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PROSIMPLUS APPLICATION EXAMPLE

INTEGRATED GASIFICATION COMBINED CYCLE (IGCC) PLANT

EXAMPLE PURPOSE
This example presents an Integrated Gasification Combined Cycle (IGCC) based on coal gasification using ProSimPlus.

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Energy

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1. PROCESS MODELING

1.1. Process presentation

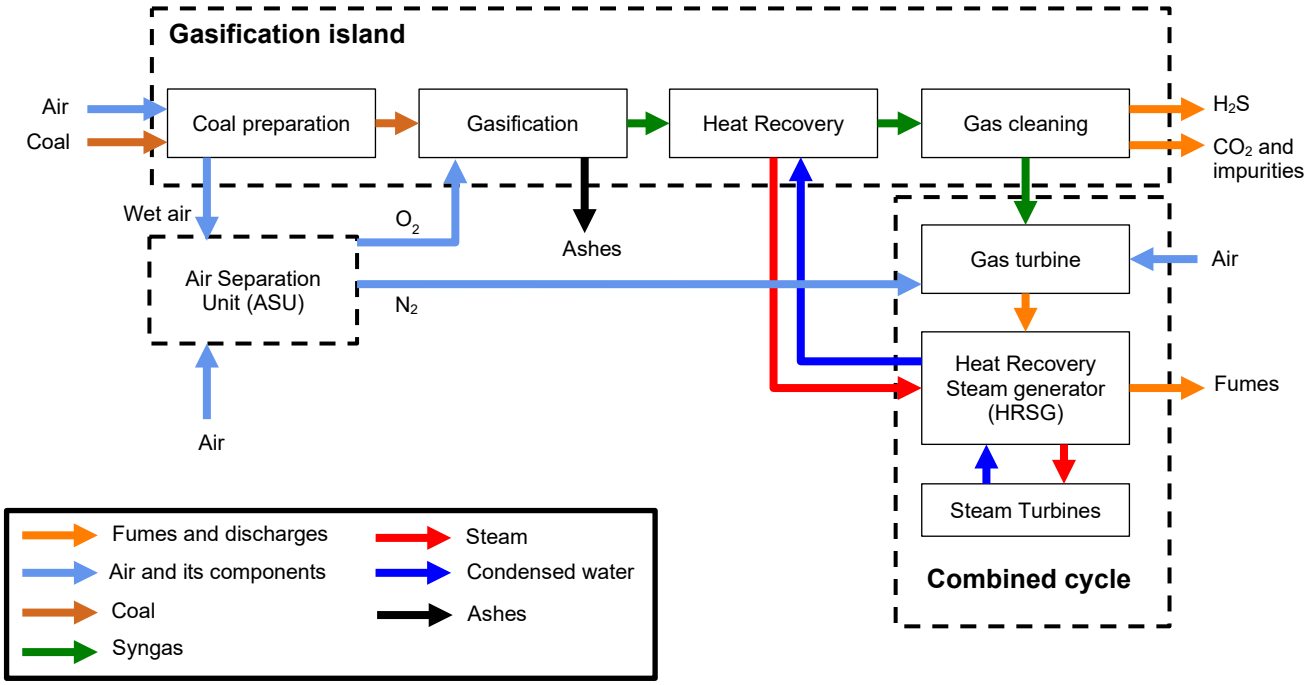
This example presents the simulation of an Integrated Gasification Combined Cycle (IGCC) plant. This process is used to turn coal and/or other carbon-based fuels into synthesis gas (also named “syngas”) by means of partial oxidation with air, oxygen or steam. The main inputs of the process are the air (as combustive) and the waste (as fuel). The coal (named “waste” in this example) is converted into syngas undergoing gasification and combustion reactions in the gasifier. The gasifier works at high pressure and with pure oxygen (separated with an Air Separation Unit, ASU).

Unlike coal combustion processes, gasification is performed with less oxygen requirement. Hence, the fuel gas obtained is composed mainly of carbon monoxide (CO) and hydrogen (H_2). The impurities are removed from the syngas prior to the power generation cycle. Some of these pollutants, such as sulfur (S), can be turned into re-usable byproducts through the “Claus” process.

With additional process equipment, a water-gas shift reaction can increase gasification efficiency and reduce carbon monoxide (CO) emissions by converting it to carbon dioxide (CO_2). The resulting carbon dioxide from the shift reaction can be separated, compressed, and stored through sequestration.

These first operations (coal preparation, gasification, gas cleaning) represents the “Gasification island” block of an IGCC plant.

Then the excess heat from the gasification and syngas fired generation is passed to a steam cycle, similar to a combined cycle gas turbine. This second block is also named “Combined cycle” block.

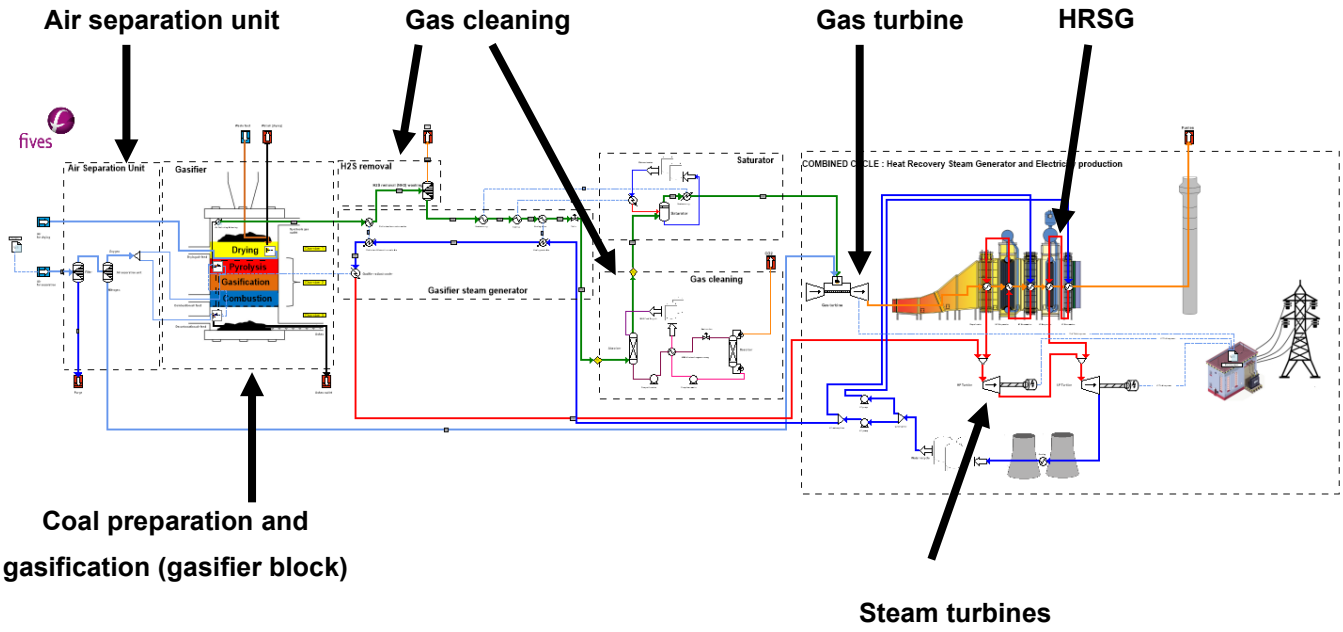


Block diagram of a typical IGCC plant

The input data and results of this example are based on different IGCC plants presented in [EDW07], [ENE17] and [NAY11].

1.2. Process flowsheet

The process flowsheet is divided in several blocks according to the process diagram shown in the previous section.



1.3. Compounds

1.3.1. Coal (“Waste”) compound

The composition of the “Coal” (“Waste”) is described below:

Element	Percentage (% wt)
Ashes	7.24
Carbon (C)	73.81
Hydrogen (H)	4.88
Nitrogen (N)	1.48
Sulfur (S)	2.13
Oxygen (O)	5.41
Moisture (H_2O)	5.05

Coal composition

Coal is a non-conventional solid and thus, the compound cannot be directly loaded from the DIPPR database embedded in Simulis Thermodynamics [ROW17]. The “Coal” (“Waste”) has to be created as a new compound and its composition has to be input in a form suitable to ProSimPlus.

