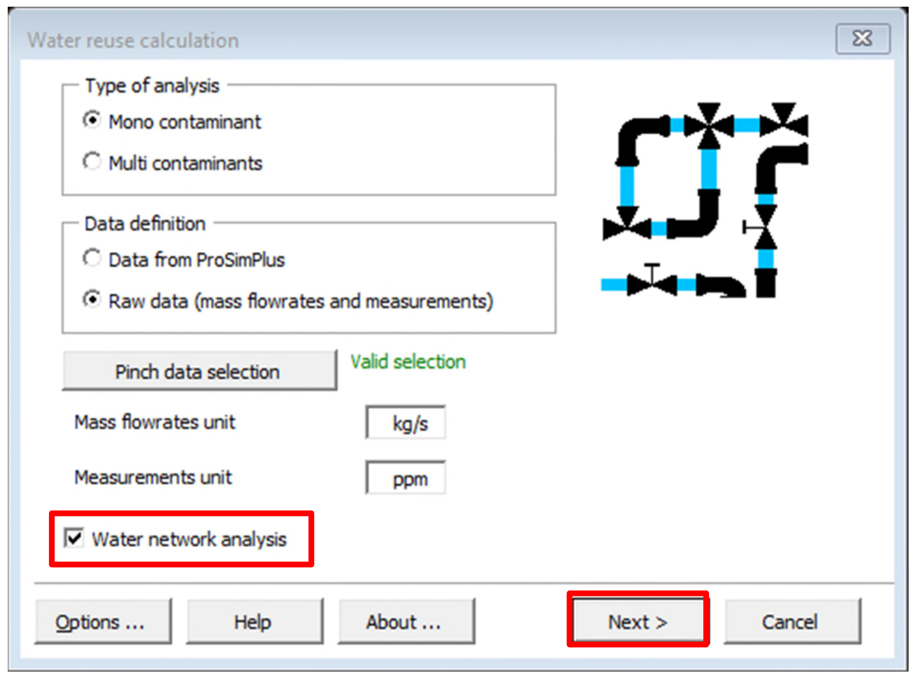


Step 2: Definition of the theoretical optimum of the process water consumptions

If the user has a license for the use of Simulis Pinch, the tool can generate a water network whose purpose is to reuse a maximum of internal water in the process



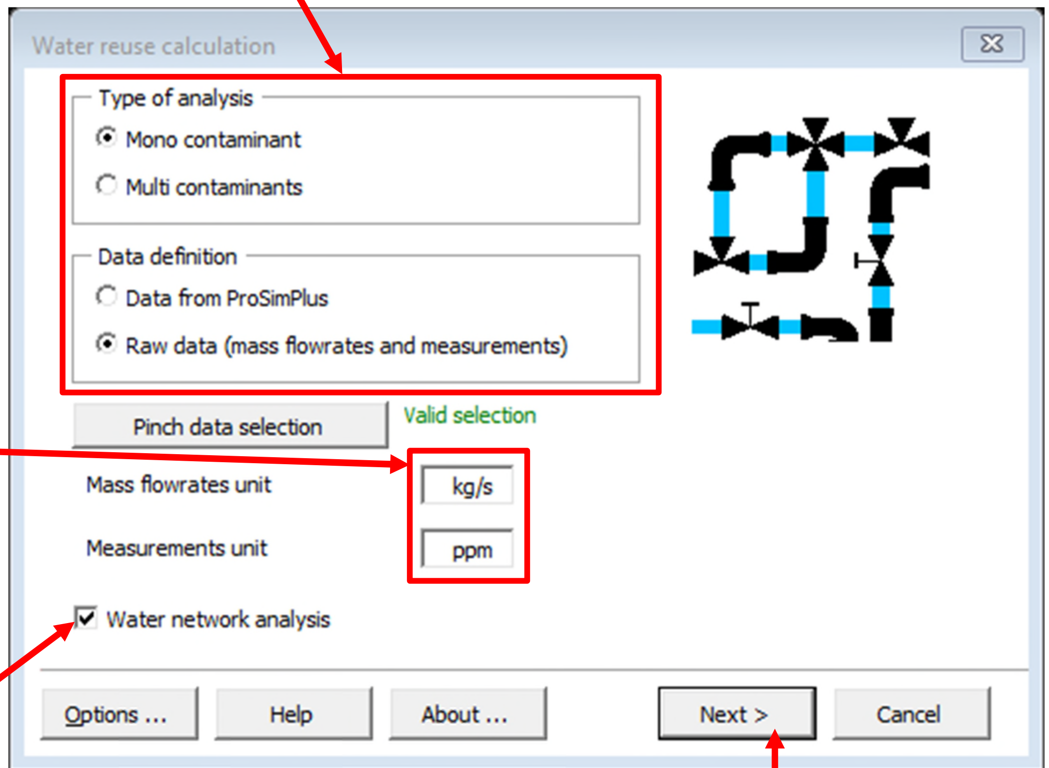
Interface **without** Simulis Pinch licence



Interface **with** Simulis Pinch licence

Step 3: Design of a water network

1. Define the type of analysis and the data definition (mono contaminant analysis from raw data for this example)



2. Provide the units of the flowrates (F) and of the measurements (C)

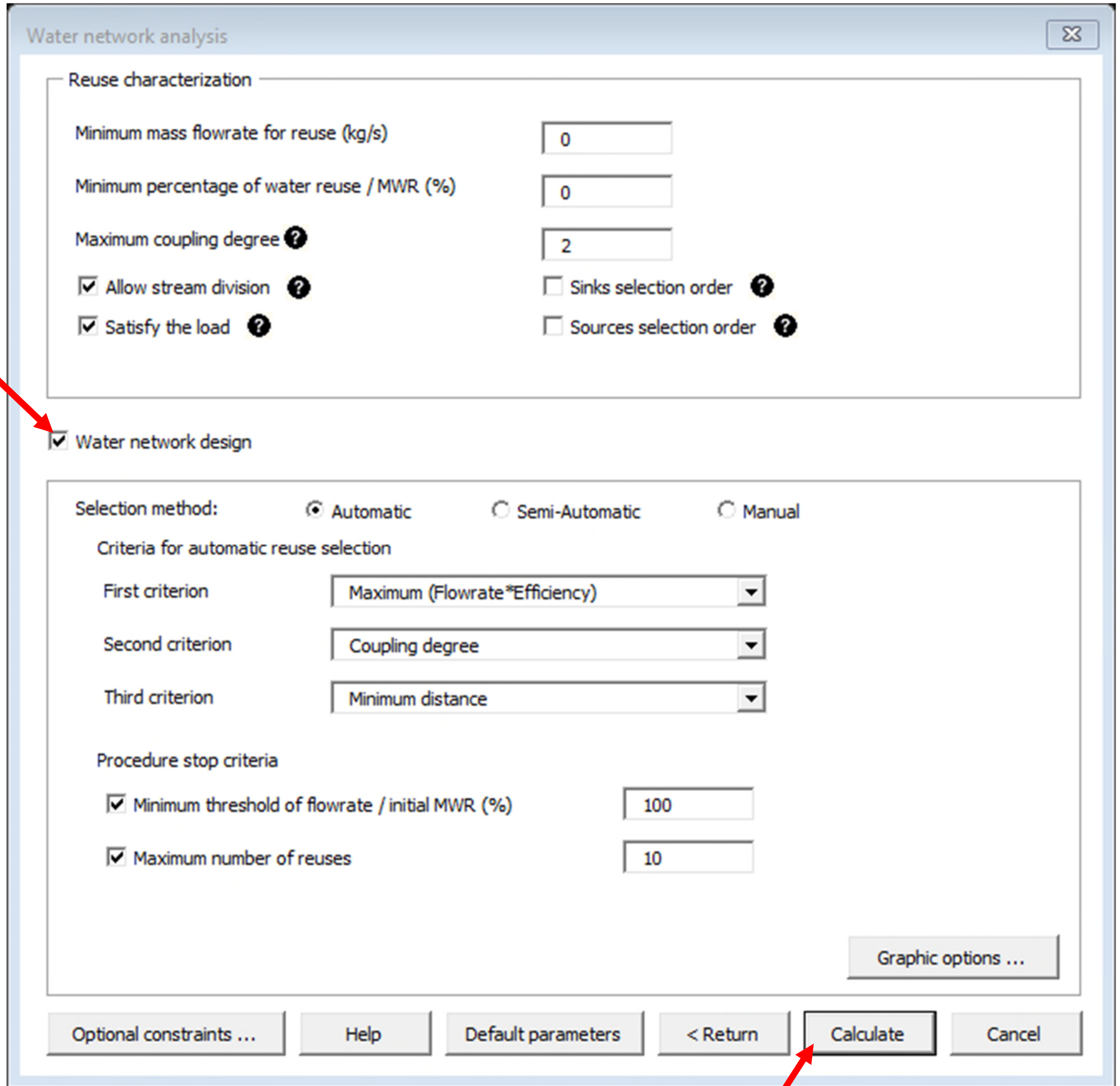
3. Check the **Water network analysis** box

