Getting started with ProSec in ProSimPlus environment

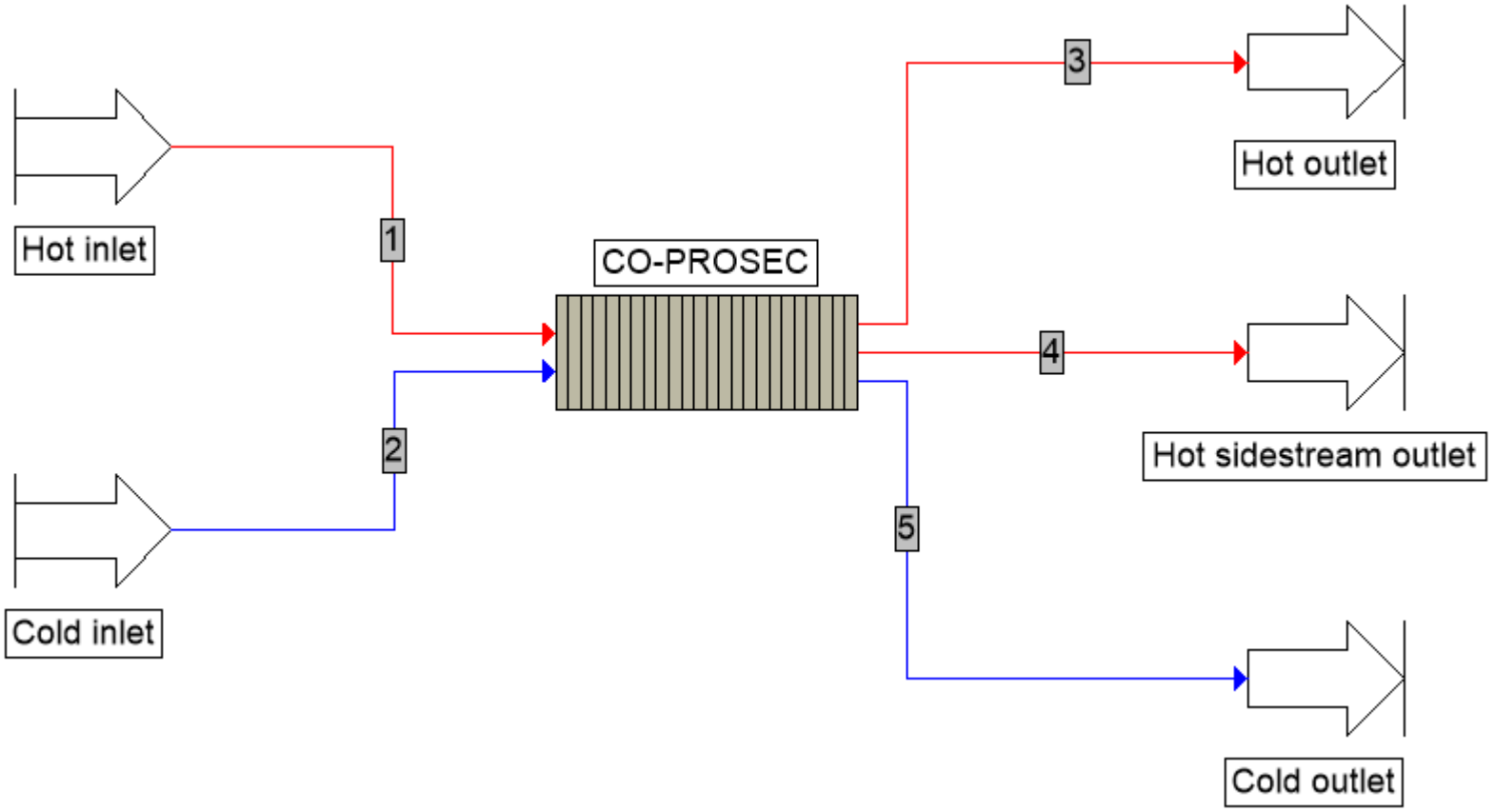
Use Case 3: Use of tabulated thermodynamic data provided by the user

Introduction

- This document shows how to provide tabulated thermodynamic data instead using the once automatically tabulated using the thermodynamic server of the host software.
- Tags will be used to display the results calculated by ProSec and those of the material stream of the host software.
- In this document, ProSec is used in ProSimPlus, Fives ProSim's steady state simulation software.
- This step-by-step guide assumes that the concepts described in the step-by-step guides of ProSec in ProSimPlus environment "Main features overview" and "Import/export parameters/results, use case study capability, define a specification" have been acquired.

Starting point

- Simulation obtained at the end of the step-by-step “Main features overview” of ProSec in ProSimPlus environment



Step 1
Generation of the tabulated thermodynamic data

- Data tabulated by the user for the enthalpy curves and the physico-chemical properties
  - In this case, the thermodynamic calculation server of the host software will not be used in ProSec calculations.

The way of description of the user tabulated data should be coherent with:

  - The type of the inlet fluid (mixture or pure compound)
  - The physical state of the fluid during the heat exchange (single-phase liquid, single-phase vapor or two-phase vapor-liquid)

  - Up to 160 tabulated points

  - The format of the data depends on:
    - The fluid type (mixture or pure compound)
    - The physical state of the fluid (single-phase liquid, single-phase vapor or two-phase vapor-liquid)
    - Whether or not to take pressure into account on enthalpy curves

Step 1
Generation of the tabulated thermodynamic data

- Pressure effect not taken into account on the enthalpy curves
  - Data needed

	Single phase		Two phases	
Property	**Liquid**	**Vapor**	**Mixture**	**Pure fluid**
Temperature	✓	✓	✓	✓
Mass enthalpy	✓	✓	✓	✓
Mass vaporization ratio	✗	✗	✓	✓
Liquid density	✓	✗	✓	✓
Liquid mass specific heat	✓	✗	✓	✓
Liquid dynamic viscosity	✓	✗	✓	✓
Liquid thermal conductivity	✓	✗	✓	✓
Vapor density	✗	✓	✓	✓
Vapor mass specific heat	✗	✓	✓	✓
Vapor dynamic viscosity	✗	✓	✓	✓
Vapor thermal conductivity	✗	✓	✓	✓

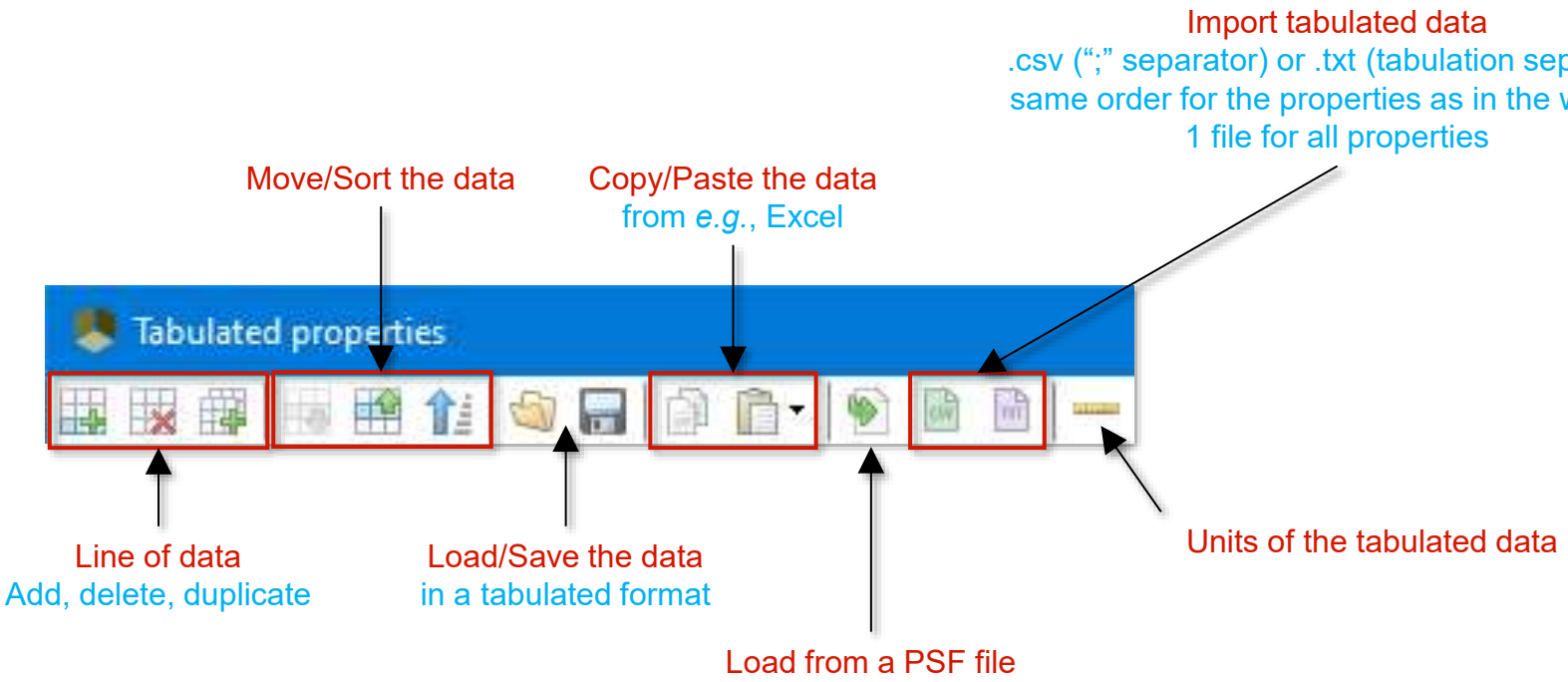
Definitions:

