Getting started with Simulis® Pinch
Water module

Use Case 3: Water integration of a refinery plant - Multi-contaminants analysis

Release Simulis Pinch 2.0.0

Software & Services In Process Simulation

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Introduction

This getting started shows you the basics of Simulis Pinch Water in order to perform a multi-contaminants analysis 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

This document follows the guide "Use Case 1: Water integration of an acrylonitrile plant – First steps with Simulis Pinch Water" based on a mono-contaminant analysis.

Step 1: Data generation in Microsoft™ Excel

The data used in this document are based on a petroleum refinery plant. This example is studied in:
Gunaratnam M., « Automated Design of Total Water Systems », Ind. Eng. Chem. Res., 2005, 44, 588-599.

There are 3 limiting contaminants for the water reuse:

- **Suspended solids:** also named Total Suspended Solids (TSS) is the dry-weight of suspended particles and refers to all insoluble solids present in suspension in a liquid. The more water contains TSS, the more the turbidity increases.
The suspension is a "matrix" capable of adsorbing various contaminants, which can transform it and be transported. Thus, TSS is the most common industrial contaminant.

- **Hydrogen sulfide (H_2S):** sulfur present in the H_2S is a contaminant for the catalysts and it is a generator of acid corrosion during combustion. It is necessary to limit its emissions as much as possible. For these reasons, methods of "hydro-desulphurization" are used in oil refineries, and "Claus" processes are performed to treat the H2S and produce pure sulfur.

- **Hydrocarbons:** hydrocarbons are contaminants for the steam stripping columns and for hydro desulphurization sections because they degrade the performance of equipment. We must therefore limit the reuse with high concentrations of hydrocarbons.

Step 1: Data generation in Microsoft™ Excel

The data are presented below:

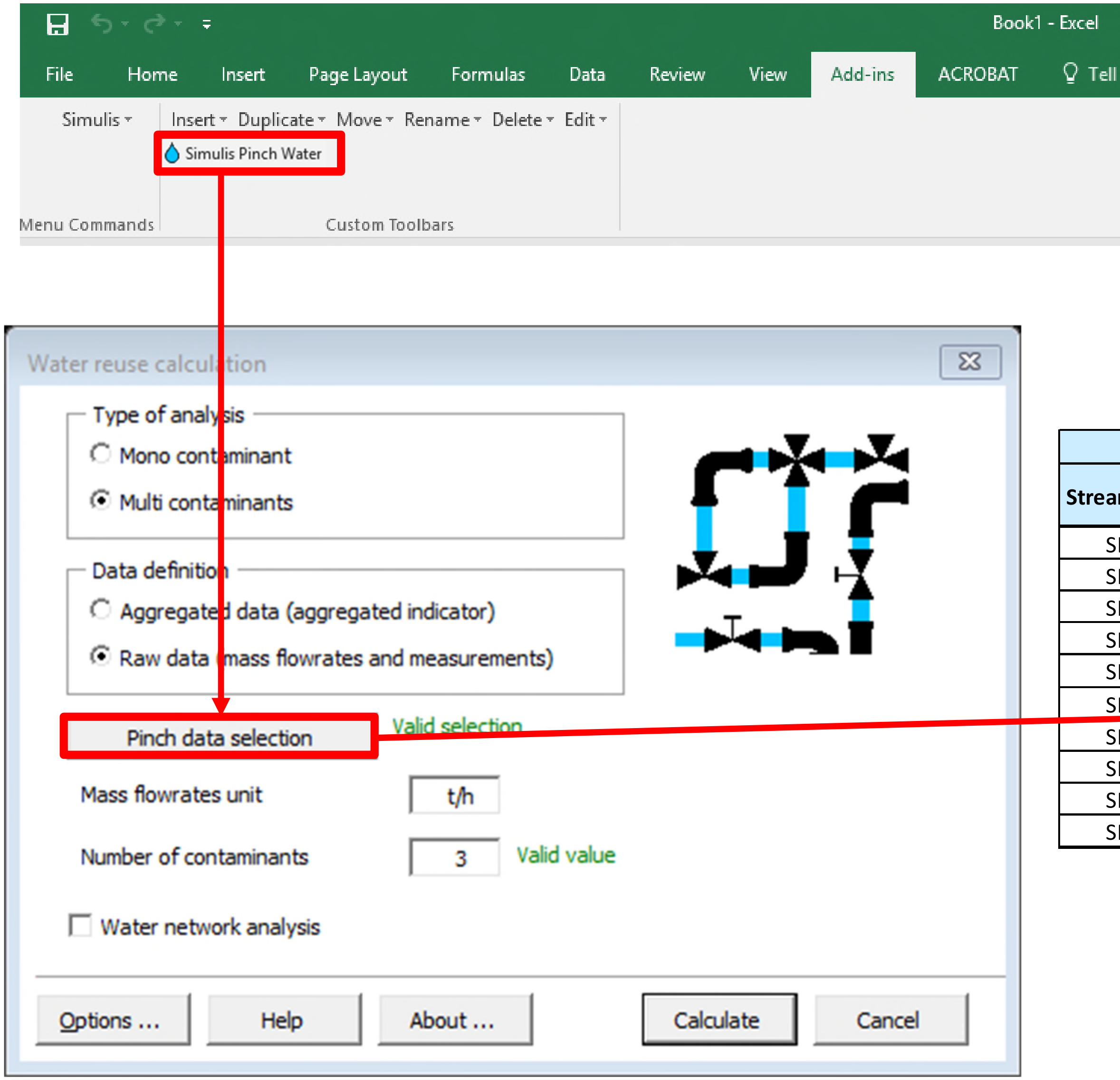
Operation	Flowrate (t/h)	Contaminant	C_{in} (ppm)	C_{out} (ppm)
Steam stripping	50	H.C.	0	15
		H_2S	0	400
		S.S.	0	35
Hydro-desulphurization I	34	H.C.	20	120
		H_2S	300	12500
		S.S.	45	180
Desalter	56	H.C.	120	220
		H_2S	20	45
		S.S.	200	9500
Ejector steam for vacuum column	8	H.C.	0	20
		H_2S	0	60
		S.S.	0	20
Hydro-sulphurization II	8	H.C.	50	150
		H_2S	400	8000
		S.S.	60	120

