

PROSIMPLUS APPLICATION EXAMPLE

CLAUDE PROCESS FOR HYDROGEN LIQUEFACTION

EXAMPLE PURPOSE

This example details a Claude process for the liquefaction of hydrogen. A method is presented to account for the ortho-para hydrogen conversion reaction for two of the multi-fluid exchangers. Criteria such as the Specific Energy Consumption (SEC) and the exergy efficiency of the multi-fluid exchangers are calculated.

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CORRESPONDING PROSIMPLUS FILES

PSPS_EX_EN-Claude-process-hydrogen-liquefaction.pmp3

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Energy

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1. PROCESS MODELING

1.1. Process description

Hydrogen is gaining more and more attention as an energy carrier because its use doesn't emit greenhouse gases, and it can be used to store renewable energy. The most competitive renewable electricity generation centers, such as wind farms in the North Sea or solar farms in the Middle East, are far from the major production sites in Europe. Therefore, supply infrastructure needs to be developed to transport hydrogen over long distances. The main obstacle is its low volumetric density, which would lead to oversized storage and transport equipment. To increase volumetric density, liquefaction is a promising option for large-scale delivery. Hydrogen liquefaction occurs at about 20 K at atmospheric pressure. It is the most energy-intensive process in the supply chain and therefore special attention must be paid to its design [RES23].

A conventional hydrogen liquefaction process consists of four consecutive steps [OHL14]:

1. Pre-compression of hydrogen feed gas, if required.
2. Pre-cooling of hydrogen gas to about 80 K.
3. Cryogenic cooling of hydrogen gas until 20-30 K, including ortho-para conversion of hydrogen.
4. Final expansion and liquefaction of hydrogen.

Most current hydrogen liquefaction technologies are characterized by the nature of the refrigeration cycle used in the cryogenic refrigeration section. In the liquefaction processes built, this cycle is based on either a helium Brayton cycle or a hydrogen Claude cycle [CAR17a]. A Brayton cycle uses a turbine instead of a Joule-Thomson valve for expansion. The classical Claude cycle is a combination of a Joule-Thomson cycle and the Brayton cycle: one stream of refrigerant is expanded in turbines while a second flow is cooled and expanded in a valve to produce a two-phase flow [CAR17a]. The Specific Energy Consumption (SEC) of liquefaction trains operating in the United States is estimated to be between 12.5 and 15 kWh/kg_{LH2} for capacities between 5.4 and 32 t_{LH2}/d [CAR17b].

Simulation makes it easy to investigate the recirculation between the heat exchangers, their temperature levels, the use of turbines or valves, the compounds used for cooling, etc. In order to take into account the ortho-para reaction of hydrogen in a non-reactive temperature controllers (HEXs) in series, one method is to add a reactor at the outlet of the current to be liquefied [RIA23]. The reactor can be at a given conversion rate, balanced or Gibbs free energy minimization [RIA23]. To take into account the exothermicity of the reaction, the reactor can be adiabatic or isothermal [RIA23]. To apply the reaction heat calculated at the reactor level in the temperature controllers (HEXs) in series, it is possible to recycle the outgoing flow from the reactor directly or indirectly in the multi-fluid exchanger, transmit it to an external flow or distribute it as a heat loss in the multi-fluid exchanger [RIA23]. To follow the choice made in [RES23], this simulation uses two adiabatic reactors whose conversion rates are calculated from the equilibrium constant of [WIL18]. In [RES23] the flows from the two reactors are not treated in the same way. The simulation is built with the same principle.

