

# Getting started with Simulis® Pinch Water module

Use Case 2: Water integration of an acrylonitrile plant  
- Advanced use of Simulis Pinch Water

Release Simulis Pinch 2.0.0

Software & Services In Process Simulation

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# Introduction

This getting started shows you the use of optional constraints with Simulis Pinch Water to perform an advanced process water integration.

This document follows the getting started “Use Case 1: Water integration of an acrylonitrile plant – First steps with Simulis Pinch Water”

This guide is organized as follows:

-  Step 1: Adding a constraint on zones
-  Step 2: Adding a distance constraint between streams
-  Step 3: Adding an incompatibility matrix
-  Step 4: Adding a constraint of "difficulty" between streams

# Introduction

A first step before the use of optional constraints is to reshape the Microsoft™ Excel sheet input data:

1. Click on the ***Optional constraints*** button

Water network analysis

Reuse characterization

Minimum mass flowrate for reuse (kg/s)

Minimum percentage of water reuse / MWR (%)

Maximum coupling degree

☒ Allow stream division

☒ Satisfy the load

☐ Sinks selection order

☐ Sources selection order

☒ Water network design

Selection method: ☒ Automatic ☐ Semi-Automatic ☐ Manual

Criteria for automatic reuse selection

First criterion

Second criterion

Third criterion

Procedure stop criteria

☒ Minimum threshold of flowrate / initial MWR (%)

☒ Maximum number of reuses

Graphic options ...

Optional constraints ... Help Default parameters < Return Calculate Cancel

# Introduction

2. Click on the **Generate tables** button

Water Network Design: Optional constraints

☐ Use constraints on zone ?

☒ none  
☐ Intrazone reuses only  
☐ Conditional interzone reuses

Stream zones selection

Selection of the authorized source zones

Selection of the authorized sink zones

☐ Incompatibility matrix ?

Selection

☐ Difficulty ?

Maximum difficulty

Selection

☐ Mapping ?

Maximum distance

Selection

Help

**Generate Tables**

Validate

Cancel

# Introduction

The input data (stream name, flowrates (F), contaminant measurement (C)) are then reshaped and optional tables are generated in a "Optional Tables" sheet:

Input data		
Stream names	Mass flowrate (F)	Contaminant (C) measurement
SK1	5,8	1,00E+01
SK2	1,2	0,00E+00
SR1	- 0,8	0,00E+00
SR2	- 5,0	1,40E+01
SR3	- 5,9	2,50E+01
SR4	- 1,4	3,40E+01

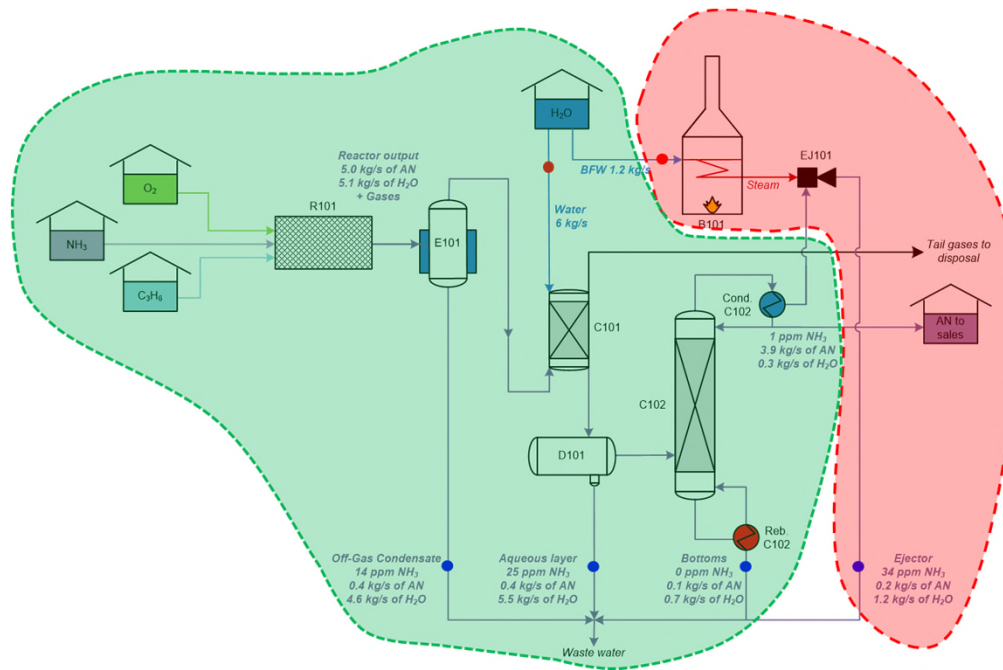
Difficulty	Geom(x)	Geom(y)	Geom(z)	Stream Zone	Authorized sources streams zones	Authorized sinks streams zones	Incompatibility matrix	SK1	SK2
							SR1	0	0
							SR2	0	0
							SR3	0	0
							SR4	0	0