**H.C.: Hydrocarbon*

**S.S.: Suspended solids (suspended matter)*

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)

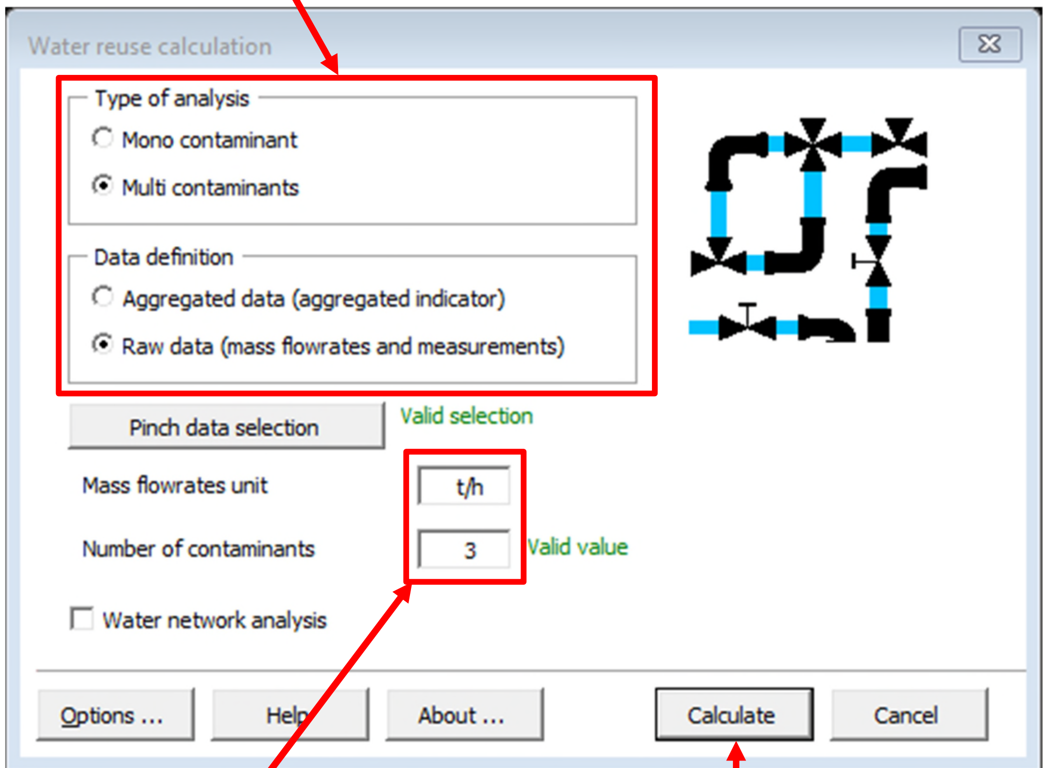


Input data				
Stream names	Mass flowrate (F)	Contaminant (C) measurement 1	Contaminant (C) measurement 2	Contaminant (C) measurement 3
SK-O1	50,0	0,00E+00	0,00E+00	0,00E+00
SK-O2	34,0	2,00E+01	3,00E+02	4,50E+01
SK-O3	56,9	1,20E+02	2,00E+01	2,00E+02
SK-O4	8,0	0,00E+00	0,00E+00	0,00E+00
SK-O5	8,0	5,00E+01	4,00E+02	6,00E+01
SR-O1	- 50,0	1,50E+01	4,00E+02	3,50E+01
SR-O2	- 34,0	1,20E+02	1,25E+04	1,80E+02
SR-O3	- 56,9	2,20E+02	4,50E+01	9,50E+03
SR-O4	- 8,0	2,00E+01	6,00E+01	2,00E+01
SR-O5	- 8,0	1,50E+02	8,00E+03	1,20E+02

Raw data

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

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



2. Provide the units of the flowrates (F) and the number of contaminants (here 3 contaminants)

3. Click on ***Calculate***

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

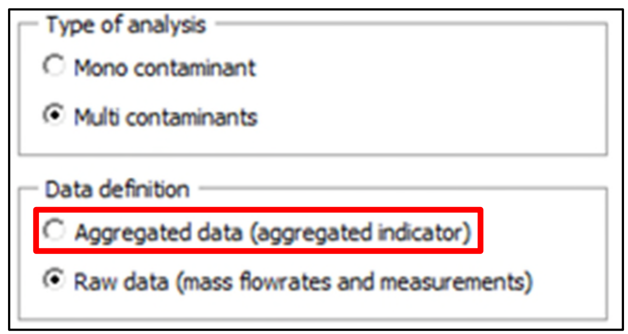
For a multi contaminants analysis (from raw data), the results of the diagnostic are provided for each contaminant taken independently of others.

