THREE-CYCLE COMBINED ELECTRICITY GENERATION PLANT

EXAMPLE PURPOSE

This example presents the simulation of a power plant with three combined cycles: a solid oxide fuel cell (SOFC), a gas turbine (GT) and a steam cycle (SC).

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1. PROCESS MODELING

1.1. Process description

This example presents the production of electricity with three combined cycles. A Solid Oxide Fuel Cell (SOFC) operates at high temperature, from 600 to 1000°C. By combining the heat of the gas leaving the SOFC with a combined cycle for the production of electricity, a very high efficiency power generation system can be obtained (around 60%). This example is inspired by a process developed by Mitsubishi Heavy Industries (MHI) as illustrated below. This process is based on fossil fuel energy with three cascade stages: SOFC, gas turbine (GT) and steam turbine (ST). For the last stage, a steam cycle will be used to maximize the energy recovery of the process [MHI11].
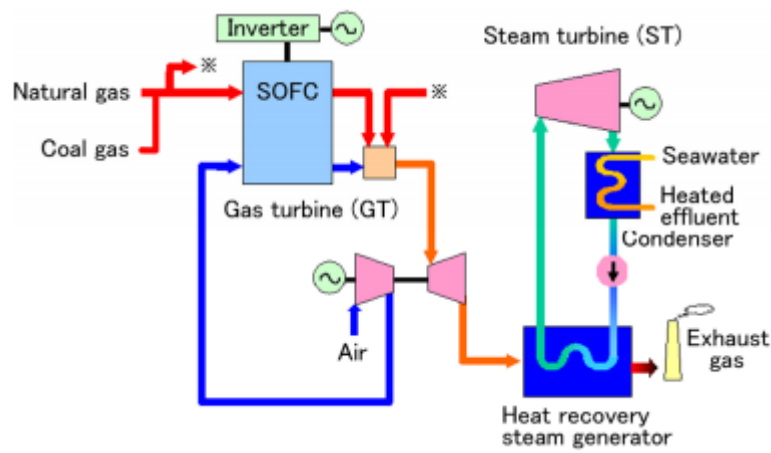
In this context, the process is therefore divided into 3 parts:

> ➢ a solid oxide fuel cell (SOFC)
> ➢ a gas turbine (GT)
> ➢ a steam cycle (SC)

The SOFC fuel cell is an interesting energetic alternative because it is efficient, and it has a low environmental impact. It is made of two electrodes (anode and cathode) separated by a solid electrolyte. The fuel, usually hydrogen, is introduced into the anode compartment where an oxidation reaction occurs. The produced electrons go into the external electrical circuit. The oxygen is introduced into the cathode compartment where it is reduced into O^{2-} oxide ions. These ions diffuse through the ionically conductive electrolyte.

For the gas turbine (GT), the air is compressed before flaming up with the gas from the SOFC in the combustion chamber. The fumes are then expanded in the turbine, which generates the physical energy into mechanical energy and finally electricity.

For the steam cycle (SC), the water is compressed and then vaporized in contact with a hot source. The water expansion through the turbine generates the physical energy converted into electricity.