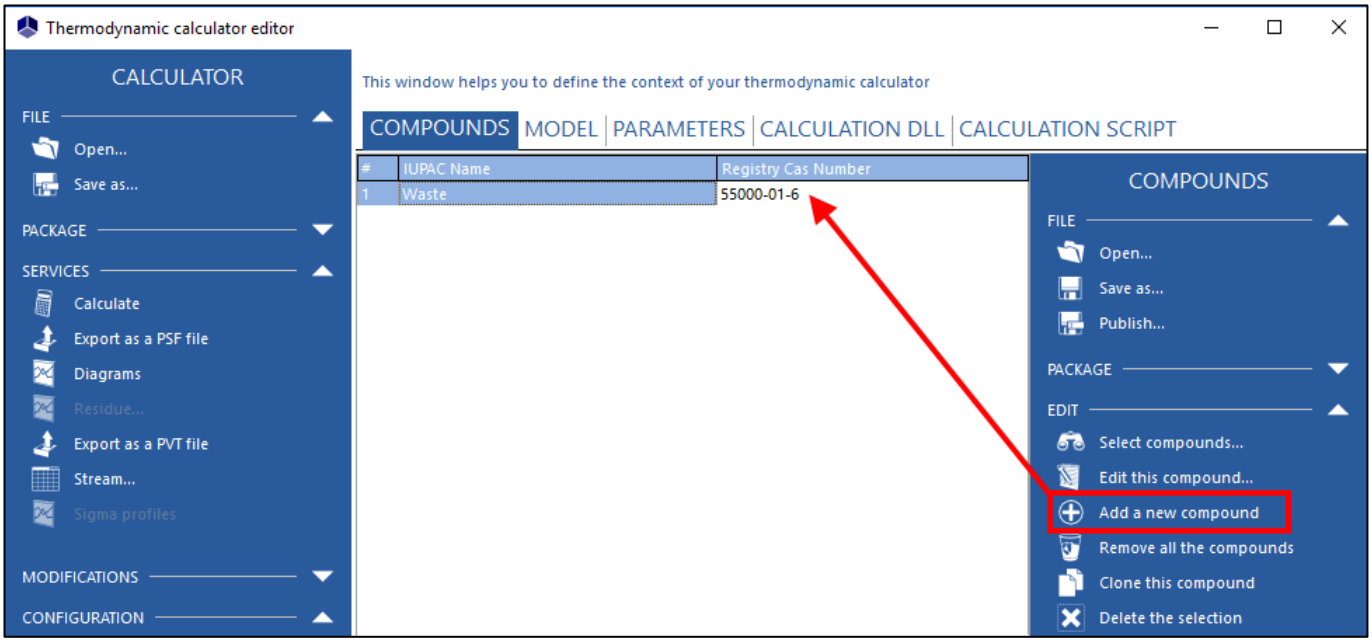
The waste is composed of 3 compounds following Simulis Thermodynamics terminology:

- Waste : CHONS compound created as a new compound;
- Ashes : In this example the ashes have been considered as silicon dioxide (SiO_2). This compound is the most commonly found in nature (“coal”) and well represent inerts of a waste stream (the critical properties (Tc, Pc, Zc, Vc) of this compound has been deleted in order to impose the solid state whatever the operating temperature of the system) ;
- Water : the moisture.

The “Waste” (coal) composition of the CHONS compound is computed as below (cf. “Coal_compound.xlsx”):

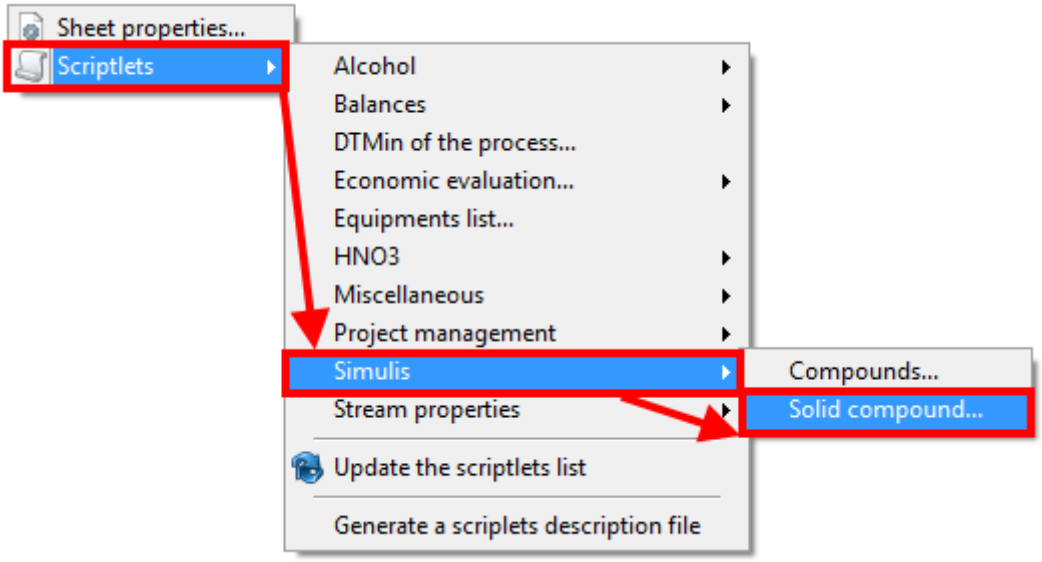
Element	Percentage (% wt)
Carbon (C)	84.15
Hydrogen (H)	5.56
Nitrogen (N)	1.69
Sulfur (S)	2.43
Oxygen (O)	6.17

The “Waste” compound is created as a new compound in the calculator editor of Simulis Thermodynamics:

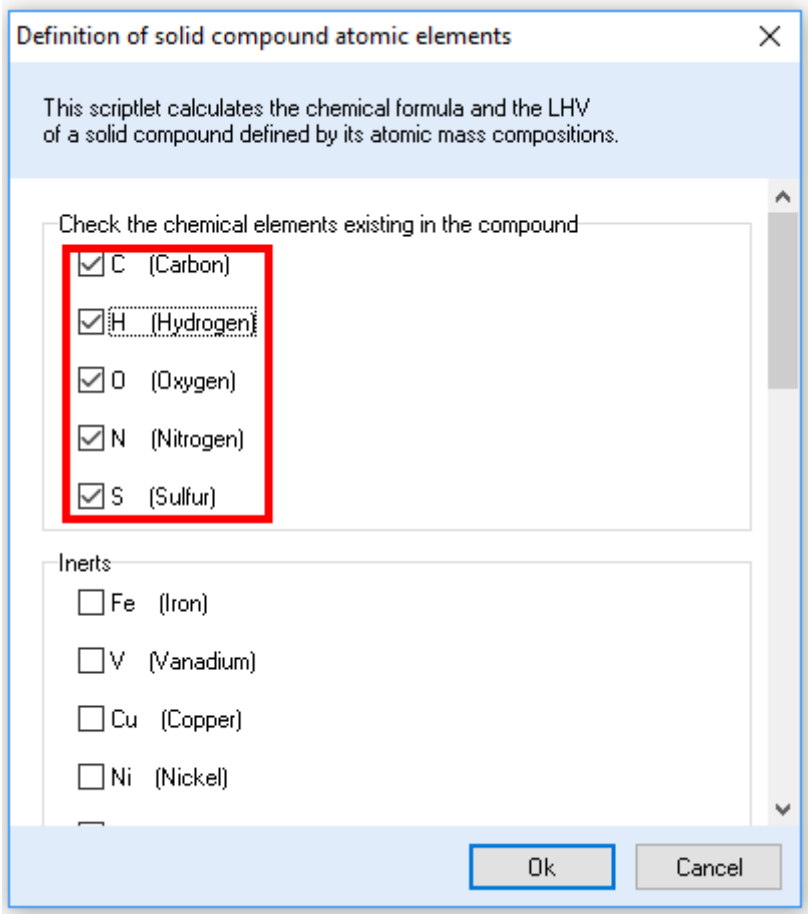


Note: The name of the new compound has been changed and a CAS number was associated to the new compound (55000-01-6).

Then, the “Waste” compound is modified using the scriptlet “Solid compound” (more details can be found in [NT172]). This scriptlet is accessible by a simple right click on the flowsheeting area of ProSimPlus.



The window below is displayed and the atomic elements are described:



In this example, only C, H, O, N, and S atomic elements are used.