Background picture size bounds			
Xmin	Xmax	Ymin	Ymax



# Step 1: Adding a constraint on zones

The user defines the areas in which the different streams are present. For this example, 2 zones are defined:



Input data		
Stream names	Mass flowrate (F)	Contaminant (C) measurement
SK1	5,8	1,00E+01
SK2	1,2	0,00E+00
SR1	- 0,8	0,00E+00
SR2	- 5,0	1,40E+01
SR3	- 5,9	2,50E+01
SR4	- 1,4	3,40E+01

Stream Zone	Authorized sources streams zones	Authorized sinks streams zones
1		
2		
1		
1		
1		
2		

# Step 1: Adding a constraint on zones

In the optional constraints window:

1. Check **Use constraints on zone** box
2. Select the constraint to have only intrazone reuses (the proposed reuses are made only between the streams of the same zone)
3. Click on the button **Stream zones selection** button

Water Network Design: Optional constraints

☒ Use constraints on zone ?

☐ none

☒ Intrazone reuses only

☐ Conditional interzone reuses

Stream zones selection

Selection of the authorized source zones

Selection of the authorized sink zones

☐ Incompatibility matrix ?

Selection

☐ Difficulty ?

Maximum difficulty

Selection

☐ Mapping ?

Maximum distance

Selection

Help

Generate Tables

Validate

Cancel

# Step 1: Adding a constraint on zones

Selection of the zones:

Input data		
Stream names	Mass flowrate (F)	Contaminant (C) measurement
SK1	5,8	1,00E+01
SK2	1,2	0,00E+00
SR1	- 0,8	0,00E+00
SR2	- 5,0	1,40E+01
SR3	- 5,9	2,50E+01
SR4	- 1,4	3,40E+01

Difficulty
1
2
1
3
2
1

Geom(x)	Geom(y)	Geom(z)
20	15	
40	25	
100	35	
80	90	
50	30	
0	60	

Stream Zone	Au
1	
2	
1	
1	
1	
2	

Background picture size bounds			
Xmin	Xmax	Ymin	Ymax

Selection of the stream zones ? X

1 column: stream zones

SLS4:SLS9

OK Cancel

☒ Use constraints on zone ?

- ☐ none  
☒ Intrazone reuses only  
☐ Conditional interzone reuses

Stream zones selection

Valid selection

Selection of the authorized source zones

Selection of the authorized sink zones



# Step 1: Adding a constraint on zones

The results obtained by Simulis Pinch Water are the following: only 1 reuse is possible and it is located in the **zone 1**:

## SUMMARY FOR THE WATER NETWORK

Initial number of possible reuse:	2
Cumulative percentage of water reuse:	83,82
Number of reuses:	1
Total water reuse (kg/s):	4,1
Water flowrate available to reuse (kg/s):	0,8
Additional required amount of fresh water(kg/s):	2,9
Amount of waste water (kg/s):	9,0
Remaining number of Sources:	4
Remaining number of Sinks:	1

## 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

**NO MORE REUSE IS POSSIBLE**

Using zones constraints, the new water network can reuse 83.82% of the initial MWR

→ *Network efficiency has been degraded when adding constraints*

# Step 2: Adding a distance constraint between streams

With Simulis Pinch Water, it is possible to go beyond the concept of zones. The user can define coordinates of streams on the industrial site. For example, on a 2D map:

Input data		
Stream names	Mass flowrate (F)	Contaminant (C) measurement
SK1	5,8	1,00E+01
SK2	1,2	0,00E+00
SR1	- 0,8	0,00E+00
SR2	- 5,0	1,40E+01
SR3	- 5,9	2,50E+01
SR4	- 1,4	3,40E+01

Difficulty
1
2
1
3
2
1

Geom(x)	Geom(y)	Geom(z)
20	15	
40	25	
100	35	
80	90	
50	30	
0	60	

# Step 2: Adding a distance constraint between streams

In the optional constraints window, the user must:

1. Select the coordinates

Input data		
Stream names	Mass flowrate (F)	Contaminant (C) measurement
SK1	5,8	1,00E+01
SK2	1,2	0,00E+00
SR1	- 0,8	0,00E+00
SR2	- 5,0	1,40E+01
SR3	- 5,9	2,50E+01
SR4	- 1,4	3,40E+01

Background picture size bounds			
Xmin	Xmax	Ymin	Ymax

Difficulty
1
2
1
3
2
1

Geom(x)	Geom(y)	Geom(z)
20	15	
40	25	
100	35	
80	90	
50	30	
0	60	



The units of coordinates information and the maximum distance are identical (it is why they do not appear)

Mapping selection ? X

3 columns : x, y, z

SH54: SJ59

OK Cancel



The zones constraint is not taken into account for this example with the distance constraint

2. Give the maximum distance between two streams

In this example, the constraint is 65 m

☒ Mapping ?