1.2.   Simulation flowsheet
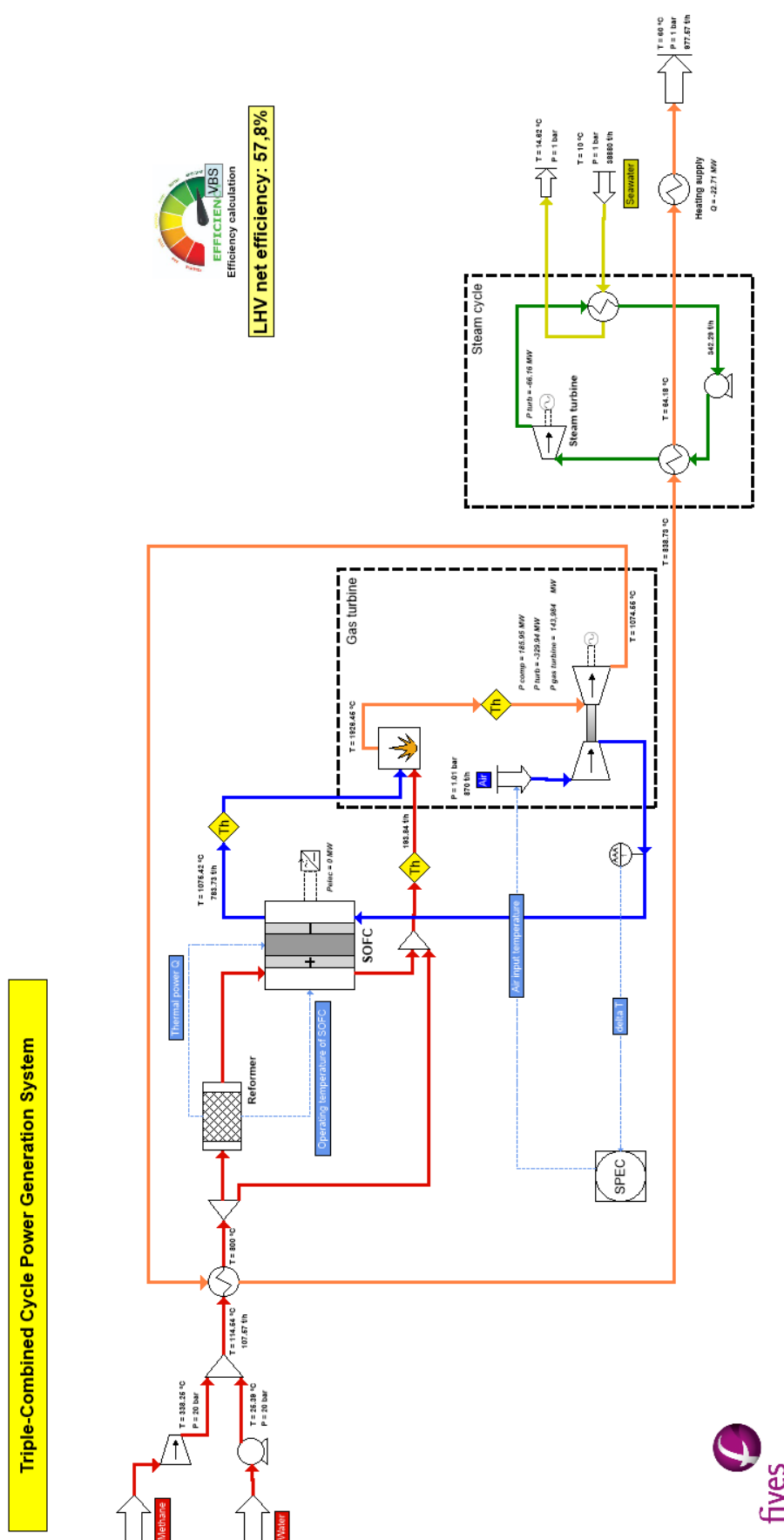
Electricity generation plant simulation of a three-cycle combined process

1.3. <u>Components</u>

The components involved 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
Nitrogen	N_2	7727-37-9
Carbon dioxide	CO_2	124-38-9
Methane	CH_4	74-82-8
Ammonia	NH_3	7664-41-7
Hydrogen sulfide	H_2S	7783-06-4
Sulphur dioxide	SO_2	7446-09-5
Nitric oxide	NO	10102-43-9
Carbon monoxide	CO	630-08-0
Sulphur trioxide	SO_3	7446-11-9

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[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**

Three thermodynamic "calculator" are defined to simulate this example:

➢ "Global calculator": this calculator is used for the global flowsheet, except for the steam cycle and the combustion module. The selected thermodynamic model is Soave-Redlich-Kwong (SRK).

➢ "Fumes – Biogas": this calculator is especially used to simulate the inlet and outlet streams (fuel, air, fumes) of the combustion unit.

➢ "Water": this calculator is especially used for the pure water streams of the steam cycle. Therefore, the "pure water" model is selected.

1.5. Chemical reactions

The following reaction takes place in the simple reactor:
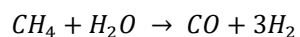
$$CH_4 + H_2O \rightarrow CO + 3H_2$$

This reformer converts part of the methane into carbon monoxide and hydrogen for the SOFC fuel cell. The methane conversion rate is 0.85 (85%).