The scriptlet “Solid compound” enables user to estimate the heat of combustion of a solid (Low Heating Value: LHV) unless the heat of combustion (LHV) is provided directly in one of the description windows of the scriptlet.

The number of carbon (C) atoms of the chemical formula of the waste is an input data of the scriptlet. This input data has no effect on mass simulation results (only molar results on the coal stream are different).
The composition and the flowrate of the coal are defined on a mass basis. Therefore, the number of carbon atoms defined in this scriptlet has no effect on the simulation results (molar results are meaningless).
Note: the stoichiometric coefficients changed following the number of carbons (C) (cf. 1.5 Reactions).

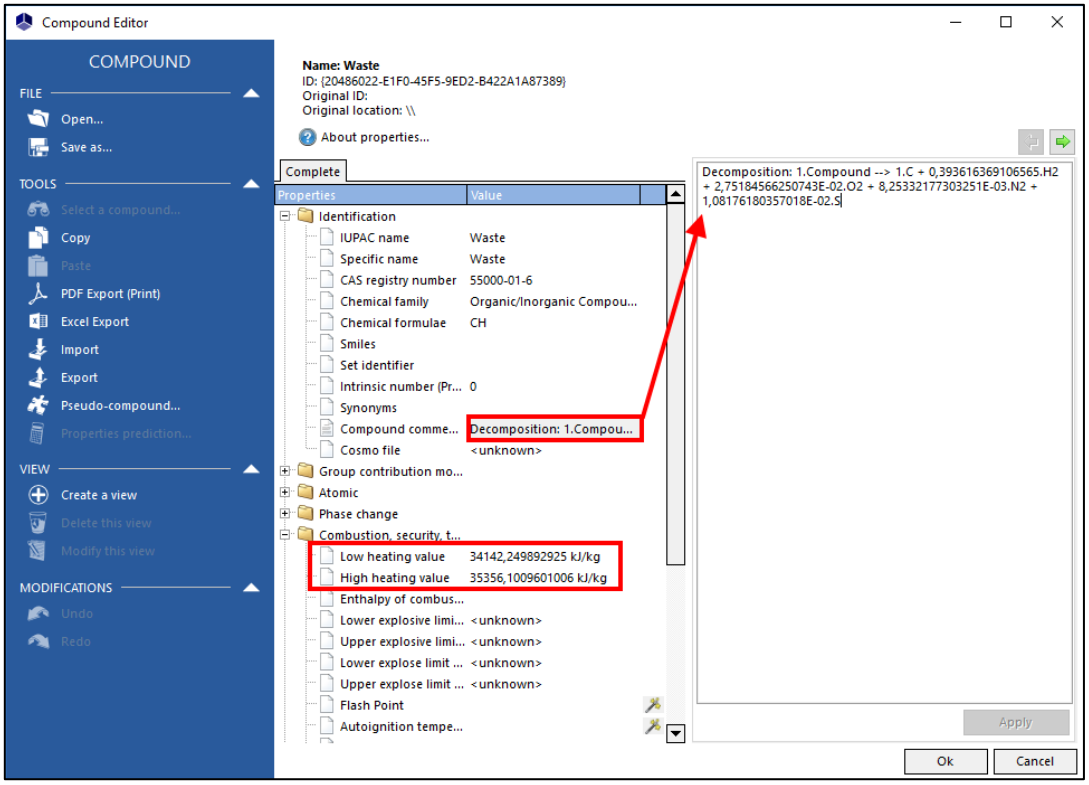
Results of the scriptlet with a number of carbon (C) atoms of 10 000:

Atom	Mass fraction (-)	Mole-fraction (-)	Chemical formula	Chemical formula (in equilibrium reactor)		Mw (g/mol)	DH0f (J/mol)	DG0f (J/mol)	LHV (kJ/kg)	HHV (kJ/kg)	Decomposition reaction in C,H2,O2,N,S	Sto. Coef.
C	0.84	0.535	10000	10000		142350	-4.413618E7	69414880	34189.7	35405.8	Compound	-1.00
H	0.055	0.421	7872	7872							C	10000
O	0.062	0.0294	550	550							H2	3936
N	0.016	0.0088	165	165							O2	275
S	0.022	0.0053	99.7	100							N2	82.5
											S	99.7

Results of the scriptlet with a number of carbon (C) atoms of 1:

Atom	Mass fraction (-)	Mole-fraction (-)	Chemical formula	Chemical formula (in equilibrium reactor)		Mw (g/mol)	DH0f (J/mol)	DG0f (J/mol)	LHV (kJ/kg)	HHV (kJ/kg)	Decomposition reaction in C,H2,O2,N,S	Sto. Coef.
C	0.84	0.535	1	1		14.235	-4413.618	6941.488	34189.7	35405.8	Compound	-1.00
H	0.055	0.421	0.7872	0.7872							C	1
O	0.062	0.0294	0.055	0.055							H2	0.3936
N	0.016	0.0088	0.0165	0.0165							O2	0.0275
S	0.022	0.0053	0.00997	0.01							N2	0.00825
											S	0.00997

The scriptlet enables the user to **automatically** change the properties data of the compound by the properties results from the scriptlet.



Compound editor of the "Waste" compound

1.3.1. Final compounds list

The compounds used in this example are listed in the table below. The order of the components has to be kept given that some scripts use this predefined order.

Name	Chemical formula	CAS number
Waste	$CH_{0,787}O_{0,055}N_{0,0165}S_{0,0099}$	55000-01-6
Char	C	7440-44-0
Oxygen	O_2	7782-44-7
Nitrogen	N_2	7727-37-9
Water	H_2O	7732-18-5
Hydrogen	H_2	1333-74-0
Carbon monoxide	CO	630-08-0
Carbon dioxide	CO_2	124-38-9
Methane	CH_4	74-82-8
Toluene	C_7H_8	108-88-3
Naphthalene	$C_{10}H_8$	91-20-3
Hydrogen sulfide	H_2S	7783-06-4
Sulfur dioxide	SO_2	7446-09-5
Nitric oxide	NO	10102-43-9
Nitrogen dioxide	NO_2	10102-44-0
Ashes	SiO_2	14808-60-7
Sulfur	S	7704-34-9
Sulfur trioxide	SO_3	7446-11-9
Monoethanolamine	C_2H_7NO	141-43-5

DIPPR compounds

1.4. Thermodynamic model

The IGCC is divided in several process blocks which deal with different components such as solid, syngas, pure water, monoethanolamine (MEA). In order to obtain realistic results, several calculators are defined to simulate the IGCC process:

- "Global calculator": contains the final compounds list defined previously and is defined with an "Ideal" thermodynamic profile. This calculator is used to simulate the syngas (different hydrocarbons) and the fumes streams for which the ideal mixture (no interaction between molecules) is considered. Indeed, these streams undergo only thermal treatment through heat exchanger and no equilibrium (flash drum) takes place on the syngas and fumes pipelines;
- "Gasification drying": contains the final compounds list defined previously and is defined with a "Bio application with solids" thermodynamic profile. This calculator is specifically used to simulate the drying of the waste with a flash drum. Indeed, the equilibrium occurring in the flash drum has to be accurate to separate the solids from the drying air;
- "Syngas cleaning": contains the final compounds list defined previously and is defined with an "Amines and acid gases" thermodynamic profile. This calculator is used to simulate the CO_2 removal using MEA ("Gas cleaning" block of the process);
- "Pure water": contains only the "water" compound and therefore, is defined with a "Pure water" thermodynamic profile (based on NBS/NRC steam tables). This calculator is used to simulate the water streams.

More information about these models can be found in the thermodynamic models' user guide, which can be accessed from the "MODEL" tab of the Simulis Thermodynamics calculator editor.