- Single-phase fluid is a fluid without phase change
- Pure fluid is a fluid with phase change containing only one compound,

  i.e. $T_{bubble} = T_{dew}$

Step 1
Generation of the tabulated thermodynamic data

- Pressure effect not taken into account on the enthalpy curves
  - Toolbar



  - Order of the columns (window or imported file)

Enthalpic curve			Vapor phase				Liquid phase			
Temperature (K)	Mass vaporization ratio	Enthalpy (kcal/kg)	Density (kg/m3)	Specific heat (J/kg/K)	Viscosity (cP)	Thermal conductivity (kcal/m/h/K)	Density (kg/m3)	Specific heat (J/kg/K)	Viscosity (cP)	Thermal conductivity (kcal/m/h/K)

Step 1
Generation of the tabulated thermodynamic data

- Pressure effect not taken into account on the enthalpy curves
  - Single vapor phase example

Tabulated properties

	Enthalpic curve			Vapor phase				Liquid phase			
	Temperature (K)	Mass vaporization ratio	Enthalpy (kcal/kg)	Density (kg/m3)	Specific heat (kcal/kg/K)	Viscosity (cP)	Thermal conductivity (kcal/m/h/K)	Density (kg/m3)	Specific heat (kcal/kg/K)	Viscosity (cP)	Thermal conductivity (kcal/m/h/K)
1	97,55	1	0	719,5295	1,67	0,0048	0,0057				
2	111,75	1	8,076	651,8975	1,419	0,0054	0,0077				
3	125,9	1	18,45	566,5927	1,298	0,0074	0,0096				
4	133,05	1	26,606	444,3427	1,05	0,0095	0,0114				
5	140,15	1	36,065	252,7588	0,8065	0,011	0,0144				
6	147,25	1	41,515	174,8096	0,622	0,0122	0,0156				
7	154,35	1	45,414	143,4968	0,451	0,0137	0,0175				

Restore Ok Cancel

  - Single liquid phase example

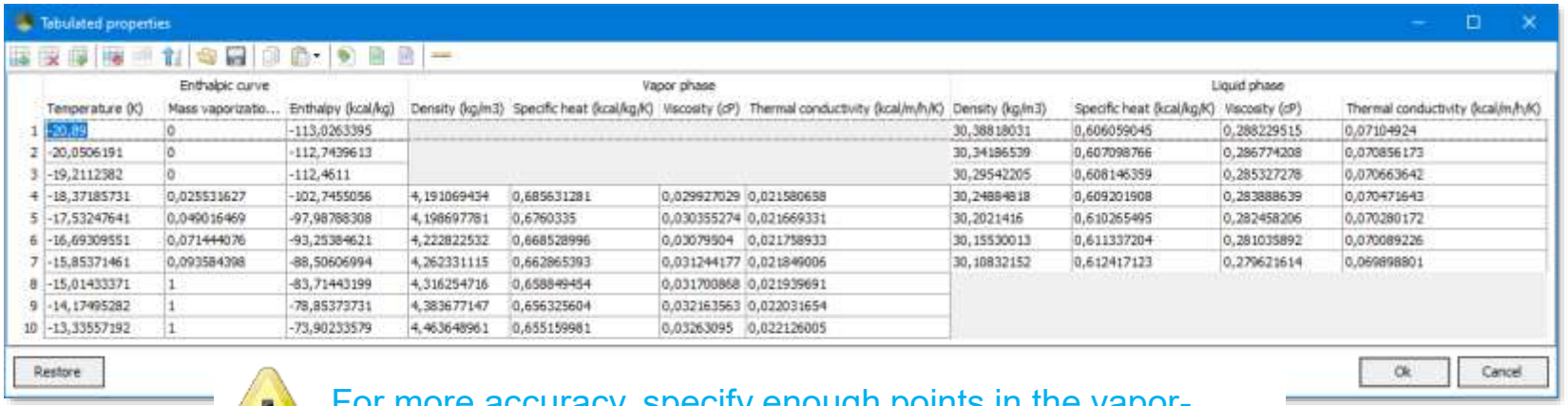
Tabulated properties

	Enthalpic curve			Vapor phase				Liquid phase			
	Temperature (°C)	Mass vaporizatio...	Enthalpy (kcal/kg)	Density (kg/m3)	Specific heat (kcal/kg/K)	Viscosity (cP)	Thermal conductivity (kcal/m/h/K)	Density (kg/m3)	Specific heat (kcal/kg/K)	Viscosity (cP)	Thermal conductivity (kcal/m/h/K)
1	-118,5	0	0					562,04	0,658	0,182	0,187
2	-106,7	0	0					551,28	0,649	0,159	0,178
3	-97,9	0	0					544,42	0,64	0,146	0,17
4	-91,8	0	0					539,3	0,634	0,137	0,165
5	-87,8	0	0					535,74	0,631	0,132	0,162
6	-85,2	0	0					533,24	0,629	0,129	0,159
7	-83,3	0	0					531,4	0,628	0,127	0,157

Restore Ok Cancel

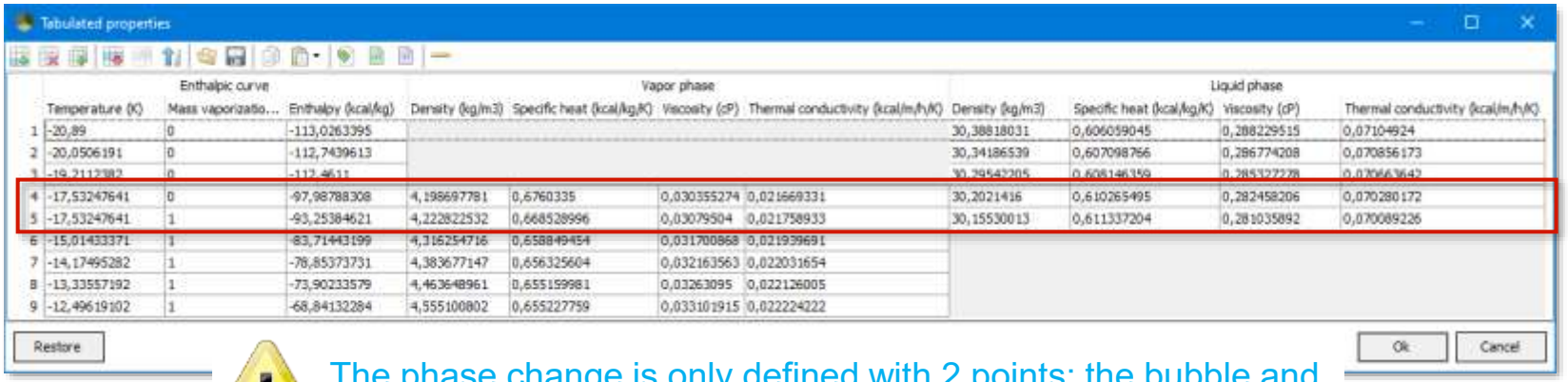
Step 1
Generation of the tabulated thermodynamic data

- Pressure effect not taken into account on the enthalpy curves
  - Two-phase vapor-liquid mixture example



For more accuracy, specify enough points in the vapor-liquid zone

  - Pure fluid with phase change example



The phase change is only defined with 2 points: the bubble and the dew points should be present

Step 1
Generation of the tabulated thermodynamic data

- Pressure effect taken into account on the enthalpy curves
  - Data needed
    - ✓ Two enthalpy curves (temperature, mass enthalpy, mass vaporization ratio) at two different pressures
    - ✓ One table at one pressure for the vapor physico-chemical properties
    - ✓ One table at one pressure for the liquid physico-chemical properties