Component	Stoichiometric coefficients
OXYGEN	0,000000
HYDROGEN	3,000000
CARBON DIOXIDE	0,000000
CARBON MONOXIDE	1,000000
NITROGEN	0,000000
WATER	-1,000000
METHANE	-1,000000
HYDROGEN SULFIDE	0,000000
SULFUR DIOXIDE	0,000000
SULFUR TRIOXIDE	0,000000
NITRIC OXIDE	0,000000
AMMONIA	0,000000

1.6. Operating conditions

1.6.1. Solid Oxide Fuel Cell

✓ Feeds

Name:	Methane	Water
Partial mass flowrate (t/h)		
Oxygen	0	0
Hydrogen	0	0
Carbon dioxide	0	0
Carbon monoxide	0	0
Nitrogen	0	0
Water	0	59.45
Methane	48.12	0
Temperature (°C)	25	25
Pressure (bar)	1.01325	1.01325

✓ Compressor "Fuel compressor"

Specification	Pressure
Exhaust pressure (bar)	20
Isentropic efficiency	0.75
Mechanical efficiency	0.95
Electrical efficiency	0.98

✓ Centrifugal pump "P1"

Specification	Pressure
Exhaust pressure (bar)	20
Volumetric efficiency	0.65
Mechanical efficiency	0.95
Electrical efficiency	0.98

✓ Generalized heat exchanger "Generalized heat exchanger"

Exchanger type	Counter current or multipass
Specification type	Outlet temperature of the cold stream
Outlet temperature (°C)	800

✓ Stream splitter "S1"

Supplied specification	Splitting ratio
Splitting ratio	0.378
Automatically calculated stream	Incoming stream in the simple reactor

✓ Simple reactor "Reformer"

Reaction set	Global set
Thermal behaviour of the reactor	Reactor with a specified output temperature
Temperature (°C)	800
Pressure specification	The lowest of the feeds
Methane conversion rate	0.85

✓ Solid Oxide Fuel Cell "SOFC"

Carbon monoxide conversion rate	0.85
Hydrogen conversion rate	0.85
Cathode-anode output deviation temperature (°C)	0.6
Energy efficiency	0.5

✓ Calculator Switch

A "Calcluator switch" module is used to change the calculator of a material stream entering in a unit operation for which the calculator is different than the stream calculator. This calculator change is necessary especially for two calculators using different enthalpy basis, different thermodynamic paths or different thermodynamic approaches (homogeneous vs heterogeneous).

	Calculator switch	Calculator switch 1
Thermodynamic model	"Fumes – Biogas"	"Fumes – Biogas"

✓ Management of constraints and recycling ("SPEC"): the "Constraints and recycles" module is used to reach a specified temperature at the compressor outlet. The module is set by default.

This "Constraints and Recycles" module uses the deviation between the measured temperature of the "Air compressor" outlet and the set point in order to adjust the temperature of the "Air" feed.

✓ Cooler/Heater "Heating supply"

Outlet temperature (°C)	60

Note: All mixers are set with default values (outlet pressure is the lowest of the supplies).

1.6.2. Gas turbine

✓ Feed

Name:	Air
Molar fractions	
Oxygen	0.21
Hydrogen	0
Carbon dioxide	0
Carbon monoxide	0
Nitrogen	0.79
Water	0
Methane	0
Mass flowrate (t/h)	870
Temperature (°C)	588.675
Pressure (bar)	1.01325

✓ Combustion "combustion"

LHV calculation	Calculated from compounds data
Heat losses (% of combustion power)	5
Combustion chamber pressure	Equal to the lowest of the feeds pressure

✓ Compressor "Air compressor"

Specification	Pressure
Exhaust pressure (bar)	20
Isentropic efficiency	0.78
Mechanical efficiency	0.95
Electrical efficiency	0.98

✓ Expander "Gas Turbine"

Supplied specification	Pressure
Exhaust pressure (bar)	1
Isentropic efficiency	0.85
Mechanical efficiency	0.95
Electrical efficiency	0.98

✓ Calculator Switch

Thermodynamic model	"Global calculator"

1.6.3. Steam cycle

✓ Feed

Name:	Seawater
Partial mass flowrate (t/h)	
Oxygen	0
Hydrogen	0
Carbon dioxide	0
Carbon monoxide	0
Nitrogen	0
Water	38800
Methane	0
Temperature (°C)	10
Pression (bar)	1

✓ Generalized heat exchangers "Generalized heat exchanger"