1.5. Reactions

Several reactions occur during the gasification process. Thereby, 6 reaction sets have to be defined:

- "Decomposition" reaction: this reaction is based on the stoichiometric coefficients computed with the "Solid compound" scriptlet:

$$CH_wO_xN_yS_z \rightarrow C + \frac{w}{2}H_2 + \frac{x}{2}O_2 + \frac{y}{2}N_2 + zS$$

Decomposition reaction in C,H2,O2,N,S	Sto. Coef.	Notation
Compound	-1.00	-
C	1	-
H2	0.3936	w/2
O2	0.0275	x/2
N2	0.00825	y/2
S	0.00997	z

- "Combustion" reaction: conventional combustion reaction of the char (C):

$$C + O_2 \rightarrow CO_2$$

- "Gasification" reactions: conventional gasification reactions of the char (C):

$$C + CO_2 \rightarrow 2CO$$

$$C + H_2O \rightarrow CO + H_2$$

- "Decarbonation" reaction: conventional combustion reaction of the char (C):

$$C + O_2 \rightarrow CO_2$$

- "WGS" reaction: water gas shift reaction:

$$CO + H_2O \leftrightarrow CO_2 + H_2$$

- "Balancing" reactions: this set of reactions represents the pyrolysis reactions. These reactions are described with distribution rates (I_1, I_2, I_3, I_4, I_5):

$$\frac{1}{2}N_2 + \frac{1}{2}(2 - I_1) * O_2 \rightarrow I_1 * NO + (1 - I_1) * NO_2 \quad (1)$$

$$S + (1 - I_2) * O_2 + I_2 * H_2 \rightarrow I_2 * H_2S + (1 - I_2) * SO_2 \quad (2)$$

$$C + \frac{1}{2}(2 - I_3) * O_2 \rightarrow I_3 * CO + (1 - I_3) * CO_2 \quad (3)$$

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O \quad (4)$$

$$(10 - 9 * I_4 - 3 * I_5 - 3 * I_4 * I_5) * C + (4 - 2 * I_4) * H_2 \rightarrow I_4 * CH_4 + I_5 * (1 - I_4) * C_7H_8 + (1 - I_5)(1 - I_4) * C_{10}H_8 \quad (5)$$

With:

I_1 : Distribution rate between NO and NO_2 (%)

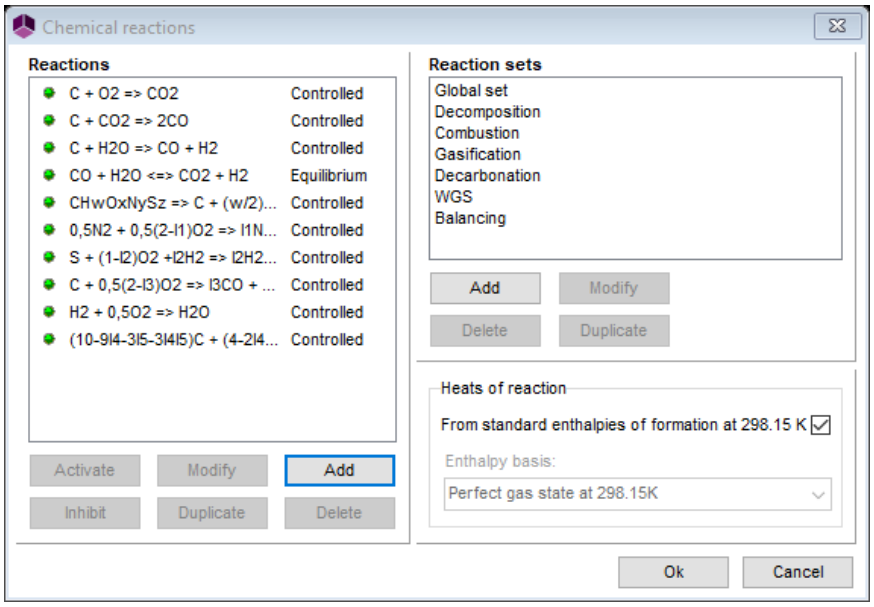
I_2 : Distribution rate between H_2S and SO_2 (%)

I_3 : Distribution rate between CO and CO_2 (%)

I_4 : Distribution rate between CH_4 and the tars (C_7H_8, $C_{10}H_8$) (%)

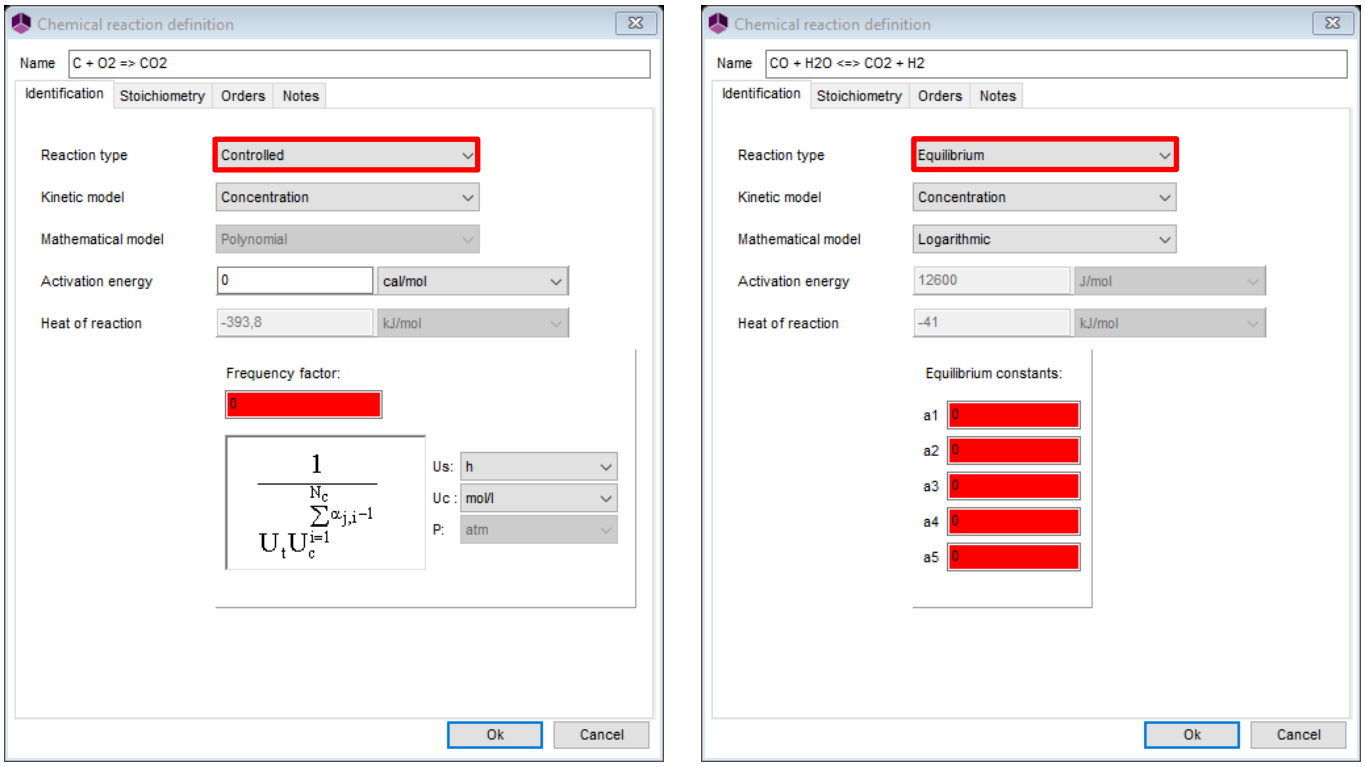
I_5 : Distribution rate between C_7H_8 and $C_{10}H_8$ (%)

Note: The order of the reactions for the "Balancing" set has to be kept given that the script of the "Balancing" reactor uses this predefined order.



Different reaction sets

All the reactions are defined as “controlled” reactions except the water gas shift (WGS) reaction defined as an equilibrium reaction:



Chemical reaction definition windows for all the reactions (left one) except for WGS reaction (right one)

1.6. Operating conditions of the "Gasification island" block

1.6.1. Air Separation Unit (ASU)

The operating conditions required to define the ASU are gathered in this part.