Thus, 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)

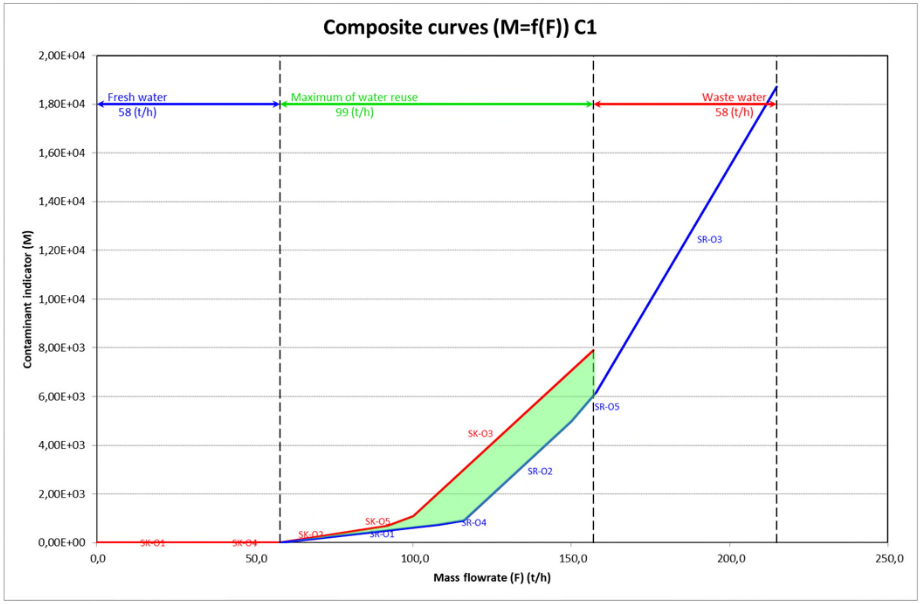
It is possible to aggregate these contaminants into a single indicator (according to an aggregation calculation defined by the user). In this case, the user chooses the “Aggregate data (aggregated indicator)” option for the definition of the data type.

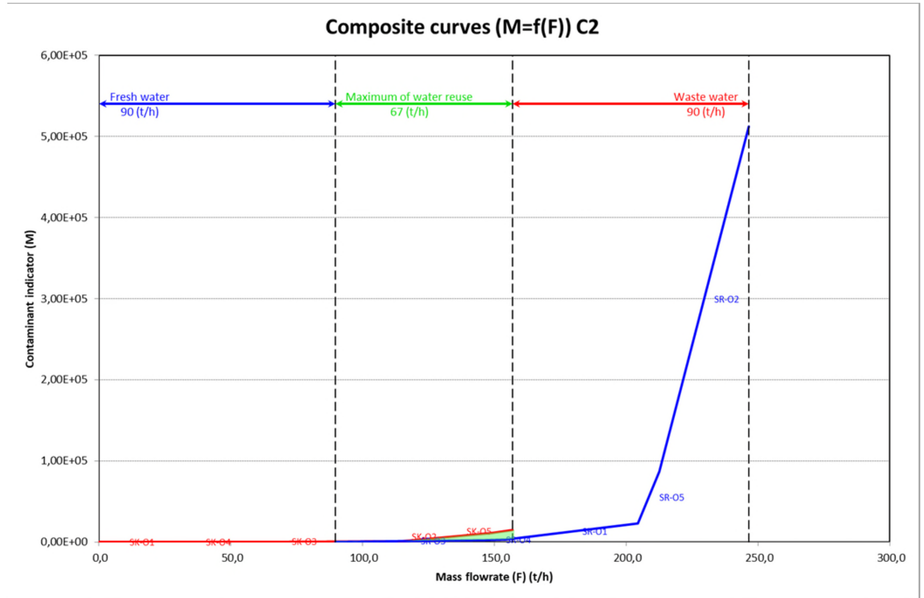
This method is used to draw a single dataset (only 1 composite curve diagram, only 1 water pinch analysis...) and thus simplify the water pinch analysis.

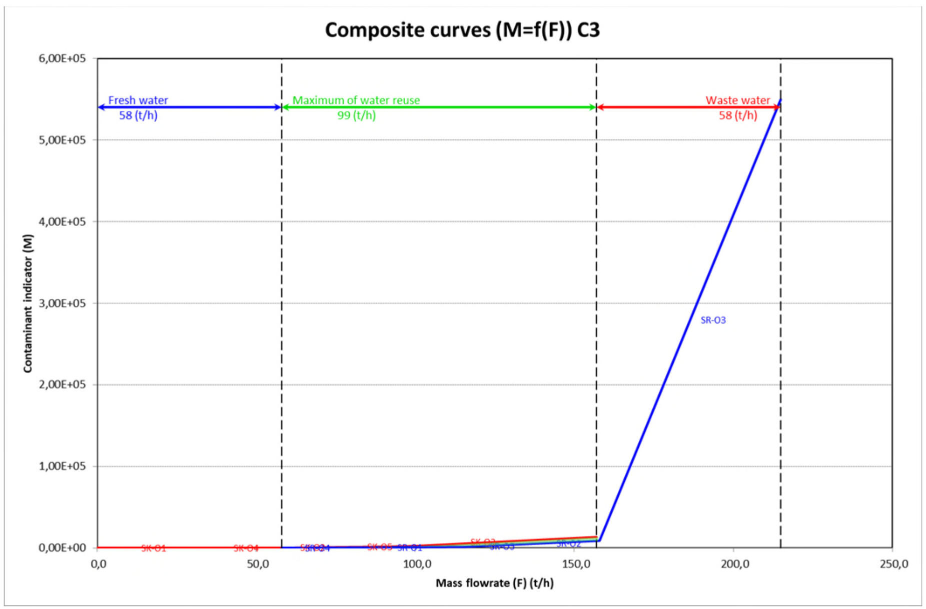


This aggregation calculation can also be performed in ProSimPlus using the “Water Pinch Analysis” module with a multi-contaminants analysis.