Maximum distance 65

Selection Valid selection

# Step 2: Adding a distance constraint between streams

It is possible to modify the selection criteria for Simulis Pinch Water by choosing the most effective reuses and the closest ones:

Water network analysis

Reuse characterization

Minimum mass flowrate for reuse (kg/s)

Minimum percentage of water reuse / MWR (%)

Maximum coupling degree

☒ Allow stream division

☒ Sinks selection order

☒ Satisfy the load

☐ Sources selection order

☒ Water network design

Selection method: ☒ Automatic ☐ Semi-Automatic ☐ Manual

Criteria for automatic reuse selection

First criterion

Second criterion

Third criterion

Procedure stop criteria

☒ Minimum threshold of flowrate / initial MWR (%)

☒ Maximum number of reuses

Graphic options ...

Optional constraints ... Help Default parameters < Return Calculate Cancel



# Step 2: Adding a distance constraint between streams

Simulis Pinch Water proposes a new water network. For each proposed reuse, the distance between the streams is displayed

## SUMMARY FOR THE WATER NETWORK

Initial number of possible reuse:	2
Cumulative percentage of water reuse:	63,12
Number of reuses:	2
Total water reuse (kg/s):	3,1
Water flowrate available to reuse (kg/s):	0,0
Additional required amount of fresh water(kg/s):	3,9
Amount of waste water (kg/s):	10,0
Remaining number of Sources:	3
Remaining number of Sinks:	0

## RESULTS FOR THE AUTOMATIC DESIGN OF THE WATER NETWORK

Reuse Item	INPUT DATA						REUSE CHARACTERISTICS				Distance
	Sink			Source 1			Source 1	Source 2	Total mass flowrate	Fresh water	
	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	0,00E+00	1,2	SR1	0,00E+00	0,8	0,8	0,0	1,2	0,4	60,8
2	SK1	1,00E+01	5,8	SR3	2,50E+01	5,9	2,3	0,0	5,8	3,5	33,5

NO MORE REUSE IS POSSIBLE



*This distance constraint will not be used later in the example presented in this document*

# Step 3: Adding an incompatibility matrix

After adding zones constraint for local integration (step 1 of the document), the user can add incompatibility constraints.

It is then possible to add incompatibility constraints between the “process” streams (SR1, SR2 and SR3) with the boiler feed water (SK2)

Input data		
Stream names	Mass flowrate (F)	Contaminant (C) measurement
SK1	5,8	1,00E+01
SK2	1,2	0,00E+00
SR1	- 0,8	0,00E+00
SR2	- 5,0	1,40E+01
SR3	- 5,9	2,50E+01
SR4	- 1,4	3,40E+01

Incompatibility matrix	SK1	SK2
SR1	0	1
SR2	0	1
SR3	0	1
SR4	0	0

Incompatibility selection ? X

0-> compatible, 1-> incompatible, sources in rows, sinks in columns

OK Cancel

☒ Incompatibility matrix ?

Selection Valid selection

# Step 4: Adding a constraint of "difficulty" between streams

The concept of **difficulty** allows to represent different concepts (viscosity, toxicity, flammability...).

In this example, some streams are more viscous and more toxic than others.

A difficulty value is given to each stream. The user then sets the maximum difficulty:

Input data		
Stream names	Mass flowrate (F)	Contaminant (C) measurement
SK1	5,8	1,00E+01
SK2	1,2	0,00E+00
SR1	- 0,8	0,00E+00
SR2	- 5,0	1,40E+01
SR3	- 5,9	2,50E+01
SR4	- 1,4	3,40E+01

Background picture size bounds			
Xmin	Xmax	Ymin	Ymax

Difficulty
1
2
1
3
2
1

Geom(x)	Geom(y)	Geom(z)
20	15	
40	25	
100	35	
80	90	
50	30	
0	60	

Difficulty selection ? X

1 column: difficulties

SF\$4:SF\$9

OK Cancel

☒ Difficulty ?

Maximum difficulty

Valid selection



*The difficulty of a reuse is the sum of the difficulties of the two streams*

# Step 5: New water network

The constraints used are:

- Interzone reuses only (step 1)
- Incompatibility between some streams (step 3)
- Difficulty constraint (step 4)

Water Network Design: Optional constraints

☒ Use constraints on zone ?

