ProSim

PROSIMPLUS APPLICATION EXAMPLE

AMMONIA SYNTHESIS PROCESS

EXAMPLE PURPOSE
This example presents the ammonia synthesis process from natural gas. This example includes two simulations: one simulation is dedicated to the entire process and another to the reactor alone to take into account its technological specificities. A pinch analysis of the process is also carried out.

ACCESS	☑ Free Internet	☐ Restricted to ProSim clients	☐ Restricted	☐ Confidential

CORRESPONDING PROSIMPLUS FILES	*PSPS_EX_EN-Ammonia-Synthesis-Process.pmp3* *PSPS_EX_EN-Ammonia-Synthesis-Reactor.pmp3*

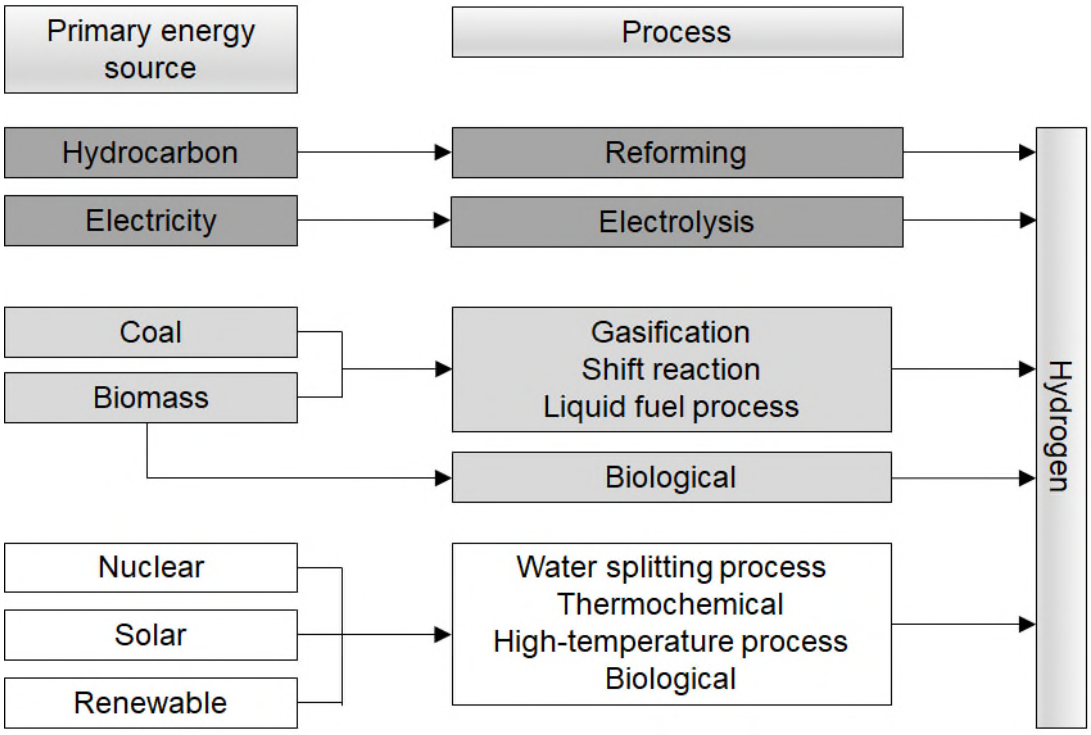
TABLE OF CONTENTS

1. PROCESS MODELING

1.1. Process description

Ammonia (NH_3) is the least expensive compound combining nitrogen with raw materials, used in more than 76% of all nitrogen-based products [AMH22]. The main categories of ammonia applications are productions of ammonium bicarbonate, ammonium nitrate, ammonium sulphate, calcium ammonium nitrate, urea, fertilizer, and other direct uses [AMH22].

There are several ways to produce hydrogen [AMH22], [GOD12], [PAT19], [ROU18]. Currently, most industrial hydrogen is produced from fossil fuels (natural gas, oil, and coal), primarily by steam reforming of natural gas. To reduce CO_2 emissions into the atmosphere, particular attention is increasingly being paid to renewable production options which include water electrolysis (see "PSPS_EX_EN-Hydrogen-Production-Electrolysis") using renewable energies (e.g.: wind, solar, hydroelectric, and geothermal), biomass gasification (see "PSPS_EX_EN-IGCC-Plant"), photoelectrochemical and biological processes and high temperature thermochemical cycles. The general routes of hydrogen production by different processes and from different primary energy sources are shown in the following figure [GOD12].



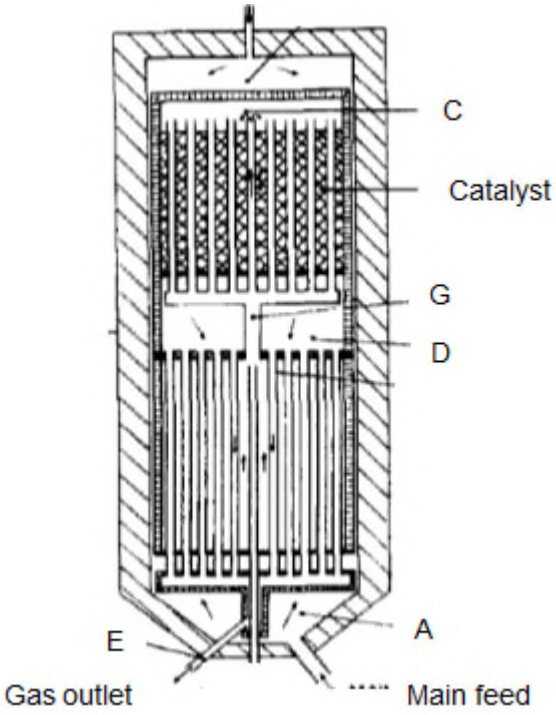
The example detailed in this document presents the production of ammonia by natural gas reforming [AMH12], [ROU18]. The "PSPS_EX_EN-Ammonia-Synthesis-Process.pmp3" simulation presents this ammonia production process. The heat exchanges between the process streams and the generation of steam necessary for reforming by a boiler are also simulated. Utility networks and any expander-compressor couplings are not simulated but can easily be added with ProSimPlus.