	Condenser	**Evaporator**
Exchanger type	Counter current or multipasses	Counter current or multipasses
Specification type	Subcooled below its bubble point	Minimal internal temperature approach
Temperature difference (°C)	5	10

✓ Expander "Steam turbine"

Specification	Pressure
Exhaust pressure (bar)	0.05
Isentropic efficiency	0.75
Mechanical efficiency	0.95
Electrical efficiency	0.98

✓ Centrifugal pump "P2"

| **Specification**	Pressure
Exhaust pressure (bar)	23
Volumetric efficiency	0.75
Mechanical efficiency	0.95
Electrical efficiency	0.98

1.7. <u>Initialization</u>

The calculation sequence is automatically determined by ProSimPlus. The tear stream "3" (output of the pump in the steam cycle) must be initialized to define the flux circulating in the loop. The following definition is used:

Stream	3
Partial mass flowrate (t/h)	
Oxygen	0
Hydrogen	0
Carbon dioxide	0
Carbon monoxide	0
Nitrogen	0
Water	342.29
Methane	0
Oxygen	0
Hydrogen	0
Carbon dioxide	0

1.8.   **"Tips and tricks"**

The "Diagram" scriptlet is used to obtain thermodynamic cycles or process points in a diagram (P-H, P-S, P-T, T-H, T-S). To use this scriptlet, one of the material streams of the cycle must be selected and then with a right click, run the scriptlet via "Scriptlets -> Diagram":
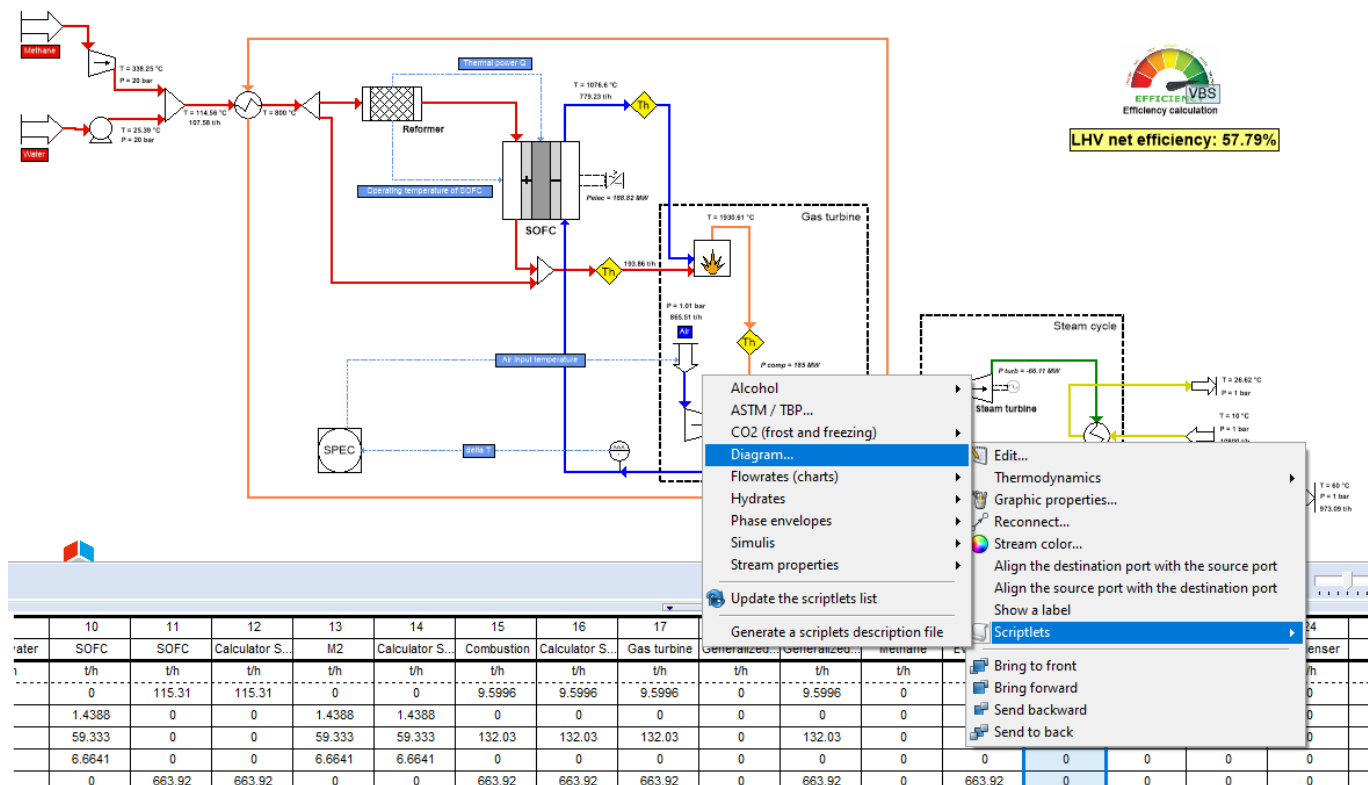
Definition of diagram type