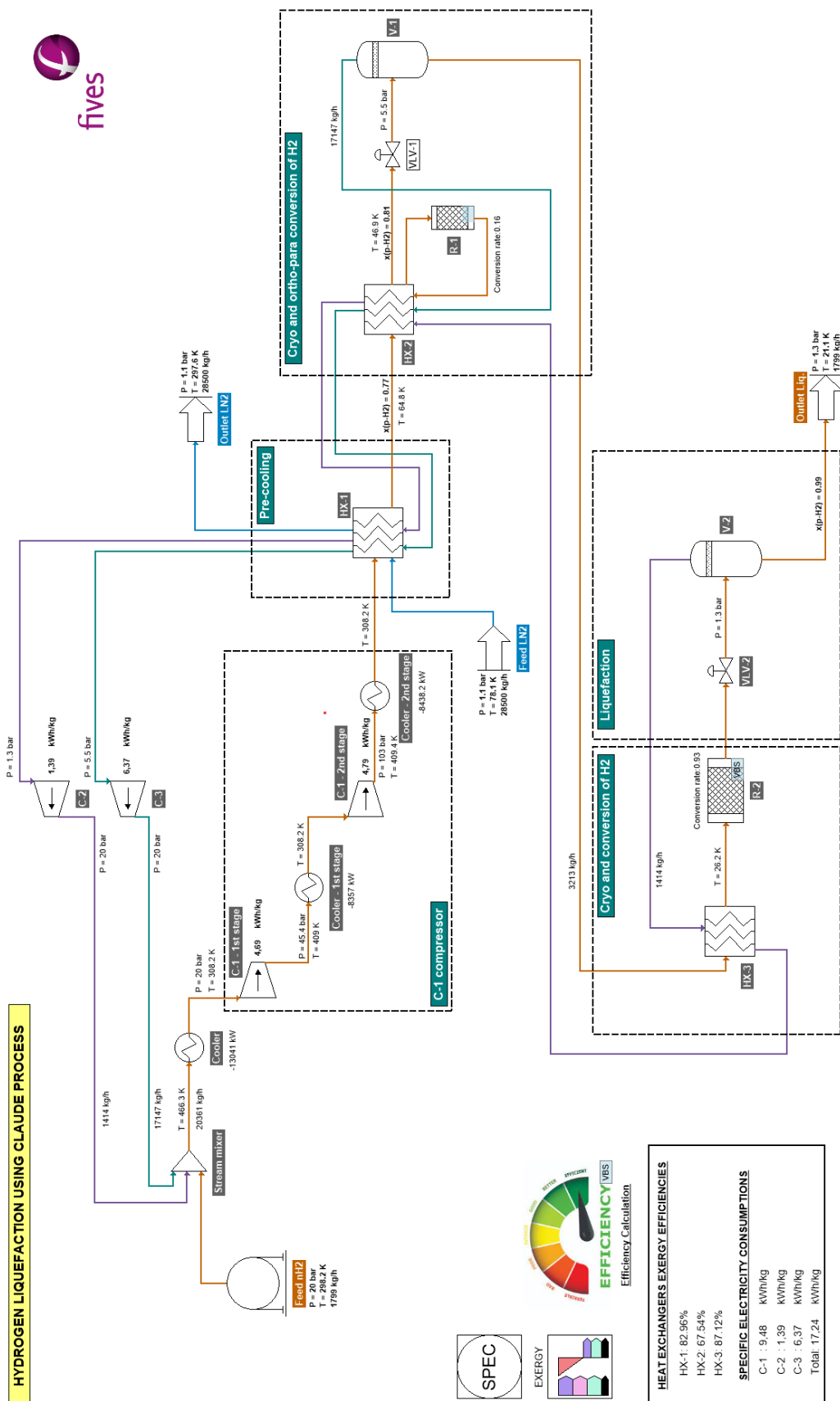
This example is based on the process described in [RES23]. It deals with the simulation of a Claude cycle pre-cooled with liquid nitrogen. The paragraph 1.2 shows the simulation flowsheet. Two of the heat exchangers, HX-2 and HX-3, are reactor exchangers which, in addition to hydrogen liquefaction, ensure ortho-para hydrogen conversion. As the MHX unit operation used to model these heat exchangers doesn't manage chemical reactions, the ortho-para

hydrogen conversion reaction is taken into account in separate reactors. In order to follow the hypothesis made in [RES23], their outflows are recycled in the HX-2 and HX-3 exchangers to take into account the exothermicity of the reaction. Still following the hypothesis made in [RES23], it is assumed that the ortho-para equilibrium is reached (no displacement of the equilibrium by the use of a catalyst). To go further, the example “COPROSEC_EX_EN-ortho-para-hydrogen-conversion” allows you to:

- ✓ Model a reactor exchanger with brazed plates and fins with a fixed-bed catalyst in certain passages,
- ✓ Model a catalytic reaction to increase the ortho-para conversion of hydrogen.