The different blocks of the process are:

- ✓ Desulfurization ("Sulfur removal"): Final desulfurization of natural gas to eliminate the last traces of sulfur: this component is poisonous for the catalysts used for this process. Desulfurization is based on the hydrogenation of sulfur compounds into hydrocarbons and H_2S. A simple reactor is used to model this part by assimilating sulfur compounds to Tetrahydrothiophene. The adsorption of H_2S is generally carried out on zinc oxides. A components splitter makes it possible to simply represent this operation.
- ✓ Primary steam reforming ("Primary reforming"): this block converts methane into hydrogen, CO, and CO_2. Steam methane reforming is performed by chemical equilibrium in a continuous stirred tank reactor. The reforming of the other hydrocarbons is done in a simple reactor with fixed conversion rates.
- ✓ Secondary reforming ("Secondary reforming"): a post-combustion of methane in air with simultaneous consideration of its air reforming and CO conversion is carried out in a continuous stirred tank reactor. This second reforming block converts as much methane as possible into hydrogen, CO, and CO_2.
- ✓ CO conversion ("Shift conversion"): this block converts CO into hydrogen and CO_2 by reaction with water. The CO conversion is done in two stages at two different temperatures in two continuous stirred tank reactors.
- ✓ Elimination of residual water ("Water removing"): this step is modeled by a vapor-liquid flash at a given temperature and pressure.
- ✓ Decarbonation of synthesis gas ("CO_2 removing"): this step removes CO_2 from the gas resulting from the reforming steps. This decarbonation process is carried out in a simple way by using a components splitter. Examples dedicated to different decarbonation methods are available:
    - o Amines process with MEA as solvent, see "PSPS_EX_EN-CO2-capture-with-amine-process;
    - o Rectisol process with methanol as solvent, see "PSPS_EX_EN-Rectisol-Process;
    - o Purisol process with NMP as solvent, see "PSPS_EX_EN-Purisol-Process;
    - o Selexsol process with Selexsol as solvent, see "PSPS_EX_EN-Selexol-Process.
- ✓ Methanation ("Methanation"): its purpose is to eliminate traces of oxygenated compounds. In this example, CO and CO_2 are the remaining oxygenated compounds to be eliminated.
- ✓ Gas compression ("3 stages synthesis gas compressor"): here in three stages with elimination of condensates.
- ✓ Ammonia synthesis loop ("Ammonia synthesis") which includes:
    - o The catalytic synthesis reactor: in the main simulation, a simple reactor with a fixed conversion rate is used. A simulation taking into account the chemical equilibrium and the technology of this reactor is carried out in the simulation "PSPS_EX_EN-Ammonia-Synthesis-Reactor.pmp3;
    - o A series of heat exchangers where the ammonia produced is condensed and then separated in liquid state;
    - o An ammonia refrigeration unit that provides the cold needed to condense and cool the ammonia produced. Since this simulation is focusing only on the process part, this loop is not included in the simulation.

The energy integration of this process is analyzed via an energy pinch analysis module (§ 2.3). Process performance is analyzed using an electrical balance module and a generalized balance module.

The modeling of the ammonia synthesis reactor follows the one proposed by [BAD65]. The gas follows the path below, as shown on the following drawing:



- ✓ Thermal transfer section:

  A ➔ G: Preheating of the incoming gas by cooling of the gas leaving the reactor. This is modeled by the cooler/heater E201a in which the temperature at point G is imposed.

- ✓ Reactive section:

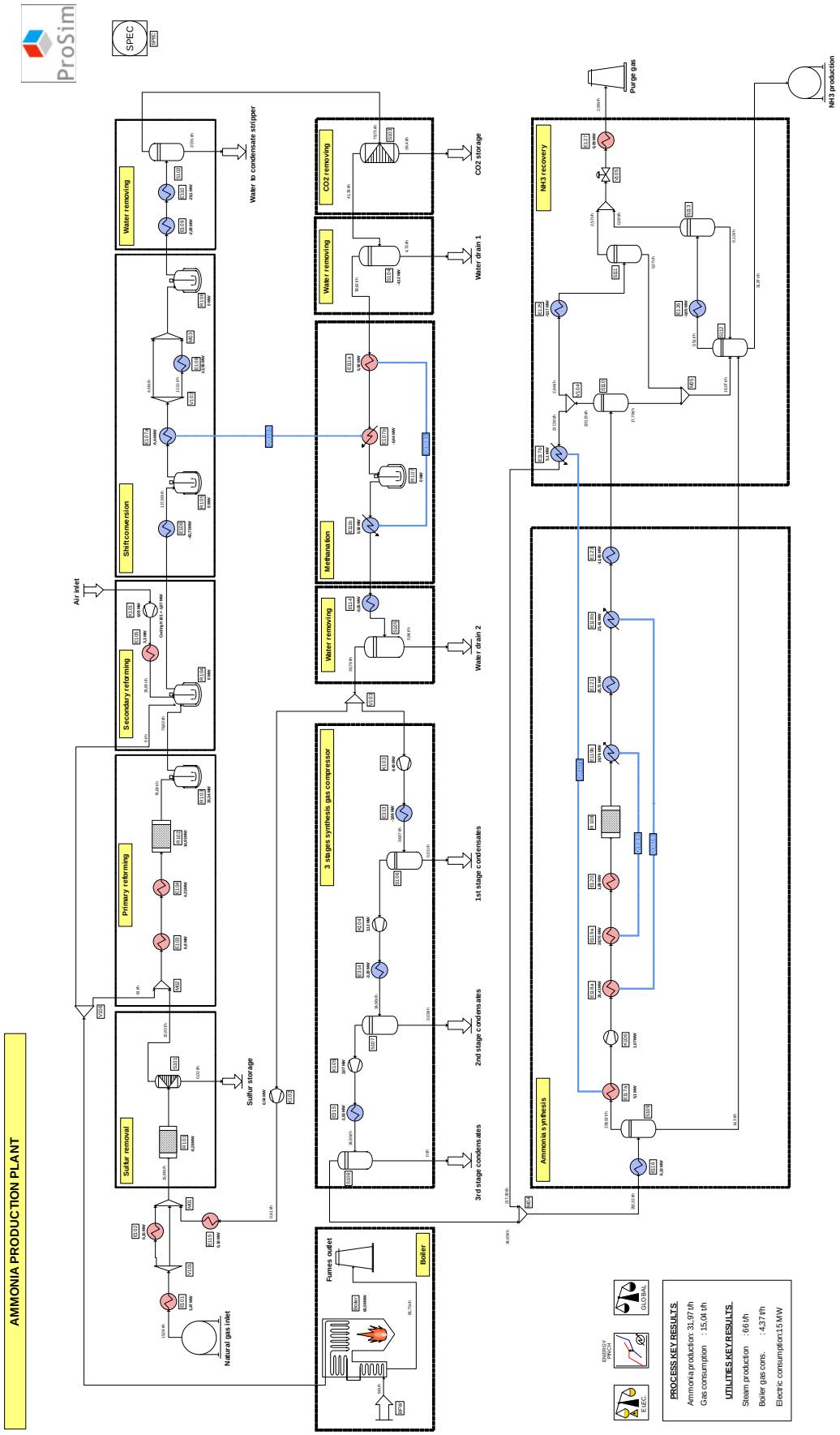
  G ➔ C: The gas after the preheating is used to contain the heat of reaction. This is modeled using the possibility of defining a heat transfer fluid (reactor with jacket) in the plug flow reactor R201.

  C ➔ D: This is the reactive section. The dimensions of the R201 reactor have been adapted to correspond to the flow characteristics considered in [BAD65].