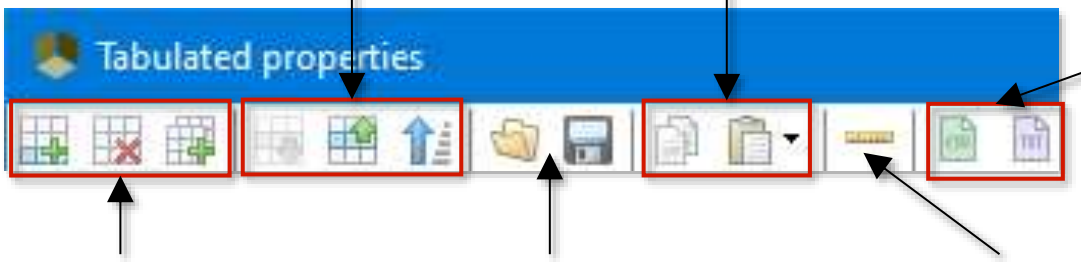
Same temperature tabulation for the two enthalpy curves

Warning messages appear in “Historic” report if there are extrapolations out of the pressure and/or temperature tabulated range

Import tabulated data
.csv (“;” separator) or .txt (tabulation separator)
same order for the properties as in the window
1 file for the 2 enthalpy curves
1 file for the liquid physico-chemical properties
1 file for the vapor physico-chemical properties

Move/Sort the data

Copy/Paste the data
from *e.g.*, Excel



Line of data
Add, delete, duplicate

Load/Save the data
in a tabulated format

Units of the tabulated data

Step 1
Generation of the tabulated thermodynamic data

- Pressure effect taken into account on the enthalpy curves
  - Two phases liquid-vapor mixture example

Enthalpy curves

Pressures of the two curves

Enthalpic curves | Vapor phase | Liquid phase

P1 31 psi P2 30 psi

		P1		P2	
	Temperature (°F)	Mass vaporizatio...	Enthalpy (cal/g)	Mass vaporizatio...	Enthalpy (cal/g)
11	-16,15375308	0	-118,244503	0	-118,2456592
12	-15,68012839	0	-118,1027211	0	-118,1038722
13	-15,2065037	0	-117,9608148	0	-117,9619608
14	-14,73287901	0	-117,8187836	0	-117,8199245
15	-14,25925432	0	-117,6766272	0	-117,677763
16	-13,78562963	0	-117,5343452	0	-117,5354757
17	-13,49135075	0	-117,4458771	0	-117,4470044
18	-13,31200494	0	-117,391937	0,020841286	-115,3648011
19	-12,83838024	0	-117,2494023	0,094654414	-108,0458567
20	-12,36475555	0	-117,1067406	0,210142252	-96,68832312
21	-11,89113086	0	-116,9639514	0,381945144	-79,88054811
22	-11,27109132	0,089682451	-108,0758328	0,638850501	-54,81519543
23	-10,65105178	0,249347004	-92,42216277	0,832225054	-35,95969671
24	-10,03101224	0,496319882	-68,34720592	0,958157273	-23,67202771
25	-9,4109727	0,732945083	-45,32496932	1	-19,51752041
26	-8,79093316	0,894131542	-29,64136734	1	-19,39458079
27	-8,17089362	1	-19,32987784	1	-19,27153634
28	-1,319793956	1	-17,96177384	1	-17,90490418
29	5,531305708	1	-16,58054482	1	-16,52508041
30	12,38240537	1	-15,18585162	1	-15,13173061
31	19,23350504	1	-13,77738115	1	-13,72454597
32	26,0846047	1	-12,35484538	1	-12,30324233
33	32,93570437	1	-10,91798025	1	-10,86755912
34	39,78680403	1	-9,466544639	1	-9,41725844
35	46,63790369	1	-8,000319419	1	-7,952124057

Vapor phase properties

Enthalpic curves | Vapor phase | Liquid phase

	Temperature (°F)	Density (lb/ft3)	Specific heat (cal/g/K)	Viscosity (lb/ft/h)	Thermal conductivity (Btu/ft/h/F)
1	-11,73113036	0,297904363	0,356530118	0,016674929	0,008263497
2	-11,17109132	0,298855359	0,35664208	0,016664042	0,008261534
3	-10,55105178	0,299683754	0,356780571	0,016656702	0,008261517
4	-9,931012241	0,300228797	0,356974475	0,016657624	0,008265785
5	-9,3109727	0,30047886	0,357225556	0,016667153	0,008274467
6	-8,69093316	0,300589321	0,35750564	0,016680716	0,008285262
7	-8,07089362	0,30056084	0,35780032	0,016697048	0,008297966
8	-1,219793956	0,295325409	0,361203169	0,016954609	0,008503583

Liquid phase properties

Enthalpic curves | Vapor phase | Liquid phase

	Temperature (°F)	Density (lb/ft3)	Specific heat (cal/g/K)	Viscosity (lb/ft/h)	Thermal conductivity (Btu/ft/h/F)
1	-20,33	34,94651041	0,533971235	0,412323787	0,073138864
2	-20,41637531	34,92588954	0,534427338	0,41112319	0,073039515
3	-19,94275062	34,90525913	0,534884999	0,409927092	0,072940318
4	-19,46912593	34,88461907	0,535344225	0,408735465	0,072841273
5	-18,99550123	34,86396925	0,535805022	0,407548283	0,07274238
6	-18,52187654	34,84330957	0,536267394	0,406365519	0,072643639
7	-18,04825185	34,82263992	0,536731349	0,405187146	0,072545049
8	-17,57462716	34,80196018	0,537196892	0,404013138	0,072446609
9	-17,10100247	34,78127025	0,537664029	0,402843469	0,072348321
10	-16,62737778	34,76057002	0,538132766	0,401678113	0,072250182

Step 1
Generation of the tabulated thermodynamic data

- Pressure effect taken into account on the enthalpy curves
  - Pure fluid with phase change example

Enthalpy curves

Enthalpic curves | Vapor phase | Liquid phase

P1 2.14 bar P2 2 bar

	Temperature (K)	Mass vaporizatio... (P1)	Enthalpy (J/kg) (P1)	Mass vaporizatio... (P2)	Enthalpy (J/kg) (P2)
1	246,15	0	-118,544	0	-118,546
2	247,714	0	-117,699	0	-117,701
3	247,714	0	-117,699	1	-20,3149
4	249,15	0	-116,919	1	-19,8055
5	249,495	0	-116,732	1	-19,6829
6	249,495	1	-19,7998	1	-19,6829
7	252,15	1	-18,8502	1	-18,7355
8	255,15	1	-17,7698	1	-17,6573
9	258,15	1	-16,6812	1	-16,5709

The bubble and the dew points should be duplicate

Bubble and dew points at the second pressure (P2)

Bubble and dew points at the second pressure (P1)

Vapor phase properties

Enthalpic curves | Vapor phase | Liquid phase

	Temperature (°F)	Density (lb/ft3)	Specific heat (cal/g/K)	Viscosity (lb/ft/h)	Thermal conductivity (Btu/ft/h/F)
1	-11,73115356	0,297904363	0,356530118	0,016674929	0,008263497
2	-11,17109132	0,298855359	0,35664208	0,016664042	0,008261534
3	-10,55105178	0,299683754	0,356780571	0,016656702	0,008261517
4	-9,931012241	0,300228797	0,356974475	0,016657624	0,008265785
5	-9,3109727	0,30047886	0,357225556	0,016667153	0,008274467
6	-8,69093316	0,300589321	0,35750564	0,016680716	0,008285262
7	-8,07089362	0,30056084	0,35780032	0,016697048	0,008297966
8	-1,219793956	0,295325409	0,361203169	0,016954609	0,008503583

Liquid phase properties

Enthalpic curves | Vapor phase | Liquid phase

	Temperature (°F)	Density (lb/ft3)	Specific heat (cal/g/K)	Viscosity (lb/ft/h)	Thermal conductivity (Btu/ft/h/F)
1	-20,33	34,94651041	0,533971235	0,412323787	0,073138864
2	-20,41637531	34,92588954	0,534427338	0,41112319	0,073039515
3	-19,94275062	34,90525913	0,534884999	0,409927092	0,072940318
4	-19,46912593	34,88461907	0,535344225	0,408735465	0,072841273
5	-18,99550123	34,86396925	0,535805022	0,407548283	0,07274238
6	-18,52187654	34,84330957	0,536267394	0,406365519	0,072643639
7	-18,04825185	34,82263992	0,536731349	0,405187146	0,072545049
8	-17,57462716	34,80196018	0,537196892	0,404013138	0,072446609
9	-17,10100247	34,78127025	0,537664029	0,402843469	0,072348321
10	-16,62737778	34,76057002	0,538132766	0,401678113	0,072250182

Step 1
Generation of the tabulated thermodynamic data

- Generate tabulated thermodynamic data in a tool external to ProSec
- For example, by using Simulis® Thermodynamics in Microsoft® Excel (see the step-by-step guide “Getting started with Simulis® Thermodynamics. Use case 1: Main features overview”)

Simulis Calculator SC1

Name	Calc!SC1

	Unit	
Quantity	Data	Results
Temperature	K	K
Pressure	bar	bar
Mass enthalpy	J/kg	J/kg
Density	kg/m3	kg/m3
Mass entropy	J/kg/K	J/kg/K
Dynamic viscosity	Pa.s	Pa.s
Thermal conductivity	W/m/K	W/m/K

	Scale	
Data	1	wt./wt.
Results	1	wt./wt.