☐ none  
☒ Intrazone reuses only  
☐ Conditional interzone reuses

Stream zones selection Valid selection

Selection of the authorized source zones

Selection of the authorized sink zones

☒ Incompatibility matrix ?

Selection Valid selection

☒ Difficulty ?

Maximum difficulty

Selection Valid selection

☐ Mapping ?

Maximum distance

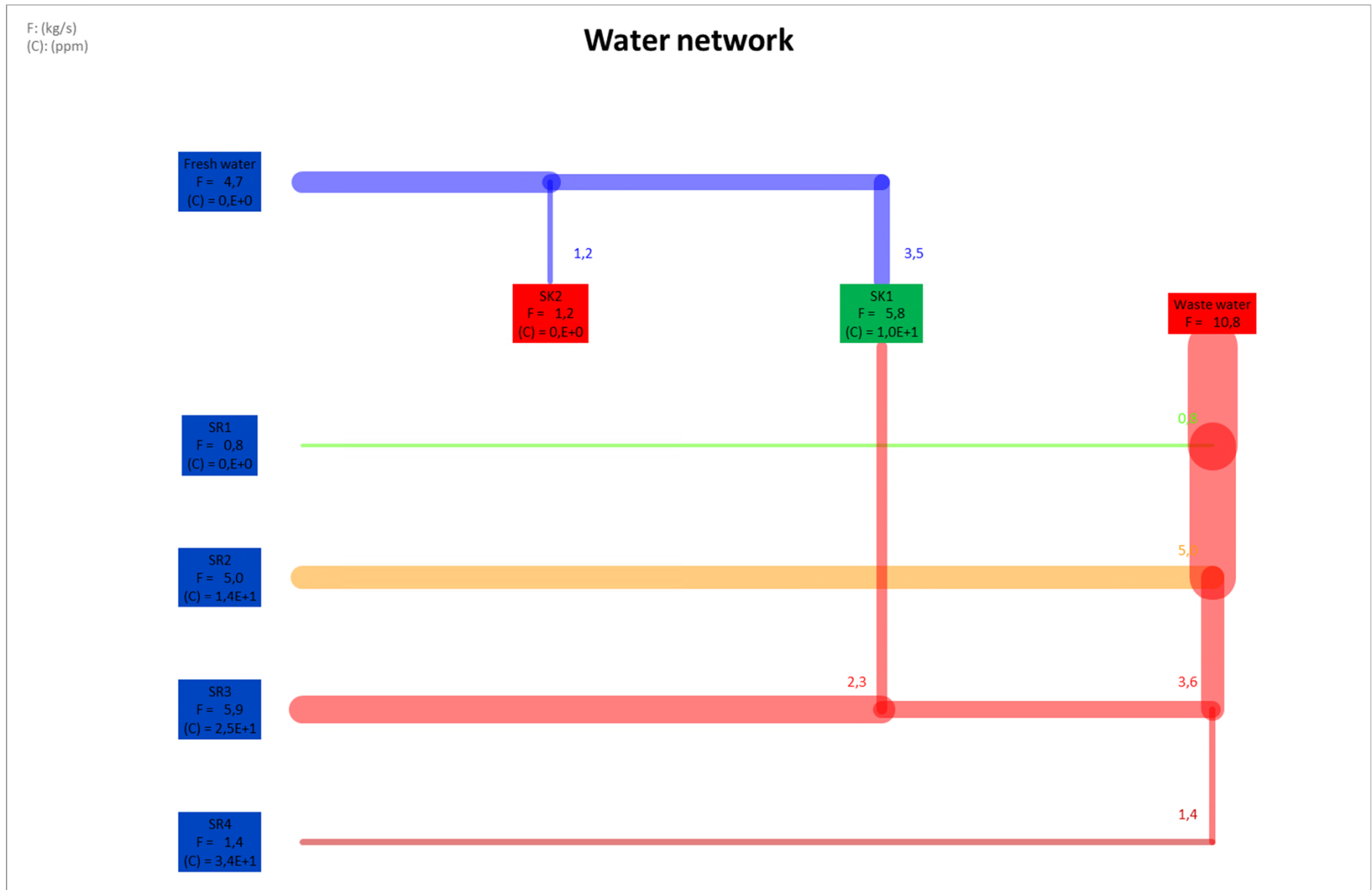
Selection

Help
 Generate Tables
 Validate
 Cancel



# Step 5: New water network

Adding different constraints modifies the water network. The proposed network has only one reuse. This network can recover  $\approx 47\%$  of MWR.





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