The normal hydrogen to be liquefied (25% p-H₂ and 75% o-H₂) enters the process via stream 01 at a pressure of 20 bars and at room temperature. It is assumed here to be free of moisture and condensable gases. This stream is mixed with high p-H₂ amount recycling streams 16 and 20 to form stream 02, which is cooled using process water (the utility part is not shown in this simulation) and then compressed to 103 bars in the C-1 two-stage compressor with two intercoolers. The output stream of C-1, 04b, is cooled in the HX-1 and HX-2 temperature controllers (HEXs) in series, to 64.8 K and then 46.9 K respectively, by heating the recycled hydrogen gas streams at low and medium pressure. The HX-1 heat exchanger includes a liquid nitrogen flow at a pressure of 1.1 bars. The HX-1 and HX-2 heat exchangers are characterized by a minimum temperature approach of 2 K. The flow of hydrogen to be liquefied is sent to the R-1 reactor. Flow 06a at the outlet of R-1 is cooled in HX-2 before reducing its pressure to 5.5 bars in the Joule-Thomson VLV-1 valve. The resulting two-phase flow is separated in the V-1 drum. The steam is recycled to cool the process stream in HX-1 and HX-2. The liquid passes through the process – process heat exchanger HX-3, which is characterized by a minimum temperature approach of 1 K. Flux 09 is sent to the R-2 reactor, then cooled through the Joule-Thomson VLV-2 valve, reaching the storage pressure of 1.3 bars. The V-2 drum separates the steam, which is recycled back as a cold stream through HX-3, HX-2 and HX-1, and the liquid, which leaves the process to be stored in an insulated tank at a pressure of 1.3 bars. For the sake of simplicity, pressure drops inside heat exchangers are neglected.

1.2. Process flowsheet



Simulation flowsheet of a Claude process for hydrogen liquefaction

1.3. Compounds

The compounds considered in the simulation, along with their chemical formulae and CAS numbers¹ are shown in the table below. The two hydrogens are imported from the “H2” database, which was developed mainly for this application, and from the standard ProSimPlus database [ROW24]. The nitrogen compound is directly imported from the standard database of ProSimPlus [ROW24].

Compound	Chemical formula	Notation	CAS number ⁽¹⁾
HYDROGEN (para, isomers model)	H ₂	p-H ₂	55000-01-6
HYDROGEN (ortho, isomers model)	H ₂	o-H ₂	88000-01-5
NITROGEN	N ₂	N ₂	7727-37-9

Normal hydrogen is also available in the “H2” database. It is therefore possible to set up the same simulation and obtain similar results by using a mixture of normal hydrogen and para hydrogen. The enthalpy of fusion and the sublimation pressure of o-H₂ are missing for this constituent. To avoid a warning message in the exergy calculation, although these properties are not used, they have been taken to be equal to those of p-H₂.

1.4. Thermodynamic model

The thermodynamic profile “Hydrogen (isomers)” is used in streams containing only hydrogen (p-H₂ and/or o-H₂). This model allows to represent the energy and transport properties of mixtures containing n-H₂, p-H₂ and o-H₂ for temperatures between 20 K and 400 K and pressures between 0.1 bar and 100 bars. The Redlich-Kwong equation of state [RED49] was selected as well as the generalized Twu-Nancy alpha function [LEG16]. For a good representation of the transport properties (vapor and liquid dynamic viscosity, and vapor and liquid thermal conductivity) the parameters of the models of [ASS11], [MUZ13], [REI77] were adjusted using experimental data.

The thermodynamic profile “PSRK” ([HOL91], [GME95], [CHE02]) is used for streams containing only nitrogen.

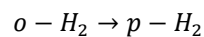
Each thermodynamic profile has its own dedicated thermodynamic calculator: “Hydrogen isomers” and “PSRK”.

¹ CAS Registry Numbers® are the intellectual property of the American Chemical Society and are used by Fives ProSim SAS with the express permission of ACS. CAS Registry Numbers® have not been verified by ACS and may be inaccurate.

1.5. Chemical reactions

The ortho-para conversion reaction of hydrogen is taken into account in a very simple way because the conversion rate between p-H₂ and o-H₂ will be calculated via a script directly in the dedicated reactive modules. This reaction is associated with the "Hydrogen isomers" calculator.

The reaction is described as an instantaneous reaction whose heat of reaction is calculated.