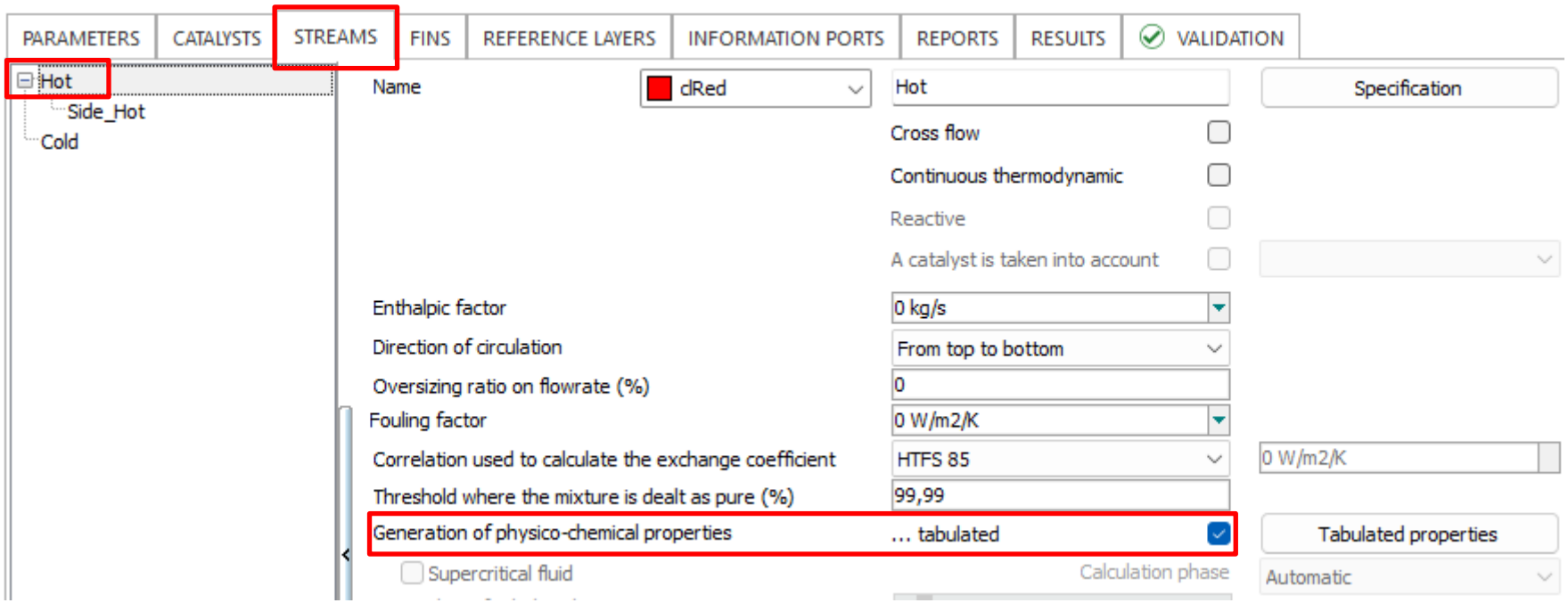
		z
Index	Compound	wt./wt.
1	METHANE	0,5
2	ETHANE	0,5

P	69,4	bar

			Vapor phase			
T	Vap. ratio	H	ρ	Cp	μ	λ
K	wt./wt.	J/kg	kg/m3	J/kg/K	Pa.s	W/m/K
262	1	-242592,420246	125,233756	5108,256591	1,425222E-05	0,041303
264	1	-232729,077692	120,205386	4766,948477	1,404855E-05	0,040822
266	1	-223482,982719	115,788987	4488,259795	1,388795E-05	0,040446
268	1	-214743,942691	111,866380	4257,836894	1,376014E-05	0,040152
270	1	-206426,643980	108,348360	4064,991132	1,365790E-05	0,039922
272	1	-198464,271619	105,166568	3901,770752	1,357599E-05	0,039746
274	1	-190803,816148	102,267793	3762,215064	1,351056E-05	0,039614
276	1	-183402,670196	99,609994	3641,805693	1,345870E-05	0,039518
278	1	-176226,158097	97,159489	3537,074675	1,341956E-05	0,039479
280	1	-169245,728898	94,888945	3445,326489	1,338999E-05	0,039467
282	1	-162437,620371	92,775917	3364,440228	1,336857E-05	0,039478
284	1	-155781,859462	90,801782	3292,727637	1,335417E-05	0,039508
286	1	-149261,505345	88,950935	3228,830160	1,334584E-05	0,039556
288	1	-142862,069365	87,210183	3171,643419	1,334282E-05	0,039619
290	1	-136571,065448	85,568282	3120,261173	1,334446E-05	0,039696
292	1	-130377,657864	84,015581	3073,933250	1,335023E-05	0,039786
294	1	-124272,382452	82,543736	3032,033620	1,335966E-05	0,039887
296	1	-118246,923885	81,145491	2994,035910	1,337238E-05	0,039998
298	1	-112293,936109	79,814498	2959,494437	1,338803E-05	0,040120
300	1	-106406,896394	78,545174	2928,029375	1,340634E-05	0,040250
302	1	-100579,985769	77,332587	2899,315060	1,342706E-05	0,040388
304	1	-94807,990361	76,172355	2873,070675	1,344994E-05	0,040534

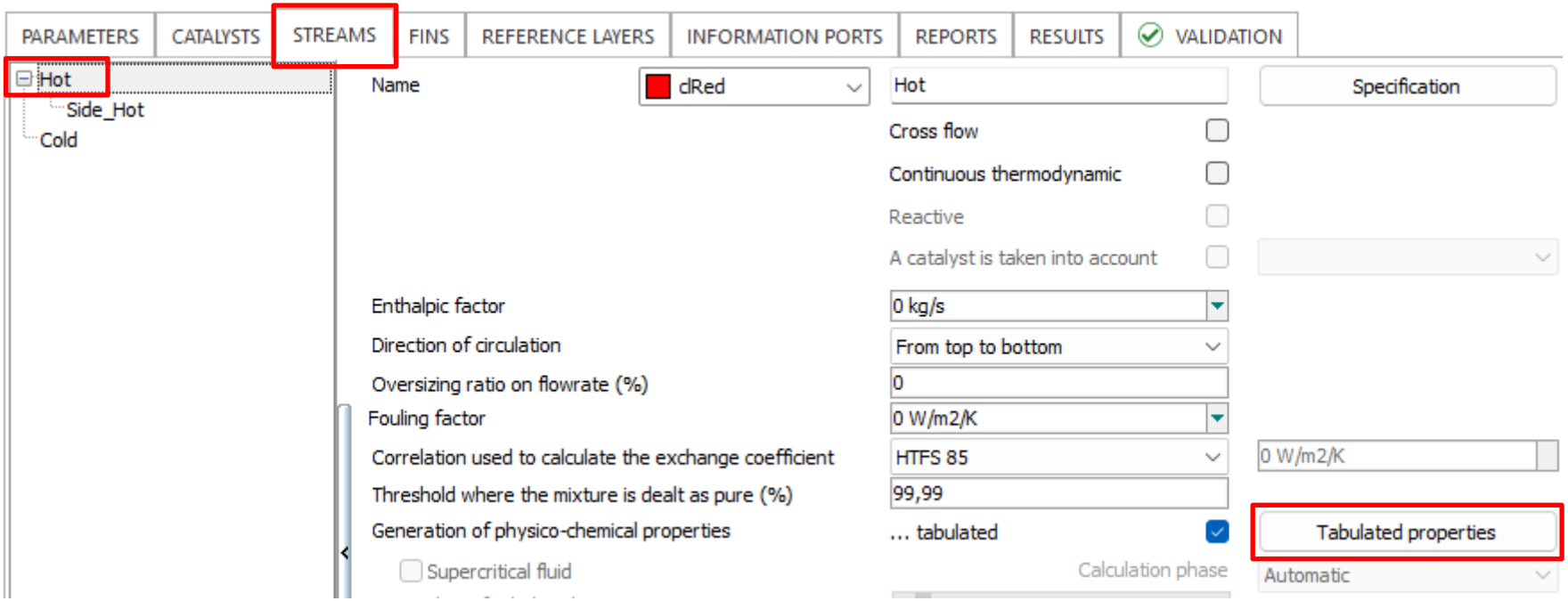
Step 2
Supply of tabulated data

- Open (edit) ProSec unit operation
- Go to “Streams” tab
- Select the stream “Hot”
  1. Activate the option “Generation of physico-chemical properties … tabulated”