- ✓ Thermal transfer section:

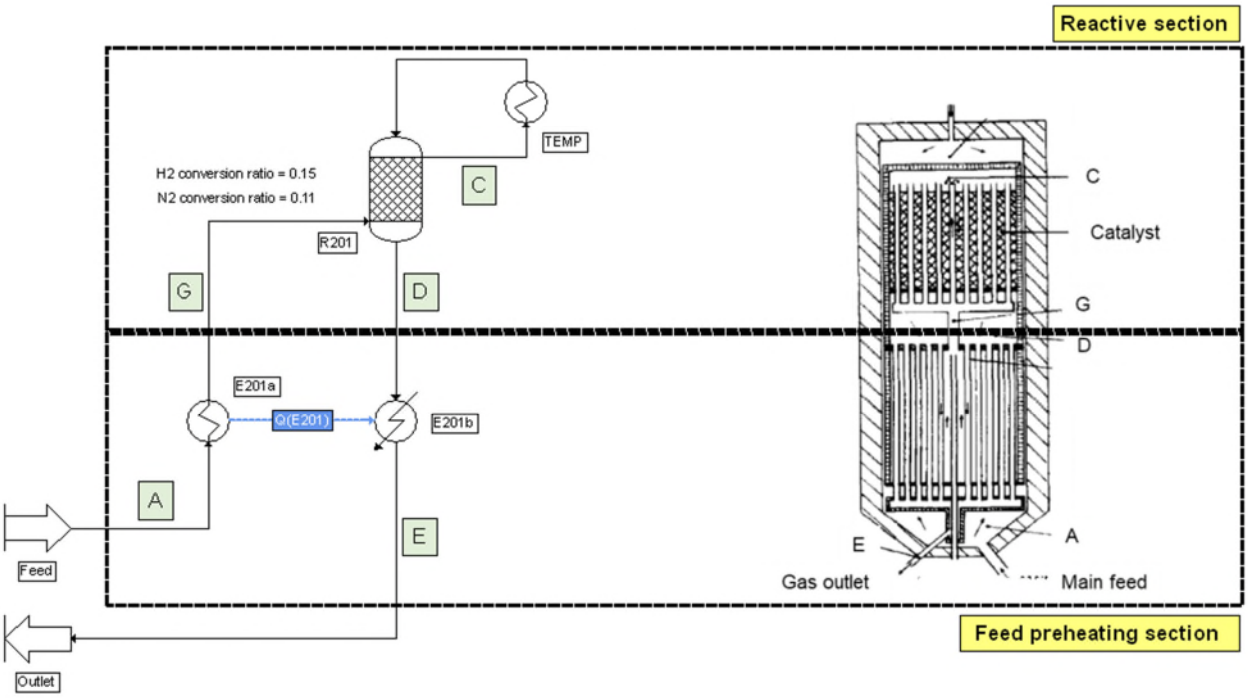
  D ➔ E: The gas leaving the reactor preheats the feed. The simple heat exchanger E201b models this heat transfer. An information stream transfers the heat duty calculated by the exchanger E201a.

1.2. Simulation flowsheet



Simulation flowsheet of an ammonia synthesis process from natural gas

AMMONIA CONVERTER



Simulation flowsheet of an ammonia synthesis reactor

1.3. Components

The components considered in the simulation are listed in the table below, as well as their chemical formula and their CAS numbers[1]. The properties of pure substances are taken from the standard ProSim database [WIL21].

Component	Chemical formula	CAS Number(1)
Water	H_2O	7732-18-5
Oxygen	O_2	7782-44-7
Hydrogen	H_2	1333-74-0
Carbon monoxide	CO	630-08-0
Carbon dioxide	CO_2	134-38-9
Nitrogen	N_2	7727-37-9
Argon	Ar	7440-37-1
Methane	CH_4	74-82-8
Ethane	C_2H_6	74-84-0
Propane	C_3H_8	74-98-6
Isobutane	C_4H_{10}	75-28-5
n-butane	C_4H_{10}	106-97-8
Isopentane	C_5H_{12}	78-78-4
Pentane	C_5H_{12}	109-66-0
n-hexane	C_6H_{14}	110-54-3
Ammonia	NH_3	7664-41-7
Tetrahydrothiophene	C_4H_8S	110-01-0
Hydrogen sulfide	H_2S	7783-06-4

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

1.4. Thermodynamic model

Two thermodynamic "calculators" are defined in this simulation:

- “Process”: this calculator is used for the entire flowsheet, except for the boiler. The selected thermodynamic profile is SRK. The binary interaction parameters are those of the database supplied with Simulis Thermodynamics.
- “Fumes”: this calculator is used for the boiler. This calculator (components and thermodynamic model) is generated automatically when configuring the boiler (“Boiler”).

1.5. Chemical reactions

All reactions are occurring in the vapor phase. The heats of reaction are calculated from the standard enthalpies of formation (1 atm, 25°C, ideal gas).

✓ The desulfurization reaction considered in this simulation is:

$$C_4H_8S + H_2 \rightarrow H_2S + C_4H_{10} \quad (1)$$

This reaction is supposed to be instantaneous: its conversation ratio is defined in the corresponding reactor.

✓ The steam reforming of methane reaction is:

$$CH_4 + H_2O \leftrightarrow CO + 3H_2 \quad (2)$$

Its equilibrium constant is:

$$Ln(K_{eq}) = 29.3014 - \frac{26248.4}{T}$$

✓ The other steam reforming reactions are:

$$C_2H_6 + 2H_2O \rightarrow 2CO + 5H_2 \quad (3)$$

$$C_3H_8 + 3H_2O \rightarrow 3CO + 7H_2 \quad (4)$$

$$C_4H_{10(iso)} + 4H_2O \rightarrow 4CO + 9H_2 \quad (5)$$

$$C_4H_{10(normal)} + 4H_2O \rightarrow 4CO + 9H_2 \quad (6)$$

$$C_5H_{12(iso)} + 5H_2O \rightarrow 5CO + 11H_2 \quad (7)$$

$$C_5H_{12(normal)} + 5H_2O \rightarrow 5CO + 11H_2 \quad (8)$$

$$C_6H_{14} + 6H_2O \rightarrow 6CO + 13H_2 \quad (9)$$

These reactions are supposed to be instantaneous their conversation ratios are defined in the corresponding reactors.

✓ The “water gas shift” reaction is:

$$CO + H_2O \leftrightarrow CO_2 + H_2 \quad (10)$$

Its equilibrium constant is:

$$Ln(K_{eq}) = -4.35369 + \frac{4593.16}{T}$$

✓ The reaction considered for the secondary reforming of methane is:

$$CH_4 + O_2 \leftrightarrow CO_2 + 2H_2O \quad (11)$$

Its equilibrium constant is:

$$Ln(K_{eq}) = 40$$

✓ The methanation reaction are:

$$CO_2 + 4H_2 \leftrightarrow CH_4 + 2H_2O \quad (12)$$

Its equilibrium constant is:

$$Ln(K_{eq}) = -24.94771 + \frac{21655.25}{T}$$

$$CO + 3H_2 \leftrightarrow CH_4 + H_2O \quad (13)$$

Its equilibrium constant is:

$$Ln(K_{eq}) = -29.3014 + \frac{26248.4}{T}$$

✓ Ammonia synthesis:

- In this first approach (“PSPS_EX_EN-Ammonia-Synthesis-Process.pmp3”), the synthesis reaction considered is:

$$N_2 + 3H_2 \rightarrow 2NH_3 \quad (14)$$

This reaction is supposed to be instantaneous: its conversation ratio is defined in the corresponding reactor.