- ✓ Coal feed

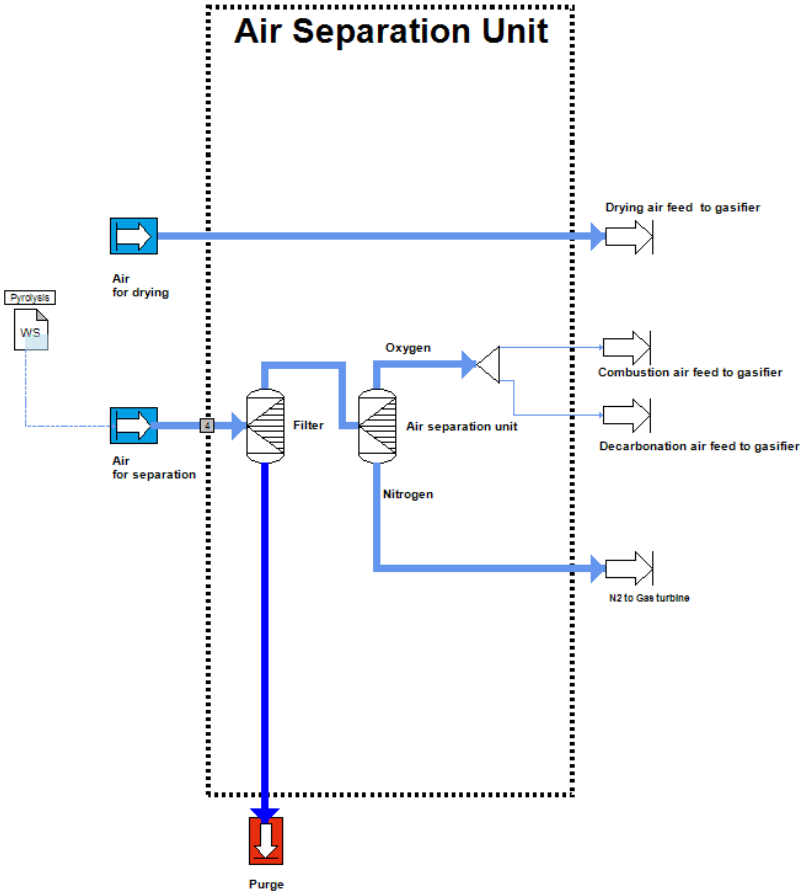
		Coal feed
Mass percentage	**Waste (Coal)**	87.71
	Ashes	7.24
	H_2O	5.05
Total mass flowrate (t/h)		6.25
Temperature (°C)		20
Pressure (atm)		1

- ✓ Air for separation

		Air feed
Molar percentage	**N_2**	0.21
	O_2	0.79
Total molar flowrate (Nm3/h)		23000
Temperature (°C)		25
Pressure (atm)		1

- ✓ Air for drying

		Air feed
Molar percentage	**N_2**	0.21
	O_2	0.79
Total molar flowrate (Nm3/h)		5000
Temperature (°C)		25
Pressure (atm)		1



ASU simulation

✓ *Component splitter*

Operating parameters	*Filter*
Recovery ratios on the overhead stream	Overhead stream feeds in the “Air separation unit” module
Nitrogen	1
Oxygen	1

The “Filter” unit operation aims to remove potential impurities or water in the input air.

Operating parameters	*Air separation unit*
Recovery ratios on the overhead stream	Overhead stream (enriched in oxygen) feeds the gasifier
Nitrogen	0.01
Oxygen	0.998
Separator temperature (°C)	25
Separator pressure (bar)	40

✓ *Stream splitter*

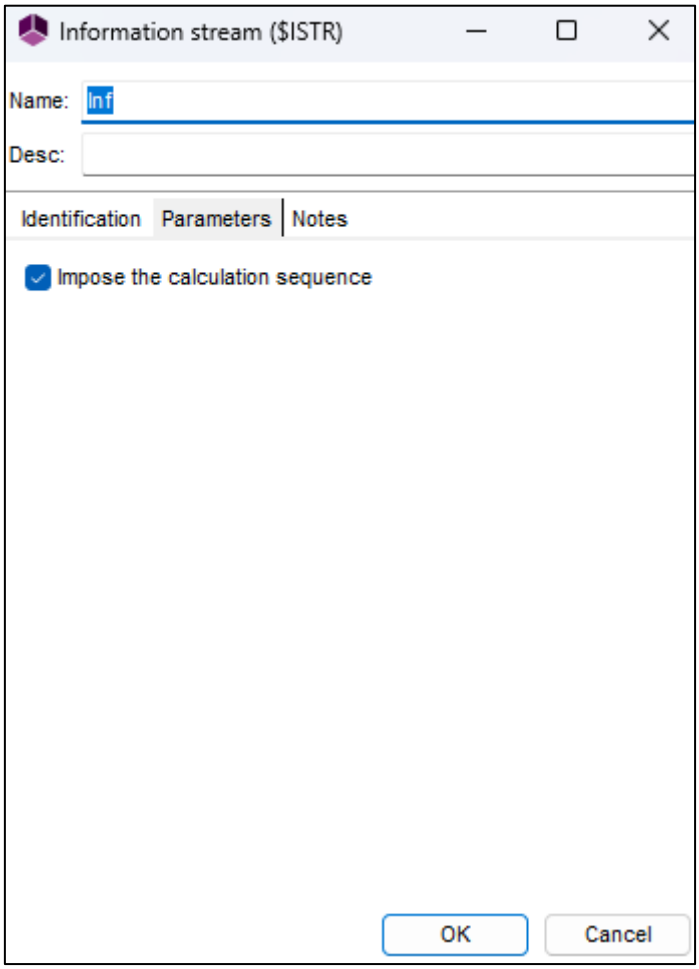
Operating parameters	***Air splitter***
Specification type	Molar flowrates
Molar flowrate of the decarbonation air feed (Nm^3/h)	320

✓ *Windows script: "Pyrolysis"*

This windows script is used to provide parameters for the gasifier. It has to be calculated as the first module in the calculation sequence that is why it is connected to the "Air for separation" feed with an information stream.

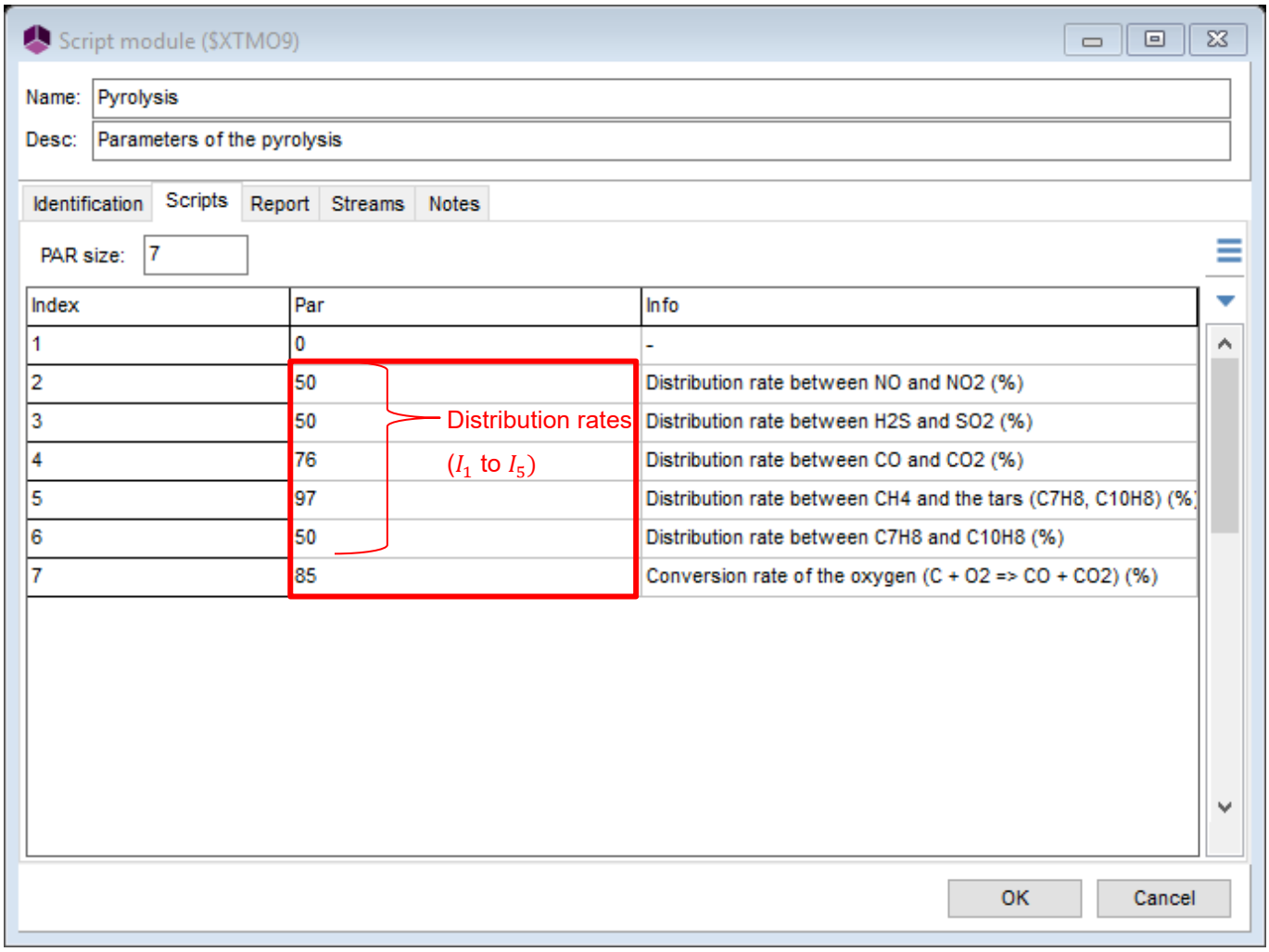
This information stream is only used to impose the calculation sequence and is configured as presented in the following screenshot.