This scriptlet is used to plot the points of the process
or the points of a thermodynamic cycle in a diagram.

Choose the diagram to plot
- ◉ P-H
- ○ P-S
- ○ P-T
- ○ T-H
- ○ T-S

Check the iso to plot
- ☐ Iso vapor ratio
- ☑ Iso temperature
- ☐ Iso pressure
- ☐ Iso enthalpy
- ☑ Iso entropy

[Ok] [Cancel]

Scriptlet parameters

Choose the type (enthalpy and entropy)
- ◉ Molar
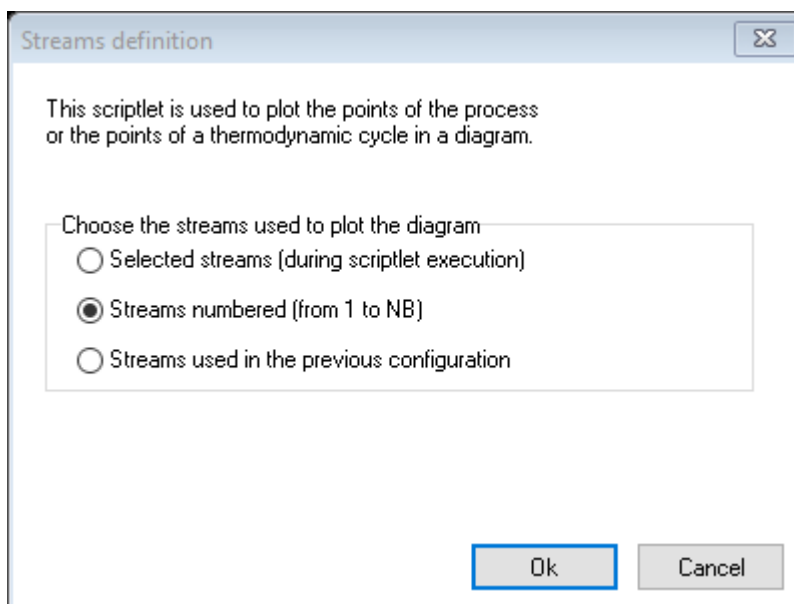- ○ Mass

Do you want to connect the points?
- ○ No
- ◉ Yes

Do you want to modify the number of iso?
- ◉ No
- ○ Yes

[Ok] [Cancel]