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





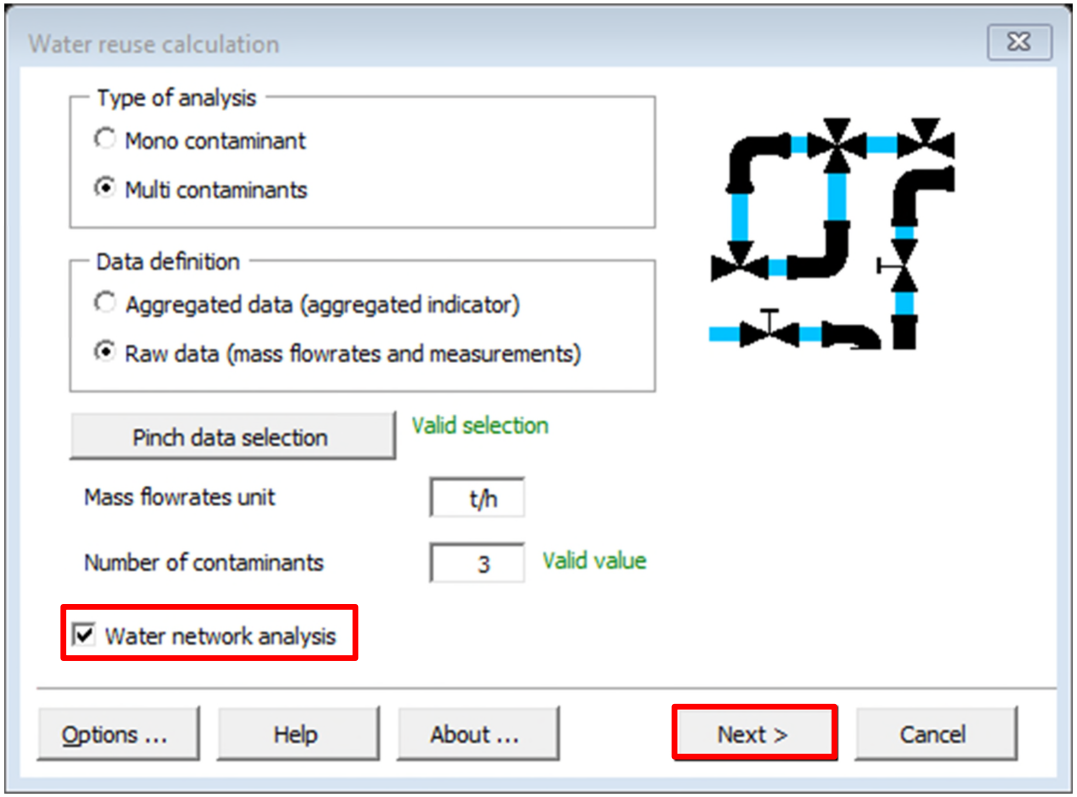


With the « multi contaminant » analysis, the results of the diagnostic are displayed for each contaminant (independently of each other).

By analyzing the composite curves, it is possible to notice a MWR (green area) for each contaminant. The minimum MWR is the C2 contaminant (*i.e.* H_2S in our case) with 67 t/h.