- In the detailed approach, for the simulation dedicated to the ammonia synthesis reactor (“PSPS_EX_EN-Ammonia-Synthesis-Reactor.pmp3”), the model proposed by Temkin-Pyzhev [MUR70] is used. It assumes the two following reactions:

$$N_2 + 3H_2 \rightarrow 2NH_3 \quad (15)$$

$$2NH_3 \rightarrow N_2 + 3H_2 \quad (16)$$

Then, the reaction rate is:

$$r = 17895{,}4exp\left(\frac{-20800}{RT}\right)\frac{P_{N_2}P_{H_2}^{1,5}}{P_{NH_3}} - 2{,}5714.10^{16}exp\left(\frac{-47400}{RT}\right)\frac{P_{NH_3}}{P_{H_2}^{1,5}}$$

Activation energy unit: kcal/kmol

Time unit: h

Pressure unit: atm

The following table details the reaction sets created to define the reactions used for each reactor.

Reaction sets	Reactions
Desulfurization	(1)
Primary reforming (part 1)	(3), (4), (5), (6), (7), (8), (9)
Primary reforming (part 2)	(2)
Secondary reforming	(2), (10), (11)
CO conversion	(10)
Methanation	(12), (13)
Ammonia synthesis (simplified)	(14)
Ammonia synthesis (detailed)	(15), (16)

1.6. Operating conditions

1.6.1. Entire simulation

✓ Feeds

	Natural gas inlet	Air inlet	BFW
Mass fraction			
Water		0.00994	1
Oxygen		0.20732	
Carbon dioxide	0.019724	0.00039	
Nitrogen	0.038600	0.	
Argon		0.00921	
Methane	0.867090		
Ethane	0.051740		
Propane	0.012590		
Isobutane	0.001537		
n-butane	0.002357		
Isopentane	0.000537		
n-pentane	0.000549		
n-hexane	0.001274		
Tetrahydrothiophene	0.004002		
Flow rate	15 042.6 kg/h	28 001.4 Nm^3/h	66 000 kg/h
Temperature (°C)	6	8	25
Pressure (bar)	45	1.01325	36

✓ Simple reactors

	Temperature (°C)	Reaction sets	Conversion ratio	
R101	304.6	Desulfurization	Tetrahydrothiophene	1
R102	755	Primary reforming (part 1)	Ethane Propane Isobutane n-butane Isopentane n-pentane n-hexane	1 1 1 1 1 1 1
R108	Adiabatic	Ammonia synthesis (simplified)	Nitrogen	0.15

Nitrogen

✓ Continuous stirred tank reactors

	Temperature	Pressure drop (bar)	Reaction sets	Approach temperature (°C)	State
R103	755°C	0.5	Primary reforming (part 1)	67	Vapor
R104	Adiabatic	1.6	Secondary reforming	37	Vapor
R105	Adiabatic	0.35	CO conversion	0	Vapor
R106	Adiabatic	0.5	CO conversion	0	Vapor
R107	Adiabatic	0	Methanation	0	Vapor

✓ Liquid-vapor separators

	Flash type	Specification
S104	Constant temperature and pressure	62°C 25.2 bar
S102	Constant pressure and enthalpy	26 bar Adiabatic
S105		24.9 bar Adiabatic
S106		The lowest of the feed streams Adiabatic
S107		
S108		
S109		
S110		
S111		
S112		25 bar Adiabatic
S113		The lowest of the feed streams Adiabatic

✓ Cooler/Heater heat exchangers

	Temperature (°C)	Pressure drop (bar)
E101	314	8.9
E102	325	2
E103	480	0
E104	560	0
E105	505	0
E106	345	0
E107a	407.232	0
E108	203	0
E109	194	0
E110	110	0
E111a	235.721	0
E114	17.7	0
E115	300	0
E116	-9.4	0
E117a	17	0
E118a	157	0
E119a	369	0
E120	379	0
E121	199.7	0
E123	18	0
E125	-21.5	0
E126	-21	0
E127	11	0
E313	28	0
E314	20	0
E315	31.2	0

For utilities without phase change, the following exchangers are defined:

	Utility	Type	Efficiency	T_{in} (°C)	T_{out} (°C)	P_{out} (bar)
E114	Water	Counter-current	0.8	15.1	22	4
E121				100	268	96.6
E123				15.1	22	5

✓ Simple heat exchangers

It's possible to "couple" a "Cooler/heater" unit operation with a "Simple heat exchanger" unit operation using an information stream. The information stream is used to transfer the heat duty calculated by the "Cooler/heater" unit operation (i.e., at a fixed outlet temperature) to the "Simple heat exchanger" unit operation. The "Simple heat exchanger" unit operation then calculates the current outlet temperature from this value. This modeling makes it possible to reduce the number of recirculation loops in the process modeled, thereby reducing the calculation time and the complexity of the resolution. The association of a "Cooler/heater" and a "Simple heat exchanger" (by an information stream) is equivalent to the use of a "Generalized heat exchanger" (see 1.8.2 Use of information streams).

	Heat duty
E107b	Value received by information stream from the cooler/heater E107a Initial value: 0 kcal/h
E111b	Value received by information stream from the cooler/heater E111a Initial value: 9 800 000 kcal/h
E117b	Value received by information stream from the cooler/heater E117a Initial value: 5 240 000 kcal/h
E118b	Value received by information stream from the cooler/heater E118a Initial value: 12 490 000 kcal/h
E119b	Value received by information stream from the cooler/heater E119a Initial value: 15 000 000 kcal/h

✓ Generalized compressors

The parameters of the air compressor K101 are:

- Type : Isentropic
- Exhaust pressure : 30.2 bar
- Efficiencies : Isentropic 0.95
  Mechanical 0.95
  Electrical 0.98
- Number of stages : 3
  Same compression ratio between stages
  Outlet temperature of intercoolers 10°C above the dew temperature

The other compressors, listed in the table below, are polytropic compressors with a mechanical efficiency of 0.95 and an electrical efficiency of 0.98.