In order to connect the points of the cycle, it is necessary to number the material streams in the order of the desired cycle, from 1 to NB.
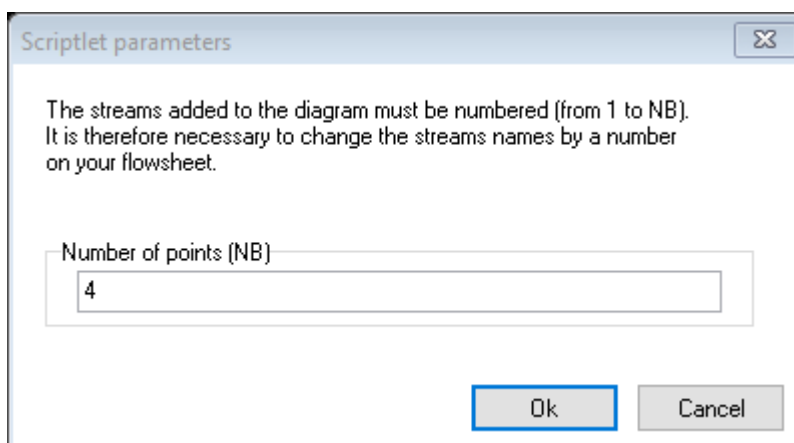
P-H diagram of stream: 1
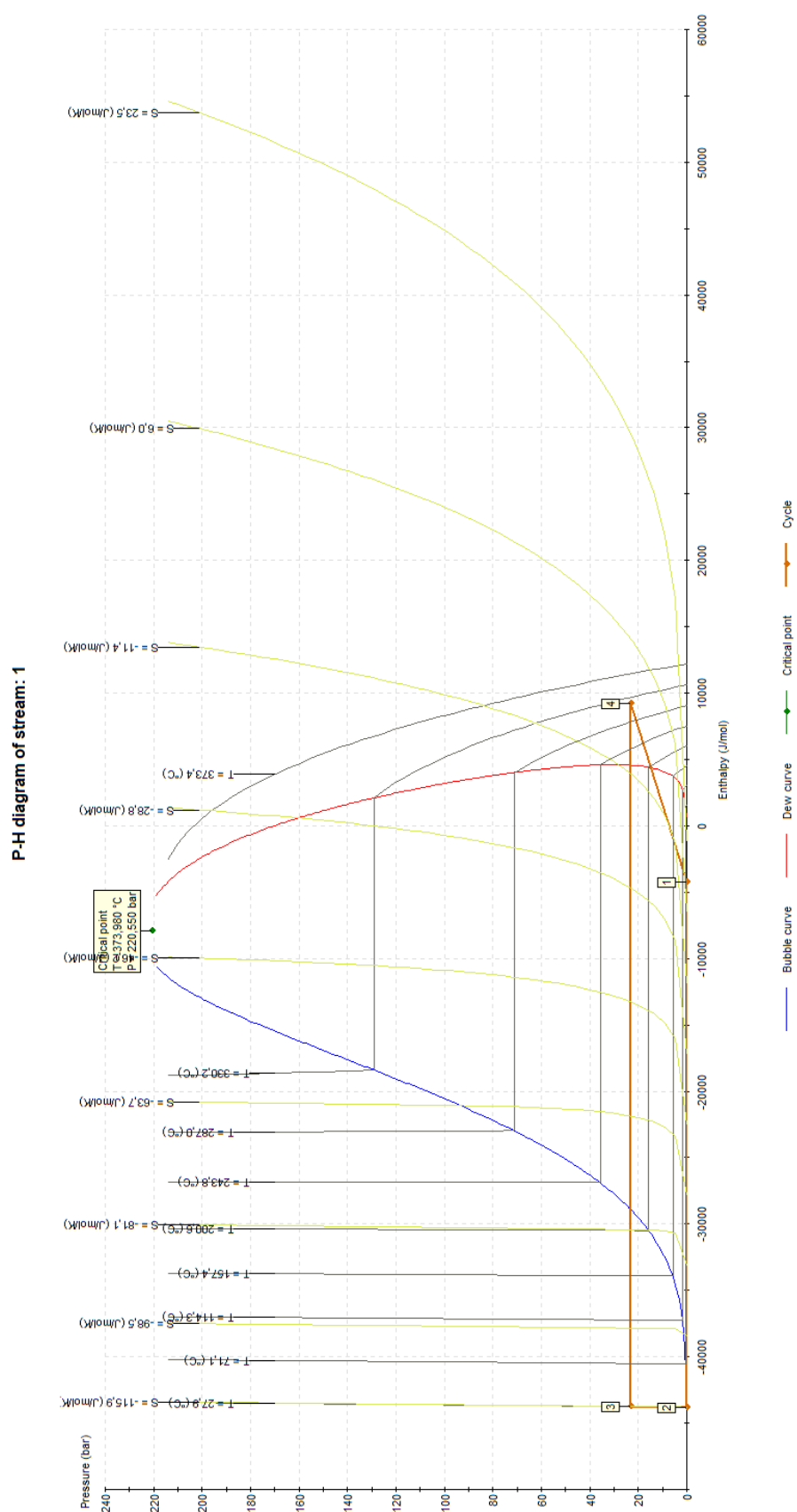
2. RESULTS

2.1. Main results

The Windows Script "Efficiency Calculation" module is used in the flowsheet and allows to summarize the performance of the process.