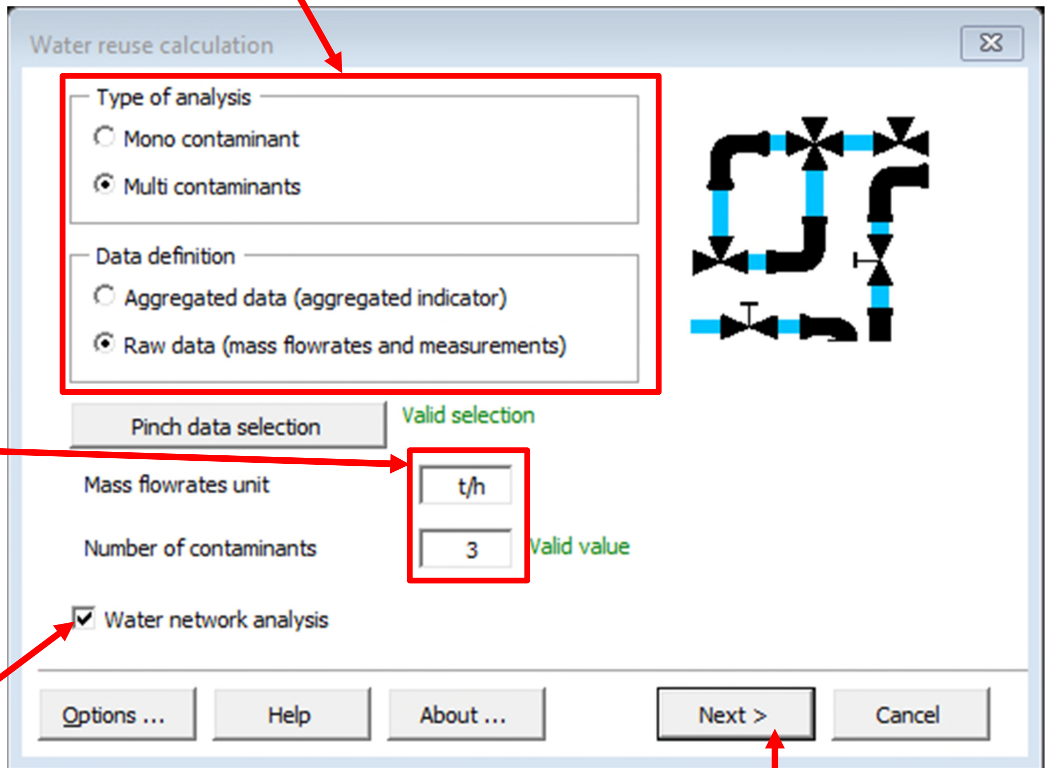
Step 3: Design of a water network

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



Step 3: Design of a water network

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



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

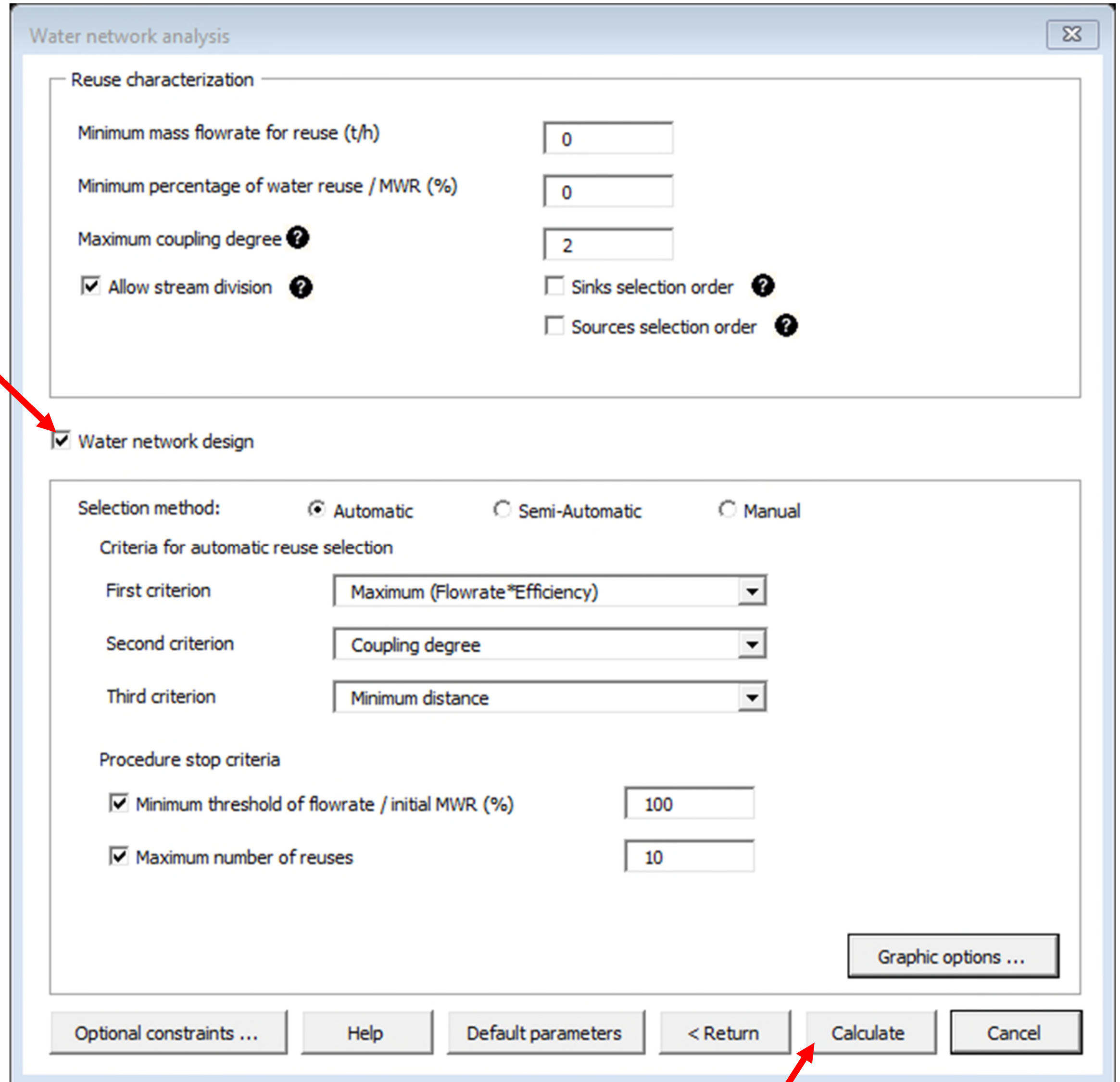
3. Check the **Water network analysis** box

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**)*

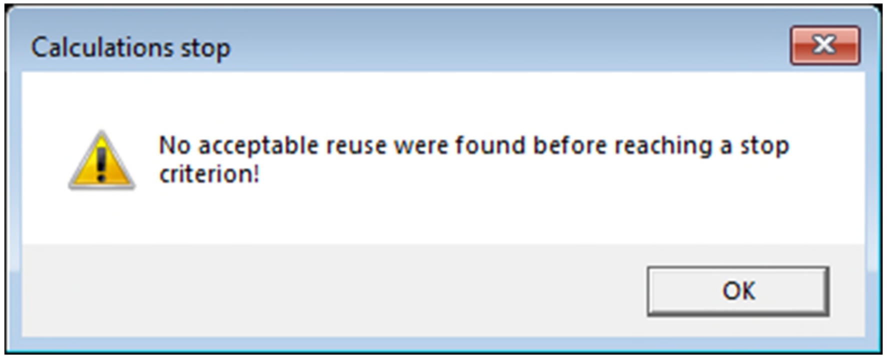


2. Click on ***Calculate***

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, Simulis Pinch Water can no longer propose additional reuse and the construction of the water network stops because no additional reuse can be determined