	Exhaust pressure (bar)	**Polytropic efficiency**
K102	69	0.90
K103	65	0.76
K104	119	0.69
K105	170	0.59
K106	180	0.90

✓ Stream mixers

	Outlet pressure (bar)
M01, M03, M04, M05, M06	Equal to the lowest of the feeds
M02	31.3

✓ Stream splitters

	Specified stream	TO	Specification type	Specification
V101	C9	M01	Splitting ratio	0
V102	C24	E108		0.961234
V103	C44	K103		0.977253
V104	C76	E125		0.0129
V106	C5	M02	Mass flow rate	61 t/h

✓ Expansion valve

	Constraint type	Specification
V105	Pressure specification	7.4 bar

✓ Component splitters

	Temperature	Components	Recovery rate
S101	294°C	Tetrahydrothiophene Hydrogen sulfide All other component	0 0 1
S103	Equal to the first feed stream temperature	Carbon dioxide All other component	0.00199714 1

- ✓ Boiler (“Boiler”)

Only the parameters different from the default ones are listed below:

Internal exchanger specification:

Fumes temperature at the outlet : 90°C

Presence of an economizer:

Calculation mode : UA model

Area : 200 m^2

Overall heat exchange coefficient : 120 $kcal/h/m^2/K$

Combustion specification:

Fuel defined by the option “Advanced description”:

Methane content : 98% mass

Ethane content : 2% mass

Update the calculation of the stoichiometric coefficients and load the fumes components.

Constraint specification:

Unit operation constraint : Useful power imposed

Utility outlet temperature : 379°C

- ✓ Constraints and recycles (“SPEC”)

Constraints and recycles module is added to the simulation in order to increase the maximum number of iterations from 20 (default value) to 50.

- ✓ Energy pinch analysis (“Energy Pinch Analysis”)

All parameters are the default ones, including the 10°C pinch. The printing of integration potentials is activated in the “Advanced options” tab of the module.

- ✓ Electrical balance (“Electrical balance”)

All parameters are the default ones.

- ✓ Generalized balance (“Generalized balance”)

All parameters are the default ones.

1.6.2. Simulation of the ammonia synthesis reactor

✓ Feed

Partial molar flow rates (kmol/h)	
Ammonia	771
Hydrogen	12 962
Nitrogen	6 179
Argon	238
Methane	865
Temperature (°C)	157
Pressure (bar)	180

✓ Plug flow reactor

The parameters of the R201 reactor are:

- Reaction set : Ammonia synthesis (detailed)
- Operating mode : Service fluid (calculated temperature)
- Service fluid flow direction : Counter-current
- Wall thermal conductivity : 16.3 W/m/K
- Tube diameter for the service fluid : 2.75 m
- Physical state : Vapor
- Reactor length : 7 m
- Tubes external diameter : 2.45 m
- Tubes internal diameter : 2.345 m
- Roughness : 10^{-6} m
- Inclination : Horizontal
- Number of tubes : 1
- Grid step for printing : 25

✓ Cooler/heater heat exchangers

	Temperature (°C)	Pressure drop (bar)
E201a	369	0
TEMP	Equal to the feed stream temperature	0

To connect the stream leaving the external jacket of the R201 reactor to the inlet of the reactive fluid of this same reactor, it is necessary in ProSimPlus to insert a unit operation. Indeed, it's not possible to connect a unit operation to itself in ProSimPlus. The role of the "TEMP" cooler/heater is therefore to be able to make this connection. For this reason, it has no thermal role.

- ✓ Simple heat exchanger

The implementation of this heat exchanger is the same as described in the corresponding part in paragraph 1.6.1.

	Heat duty
E107b	Value received by information stream from the cooler/heater E201a Initial value: 0 kcal/h

1.7. Initializations

The calculation sequence is automatically determined by ProSimPlus.

1.7.1. Entire simulation

Three tear streams are detected for the entire simulation:

- ✓ C47: Outlet stream of the E115 heat exchanger
- ✓ C78: Outlet stream of the E117b heat exchanger
- ✓ C88: Outlet liquid stream of the S113 vapor-liquid separator (flash)

These tear streams are not initialized. The initialization of these steams can make it possible to reduce the calculation time but it is not necessary in this case to reach convergence.

1.7.2. Ammonia synthesis reactor

One tear stream is detected for the simulation of the reactor alone:

- ✓ C104: Inlet stream of the R201 reactor

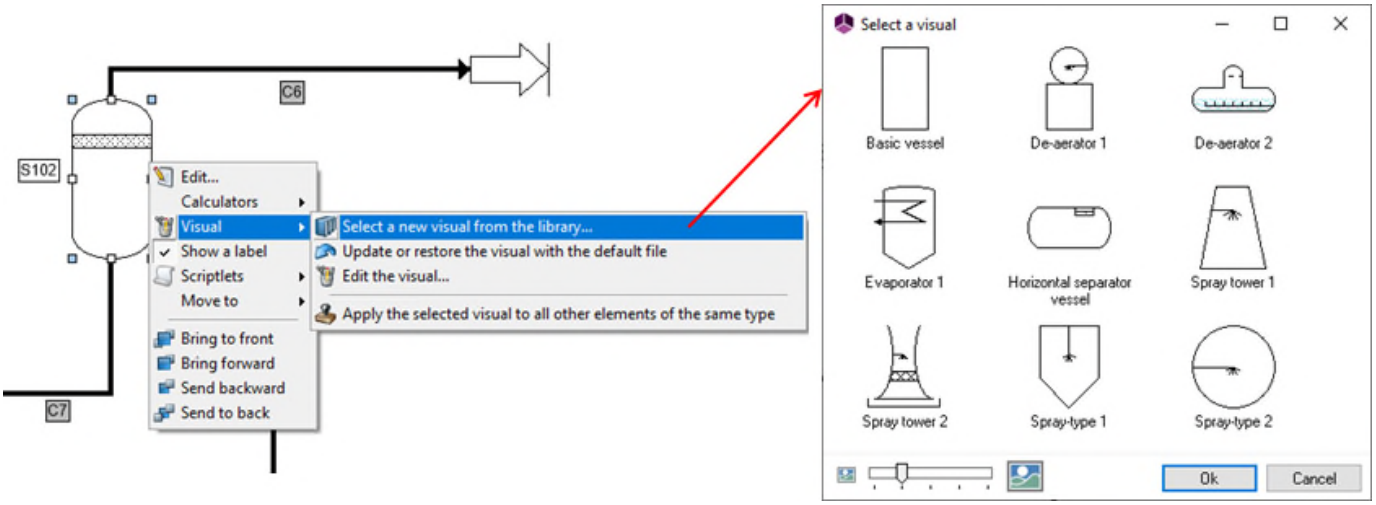
The initialization of this stream is provided in the table below (the partial molar flow rates and the pressure are identical to the inlet, only the temperature is different):

Partial molar flow rates (kmol/h)	
Ammonia	771
Hydrogen	12 962
Nitrogen	6 179
Argon	238
Methane	865
Temperature (°C)	370
Pressure (bar)	180

1.8. “Tips and tricks”

1.8.1. Change visuals of unit operations

It's possible to change the display of the unit operations to adapt them to the equipment of the process simulated. This can be done thanks to “Visual” sub-menu of the unit operations contextual menu. In the simulation file associated with this document, the visuals of the natural gas supply, of the “Fumes outlet”, of the “Purge gas” and of the “NH3 production”, of the heat exchangers as well as the one of the boiler have been changed from another one taken from the visual database:



1.8.2. Use of information streams

The use of an information stream to “couple”" a cooler/heater heat exchanger and a simple heat exchanger unit operation makes it possible to represent a 2-fluids heat exchanger. The combination of a “Cooler/heater” and a “Simple heat exchanger” (by an information stream) is equivalent to the use of a “Generalized heat exchanger”. This modeling technique for heat integration exchangers (i.e., heat exchangers between two process streams) avoids the creation of a recirculation loop.