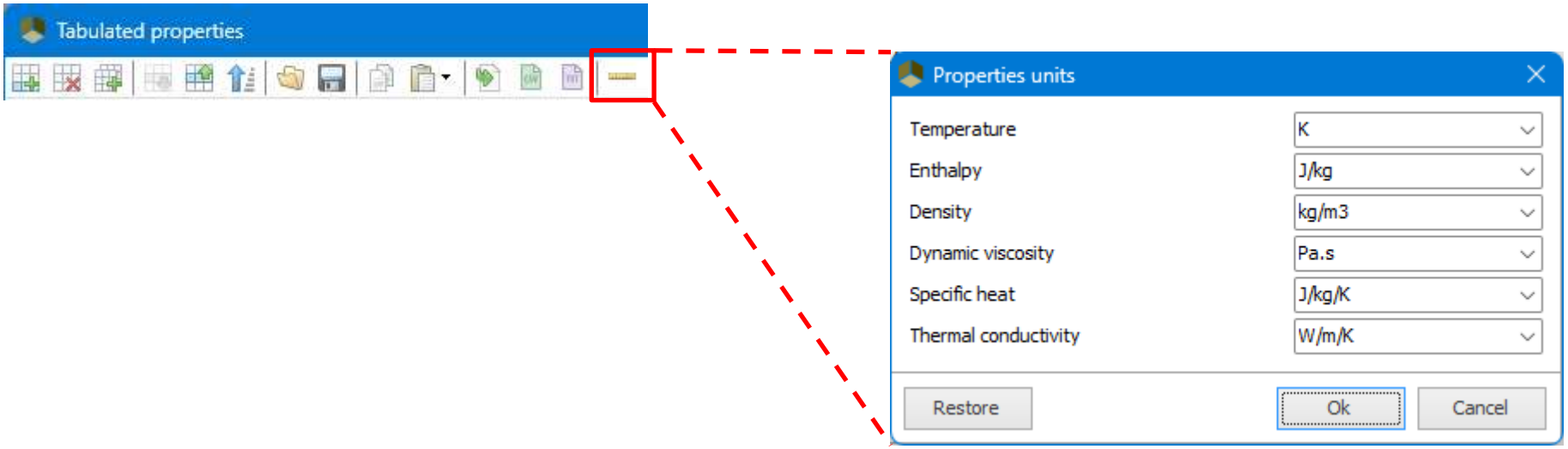
Step 2
Supply of tabulated data

- Select the stream “Hot”
  2. Click on the button “Tabulated properties”



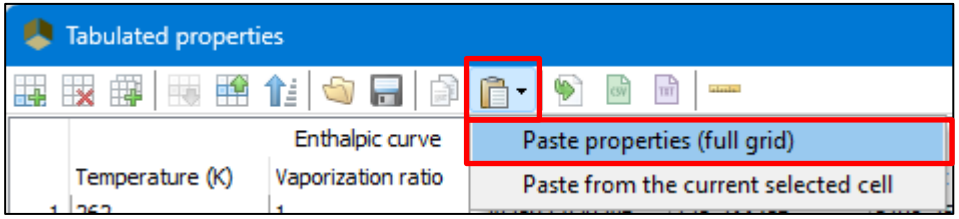
Step 2
Supply of tabulated data

- Select the stream “Hot”
  3. Click on the icon “Edit units”
  4. Select the units chosen during the generation of the tabulated thermodynamic data (step 1), for this example:
     - Temperature K
     - Enthalpy J/kg
     - Sensity kg/m3
     - Dynamic viscosity Pa.s
     - Specific heat J/kg/K
     - Thermal conductivity W/m/K



Step 2
Supply of tabulated data

- Select the stream “Hot”
  5. Enter or copy the tabulated data. For example, once copied from Microsoft® Excel (ctrl + C), the icon “paste properties (full grid)” allows to copy them directly in the window “Tabulated properties”



Tabulated properties

	Enthalpic curve			Vapor phase				Liquid phase			
	Temperature (K)	Vaporization ratio	Enthalpy (J/kg)	Density (kg/m3)	Specific heat (J/k...	Viscosity (Pa.s)	Thermal conducti...	Density (kg/m3)	Specific heat (J/k...	Viscosity (Pa.s)	Therm
1	262	1	-242592,420246	125,233756	5108,256591	1,425222E-5	0,041303				
2	264	1	-232729,077692	120,205386	4766,948477	1,404855E-5	0,040822				
3	266	1	-223482,982719	115,788987	4488,259795	1,388795E-5	0,040446				
4	268	1	-214743,942691	111,86638	4257,836894	1,376014E-5	0,040152				
5	270	1	-206426,64398	108,34836	4064,991132	1,36579E-5	0,039922				
6	272	1	-198464,271619	105,166568	3901,770752	1,357599E-5	0,039746				
7	274	1	-190803,816148	102,267793	3762,215064	1,351056E-5	0,039614				
8	276	1	-183402,670196	99,609994	3641,805693	1,34587E-5	0,039518				
9	278	1	-176226,158097	97,159489	3537,074675	1,341956E-5	0,039479				
10	280	1	-169245,728898	94,888945	3445,326489	1,338999E-5	0,039467				
11	282	1	-162437,620371	92,775917	3364,440228	1,336857E-5	0,039478				
12	284	1	-155781,859462	90,801782	3292,727637	1,335417E-5	0,039508				
13	286	1	-149261,505345	88,950935	3228,83016	1,334584E-5	0,039556				
14	288	1	-142862,069365	87,210183	3171,643419	1,334282E-5	0,039619				
15	290	1	-136571,065448	85,568282	3120,261173	1,334446E-5	0,039696				
16	292	1	-130377,657864	84,015581	3073,93325	1,335023E-5	0,039786				
17	294	1	-124272,382452	82,543736	3032,03362	1,335966E-5	0,039887				
18	296	1	-118246,923885	81,145491	2994,03591	1,337238E-5	0,039998				
19	298	1	-112293,936109	79,814498	2959,494437	1,338803E-5	0,04012				
20	300	1	-106406,896394	78,545174	2928,029375	1,340634E-5	0,04025				
21	302	1	-100579,985769	77,332587	2899,31506	1,342706E-5	0,040388				
22	304	1	-94807,990361	76,172355	2873,070675	1,344994E-5	0,040534				

Step 2
Supply of tabulated data

- Select the stream “Hot”
  6. Validate all windows
  7. Follow the same procedure for the stream “Cold”
  8. Save the file before running the simulation