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:	18
Cumulative percentage of water reuse:	41,13
Number of reuses:	3
Total water reuse (t/h):	36,3
Water flowrate available to reuse (t/h):	0,0
Additional required amount of fresh water(t/h):	120,6
Amount of waste water (t/h):	120,6
Remaining number of Sources:	4
Remaining number of Sinks:	2

RESULTS FOR THE AUTOMATIC DESIGN OF THE WATER NETWORK

Reuse Item	Sink						
	Name	Contaminant measurement (C1)	Contaminant measurement (C2)	Contaminant measurement (C3)	Target F (t/h)	Name	Contaminar measurement
1	SK-O2	2,00E+01	3,00E+02	4,50E+01	34,0	SR-O1	1,50E+01
2	SK-O5	5,00E+01	4,00E+02	6,00E+01	8,0	SR-O4	2,00E+01
3	SK-O3	1,20E+02	2,00E+01	2,00E+02	56,9	SR-O1	1,50E+01

NO MORE REUSE IS POSSIBLE

LIST OF THE STREAMS STILL REMAINING AFTER THE WATER NETWORK DESIGN

Stream names	Mass flowrate (F) (t/h)	Contaminant measurement (C1)	Contaminant measurement (C2)	Contaminant measurement (C3)
SR-O2	34,0	1,20E+02	1,25E+04	1,80E+02
SR-O5	8,0	1,50E+02	8,00E+03	1,20E+02
SR-O3	56,9	2,20E+02	4,50E+01	9,50E+03
SR-O1	21,7	1,50E+01	4,00E+02	3,50E+01
SK-O1	50,0	0,00E+00	0,00E+00	0,00E+00
SK-O4	8,0	0,00E+00	0,00E+00	0,00E+00

FRESH WATER CHARACTERISTICS

Stream	Mass flowrate (F)	Contaminant	Contaminant	Contaminant

... | Streams C1 | Water Pinch results C1 | Reuse #3 | Reuse #2 | Reuse #1 | Water network | Water network results | Input data | Optional 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:	18
Cumulative percentage of water reuse:	41,13
Number of reuses:	3
Total water reuse (t/h):	36,3
Water flowrate available to reuse (t/h):	0,0
Additional required amount of fresh water(t/h):	120,6
Amount of waste water (t/h):	120,6
Remaining number of Sources:	4
Remaining number of Sinks:	2

In the present case, with 2 reuses, the water network proposed by Simulis Pinch Water recovers ≈ 41% of average MWR (**M**aximum of **W**ater **R**ecovery). For a multi contaminant analysis, the average MWR is the average of the MWR of each contaminant.

This water recovery is not relevant for a multi contaminant analysis. It is better to compare the actual water consumption of the process (157 t/h) with those obtained by the new water network (120 t/h).
A water saving of 37 t/h is reached for this process (23.5% of actual process consumption).