In the rest of this document a so configured information stream will be called "empty".



The following script has been used (“Pyrolysis” windows script):

```
'-------------------------------------------------------------------------------
' Validation of module
'-------------------------------------------------------------------------------
Function OnCalculation()
  OnCalculation = True
End Function
'-------------------------------------------------------------------------------

'-------------------------------------------------------------------------------'
' CALL OF "UNIT CONVERSION" SCRIPT
'-------------------------------------------------------------------------------'
With CreateObject("Scripting.FileSystemObject")
  ExecuteGlobal .OpenTextFile(Project.ApplicationPath & "Scripts\UnitConversion.vbs", 1).ReadAll()
End With
'-------------------------------------------------------------------------------

'-------------------------------------------------------------------------------
' Print of results/parameters
'-------------------------------------------------------------------------------
Sub OnPrintResults()

  Temperature_Unit = ReportUnit("Temperature")

  With Module
    .PrintReport(" ")
    .PrintReport(" PROVIDED DATA FOR PYROLYSIS")
    .PrintReport(" ---------------------------" & vbLf)

    .PrintReport(" Conversion rate of char for pyrolysis")
    .PrintReport("      - Conversion rate : " & FormatNumber(.Parameter(1),2) & " % mass" & vbLf)

    .PrintReport(" Reactions parameters for synthesis gas")
    .PrintReport("           - Distribution rate between NO and NO2                  : " &
    FormatNumber(.Parameter(2),2) & " %")
    .PrintReport("           - Distribution rate between H2S and SO2                 : " &
    FormatNumber(.Parameter(3),2) & " %")
    .PrintReport("           - Distribution rate between CO and CO2                  : " &
    FormatNumber(.Parameter(4),2) & " %")
    .PrintReport("            - Distribution rate between CH4 and the tars           : " &
    FormatNumber(.Parameter(5),2) & " %")
    .PrintReport("            - Distribution rate between C7H8 and C10H8             : " &
    FormatNumber(.Parameter(6),2) & " %")
    .PrintReport("          - Conversion rate of the oxygen                          : " &
    FormatNumber(.Parameter(7),2) & " %" & vbLf)

  End with
End Sub
'-------------------------------------------------------------------------------
```

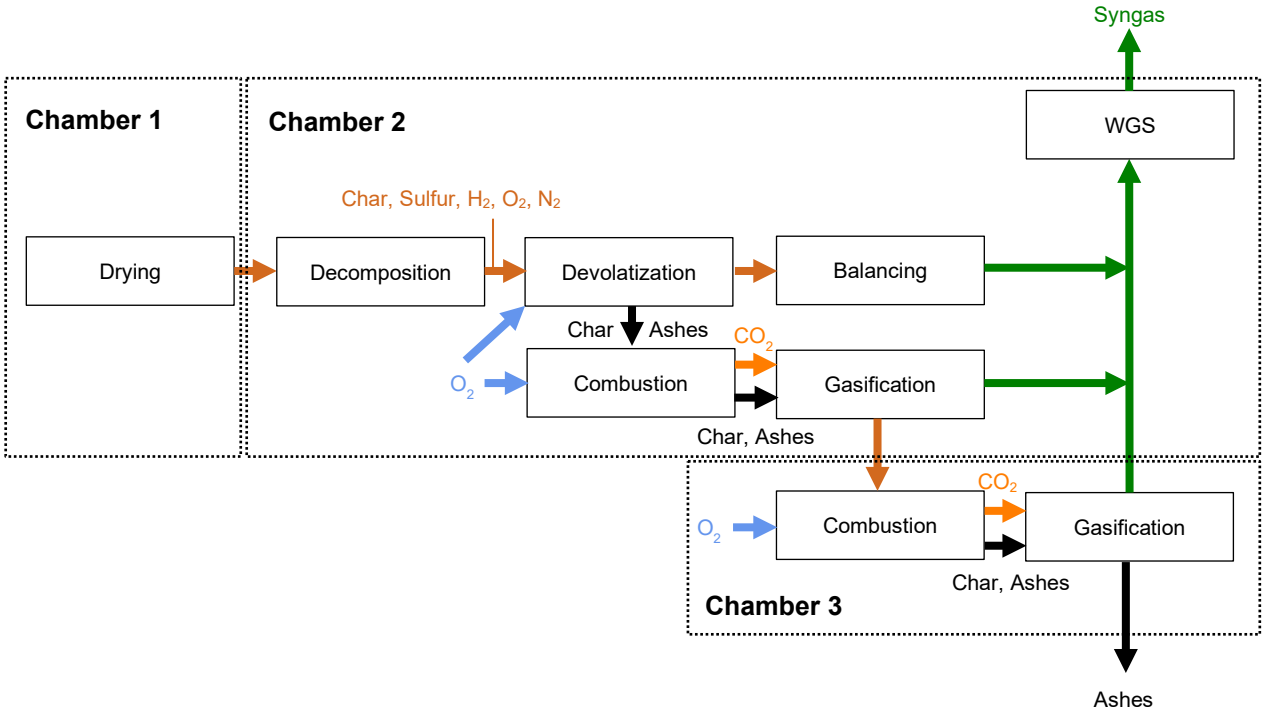


1.6.2. Gasifier

In the gasifier, coal undergoes a series of chemical and physical changes:

- Coal Drying (Chamber 1);
- Decomposition, Devolatilization (Pyrolysis) (Chamber 2);
- Combustion (Chamber 2 and 3);
- Char Gasification (Chamber 3).

Each chemical change is associated to a reaction set (cf.1.5 Reactions) and to a reactor.



Gasifier block diagram for simulation

The Devolatilization or Pyrolysis accounts for a large percentage coal weight loss and occurs rapidly during the initial stages of coal heat up. During this process, the labile bonds between the aromatic clusters in coal are cleaved, generating fragments of molecular weight much smaller than coal. This process is simulated with the “Decomposition” reaction set.

Then, fragments with low molecular weights vaporize and escape from the coal particle to constitute light gases and tar. This part is dealt with the “Devolatization” and “Balancing” blocks.