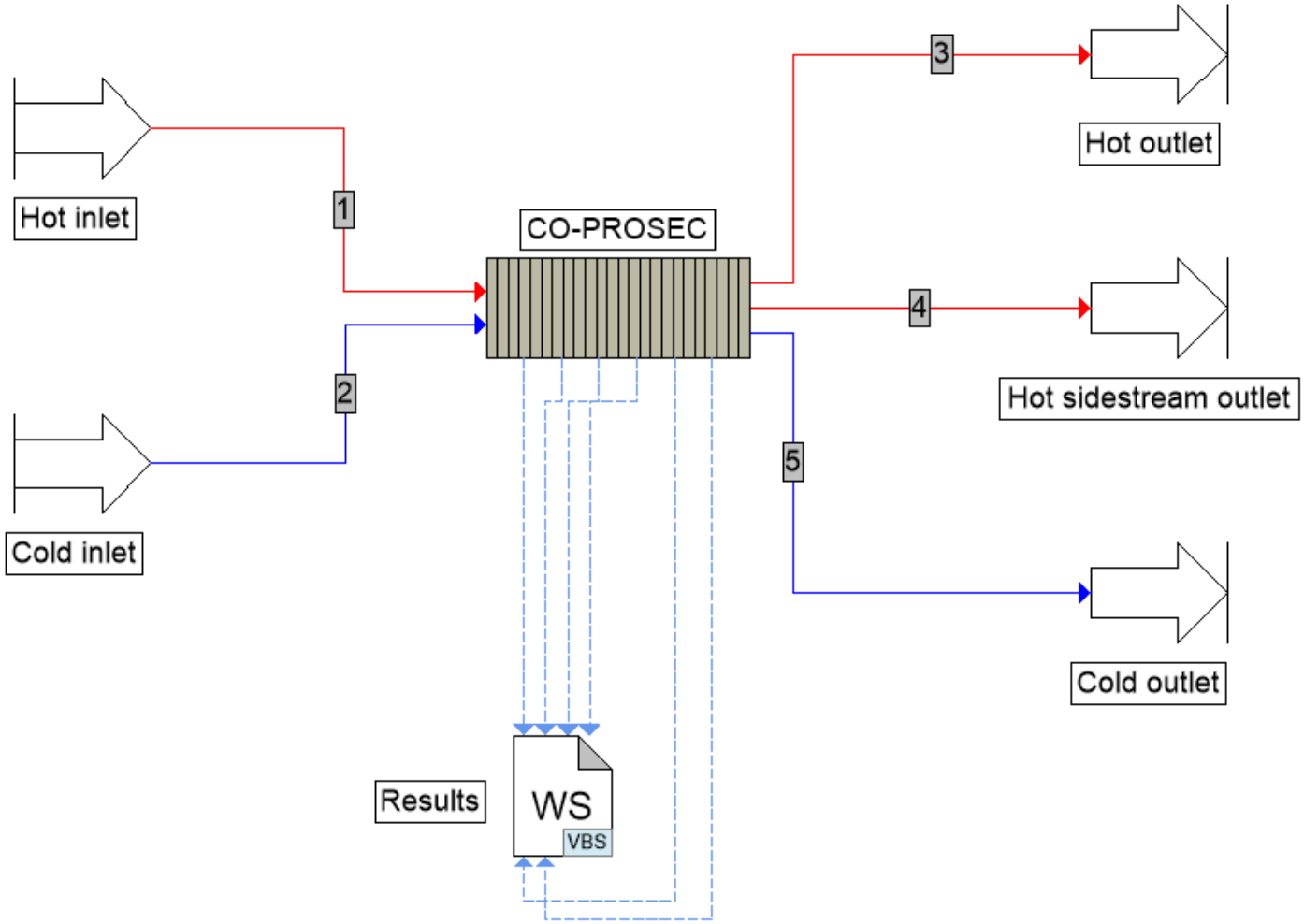
Step 3
Export of ProSec results

- Add outlet information ports to store the temperatures and vaporization rates of the outlets (hot fluid, side-stream of the hot fluid, and cold fluid) in a Windows Script module to display them via tags.

- The step-by-step guide of ProSec in the ProSimPlus environment “Import/export parameters/results, use case study capability, define a specification” describes how to export results.

Step 3
Export of ProSec results

- Simulation flowsheet at the end of the step 3



Step 4
Display results with tags

- Tags are used to display information of the simulation directly on the simulation flowsheet (for example: input data and/or results of unit operations and streams).

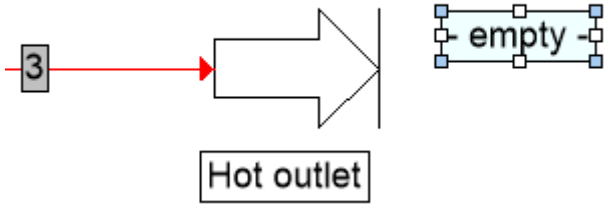
- For this example, the objective is to display the following results:
  - Outlet temperatures and vaporization ratios calculated by ProSec
  - Temperatures and vaporization ratios displayed in ProSimPlus streams

Step 4
Display results with tags

- The results calculated by ProSec to be displayed are stored in the Windows Script module.

1. Click on the icon “Add a tag”

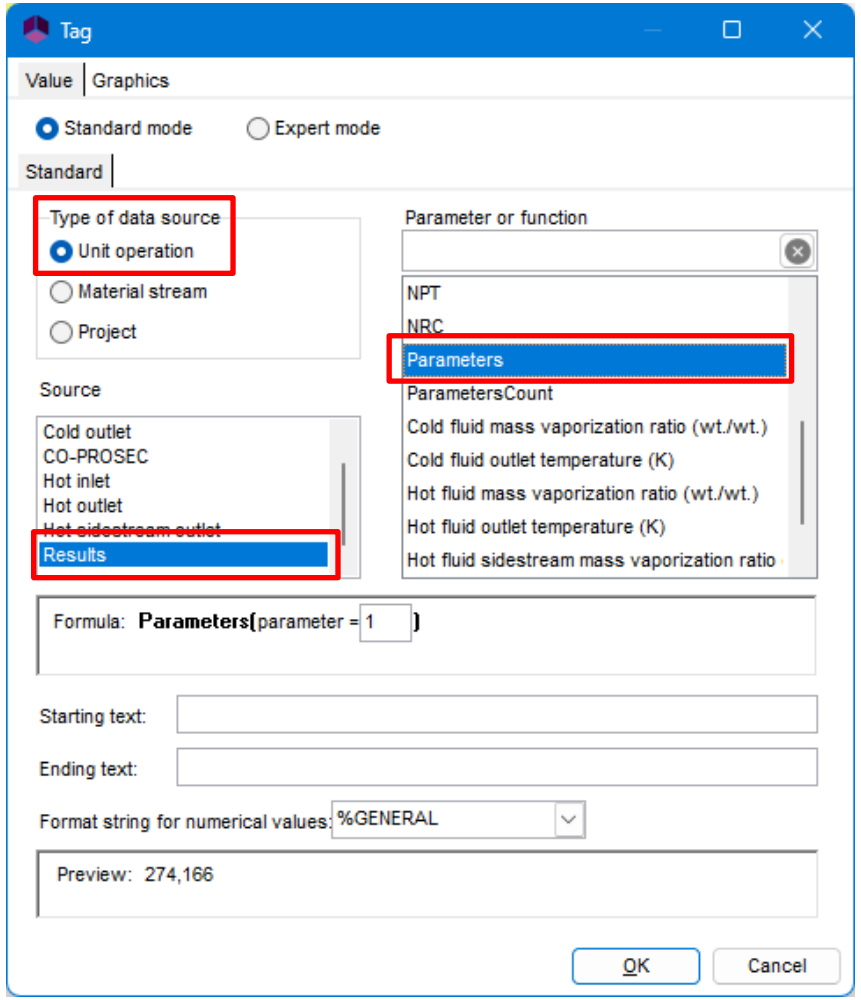
2. Click on the simulation flowsheet to place the tag



Step 4
Display results with tags

- The results calculated by ProSec to be displayed are stored in the Windows Script module.

3. Double-click on the tag
   a) Select “Unit operation” as type of data source
   b) Select the Windows Script module in the “Source” list, here “Results”
   c) Select “Parameters” in the “Parameter or function” list

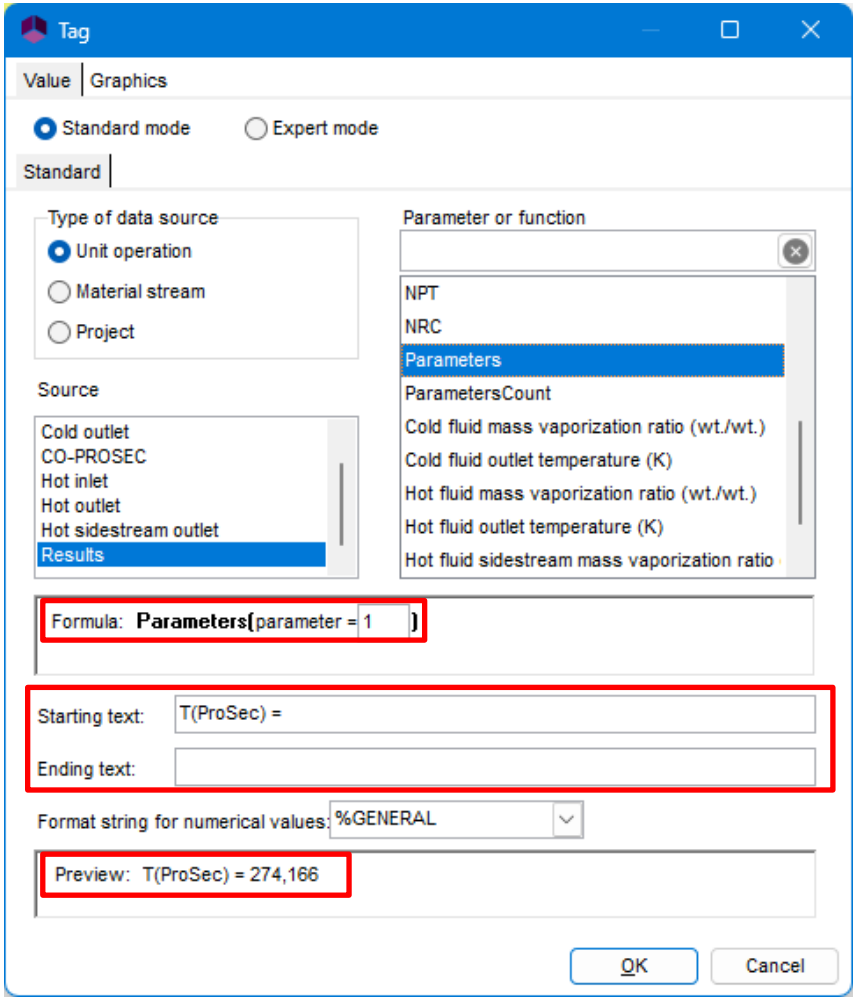


Step 4
Display results with tags

- The results calculated by ProSec to be displayed are stored in the Windows Script module.