Step 3: Design of a water network

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

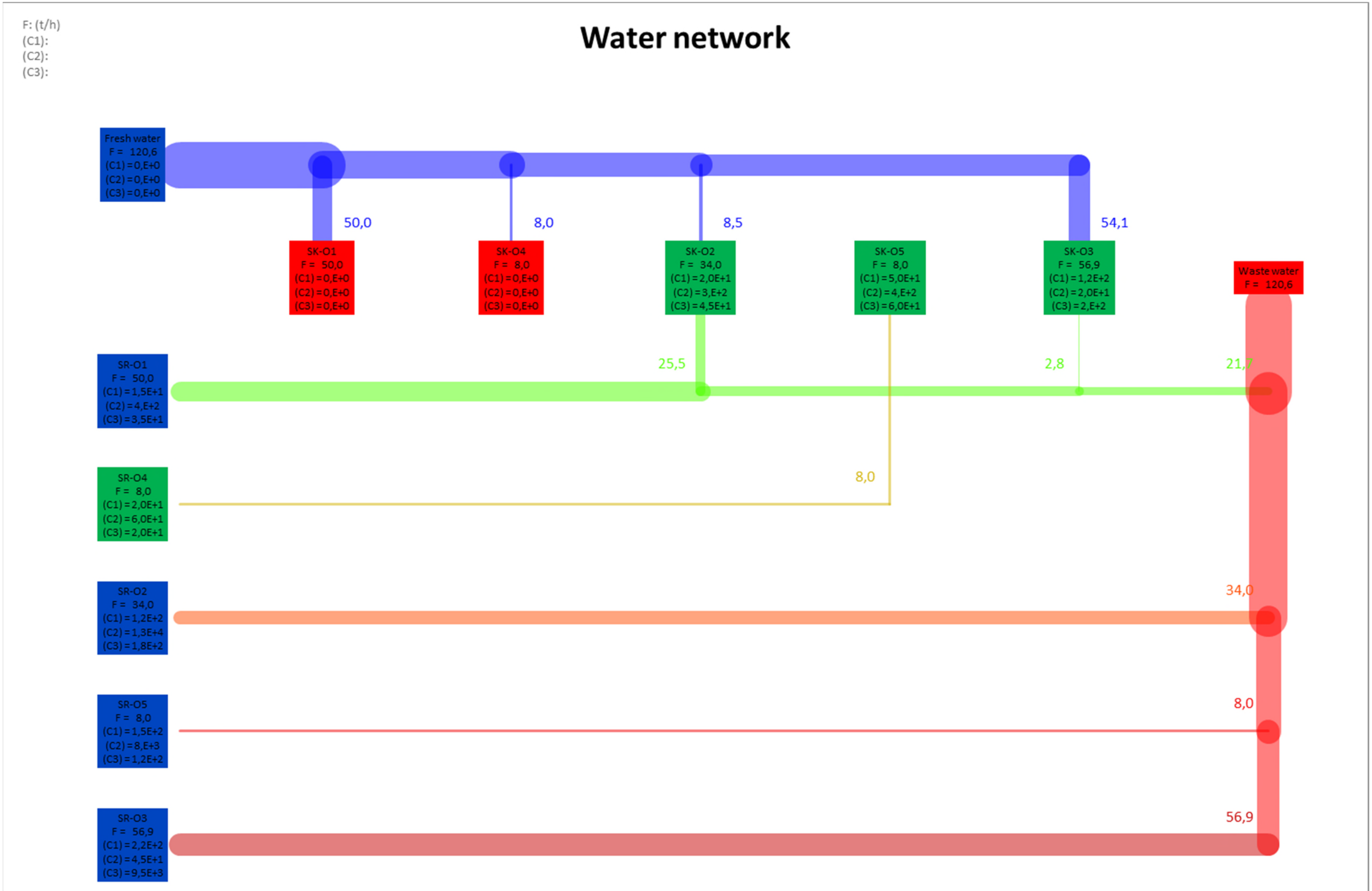
RESULTS FOR THE AUTOMATIC DESIGN OF THE WATER NETWORK

Reuse Item	INPUT DATA									
	Sink					Source 1				
	Name	Contaminant measurement (C1)	Contaminant measurement (C2)	Contaminant measurement (C3)	Target F (t/h)	Name	Contaminant measurement (C1)	Contaminant measurement (C2)	Contaminant measurement (C3)	Target F (t/h)
1	SK-O2	2,00E+01	3,00E+02	4,50E+01	34,0	SR-O1	1,50E+01	4,00E+02	3,50E+01	50,0
2	SK-O5	5,00E+01	4,00E+02	6,00E+01	8,0	SR-O4	2,00E+01	6,00E+01	2,00E+01	8,0
3	SK-O3	1,20E+02	2,00E+01	2,00E+02	56,9	SR-O1	1,50E+01	4,00E+02	3,50E+01	24,5

REUSE CHARACTERISTICS				INFORMATION ON WATER REUSE					
Source 1	Source 2	Total mass flowrate (t/h)	Fresh water (t/h)	% of water reuse / MWR	Degree of coupling	Efficiency	Splitting ratio		Mass Flowrate* efficiency
Mass flowrate (t/h)	Mass flowrate (t/h)						Source 1	Source 2	
25,5	0,0	34,0	8,5	28,9	1	1,00	0,5	0,0	25,5
8,0	0,0	8,0	0,0	14,7	1	1,00	1,0	0,0	8,0
2,8	0,0	56,9	54,1	6,1	1	0,06	0,1	0,0	0,2