1.6. Operating conditions

1.6.1. Process feeds

The "Feed nH₂" feed is the normal hydrogen feed that will be liquefied and converted to para hydrogen as much as possible. The "Feed LN₂" feed is the liquid nitrogen feed that constitutes the cold make-up of one of the heat exchangers.

	Feed nH ₂	Feed LN ₂
Molar fractions		
p-H ₂	0.25	0
o-H ₂	0.75	0
N ₂	0	1
Flow rate (kg/h)	1 798.8	28 500
Temperature (K)	298.15	Bubble temperature
Pressure (bar)	20	1.1

1.6.2. Mixer

The "Stream mixer" mixer is an adiabatic mixer at the lowest pressure of the feeds.

1.6.3. Cooler

The "Cooler" cooler is represented by a "Temperature controller (HEX)" unit operation whose outlet temperature is set at 308.15 K. No pressure drop is specified.

1.6.4. Compressors

The “C-1” compressor is a two-stage compressor with intercooler. In order to enable the use of the “Exergy balance” module, this compressor is represented by different unit operations.

Compressor	C-1 - 1st stage	C-1 - 2nd stage
Unit operation	Compressor	
Modeling	1 st stage of compression	2 nd stage of compression
Exhaust pressure (bar)	45.3872	103
Isentropic efficiency	0.8	
Mechanical efficiency	1	
Electrical efficiency	1	

Intercooler	Cooler - 1st stage	Cooler - 2nd stage
Unit operation	Temperature controller (HEX)	
Modeling	Intercooler	Outlet cooler
Temperature (K)	308.15	

The “C-2” and “C-3” compressors are single-stage compressors represented by "Compressor" unit operations.

Compressor	C-2	C-3
Exhaust pressure (bar)	20	
Isentropic efficiency	0.8	
Mechanical efficiency	1	
Electrical efficiency	1	

1.6.5. Temperature controllers (HEXs) in series

The three temperature controllers (HEXs) in series are represented by "MHX" unit operations. The parameters other than those in the following tables have their default values.

Heat exchanger HX-1		
Inlet stream	Outlet stream	Specification
04d	05	Outlet temperature = 64.8 K
18	19	No specification Initialization type: Temperature = 280 K
14	15	
21	22	

Heat exchanger HX-2		
Inlet stream	Outlet stream	Specification
17	18	No specification Initialization type: Temperature = 55 K
13	14	Outlet temperature = 62.8 K
05	06	Outlet temperature = 46.855 K
06a	06b	

Heat exchanger HX-3		
Inlet stream	Outlet stream	Specification
12	13	Delta T (outlet – reference inlet) = -1 K Reference stream: "08"
08	09	No specification Initialization type: Temperature = 293.15 K



Specification "No specification"

This specification indicates that there is no constraint on the value of the stream outlet temperature. It will be calculated to satisfy the enthalpy balance on the heat exchanger. If multiple outlet streams are not specified, their temperatures will be equal.

1.6.6. Reactors

The R-1 and R-2 reactors are used to represent the ortho-para hydrogen conversion reaction in the reactive layers of the HX-2 and HX-3 multi-fluid exchangers, respectively. These are “Simple Reactor” unit operations. Their conversion rates will be calculated from the formulation of [WIL18] giving the equilibrium composition between p-H₂ and o-H₂.

$$x_{p-H_2}^{eq} = \frac{0.1}{\exp\left(\frac{-5.313}{T/T_c}\right) + 0.1} - 2.52 \times 10^{-4} \left(\frac{T}{T_c}\right)^3 + 3.71 \times 10^{-3} \left(\frac{T}{T_c}\right)^2 - 2.04 \times 10^{-3} \frac{T}{T_c} - 0.00227$$

$$\tau_{p-H_2} = \frac{x_{p-H_2}^{eq} - x_{p-H_2,in}}{1 - x_{p-H_2,in}}$$

	R-1	R-2
Thermal behavior	Adiabatic	
Pressure	The lowest of the feeds	
Conversion rate (initialization)	0.191132	0.885364
Key component	o-H ₂	