Windows Script ($XTMO)		
Name:	Efficiency calculation	
Desc:		

Identification | **Scripts** | Report | Streams | Notes

PAR size: 20

Index	Par	Info
1	0	Electricity produced
2	0	Heating supply
3	0	Auxiliary power
4	0	LHV of fuel
5	0	SOFC output power
6	0	Gas turbine output power
7	0	Steam turbine output power
8	0	Fuel
9	0	
10	0	Efficiency
11	0	
12	0	
13	0	
14	0	

OK   Cancel

The following script is used:

```vbs
'----------------------------------------------------------------------------'
' CALL OF "UNIT CONVERSION" SCRIPT
'----------------------------------------------------------------------------'
with CreateObject("Scripting.FileSystemObject")
  ExecuteGlobal .OpenTextFile(Project.ApplicationPath & "Scripts\UnitConversion.vbs", 1).ReadAll()
  ExecuteGlobal .OpenTextFile(Project.ApplicationPath & "Scripts\FormatDouble.vbs", 1).ReadAll()
  ExecuteGlobal .OpenTextFile(Project.ApplicationPath & "Scripts\StreamProperties.vbs", 1).ReadAll()
end with

Function OnCalculation()

   'Calculation of electrical power produced
   Module.parameter(5) = Project.Modules("SOFC").RealElectricPower
   Module.parameter(6) = abs(Project.Modules("Gas turbine").Power) - Project.Modules("Air
compressor").TotalUsefulPower
   Module.parameter(7) = abs(Project.Modules("Steam turbine").Power)
   Module.parameter(1) = Module.parameter(5) + Module.parameter(6) + Module.parameter(7)

   'Calculation of amount of heat recovered
   Module.parameter(2) = abs(Project.Modules("Heating supply").HeatDuty)

   'Calculation of auxiliary power
   Module.parameter(3) = Project.Modules("Fuel compressor").TotalUsefulPower +
Project.Modules("P1").UsefulPower + Project.Modules("P2").UsefulPower

   'Calculation of the methane LHV and net efficiency of the process
   Module.parameter(4)= LHVStream(Project.Modules("Methane").OutputStream(1),1)
   Module.parameter(8) = (Project.Modules("Methane").OutputStream(1).MassFlowRate *
Module.parameter(4))

   Module.parameter(10) = ((Module.parameter(1) - Module.parameter(3))*100) / Module.parameter(8)

OnCalculation = true
end Function


'----------------------------------------------------------------------------
' Print results
'----------------------------------------------------------------------------
Sub OnPrintResults()
with Module
   .PrintReport("SOFC output power                                       = " &
NiceFloat(ConvertFromProSim("Power", Module.parameter(5), "MW"))& "(MW)")
   .PrintReport("Gas turbine output power                                = " &
NiceFloat(ConvertFromProSim("Power", Module.parameter(6), "MW"))& "(MW)")
   .PrintReport("Steam turbine output power                              = " &
NiceFloat(ConvertFromProSim("Power", Module.parameter(7), "MW"))& "(MW)")
   .PrintReport("----------------------------------------------------------------------------")
   .PrintReport("Total electrical power produced                         = " &
NiceFloat(ConvertFromProSim("Power", Module.parameter(1), "MW"))& "(MW)")
   .PrintReport("")
   .PrintReport("Auxiliary power                                         = " &
NiceFloat(ConvertFromProSim("Power", Module.parameter(3), "MW"))& "(MW)")
   .PrintReport("")
   .PrintReport("Fuel power                                              = " &
NiceFloat(ConvertFromProSim("Power", Module.parameter(8), "MW"))& "(MW)")
   .PrintReport("")
   .PrintReport("Heating supply                                          = " &
NiceFloat(ConvertFromProSim("Power", Module.parameter(2), "MW"))& "(MW)")
   .PrintReport("")
   .PrintReport("")
   .PrintReport("LHV net efficiency                                      = " &
NiceFloat(FormatNumber(Module.parameter(10),2)) & "(%)")


end with
End Sub
```