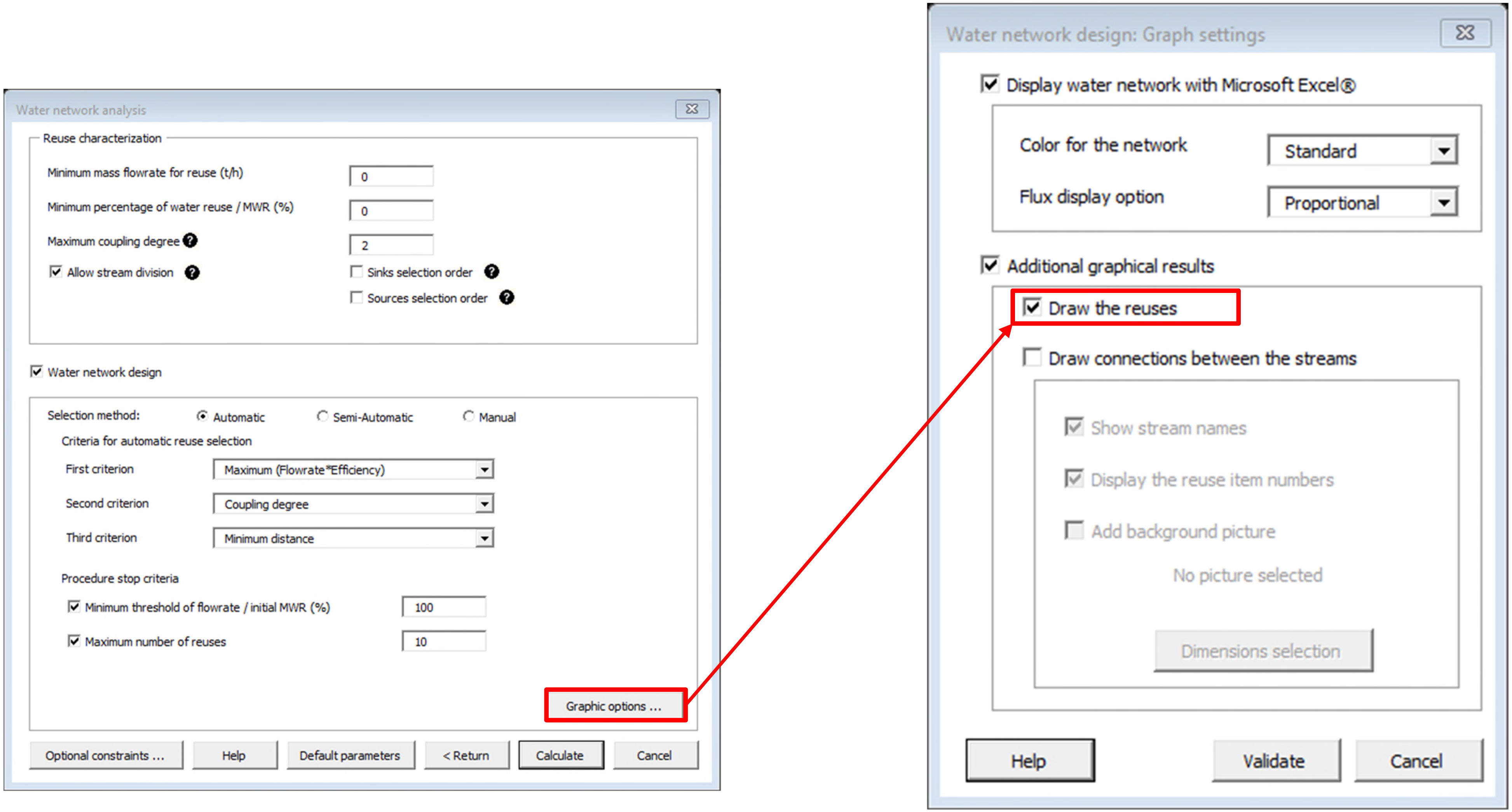
Step 3: Design of a water network

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



Step 3: Design of a water network

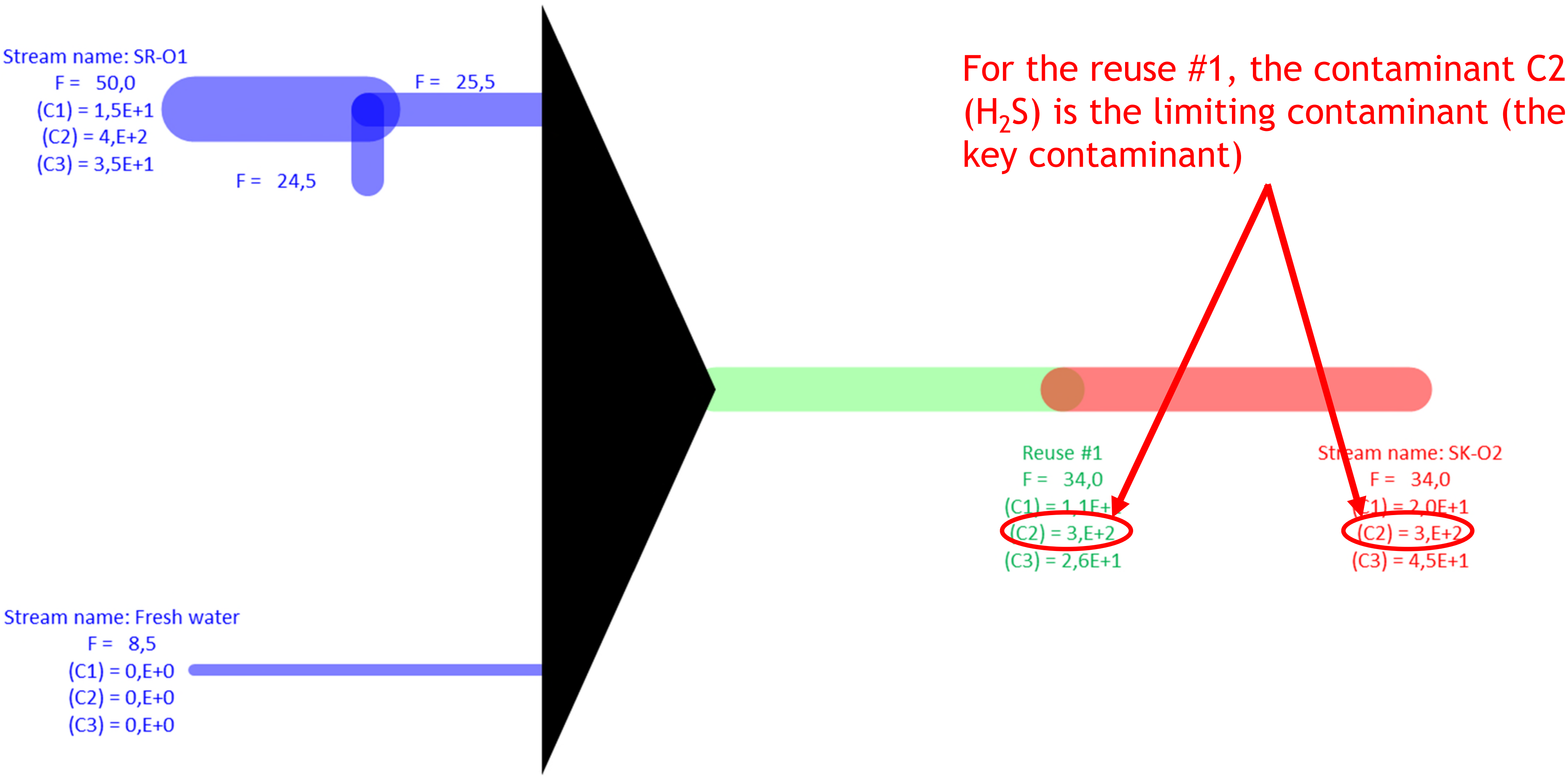
The **graphic options** of Simulis Pinch Water can be handled to draw the diagram for each reuse:



Step 3: Design of a water network

F: (t/h)
(C1):
(C2):
(C3):

Specification of reuse #1
Sink: SK-O2
Source Stream: SR-O1



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