The calculation script, common to both reactors, is presented below.

```

Sub OnCalculationStart()

'-----'
' RECOVERY OF THE INLET STREAM DATA'
'-----'
TK_in   = Module.InputStream(1).Temperature      'K
QpH2_in = Module.InputStream(1).PartialMolarFlowrate(1) 'kmol/hr
Qtot_in = Module.InputStream(1).MolarFlowrate      'kmol/hr

'-----'
' CALCULATION OF THE INLET p-H2 MOLAR FRACTION'
'-----'
xpH2_in = QpH2_in/Qtot_in

'-----'
' CALCULATION OF THE EQUILIBRIUM CONSTANT'
' WILHELMSSEN ET AL., REDUCING THE EXERGY DESTRUCTION IN THE CRYOGENIC HEAT'
' EXCHANGERS OF H2 LIQUEFACTION PROCESSES'
' INTER. J. HYDROGEN ENERGY, 43(10), 5033-5047 (2018)'
'-----'

'-----'
' CALCULATION OF THE REDUCED TEMPERATURE'
'-----'
Tcrit = 32.937      'K critical temperature from Wilhelmsen
Tr      = TK_in/Tcrit

'-----'
' CALCULATION OF THE OUTLET p-H2 MOLAR FRACTION'
'-----'
xpH2_out = 0.1/(exp(-5.313/Tr) + 0.1) - 2.52e-4*Tr^3 + 3.71e-3*Tr^2 - 2.04e-3*Tr - 0.00227

'-----'
' CALCULATION OF THE CONVERSION RATIO'
'-----'
ConvRatio = (xpH2_out - xPH2_in)/(1. - xPH2_in)

'-----'
' AFFECTATION OF THE VALUE'
'-----'
Module.ConversionRatios(1) = ConvRatio

End Sub

```

1.6.7. Joule-Thomson expansions

The Joule-Thomson expansions are represented by “Expansion valve” unit operations.

	VLV-1	VLV-2
Constraint type	Pressure specification	
Pressure (bar)	5.5	1.3

1.6.8. Separation drums

The V-1 and V-2 separation drums are represented by “Vapor-liquid separator (2-phase flash)” unit operations. They are adiabatic at the lowest pressure of the feed streams.

1.6.9. Exergy balances

All parameters remain default, except the convergence criterion for primary exergy calculations which is increased to 10^{-4} . This degradation of convergence will only be slightly noticeable for the evaluation of the exergy of temperature controllers (HEXs) in series.

1.6.10. Numerical method

In order to achieve the convergence of the simulation as quickly as possible, the numerical method is modified. To do this, a “Constraints and recycles management” module is added to the simulation. Only the following settings are changed:

- ✓ Numerical methods: Broyden
- ✓ Acceleration operator: Jacobian matrix by finites differences

Optionally, to access to the information relating to this module, it is necessary to select the tear streams via the corresponding button of this module: 04d, 05, 06, 06b and 09.

1.6.11. Tear streams

The resolution of this simulation requires 5 tear streams. Their initializations are shown in the table below.

Streams	04d	05	06	06b	09
Molar fractions					
p-H ₂	0.71				
o-H ₂	0.29				
N ₂	0				
Flow rate (kg/h)	20 383				4 174
Temperature (K)	308.15	64.8	45.8		25.7
Pressure (bar)	103				5.5

1.6.12. Custom module (script): Efficiency Calculation

The specific electricity consumptions is defined as the ratio between total useful powers of compressors and flowrate of produced liquid hydrogen as expressed by the following relation:

$$SEC = \frac{\sum_i^{stages} P_{tot,i}}{F_{H_2,liq}}$$

The following script allows to calculate this specific electricity consumption of process compressors and to convert them into units of the report.

```
'-----'
' CALL OF PREDEFINED SCRIPT
'-----'

ExecuteGlobal CreateObject("Scripting.FileSystemObject").OpenTextFile(Project.ApplicationPath &
"Scripts\IncludeScript.vbs", 1).ReadAll()
IncludeScript "UnitConversion.vbs"

function OnCalculation()
    Name1 = "C-1 - 1st stage"
    Name2 = "C-1 - 2nd stage"
    Name3 = "C-2"
    Name4 = "C-3"
    Outlet = "11"

'-----'
' CALCULATION OF THE SPECIFIC ELECTRICITY CONSUMPTIONS OF THE COMPRESSORS
'-----'

Module.Parameter(1) = ProSimToReport("Mass enthalpy",
Project.Modules(Name1).TotalUsefulPower/Project.Streams(Outlet).MassFlowRate)
Module.Parameter(2) = ProSimToReport("Mass enthalpy",
Project.Modules(Name2).TotalUsefulPower/Project.Streams(Outlet).MassFlowRate)
Module.Parameter(3) = ProSimToReport("Mass enthalpy", (Project.Modules(Name1).TotalUsefulPower
+ Project.Modules(Name2).TotalUsefulPower)/Project.Streams(Outlet).MassFlowRate)
Module.Parameter(4) = ProSimToReport("Mass enthalpy",
Project.Modules(Name3).TotalUsefulPower/Project.Streams(Outlet).MassFlowRate)
Module.Parameter(5) = ProSimToReport("Mass enthalpy",
Project.Modules(Name4).TotalUsefulPower/Project.Streams(Outlet).MassFlowRate)
sum = 0
For i = 1 to 3
    sum = sum + Module.Parameter(i+2)
Next
Module.Parameter(6) = sum

OnCalculation = True

end function
```

1.7. “Tips and tricks”

“Tags” are used to display, on the simulation flowsheet, the p-H₂ mole fractions at the outlet of the HX-1, HX-2 and HX-3 temperature controllers (HEXs) in series, the exergy efficiencies of these heat exchangers and the Specific Energy Consumption of the C-1, C-2 and C-3 compressors.

The tag expert mode allows you to code it in VBS the formatting of the value as well as displaying the unit of the report (e.g., for the C-2 compressor).

The screenshot shows the 'Tag' dialog box with the 'Expert' tab selected. The 'Expert mode' radio button is checked. The 'Parameters of the unit operation usable in the script' section is expanded, showing 'Unit operation:' and 'Parameter:' dropdown menus. Below these is a 'Syntax:' section with a 'Paste' button and an 'Info' icon. The main area contains a VBS script for formatting and reporting the mass enthalpy of the C-2 compressor. The 'Starting text:' field is set to 'C-2 :'. The 'Ending text:' field is empty. The 'Format string for numerical values:' dropdown is set to '###0.00'. The 'Preview:' field shows 'C-2 : 1,39 kWh/kg'. The 'OK' and 'Cancel' buttons are at the bottom right.

Tag

Value | Graphics

☐ Standard mode ☒ Expert mode

Expert

Parameters of the unit operation usable in the script

Unit operation:

Parameter:

Syntax:

Paste Info More

```
1 ExecuteGlobal CreateObject("Scripting.FileSystemObject").OpenTextFile(Project.ApplicationPath & "Scripts\IncludeScript.vbs", 1).ReadAll()  
2 IncludeScript "UnitConversion.vbs"  
3 IncludeScript "FormatDouble.vbs"  
4 function ExpertTag()  
5     ExpertTag = FormatDouble(project.modules("Efficiency Calculation").Parameter(4),0,3) & " " & ReportUnit("Mass enthalpy")  
6  
7 end function
```

Starting text: C-2 :

Ending text:

Format string for numerical values: ###0.00

Preview: C-2 : 1,39 kWh/kg

OK Cancel

2. RESULTS OF THE SIMULATION

This document presents only a few results. However, ProSimPlus provides complete results on all process streams and unit operations.

2.1. Process performance

The table below summarizes some of the process performances.

Flow rate of liquefied hydrogen (kg/h)	1 798.8
Outlet temperature of the liquefied hydrogen (K)	21.1
Molar fraction in p-H ₂ (mol./mol.)	0.99

The following table shows the Specific Energy Consumption of each compressor as well as the total one.

	Specific Energy Consumption (kWh/kg _{LH2})
Compressor C-1	9.48
Compressor C-2	1.39
Compressor C-3	6.37
Total	17.24

The following table shows the exergy efficiency of the three temperature controllers (HEXs) in series. A complete exergy analysis is detailed in the example "PSPS_EX_EN-PRICO-Process-natural-gas-liquefaction".

	Exergy efficiency (%)
Heat exchanger HX-1	82.96
Heat exchanger HX-2	67.54
Heat exchanger HX-3	87.12

The values obtained are consistent with those of [RES23]. The discrepancies can be explained by the discrepancies between the thermodynamic model used in this example and the model used in [RES23].