2.2. <u>Solid Oxide Fuel Cell performance</u>

Simulation results	Notation	Value
Temperature increase on cathode side (°C)	se	275.42
Electric current generated (A)	B	$2.89.10^8$
Electric power in real operation (MW)	C	188.80
Elementary cell constituting the battery in reversible operation (V)	D	1.02
Elementary cell constituting the battery in real operation (V)	E	0.65
LHV of the anode gas* (kWh/Nm^3)	F	2.79
Heat duty generated by the combustion of the fuel by the SOFC $(\dot{m}_{CO}\, LHV_{CO} + \dot{m}_{H_2}\, LHV_{H_2})$ (MW)	G	377.6
Fuel Cell efficiency η (%)	H	50.0

* Only the hydrogen and the carbon monoxide are taken into account for the LHV calculation

Note: the fuel cell efficiency is calculated using the following formula:

$$\eta = \frac{P_{elec}}{\dot{m}_{CO}\, LHV_{CO} + \dot{m}_{H_2}\, LHV_{H_2}} * 100$$

With:

η : Energy efficiency of the fuel cell (%)

$\dot{m}_{CO}$: Fuel flowrate of the carbon monoxide CO consumed by the SOFC (mol/s)

$\dot{m}_{H_2}$: Fuel flowrate of the hydrogen H$_2$ consumed by the SOFC (mol/s)

LHV_{CO} : Low Heating Value (LHV) of the carbon monoxide CO consumed by the SOFC (J/mol)

LHV_{H_2} : Low Heating Value (LHV) of the hydrogen H$_2$ consumed by the SOFC (J/mol)

P_{elec} : Electric power (W)

2.3. Gas turbine performance

Simulation results	Notation	Value
Power used by the compressor (MW)	I	185.95
Power of the turbine equipment (MW)	J	329.94
Net power generated by the gas turbine (MW)	K (=J-I)	143.98
Consumed fuel LHV (kWh/Nm³)	L	1.80
Gas turbine efficiency η (%)	M	37.8

Note: Gas turbine efficiency is calculated using the following formula:

$$\eta = \frac{P_{elec}}{\dot{m}\,LHV} * 100$$

With:

η : Energy efficiency of the gas turbine (%)

$\dot{m}$: Fuel flowrate (mol/s)

LHV : Low Heating Value (LHV) of the consumed fuel (J/mol)

P_{elec} : Electric power (W)

2.4. <u>Steam cycle performance</u>

Simulation results	Notation	Value
Power generated by the expander (MW)	N	66.16
Power consumed by the pump (MW)	O	0.31
Net power generated by the steam cycle (MW)	P (=N-O)	65.85
Heat consumed by the evaporator (MW)	Q	279.5
Cycle performance coefficient (%)	R (=P/Q)	23.6

Note: Steam cycle efficiency is calculated using the following formula:

$$COP = \frac{P_{elec\ net}}{E_c} * 100$$

With:

COP : Cycle performance coefficient (%)

P_{elec} : Electric power (W)

E_c : Amount of heat consumed by the evaporator (W)

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2.5. Global process performance

Simulation results	Notation	Value
Power generated by SOFC (MW)	S	188.80
Power generated by gas turbine (MW)	T	143.98
Power generated by the expander of the steam cycle (MW)	U	66.16
Electric power produced (MW)	V (=S+T+U)	398.94
Exchanged heat (MW)	W	22.71
Power used by « Fuel compressor » and pumps (MW)	X	12.67
Fuel power (MW)	Y	668.75
Process efficiency η (%)	Z	57.76

Note: Global process efficiency is calculated using the following formula:

$$\eta = \frac{P_{elec} - P_{aux}}{\dot{m}\ LHV} * 100$$

With:

η : Energy efficiency of global process (%)

P_{elec} : Total electric power generated (W)

$\dot{m}$: Fuel flowrate (mol/s)

LHV : Low Heating Value (LHV) of the consumed fuel (J/mol)

P_{aux} : Electric power used by compressor and pumps (W)

3. REFERENCES

[KOB11]   Y. Kobayashi, Y. Ando, T. Kabata, M. Nishiura, K. Tomida, N. Matake, *Extremely High-efficiency Thermal Power System-Solid Oxide Fuel Cell (SOFC) Triple Combined-cycle System*, Mitsubishi Heavy Industries Technical Review, Vol.48, No. 3 (2011).

[WIL21]   Wilding, W. V.; Knotts, T. A., Giles, N. F., Rowley, R. L. DIPPR Data Compilation of Pure Chemical Properties; Design Institute for Physical Properties, AIChE: New York, NY (2021).

3. REFERENCES