1.8.3. Balance unit operations

The balance unit operations (electrical balance, water balance, utility balance, generalized balance) allow to perform quickly balances on the flowsheet. In this example, the electrical balance unit operation is used to obtain the electrical consumption of the process. The generalized balance unit operation allows in this simulation to have a complete material balance.

2. RESULTS

2.1. Process performance

The following table presents the key results on the process side:

Natural gas consumption (t/h)	15.04
Ammonia production (t/h)	31.97
Purity of the produced ammonia (% mass)	99.12

The following table presents the key results on the utility side:

Steam production (t/h)	66
Boiler gas consumption (t/h)	4.37
Electrical consumption (MW)	15

2.2. Ammonia synthesis reactor

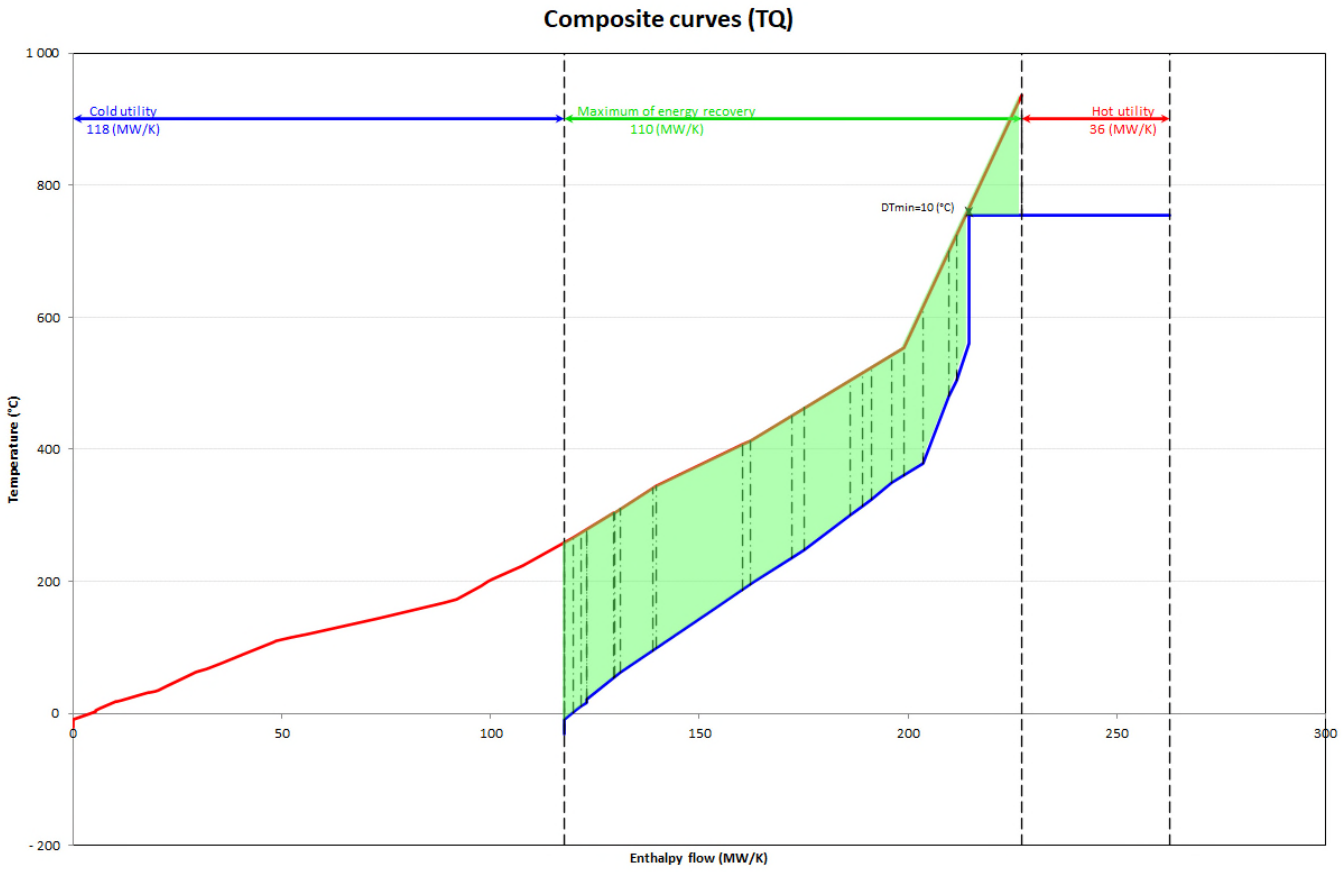
The simulation of the ammonia synthesis reactor calculates a conversion rate of the hydrogen of 15% and of the nitrogen of 11%. This value should be compared to the value of 15% specified for the nitrogen conversion rate in the complete simulation (§ 1.6.1).

It's possible to integrate the simulation of the ammonia synthesis reactor into the simulation of the entire process to represent the synthesis of ammonia more finely.

Note: It should be noted that "copy-paste" is entirely possible between the two simulations in order to directly reuse the flowsheet of "PSPS_EX_EN-Ammonia-Synthesis-Process.pmp3" in the file "PSPS_EX_EN-Ammonia-Synthesis-Reactor.pmp3".

2.3. Pinch analysis

The hot and cold composite curves plotted below are used to identify the relevant energy recoveries using the pinch method (see 4 4).



The overlap zone between the two curves (green zone) indicates the quantity of energy that it will be possible to save with internal energy recoveries by associating in the most judicious way the “energy sources streams” (hot streams) with “energy sinks streams” (cold streams). This overlap zone is named “MER” for Maximum of Energy Recovery. On the left side of the diagram, the deviation between the two curves shows the minimum cold utility requirement necessary for the process if 100% of the MER is recovered by an efficient network of heat exchangers. On the right side of the diagram, the deviation between the two curves shows the minimum hot utility requirement necessary for the process if 100% of the MER is recovered by an efficient network of heat exchangers.

Maximum energy recovery (MW)	110
Minimum cold utility heat duty (MW)	118
Minimum not utility heat duty (MW)	36

By checking the “Integration potential printing” box in the “Advanced options” tab of the “Energy Pinch Analysis” unit, it’s possible to know the heat duties currently required for the cold and hot utilities of the simulated process. Here, ≈ 151 MW is currently supplied by the cold utilities (the heat duty recovered cover ≈ 34% of needs) and ≈ 68 MW by the hot utilities (the heat duty recovered ≈ 53% of needs, ≈ 77 MW recovered by integration heat exchangers). The current integration rate reaches ≈ 70%. The thermal integration of the process is therefore interesting, but energy savings are still achievable.