2.2. Temperature controllers (HEXs) in series

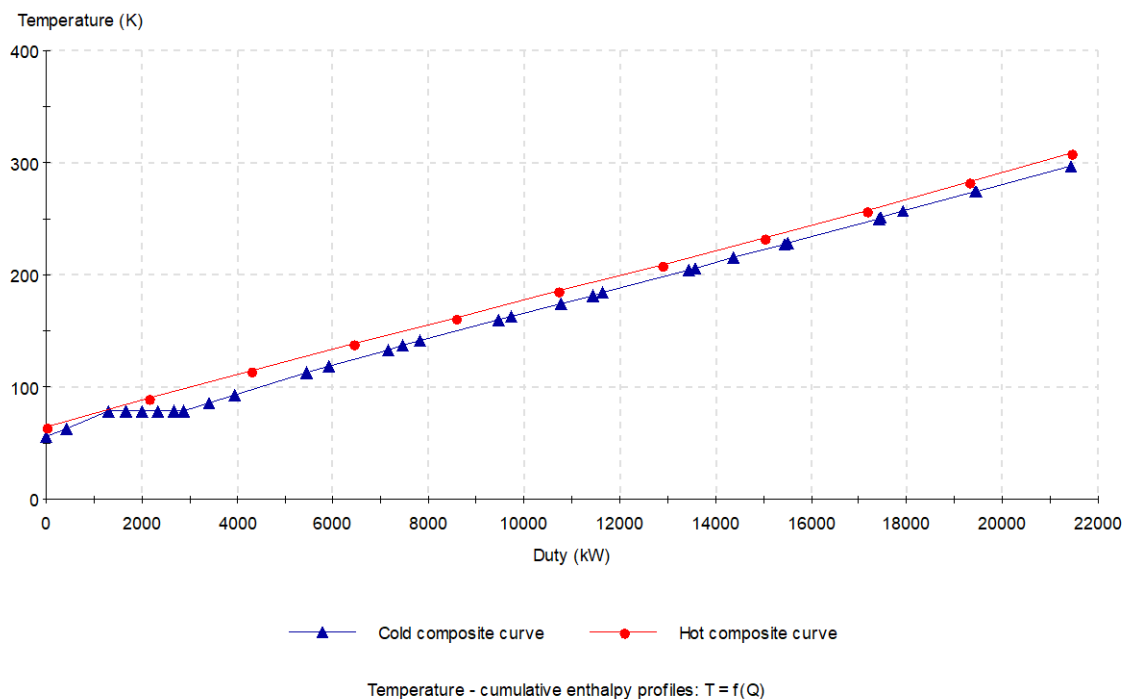
The following table shows the pinch of each of the 3 temperature controllers (HEXs) in series.

	Pinch (K)
Heat exchanger HX-1	2.05
Heat exchanger HX-2	2.00
Heat exchanger HX-3	1.00

A flow rate of 28 500 kg/h of liquid nitrogen at its bubble temperature at 1.1 bars is required to achieve the 2 K pinch in the HX-1 temperature controllers (HEXs) in series.

Cold and hot composite curves are available for each temperature controllers (HEXs) in series. They are built from the enthalpy curves of cold and hot streams. The principle of construction of the composite curves and the calculation of the temperature controllers (HEXs) in series are based on the pinch method (e.g., "PSPS_EX_EN-PRICO-Process-natural-gas-liquefaction"). The figure below shows the curves obtained for the HX-1 temperature controllers (HEXs) in series

HX-1 - Hot and cold composite curves



3. NOMENCLATURE

$F_{H_2,liq}$	Flow rate of produced liquid hydrogen	kg/h
i	Loops counter	(-)
LH_2	Liquid hydrogen	(-)
$P_{tot,i}$	Total useful power uses at the compression stage i	kW
SEC	Specific Energy Consumption	kWh/kg _{LH2}
$stages$	Number of compression stages	(-)
T	Temperature	K
T_c	Critical temperature of p-H ₂	K
$x_{p-H_2,in}$	Molar fraction of p-H ₂ at the reactor inlet	mol./mol.
$x_{p-H_2}^{eq}$	Molar fraction in p-H ₂ at equilibrium	mol./mol.
τ_{p-H_2}	Conversion ratio of p-H ₂	mol./mol.

4. REFERENCE

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