3. Double-click on the tag
   d) Select the number of the parameter to display. It's the position of the parameter in the "PAR" zone of the Windows Script module.
   e) It's possible to add a text before and/or after the value to display.
   f) A preview is available.

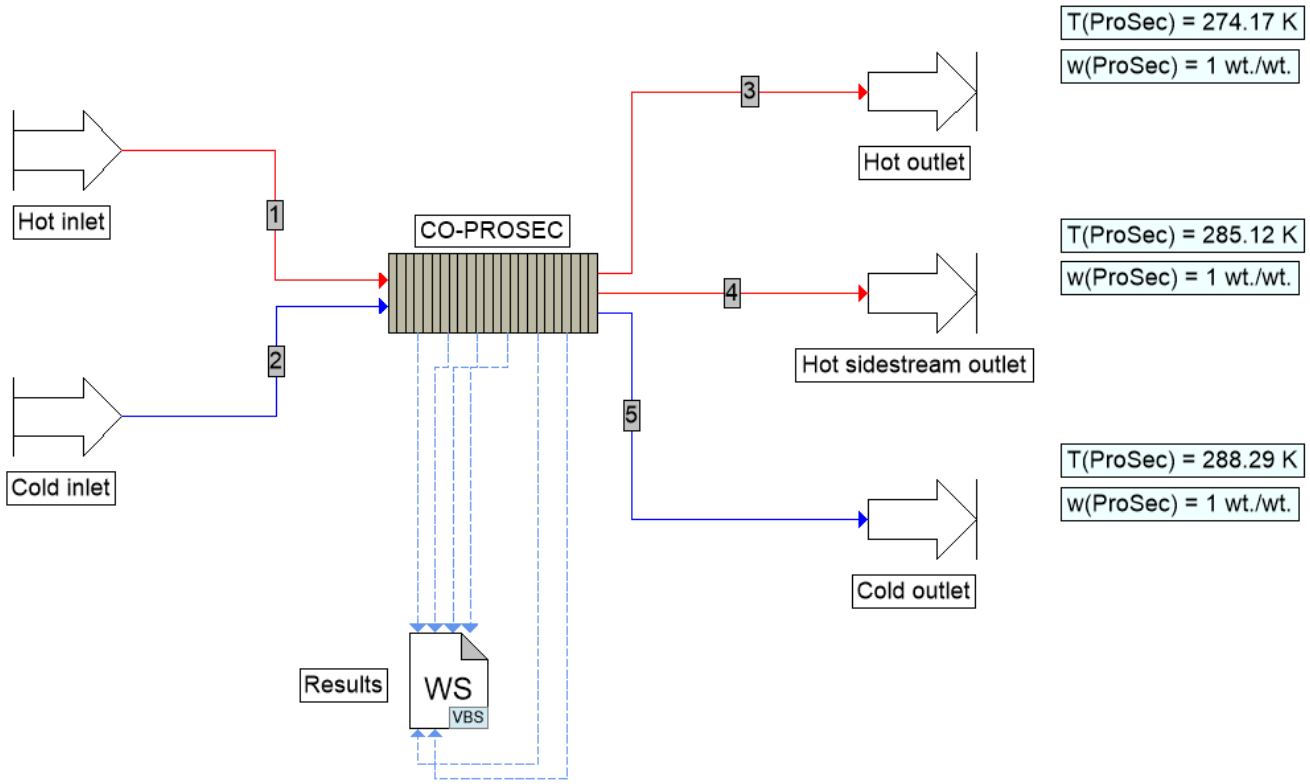
4. Click on "OK" to validate the specified parameters.



Step 4
Display results with tags

- The results calculated by ProSec to be displayed are stored in the Windows Script module.
  5. Repeat the previous procedure to display the other results calculated by ProSec.

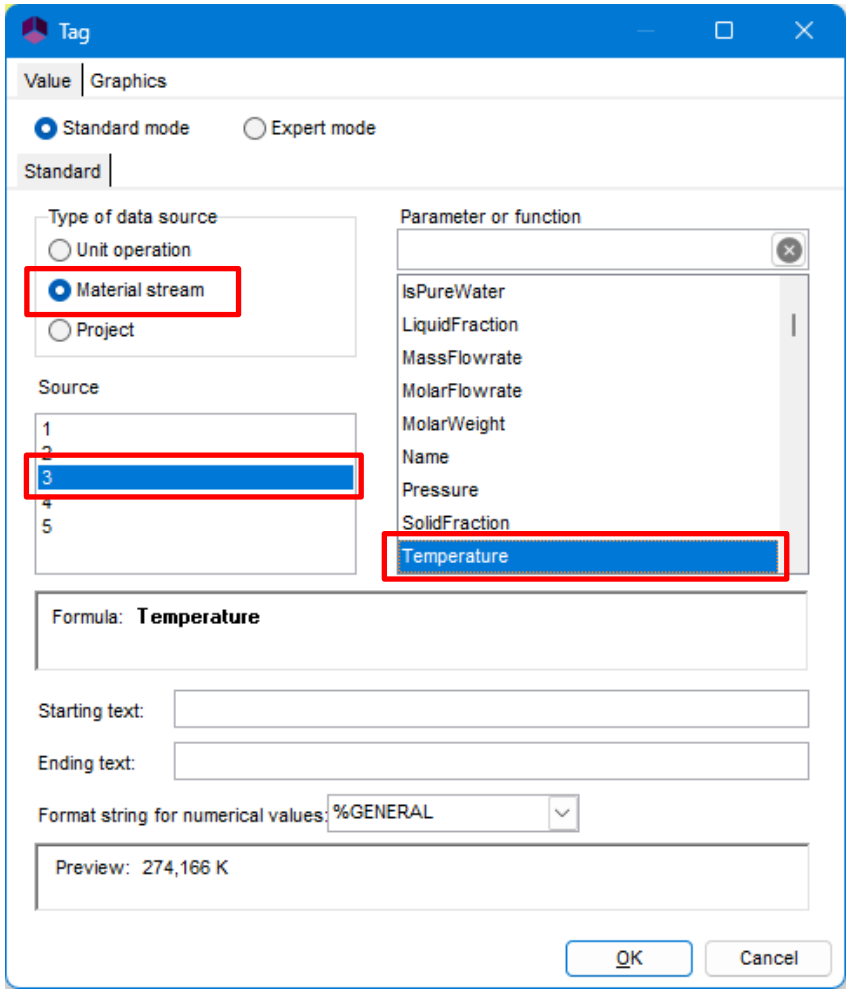
- Simulation flowsheet at this point



Step 4
Display results with tags

- Display the results of ProSimPlus streams

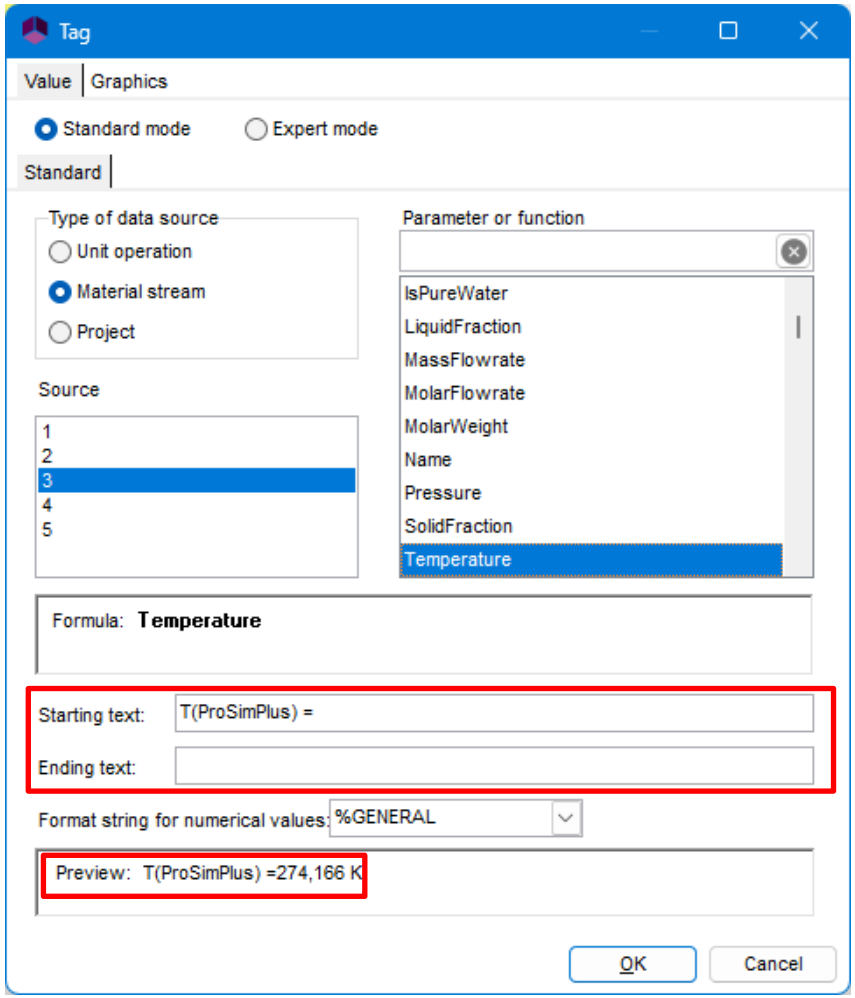
1. Add a new tag
2. Place the tag on the flowsheet
3. Double-click on the tag
   a) Select “Material stream” as type of data source
   b) Select one of the stream of interest. Here the stream “3”, stream of the hot outlet
   c) Select “Temperature” in the “Parameter or function” list



Step 4
Display results with tags

- Display the results of ProSimPlus streams

3. Double-click on the tag
   d) It's possible to add a text before and/or after the value to display.
   e) A preview is available.