	HEAT DUTY (MW)			SATISFACTION RATIO (%)
	MINIMUM	ACTUAL	MAXIMUM	
COLD FLUID	117.687	150.590	227.209	33.722
HOT FLUID	35.5664	68.4688	145.088	52.809

Maximum energy recovery	=	109.522	(MW)
Pinch temperature	=	759.990	(°C)
Real integration ratio	=	69.958	(%)
Integration potential indicator #1	=	58.836	(%)
Integration potential indicator #2	=	41.679	(%)

ACTUAL INTEGRATION HEAT EXCHANGER NETWORK

HEAT EXCHANGER	Q (MW)
E107b - E107a	0.440599
E111b - E111a	5.91717
E119b - E119a	39.7584
E118b - E118a	25.4059
E117b - E117a	5.09740
TOTAL	76.6195

.

3. REFERENCES

[AMH22] AMHAMED A.I., QARNAIN S.S., HEWLETT S., SODIQ A., ABDELLATIF Y., ISAIFAN R.J., ALREBEI O.F., “Ammonia Production Plants – A Review”, Fuels, 3, 408-435 (2022).

[BAD65] BADDOUR R.F., BRIAN P.L.T., LOGEAIS B.A., EYMERY J.P., “Steady-State Simulation of an Ammonia Synthesis Converter”, Chem. Eng. Sci., 20, 281-292 (1965).

[CAN03] RESSOURCES NATURELLE DU CANADA, “L’analyse Pinch : pour l’utilisation efficace de l’énergie, de l’eau, de l’hydrogène” (2003).

[GOD12] GODULA-JOPEK A., JEHLE W., WELLNITZ J., “Hydrogen Storage Technologies”, Wiley-VCH (2012).

[KAI99] KAISER V., FILIPPI E., LEGER H.D., LESUR P., “Calcul des réacteurs catalytiques. Synthèse d’ammoniac”, Techniques de l’Ingénieur, J4040 (1999).

[MUR70] MURASE A., ROBERTS H.L., CONVERSE A.O., “Optimal Thermal Design of an Autothermal Ammonia Synthesis Reactor”, Ind. End. Chem. Process Des. Develop., 9, 503-513 (1970).

[PAT19] PATTABATHULA V., “Ammonia”, Kirk-Othmer Encyclopedia of Chemical Technology (2019).

[ROU18] ROUWANE A., “Ammoniac”, Techniques de l’Ingénieur, J6135 (2018).

4. Appendix

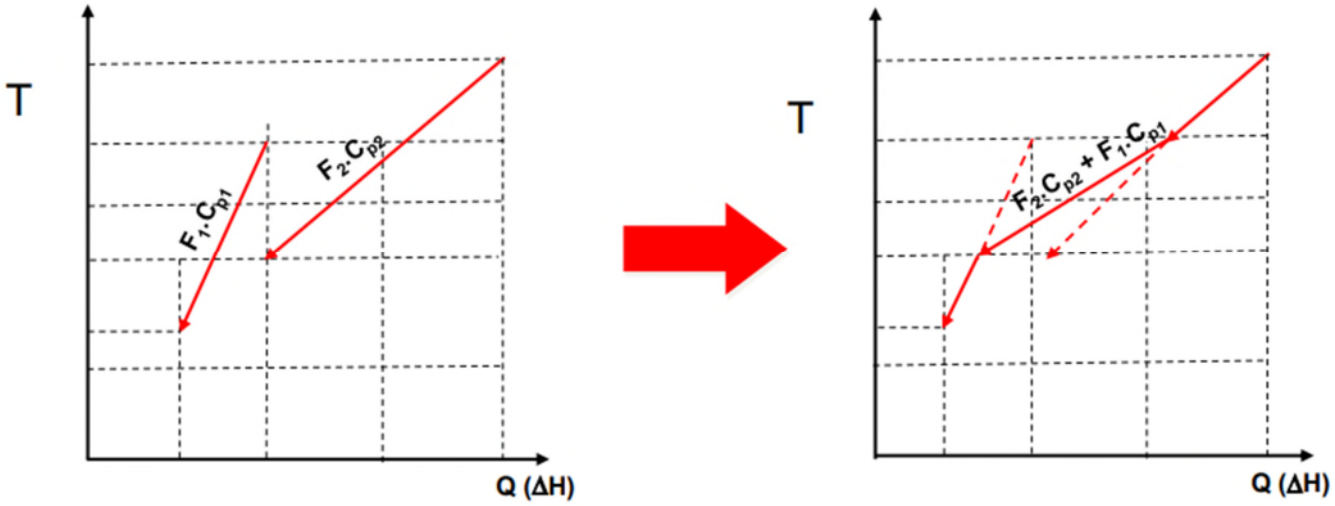
Pinch analysis or Pinch technology is a rigorous and structured method for optimizing the energy expenditure of a process.

The main characteristic of Pinch analysis is to determine, for a particular process or for the whole plant, the minimum consumption of energy, water, and hydrogen necessary for its operation. It is therefore possible to assess the maximum potential for improvement, even before starting detailed design work. The method can be applied systematically for each process of the plant or globally for the entire site.

Typical savings identified with a Pinch analysis in industrial sectors such as petroleum refining, chemicals, steel, pulp and paper, petrochemicals, and agribusiness are in the range of 10-35% [CAN03].

The first step of the pinch method is to construct the composite curves. To draw these curves, it is necessary to know the values of the flow rates of the streams F, their specific heat capacity C_p, and the inlet and outlet temperatures (ΔT) for each heating and cooling of the process. The composite curves represent the profile of the available heat sources ("hot composite curve") and the profile of the thermal requirements of the process ("cold composite curve"). Depending on their shape and location, these curves provide information on the possibilities for heat recovery within the process.

The following figure shows the construction of the hot composite curve on a Temperature-Quantity of heat exchanged diagram. The hot composite curve is constructed simply by adding, for each temperature interval, the changes in thermal load of each of the streams taken individually.



