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



We guide You to efficiency

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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.

The data are presented below:

Operation	Flowrate (t/h)	Contaminant	C _{in} (ppm)	C _{out} (ppm)
Steam stripping	50	H.C. H ₂ S S.S.	0 0 0	15 400 35
Hydro-desulphurization I	34	H.C. H ₂ S S.S.	20 300 45	120 12500 180
Desalter	56	H.C. H ₂ S S.S.	120 20 200	220 45 9500
Ejector steam for vacuum column	8	H.C. H ₂ S S.S.	0 0 0	20 60 20
Hydro-sulphurization II	8	H.C. H ₂ S S.S.	50 400 60	150 8000 120

*H.C.: Hydrocarbon

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

Step 2: Definition of the theoretical optimum⁵ 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)

₽ 5° °°	Ŧ							Book	1 - Excel	
File Home	Insert	Page Layout	Formulas	Data	Review	View	Add-ins	ACROBAT	Q Tell	
Simulis * Ir	isert ▼ Duplio Simulis Pinch \	cate ▼ Move ▼ Rei Water	name + Delete	∗ Edit ×						
Menu Commands	culition	Custom Toolb	bars					X		
Type of a	nalysis — contaminan	t				 -X				
• Multi co	ontaminant	S			l 🖡		ſ		Stream name	s Mass flowrate
- Data defi	nition —					▁J	. 🚽		SK-01	
O Angreg	ated data	(apprenated in	dicator)				· 🔺		SK-02	
			alcotory				. I		SK-O4	
• Raw da	ata (mass f	lowrates and m	easurements)					SK-O5	
	•	Vali	d coloction		1				SR-O1	-
Pinch	data select	ion	d selection						SR-O2	-
Mass flowr	atec unit	Г	+ /h						SR-O3	-
Mass nown	ates unit	I_	yn						SR-04	
Number of	contaminar	nts 🗌	3 Val	id value					SR-05	-
🗌 Water ne	twork ana	ysis	_							
Options	He	lp Al	bout		Calcu	late	Cance	ł		

Input data								
Stroom nomos	Mass flowrate (E)	Contaminant (C)	Contaminant (C)	Contaminant (C)				
Stream names	Widss HOwfale (F)	measurement 1	measurement 2	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 optimum⁶ of the process water consumptions

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

Water reuse calculation	×
Type of analysis	
C Mono contaminan	
Multi contaminant	s f
Data definition	
C Aggregated data	(aggregated indicator)
Raw data (mass f	owrates and measurements)
Pinch data select	tion Valid selection
Mass flowrates unit	t/h
Number of contamina	nts 3 Valid value
Uater network ana	lysis
Options He	elo About Calculate Cancel
2. Provide the units of the flowrates and the number of contaminants (he contaminants)	(F) 3. Click on <i>Calculate</i>

Step 2: Definition of the theoretical optimum⁷ 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)

Streams C2	Water Pinch results C2	Composite curves (C=f(dM)) C1	Grand composite curve C1	Composite curves (M=f(F)) C1	Streams C1	Water Pinch results C1

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.

~	be of analysis
2	Mono contaminant
۲	Multi contaminants
Da	ta definition
O	Aggregated data (aggregated indicator)

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.

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

Water reuse calculation
Type of analysis
C Mono contaminant
Multi contaminants
Data definition
C Aggregated data (aggregated indicator)
Raw data (mass flowrates and measurements)
Pinch data selection Valid selection
Mass flowrates unit t/h
Number of contaminants 3 Valid value
✓ Water network analysis
Options Help About Next > Cancel

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



1. Check the box *water network design*

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

Water network analysis				23
Reuse characterization				
Minimum mass flowrate for reuse (t/h)	0			
Minimum percentage of water reuse / MWR (%)	0			
Maximum coupling degree 🕖	2			
Allow stream division	Sinks select	tion order 🔞		
	Sources se	lection order		
Water patwork darian				
Vater network design				
Selection method: Automatic 	C Semi-Automatic	C Manual		
Criteria for automatic reuse selection				
First criterion Maximum (Flowrat	e*Efficiency)	-		
Second criterion Coupling degree		•		
Third criterion Minimum distance		•		
Procedure stop criteria				
Minimum threshold of flowrate / initial MWR (%) 10	00		
Maximum number of reuses	10)		
	1			
			Graphic	options
Optional constraints Help Def	ault parameters	< Return	Calculate	Cancel
		•		
	:к ()н сан	cinate		

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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



Three additional sheets were generated:

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

Initial number of possible reuse:18Cumulative percentage of water reuse:41,13Number of reuses:3Total water neuse (t/h):36,3Water flowrate available to reuse (t/h):0,0Additional required amount of fresh water(t/h):120,6Amount of waste water (t/h):120,6	NAV FOR THE WATER NETWORK	
Initial number of possible reuse:18Cumulative percentage of water reuse:41,13Number of reuses:3Total water reuse (t/h):36,3Water flowrate available to reuse (t/h):0,0Additional required amount of fresh water(t/h):120,6Amount of waste water (t/h):120,6		
Cumulative percentage of water reuse:41,13Number of reuses:3Total water reuse (t/h):36,3Water flowrate available to reuse (t/h):0,0Additional required amount of fresh water(t/h):120,6Amount of waste water (t/h):120,6	Init number of possible reuse:	18
Number of reuses:3Total water reuse (t/h):36,3Water flowrate available to reuse (t/h):0,0Additional required amount of fresh water(t/h):120,6Amount of waste water (t/h):120,6	Cumulative percentage of water reuse:	41,13
Total water reuse (t/h):36,3Water flowrate available to reuse (t/h):0,0Additional required amount of fresh water(t/h):120,6Amount of waste water (t/h):120,6	Number of reuses:	3
Water flowrate available to reuse (t/h):0,0Additional required amount of fresh water(t/h):120,6Amount of waste water (t/h):120,6	Total water veuse (t/h):	36,3
Additional required amount of fresh water(t/h): 120,6 Amount of waste water (t/h): 120.6	Water flowrate available to reuse (t/h):	0,0
Amount of waste water (t/h): 120.6	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 ources:	4
Remaining number of Sink: 2	Remaining number of Sing:	2

RESULTS FOR THE AUTOMATIC DESIGN OF THE WATER NETWORK

		Sink				
Name	Conteminant measurement (C1)	Contaminant measurement (C2)	Contaminant measurement (C3)	Target F (t/h)	Name	Contamina measurement
SK-O2	2,00E+0	3,00E+02	4,50E+01	34,0	SR-O1	1,50E+01
SK-O5	5,00E+01	4,00E+02	6,00E+01	8,0	SR-O4	2,00E+01
SK-O3	1,20E+02	2,00E+01	2,00E+02	56,9	SR-O1	1,50E+01
	Name SK-O2 SK-O5 SK-O3	Name Contaminant measurement (C1) SK-O2 2,00E+0 SK-O5 5,00E+01 SK-O3 1,20E+02	Sink Name Contininant measurement (C1) Contaminant measurement (C2) SK-02 2,00E+01 3,00E+02 SK-05 5,00E+01 4,00E+02 SK-03 1,20E+02 2,00E+01	Sink Name Contininant measurement (C1) Contaminant measurement (C2) Contaminant measurement (C3) SK-O2 2,00E+0 3,00E+02 4,50E+01 SK-O5 5,00E+01 4,00E+02 6,00E+01 SK-O3 1,20E+02 2,00E+01 2,00E+02	Sink Contaminant Contaminant Contaminant Contaminant Target F Name Contaminant Contaminant Contaminant Target F (t/h) SK-O2 2,00E+0 3,00E+02 4,50E+01 34,0 SK-O5 5,00E+01 4,00E+02 6,00E+01 8,0 SK-O3 1,20E+02 2,00E+01 2,00E+02 56,9	Sink Contininant Contaminant Contaminant Contaminant Target F Name Nsk-02 2,00E+01 3,00E+02 4,50E+01 34,0 SR-01 SK-05 5,00E+01 4,00E+02 6,00E+01 8,0 SR-04 SK-03 1,20E+02 2,00E+01 2,00E+02 56,9 SR-01

NO MORE REUSE IS POSSIBLE

LIST OF THE STREAMS STILL REMAINING AFTER THE WATER NETWORK DESIG

Stream	Mass flowrate (F)	Contaminant Contaminant		Contaminant
names	(t/h)	measurement (C1)	measurement (C2)	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		Contaminan	Conte	minant		
S	treams C1	Water Pinch results C1	Reuse #3	Reuse #2	Reuse #1	Water network	Water network results	Input data	Optional data

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 \approx 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).

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

RESULTS FOR THE AUTOMATIC DESIGN OF THE WATER NETWORK

ſ								INPUT DATA					
	Reuse	Sink				Source 1							
	Item	Name	Contaminant	Contaminant	Contaminant	Target F	Namo	Contaminant	Contaminant	Contaminant	Target F		
L		Name	measurement (C1)	measurement (C2)	measurement (C3)	(t/h)	Name	measurement (C1)	measurement (C2)	measurement (C3)	(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		

	INFORMATION ON WATER REUSE								
Source 1	Source 2	Total mass flowrate	Fresh water (t/h)	% of water reuse / MWR	Degree of coupling	Efficiency	Splitting ratio		Mass Elourato*
Mass flowrate (t/h)	Mass flowrate (t/h)	(t/h)					Source 1	Source 2	efficiency
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

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



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

	Water network design: Graph settings
	Display water network with Microsoft Excel®
Water network analysis	
Reuse characterization	Color for the network
Minimum mass flowrate for reuse (t/h) 0	
Minimum percentage of water reuse / MWR (%) 0	Flux display option Proportional
Maximum coupling degree 🚱 2	
Allow stream division 🕐 🗌 Sinks selection order 📀	Additional graphical results
Sources selection order 🔞	✓ Draw the reuses
✓ Water network design	Draw connections between the streams
Selection method: © Automatic © Semi-Automatic © Manual Criteria for automatic reuse selection	Show stream names
First criterion Maximum (Flowrate*Efficiency)	Display the reuse item numbers
Second criterion Coupling degree	
Third criterion Minimum distance	Add background picture
Procedure stop criteria	No picture selected
Minimum threshold of flowrate / initial MWR (%) 100	
Maximum number of reuses 10	Dimensions selection
Graphic options	
Optional constraints Help Default parameters < Return Calculate Cancel	Help Validate Cancel









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