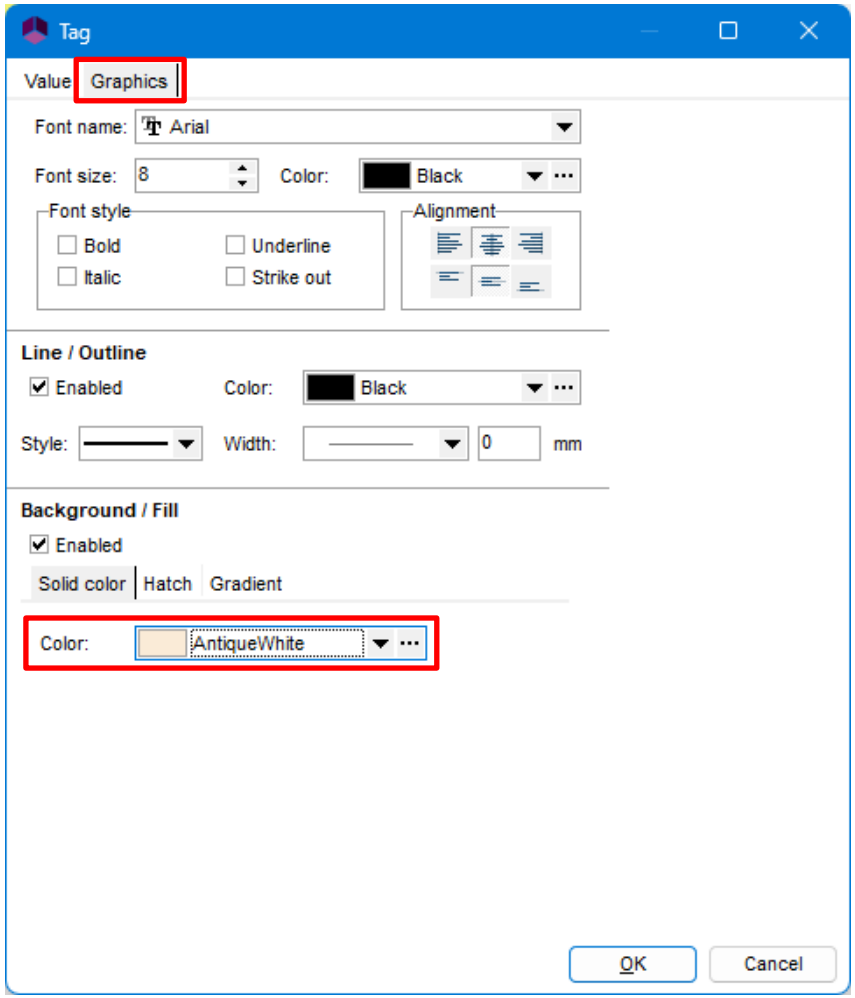


Step 4
Display results with tags

- Display the results of ProSimPlus streams

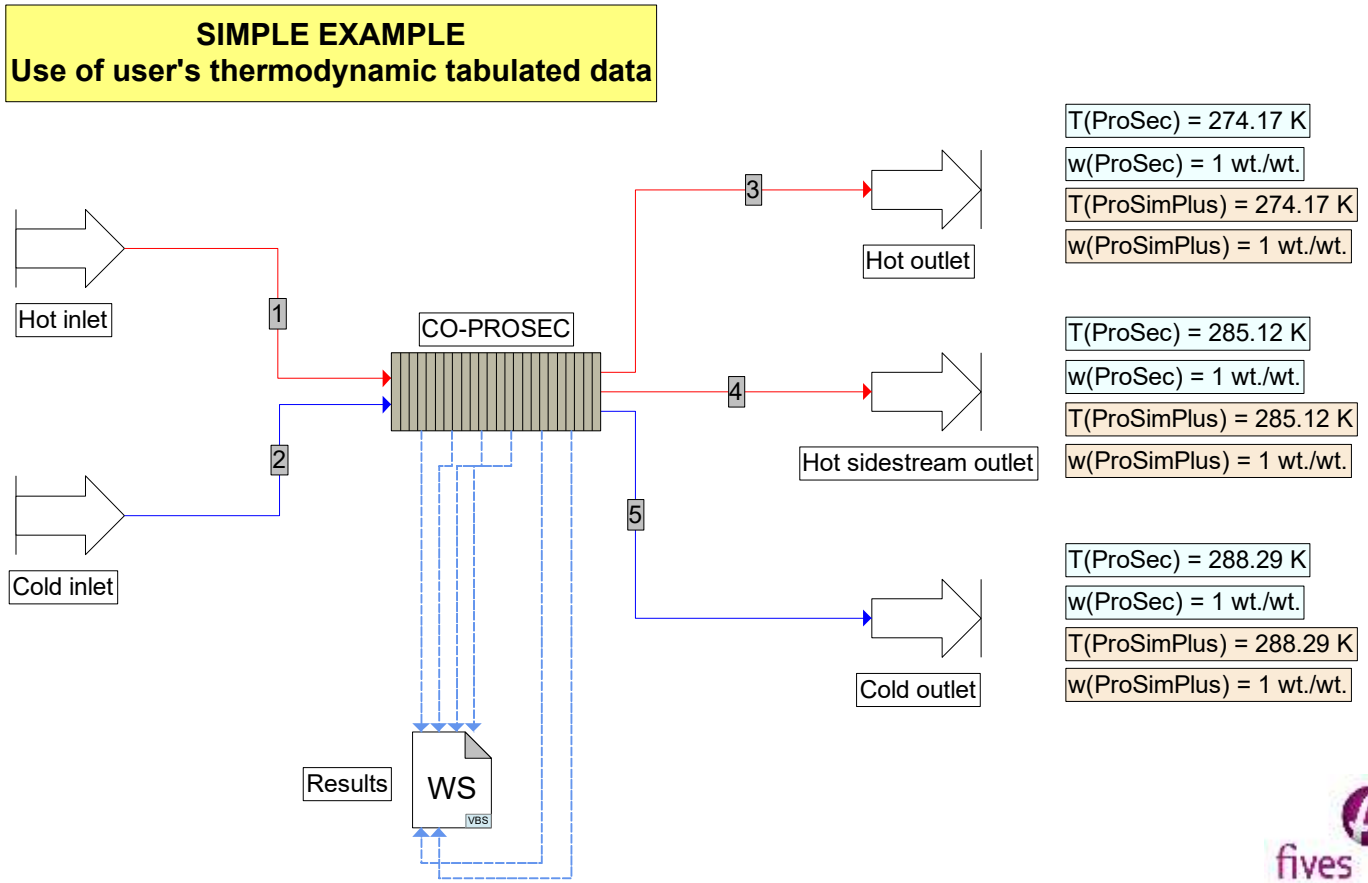
3. Double-click on the tag
   f) The “Graphics” tab allows to change the visual aspect of the tags to differentiate them for example.

4. Click on “OK” to validate the specified parameters.



Step 4
Display results with tags

- Display the results of ProSimPlus streams
  5. Repeat the previous procedure to display the results calculated for the other ProSimPlus streams of interest.
- Final simulation flowsheet



Analysis of the results

- In this example, the temperatures and vaporization rates calculated in the ProSimPlus streams are the same as those calculated in ProSec module.

- Possible differences can be explained by: :
  - Differences between the thermodynamic profile used to tabulate the thermodynamic data and the one selected in the host software (different compounds, different compositions, different models, etc.).
  - By default, ProSec calculations are isobaric to the inlet pressure. Pressure drops, *i.e.* outlet pressures, are calculated after the thermal resolution. ProSec transmits the enthalpies and pressures of the outlet streams to the host software. If the pressure drops are important, a deviation may then appear (the calculations of the host software being made at a pressure different from that of ProSec).

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