The construction is based on the following equation:

$$Q = FC_p\Delta T$$

With:

Q : Heat duty exchanged (W)

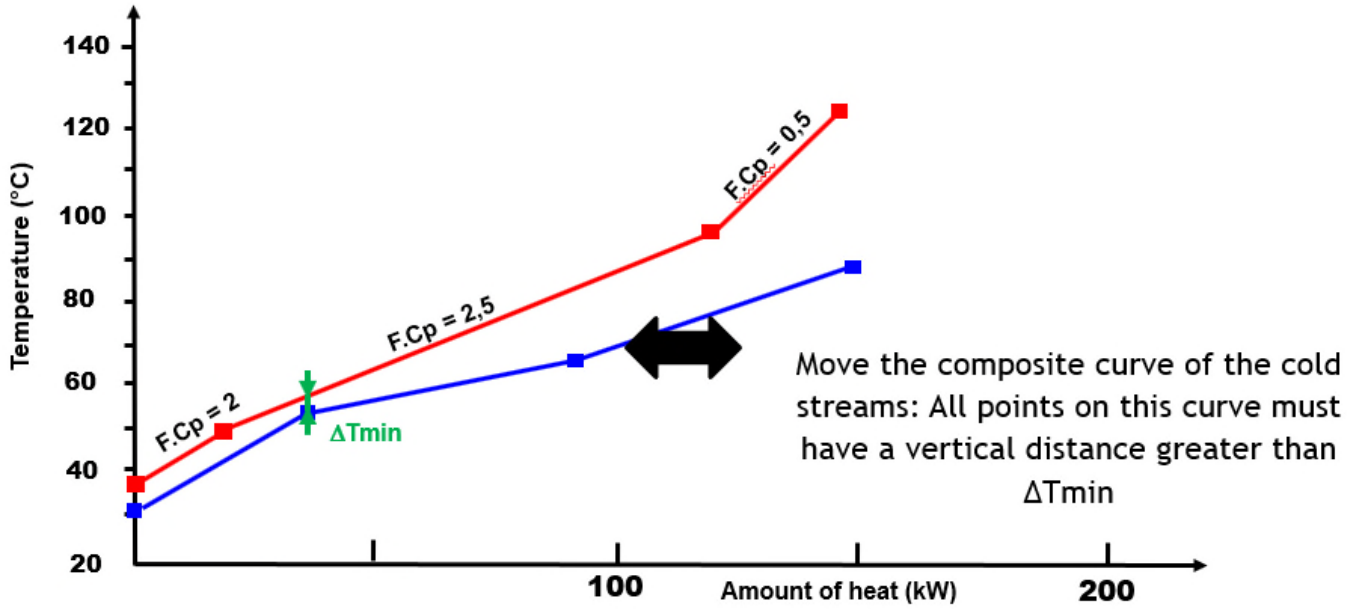
F : Flow rate of the heated stream or the cooled stream (kg/s)

C_p : Specific heat of the stream (J/kg/°C)

ΔT : Temperature difference between the inlet and the outlet of the heating or cooling (°C)

The cold composite curve is obtained in the same way.

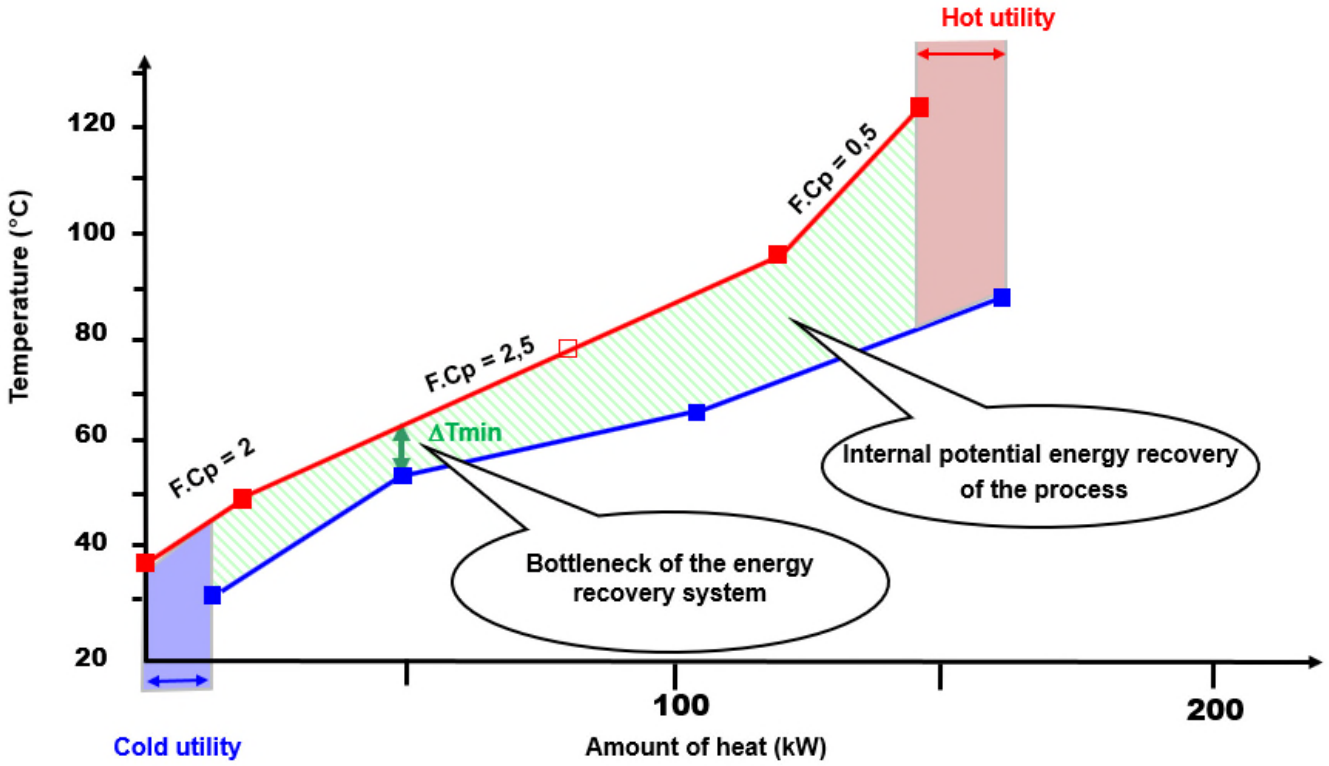
To establish the minimum energy consumption target for the process under study, the cold composite curve is positioned on the same diagram as that of the hot composite curve.



The 2 curves are slid horizontally until there is a certain difference between the 2 curves. The hot composite curve must be above the cold composite curve (for heat exchange to be possible). The smallest difference between the two curves (the locus where they are close) is the temperature difference ΔTmin also called the pinch. This value indicates the minimum temperature difference that is acceptable between the two fluids in a heat exchanger. This pinch value varies depending on the processes and heat exchanger technologies used in each process (from 10 to 20°C for petrochemicals, from 3 to 5°C for cryogenics...).

The overlap area of the two curves represents the Maximum of Energy Recovery (MER). The areas outside the overlap area represent the amounts of energy requirement to be supplied by the utilities.

Pinch analysis therefore makes it possible to establish targets for the minimum energy consumption necessary to meet the needs of a process, even before starting the design of the heat exchanger network. This allows to quickly identify the extent of energy savings that can be considered at an early stage of the analysis. This advantage is probably the most interesting that Pinch analysis offers.



As the two composite curves move apart, the pinch increases, and therefore the temperature differences between hot streams and cold streams increase. It then becomes possible to reduce the exchange surfaces of the heat exchangers for the recovery of MER and therefore to reduce the cost of heat exchangers (investment). Conversely, the greater the pinch is, the lower the MER (overlap zone) is. The process then consumes more hot and cold utilities, and the energy cost increases when pinch increases too.

The following figure shows that there is an optimal value for the pinch, which minimizes the total cost, taking into account the expenses related to the investment and those related to energy [CAN03].