4. Click on ***Next***

Step 3: Design of a water network

1. Check the box ***water network design***

*Firstly, the default values will be kept (**Automatic selection of the reuses**)*

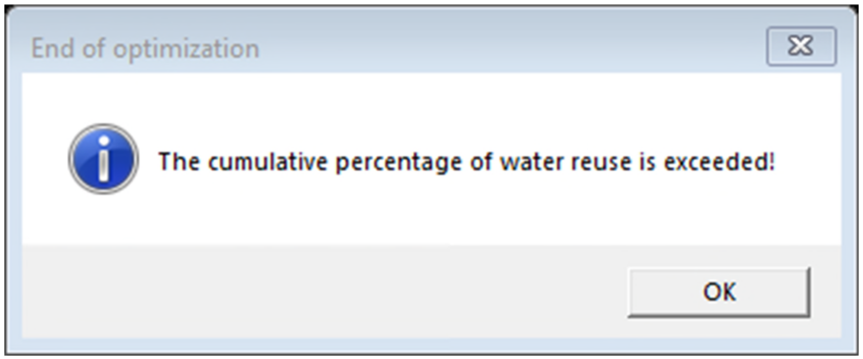


2. Click on ***Calculate***

Step 3: Design of a water network

A message will indicate the end of the calculations (when a stop criterion is met)

For this example, the cumulative percentage of water reuse (compared to the initial Maximum Water Reuse MWR) is reached (100% of the water is reused)



Step 3: Design of a water network

Three additional sheets were generated:

1. ***Input Data***
2. ***Water network results***
3. ***Water network***

SUMMARY FOR THE WATER NETWORK

Initial number of possible reuse:	3
Cumulative percentage of water reuse:	100,00
Number of reuses:	2
Total water reuse (kg/s):	4,9
Water flowrate available to reuse (kg/s):	0,0
Additional required amount of fresh water(kg/s):	2,1
Amount of waste water (kg/s):	8,2
Remaining number of Sources:	3
Remaining number of Sinks:	0

RESULTS FOR THE AUTOMATIC DESIGN OF THE WATER NETWORK

Reuse Item	INPUT DATA Sink			Source 1			
	Name	Contaminant measurement (C) (ppm)	Target F (kg/s)	Name	Contaminant measurement (C) (ppm)	Target F (kg/s)	Name
1	SK1	1,00E+01	5,8	SR2	1,40E+01	5,0	
2	SK2	0,00E+00	1,2	SR1	0,00E+00	0,8	

NO MORE REUSE IS POSSIBLE

LIST OF THE STREAMS STILL REMAINING AFTER THE WATER NETWORK DESIGN

Stream names	Mass flowrate (F) (kg/s)	Contaminant measurement (C) (ppm)
SR3	5,9	2,50E+01
SR4	1,4	3,40E+01
SR2	0,9	1,40E+01

FRESH WATER CHARACTERISTICS

Stream names	Mass flowrate (F) (kg/s)	Contaminant measurement (C) (ppm)
Fresh water	2,1	0,00E+00

RESULTS FOR THE INITIAL POSSIBLE COUPLINGS

... | Streams | Water Pinch results | Reuse #2 | Reuse #1 | Water network | Water network results | Input data | Data

Step 3: Design of a water network

The first part of the “Water network results” sheet summarizes the global information on water integration and on the water network

SUMMARY FOR THE WATER NETWORK

Initial number of possible reuse:	3
Cumulative percentage of water reuse:	100,00
Number of reuses:	2
Total water reuse (kg/s):	4,9
Water flowrate available to reuse (kg/s):	0,0
Additional required amount of fresh water(kg/s):	2,1
Amount of waste water (kg/s):	8,2
Remaining number of Sources:	3
Remaining number of Sinks:	0

In the present case, with 2 reuses, the water network proposed by Simulis Pinch Water recovers 100% of MWR (**M**aximum of **W**ater **R**ecovery)

Step 3: Design of a water network

The 2 reuses are described in a table showing their characteristics:

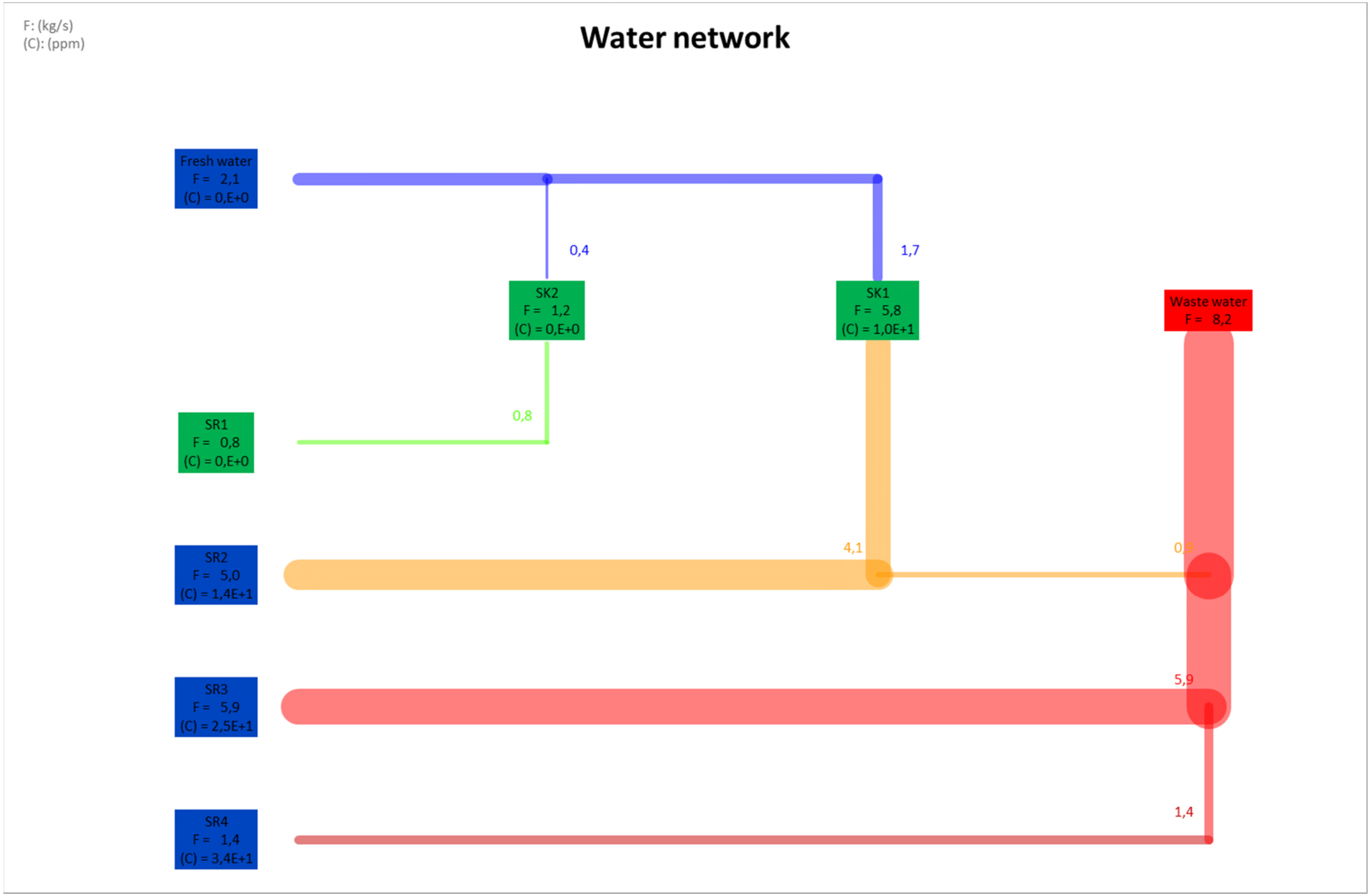
RESULTS FOR THE AUTOMATIC DESIGN OF THE WATER NETWORK

Reuse Item	INPUT DATA					
	Sink			Source 1		
	Name	Contaminant measurement (C) (ppm)	Target F (kg/s)	Name	Contaminant measurement (C) (ppm)	Target F (kg/s)
1	SK1	1,00E+01	5,8	SR2	1,40E+01	5,0
2	SK2	0,00E+00	1,2	SR1	0,00E+00	0,8

REUSE CHARACTERISTICS				INFORMATION ON WATER REUSE					
Source 1	Source 2	Total mass flowrate (kg/s)	Fresh water (kg/s)	% of water reuse / MWR	Degree of coupling	Efficiency	Splitting ratio		Mass Flowrate* efficiency
Mass flowrate (kg/s)	Mass flowrate (kg/s)						Source 1	Source 2	
4,1	0,0	5,8	1,7	83,8	1	1,00	0,8	0,0	4,1
0,8	0,0	1,2	0,4	100,0	1	1,00	1,0	0,0	0,8

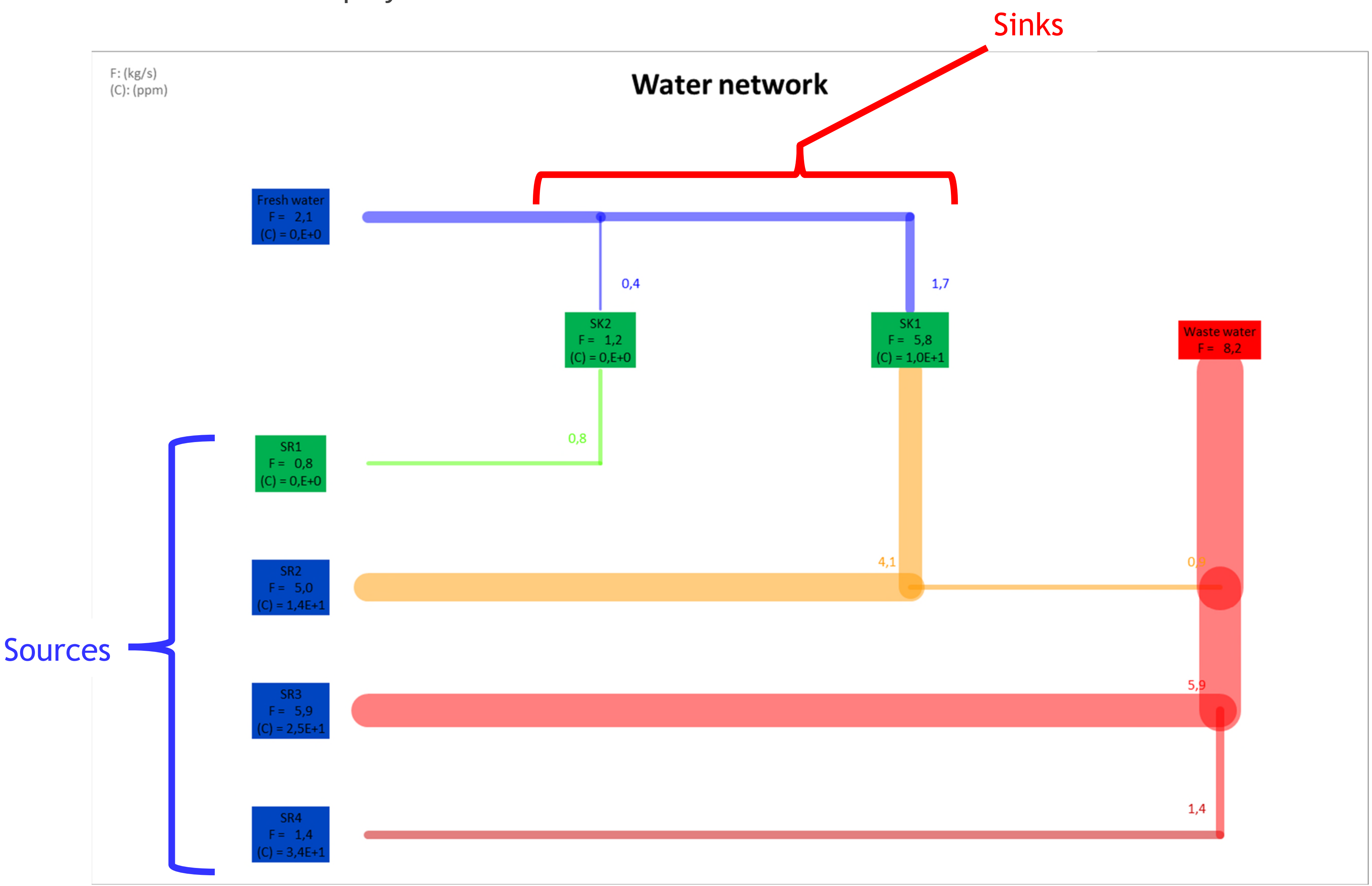
Step 3: Design of a water network

The water network is displayed in the « Water network » sheet:



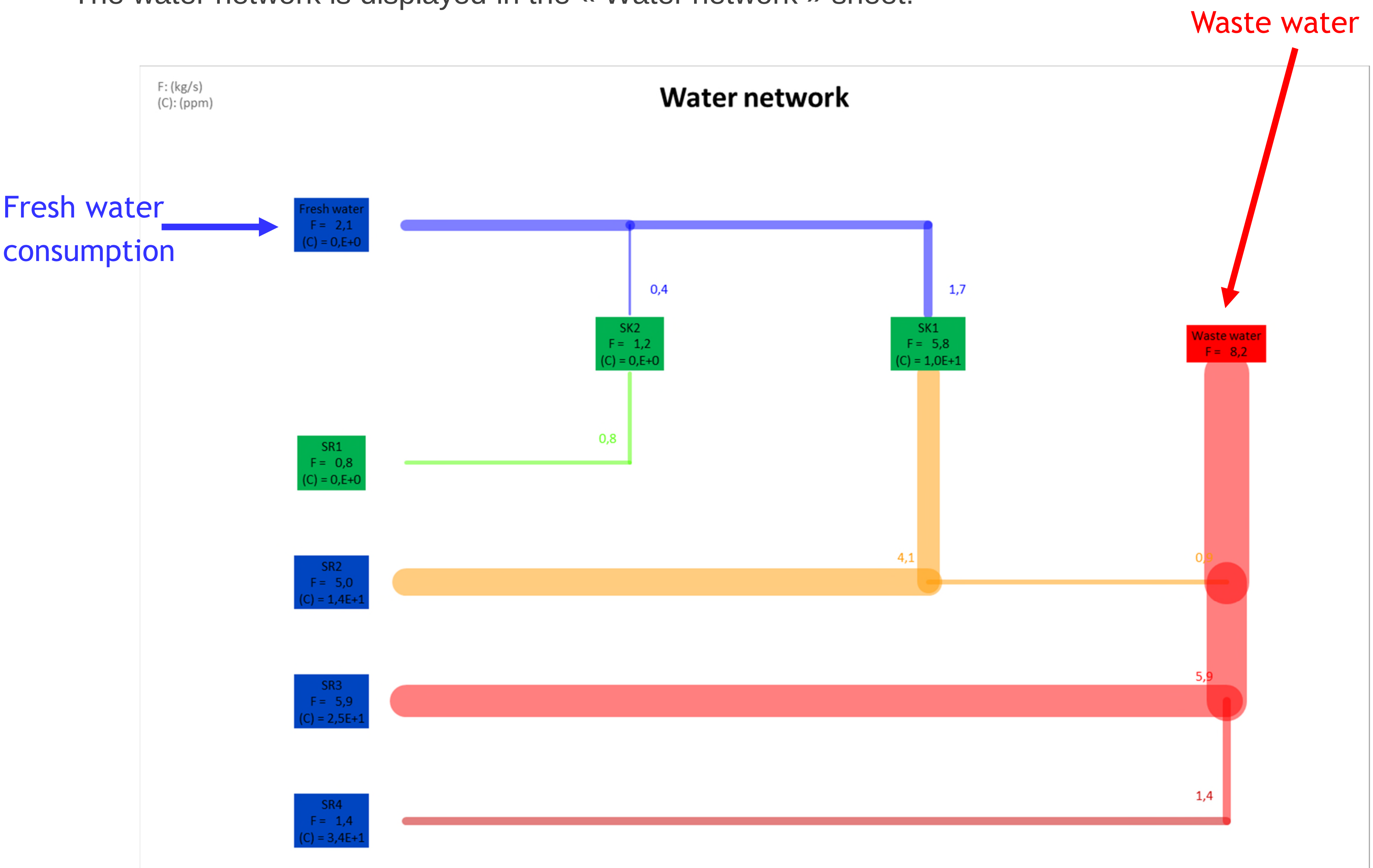
Step 3: Design of a water network

The water network is displayed in the « Water network » sheet:



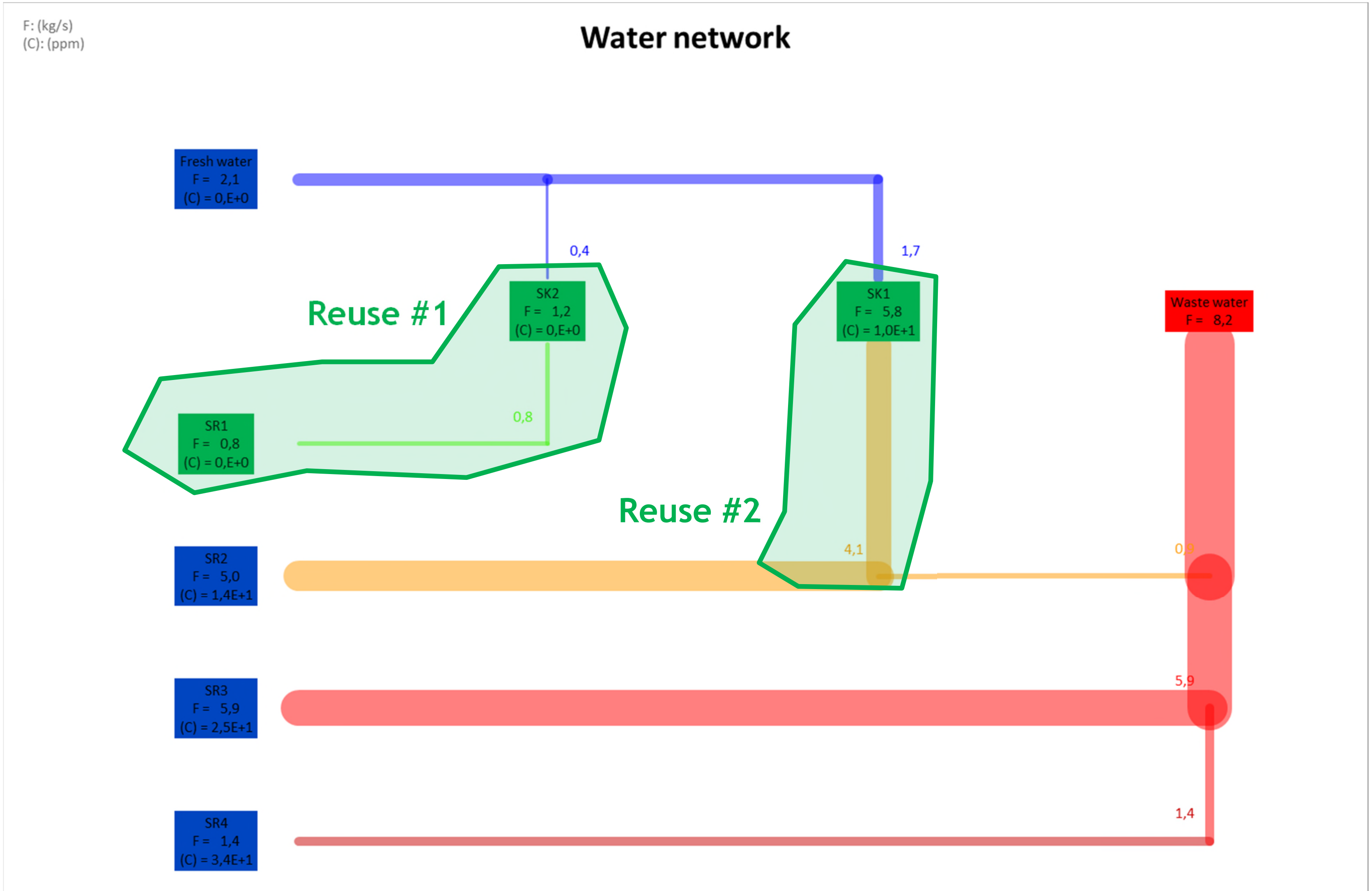
Step 3: Design of a water network

The water network is displayed in the « Water network » sheet:



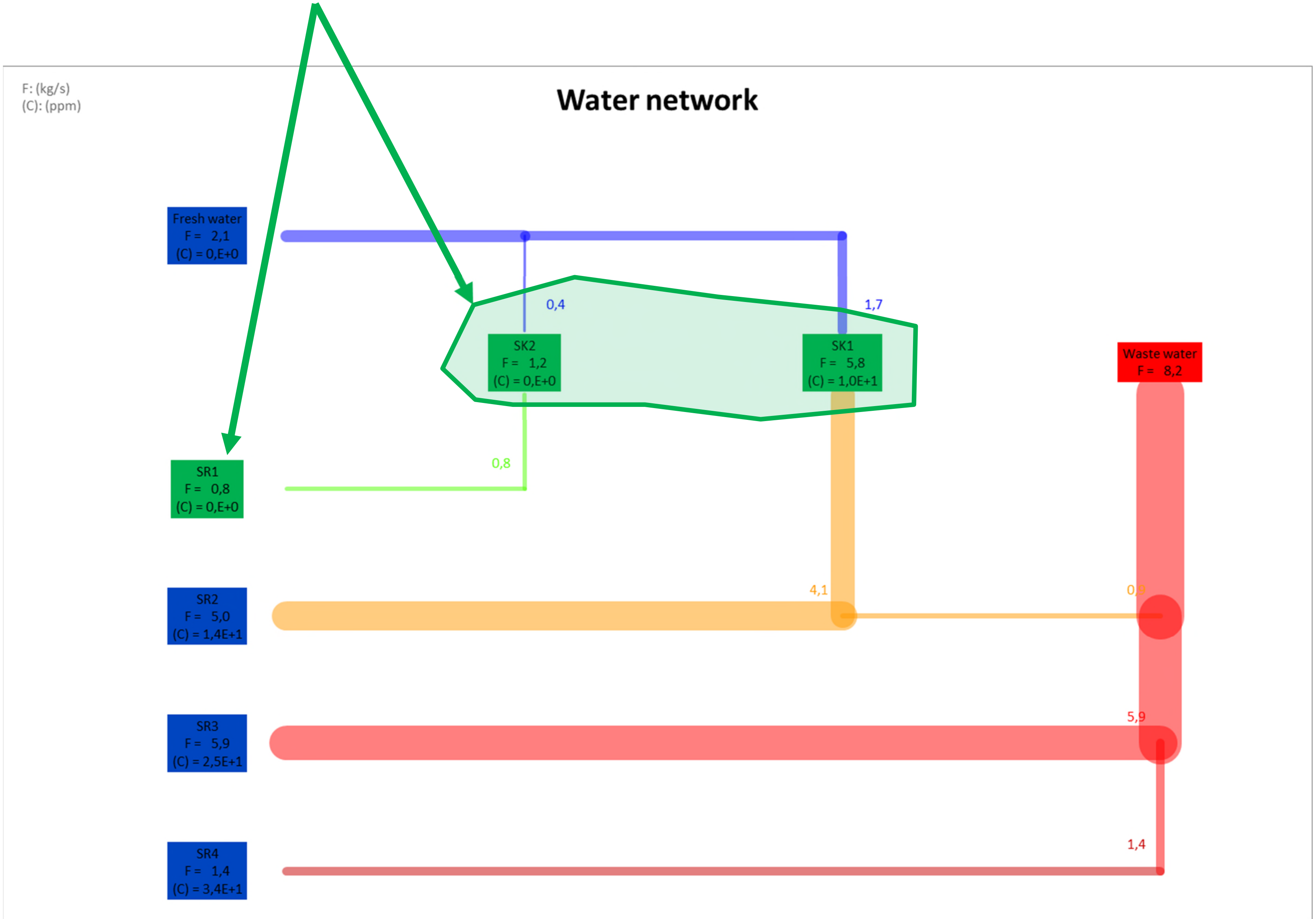
Step 3: Design of a water network

The water network is displayed in the « Water network » sheet:

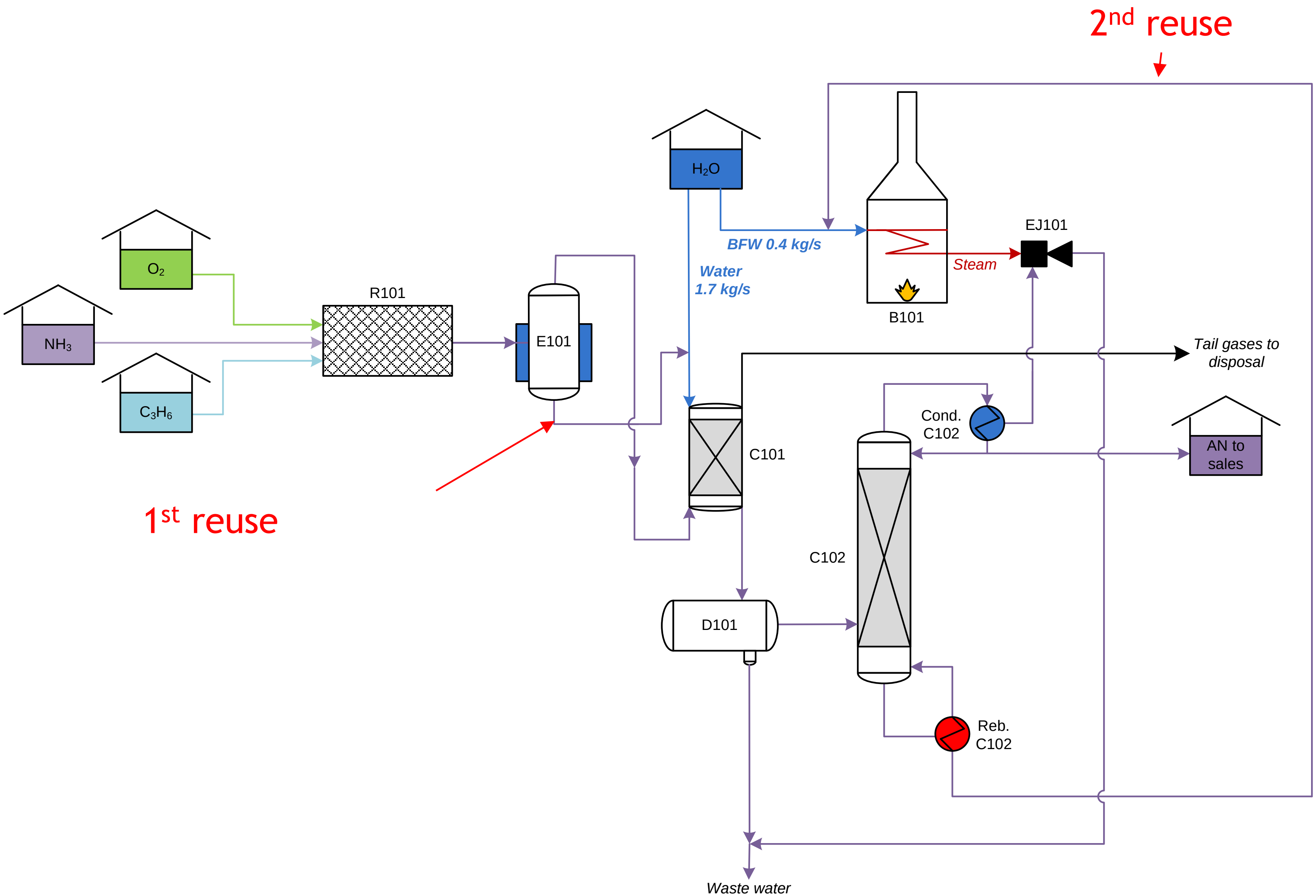


Step 3: Design of a water network

The sinks and sources streams totally coupled are displayed in green



Step 3: Design of a water network



Step 3: Design of a water network

The first result shows that 100% of reusable water (MWR) have been recovered using 2 reuses.

Is this solution the most suitable? Is there a more interesting configuration?

From the water reuse point of view, 100% of the reusable water (MWR) have been recovered, it seems hard to go further!

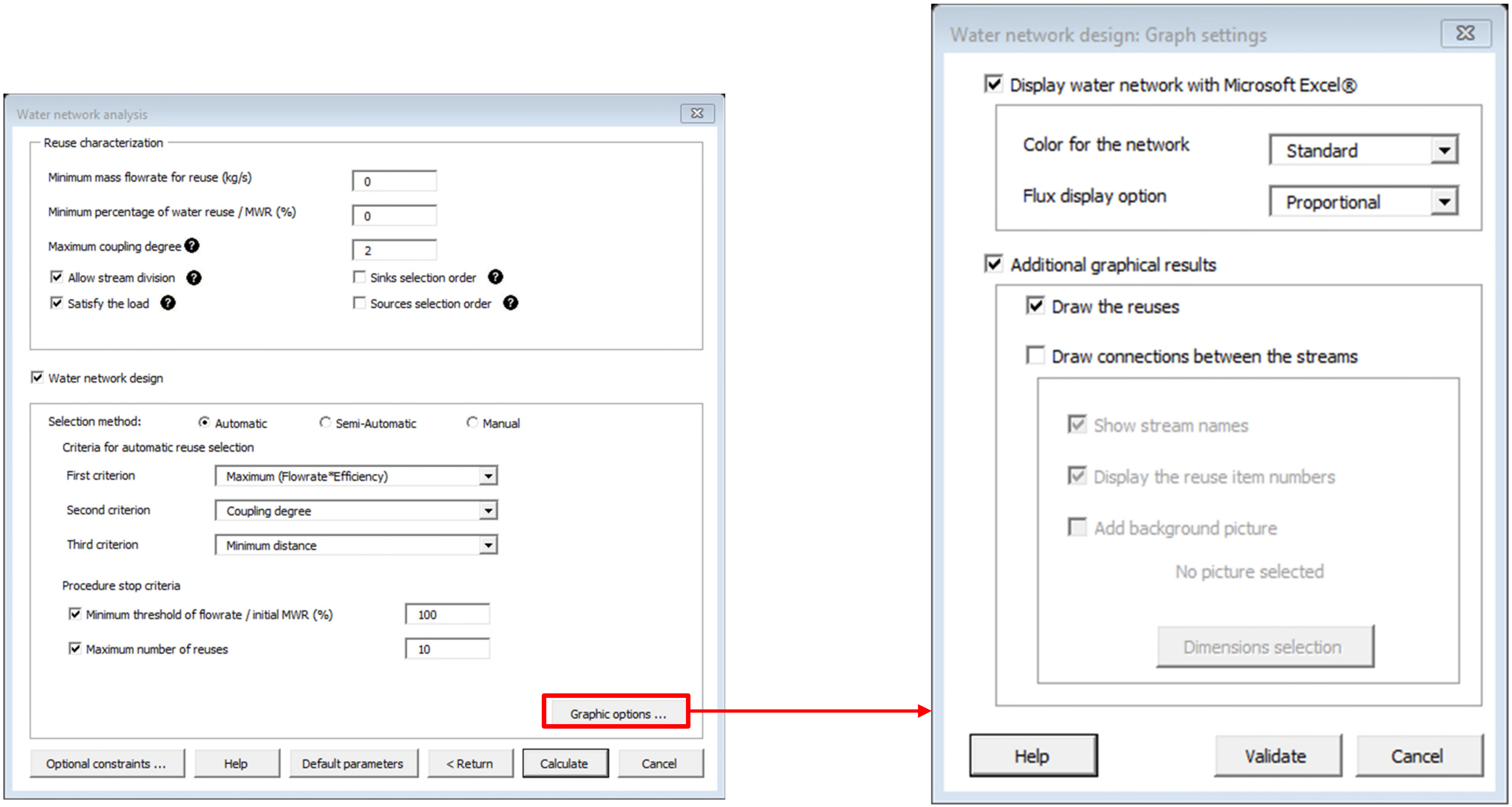
From the design point of view, there may be site constraints:

- Two streams can not be coupled because they are too viscous (reuses design problem)
- Two streams can not be coupled because they are too far from each other
- The user prefers a local integration
- The user does not want stream division
- The user wants to reduce the capital cost of reuses
- ...

These additional constraints are presented in the getting started “Use Case 2: Water integration of an acrylonitrile plant – Advanced use of Simulis Pinch”.

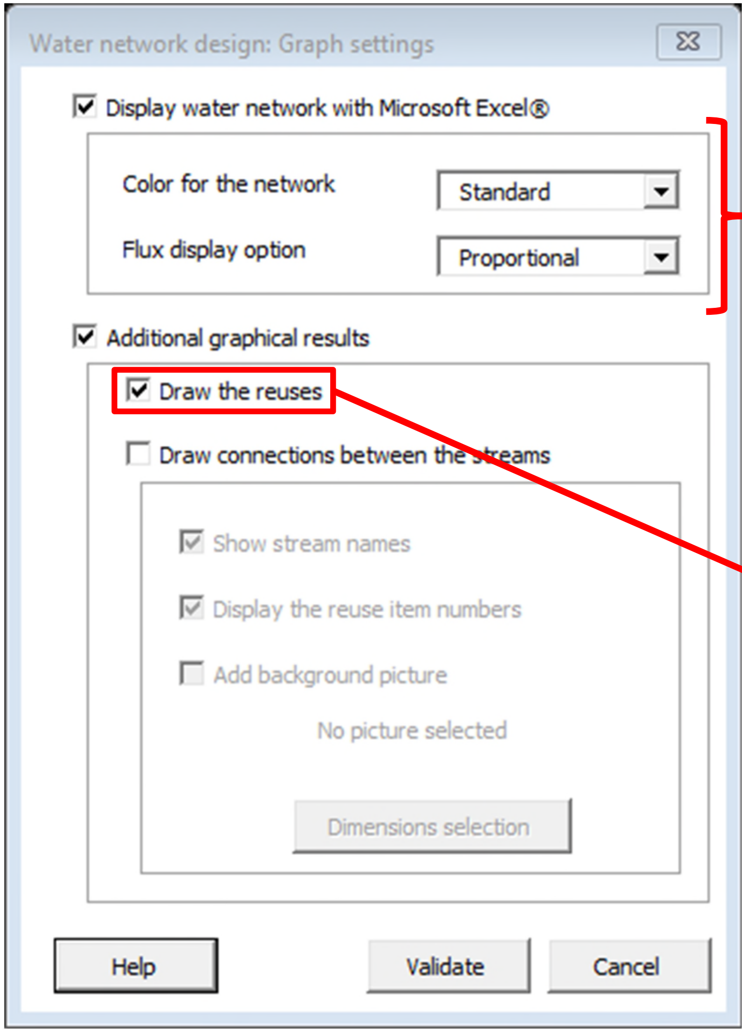
Step 3: Design of a water network

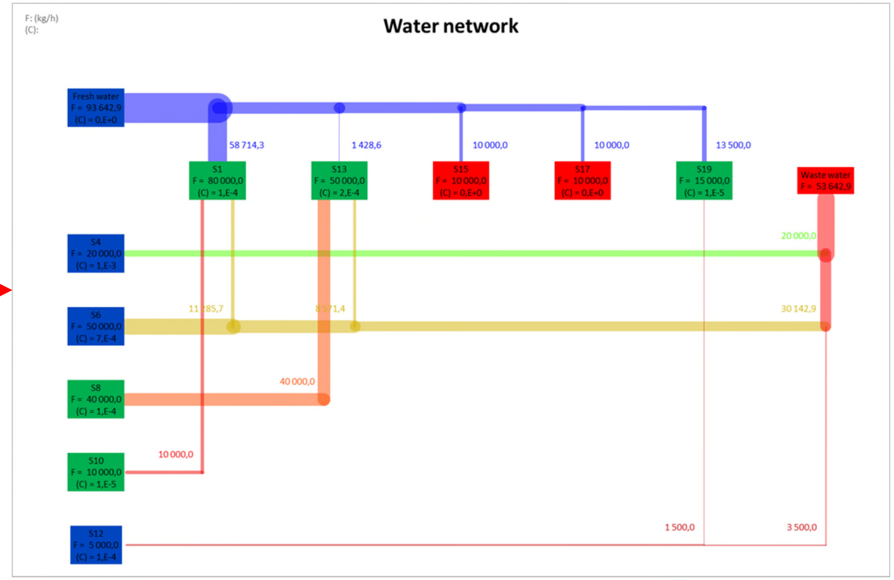
The **Graphic options** of Simulis Pinch Water:

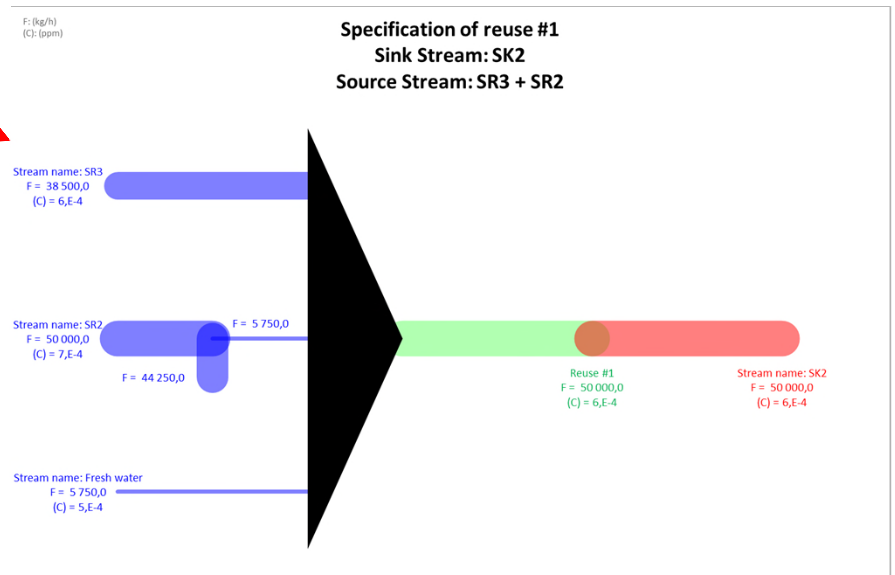


Step 3: Design of a water network

The **Graphic options** of Simulis Pinch Water:



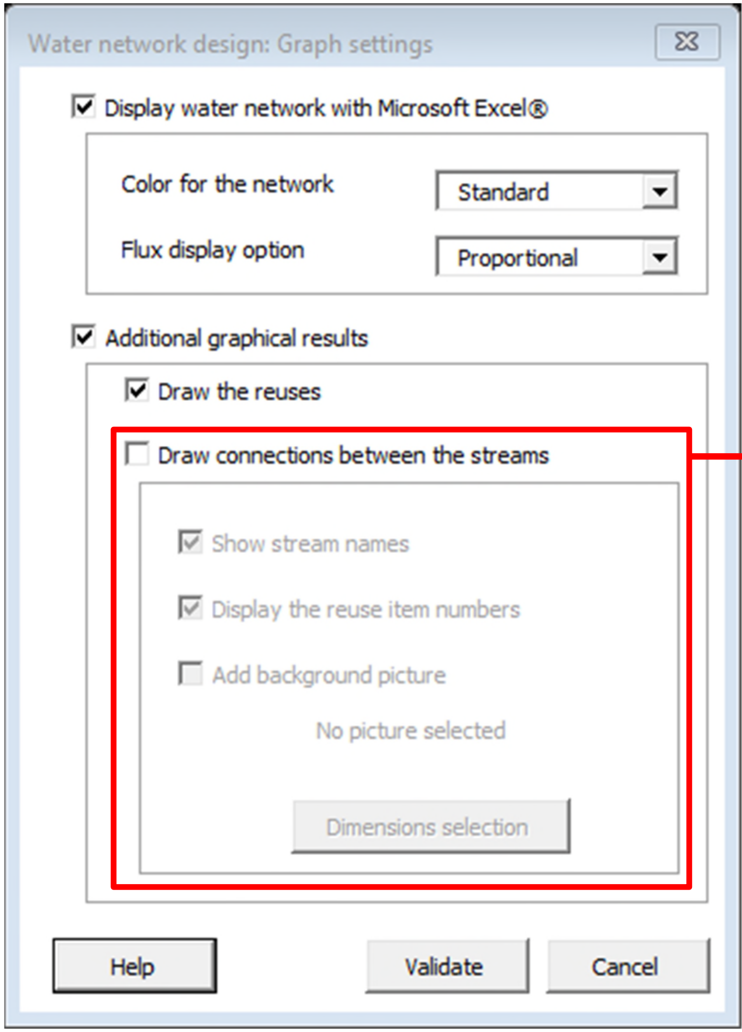


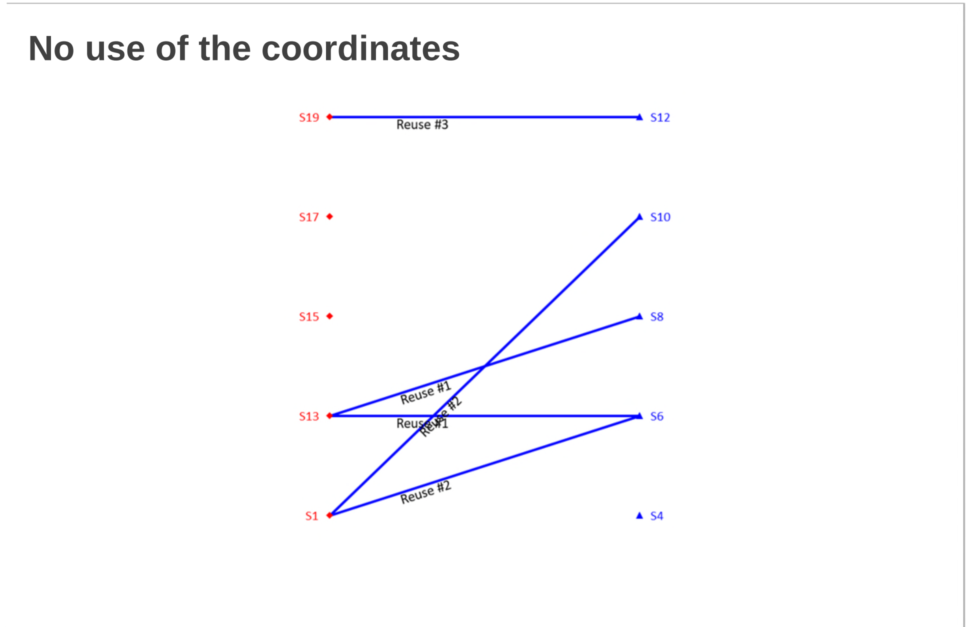


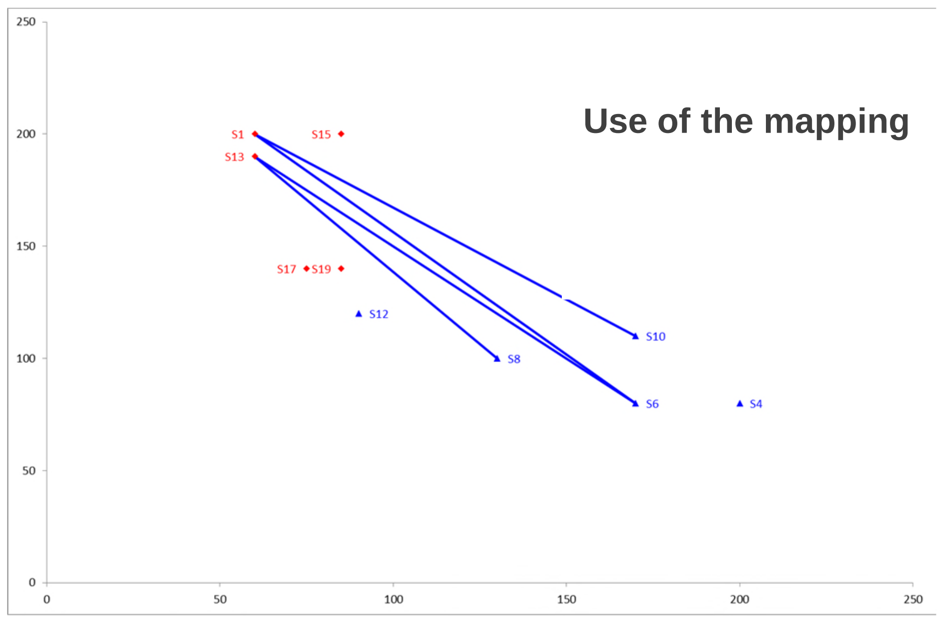
*Colors used for the water network can be modified by clicking on the option "**Color for the network**" ("Standard" by default)*

Step 3: Design of a water network

The **Graphic options** of Simulis Pinch Water:
A diagram display for each reuse is available.



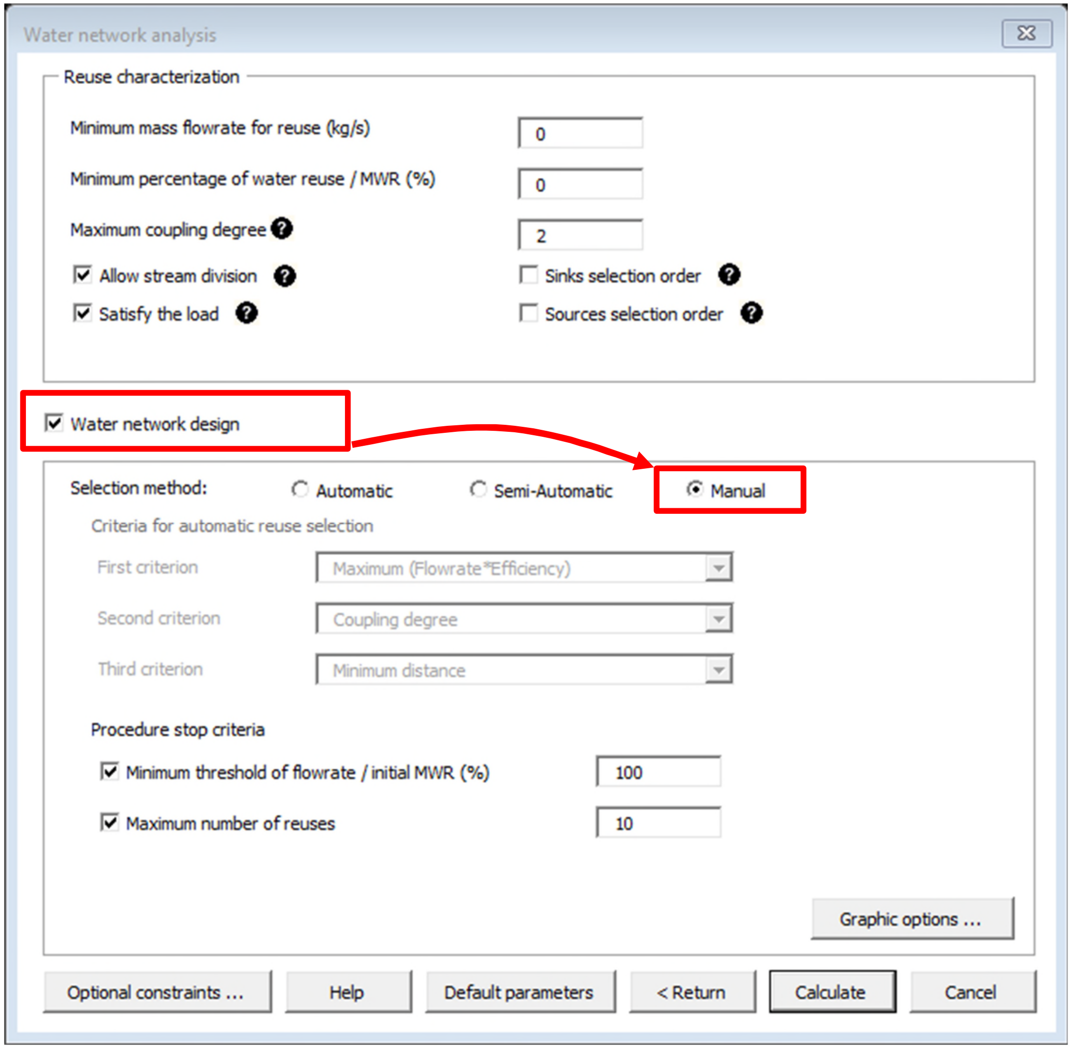




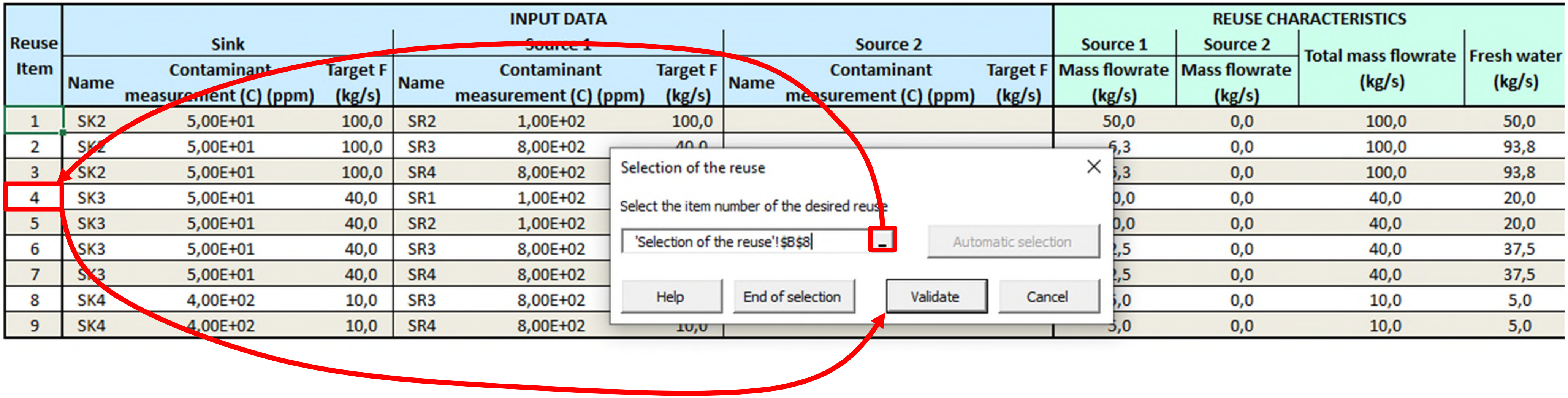
Step 3: Design of a water network

Simulis Pinch Water proposes **Manual** or **Semi-Automatic** selection modes:

1. Select the data and find the next window
2. Check the **Water network design**
3. Selection method: **Manual**



Step 3: Design of a water network



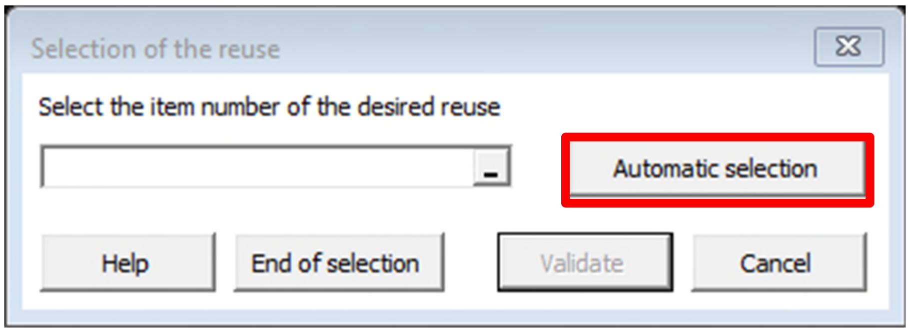
Reuse Item	INPUT DATA									REUSE CHARACTERISTICS			
	Sink			Source 1			Source 2			Source 1	Source 2	Total mass flowrate (kg/s)	Fresh water (kg/s)
	Name	Contaminant measurement (C) (ppm)	Target F (kg/s)	Name	Contaminant measurement (C) (ppm)	Target F (kg/s)	Name	Contaminant measurement (C) (ppm)	Target F (kg/s)	Mass flowrate (kg/s)	Mass flowrate (kg/s)		
1	SK2	5,00E+01	100,0	SR2	1,00E+02	100,0				50,0	0,0	100,0	50,0
2	SK2	5,00E+01	100,0	SR3	8,00E+02	40,0	[illegible]	[illegible]	[illegible]	6,3	0,0	100,0	93,8
3	SK2	5,00E+01	100,0	SR4	8,00E+02	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0,0	100,0	93,8
4	SK3	5,00E+01	40,0	SR1	1,00E+02	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0,0	40,0	20,0
5	SK3	5,00E+01	40,0	SR2	1,00E+02	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0,0	40,0	20,0
6	SK3	5,00E+01	40,0	SR3	8,00E+02	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0,0	40,0	37,5
7	SK3	5,00E+01	40,0	SR4	8,00E+02	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0,0	40,0	37,5
8	SK4	4,00E+02	10,0	SR3	8,00E+02	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	0,0	10,0	5,0
9	SK4	4,00E+02	10,0	SR4	8,00E+02	10,0	[illegible]	[illegible]	[illegible]	[illegible]	0,0	10,0	5,0

1. Select the reuse in the column ***Reuse item***
2. Click on ***Validate***

Step 3: Design of a water network

In ***Manual*** selection mode, Simulis Pinch Water offers the user a list of reuses.
The user selects the reuses until one of the stop criteria is reached.

In ***Semi-Automatic*** selection mode, the user starts to select the reuses like for ***Manual*** selection mode. With this method, the user can at all time request Simulis Pinch Water to select automatically reuses (***Automatic*** method) by clicking on the ***Automatic selection*** button.



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