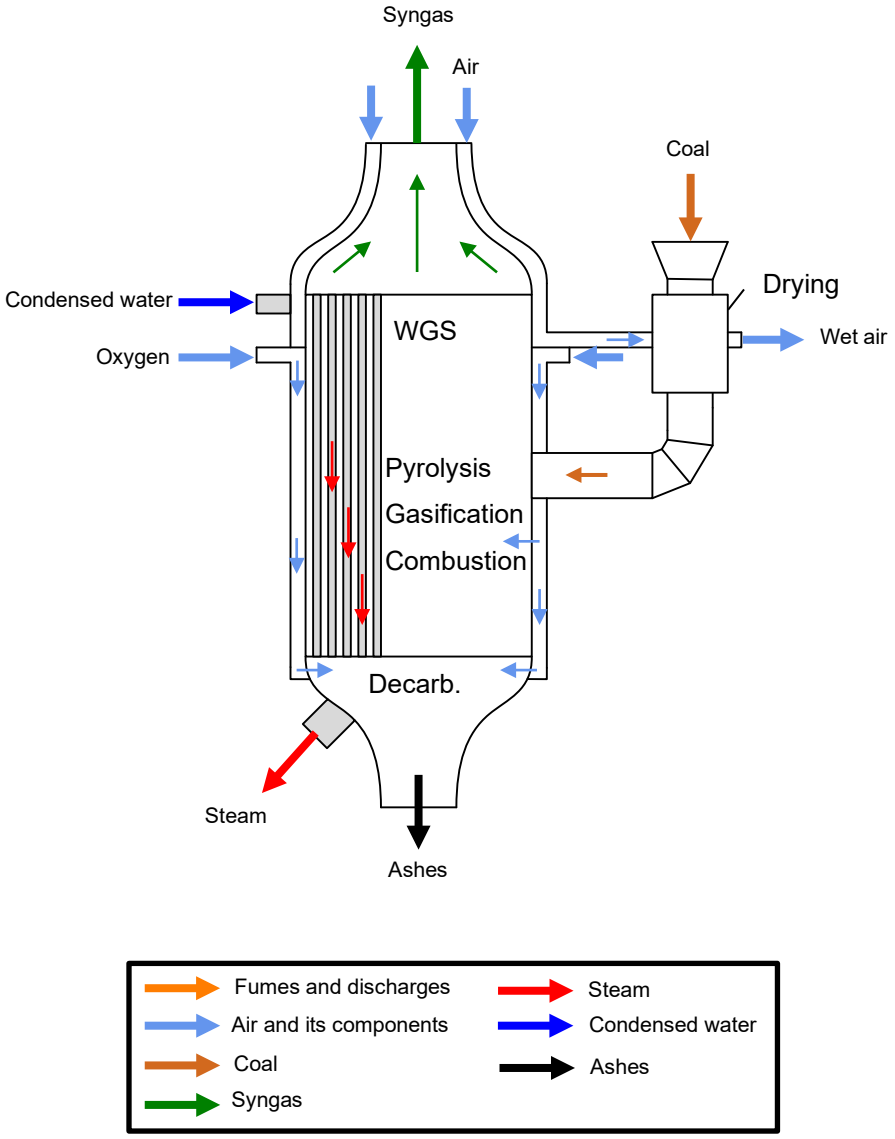
The fragments with high molecular weight, and hence low vapor pressures, remain in the coal under typical devolatilization conditions until they reattach to the char lattice. The solid product left over from devolatilization and undergoes 2 successive steps of “Combustion” and “Gasification”.

The raw syngas from the pyrolysis (“Balancing” reactor), from the first and second gasification of the char are mixed and sent to a “WGS” reactor. The pyrolysis (“Balancing” reactor) and the “WGS” reactor are assumed to be at the same temperature of 600°C.

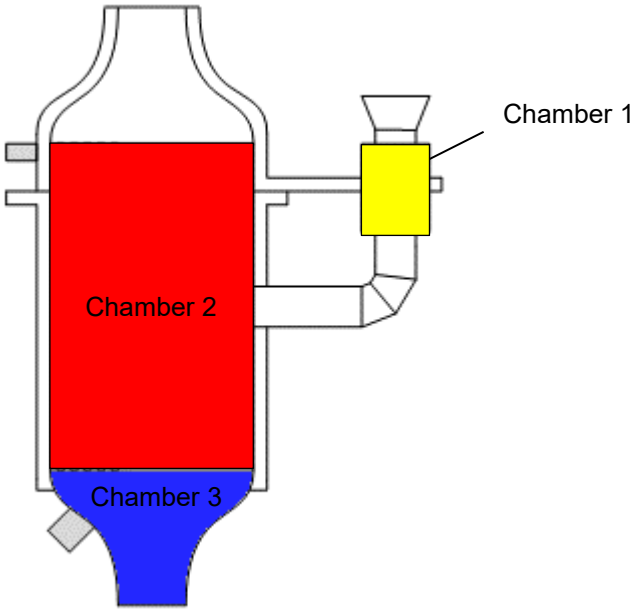
The gasifier is working on exothermic process that is why it is cooled using a condensed water through a radiant syngas cooler (bundle of tubes for the cooling system). Thereby, the gasifier produced both syngas and high-pressure steam.

The air and the pure oxygen used respectively for drying and pyrolysis/combustion are preheated before entering into the gasifier.

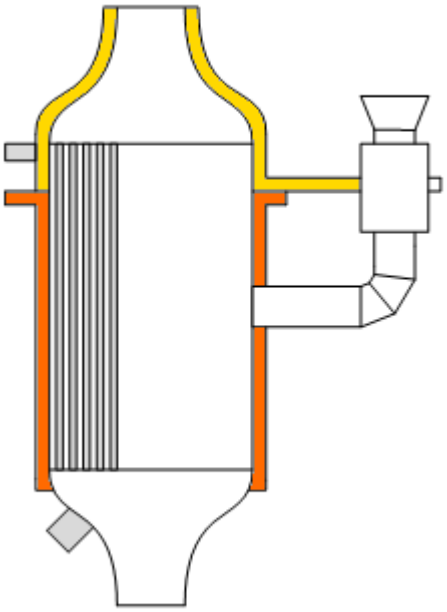
From a technical point of view, the gasifier is presented below:



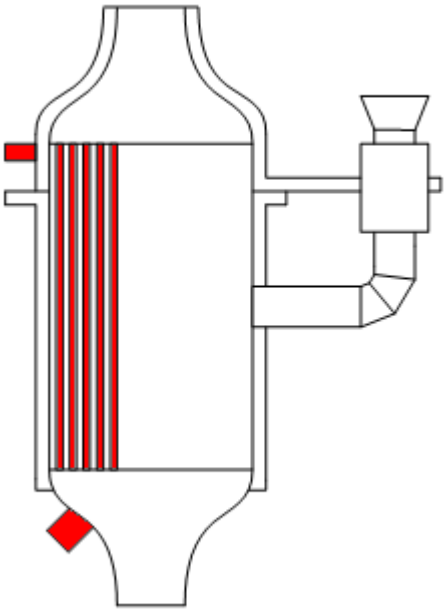
Schematic of a Gasifier



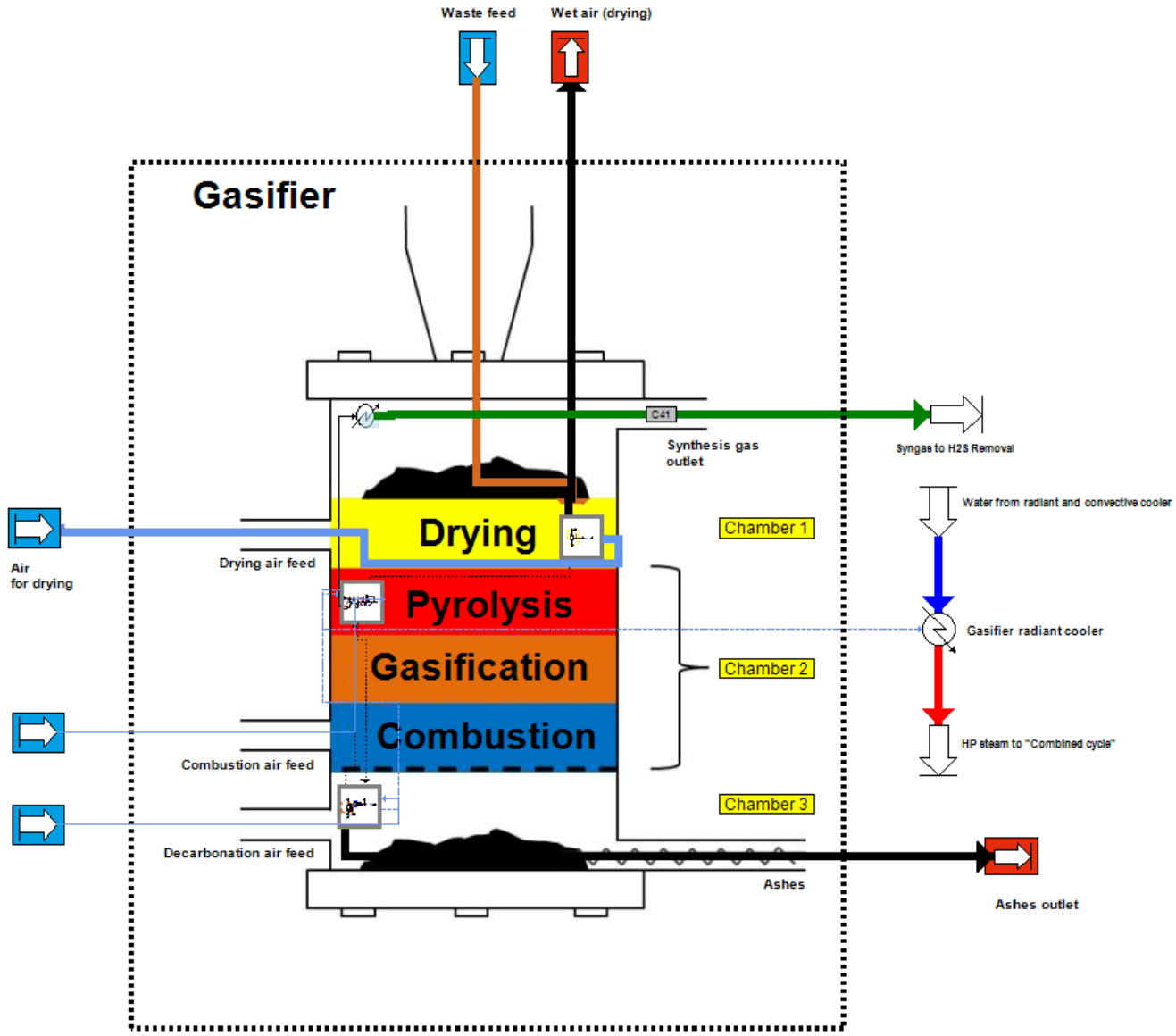
Chamber layout in the gasifier



Process flow paths of the drying air (yellow) and oxygen (orange)

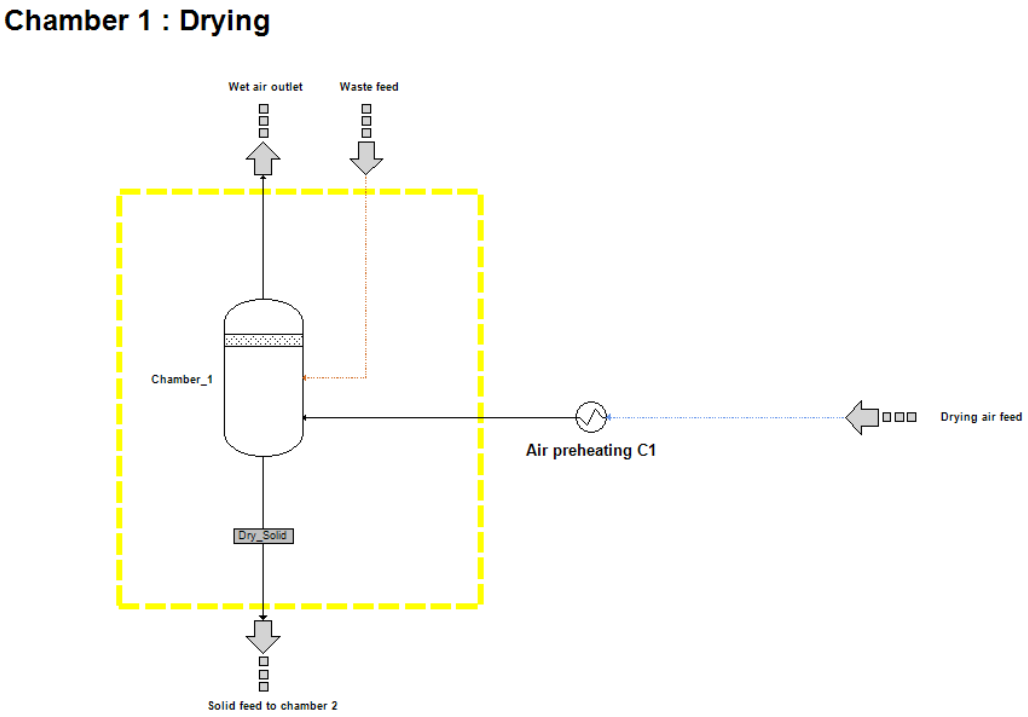


Process flow path of the cooling system



Gasifier modeling

1.6.2.1. Chamber 1: Drying



Chamber 1 modeling

✓ Cooler/Heater

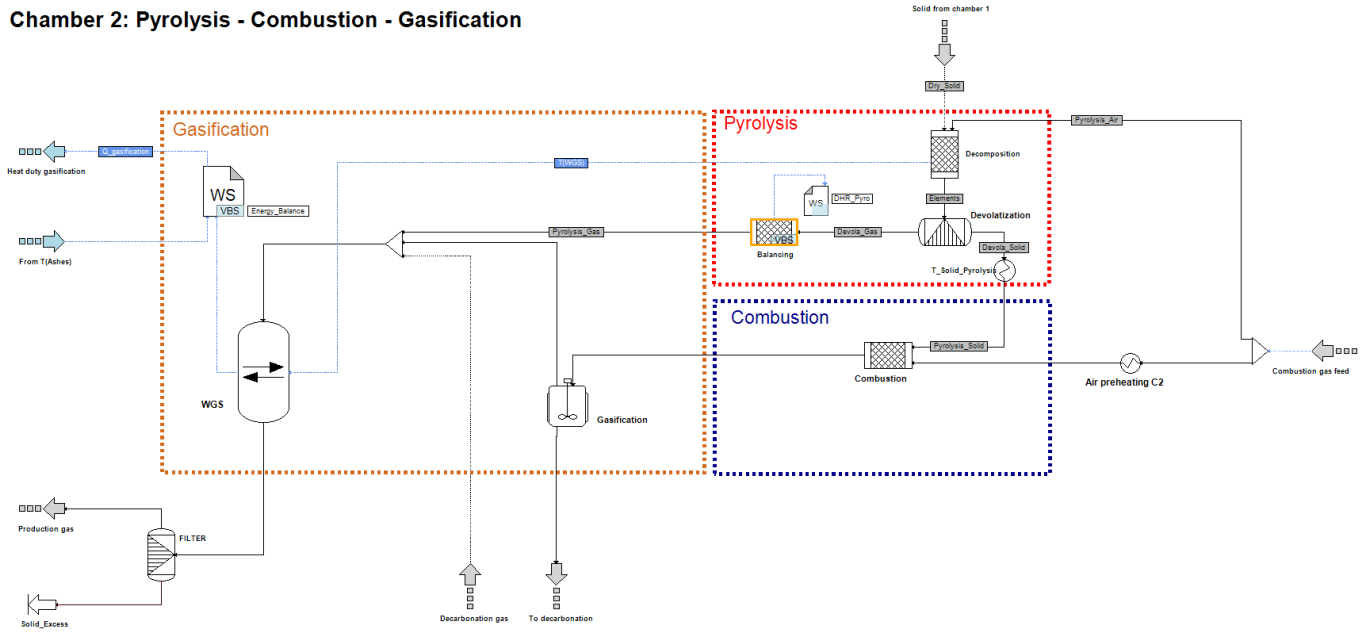
Name	*Outlet temperature (°C)*	*Pressure drop (bar)*
Air preheating C1	280	0

✓ Separator

Operating parameters	*Chamber_1*
Separator type	Liquid-vapor separator
Pressure (bar)	40
Pressure drop (bar)	0.2
Heat duty (W)	Adiabatic

Note: The "calculator" is changed for the separator calculation. In the "Identification" tab of the separator, the calculator "Gasification drying" is selected:

1.6.2.2. Chamber 2: Pyrolysis - Gasification - Combustion



Chamber 2 modeling

✓ Coolers/Heaters

Name	***Outlet temperature (°C)***	***Pressure drop (bar)***
Air preheating C2	600	0
T_Solid_Pyrolysis	200	0

✓ *Component splitter*s

Operating parameters	***Devolatization***
Recovery ratios on the overhead stream	Overhead stream goes to the combustion: “Devola_Solid” stream
Waste	1
Char	0.765

Operating parameters	***Filter***
Recovery ratios on the overhead stream	Overhead stream is the “Solid_Excess”
Ashes	1
Char	1

Note: In this example, the "Solid_Excess" has a zero flowrate (no excess of solid)

✓ *Stream splitter*

Operating parameters	***Air splitter C2***
Specification type	Molar flowrates
Molar flowrate of the combustion air feed (Nm^3/h)	3000

✓ *Simple reactors*

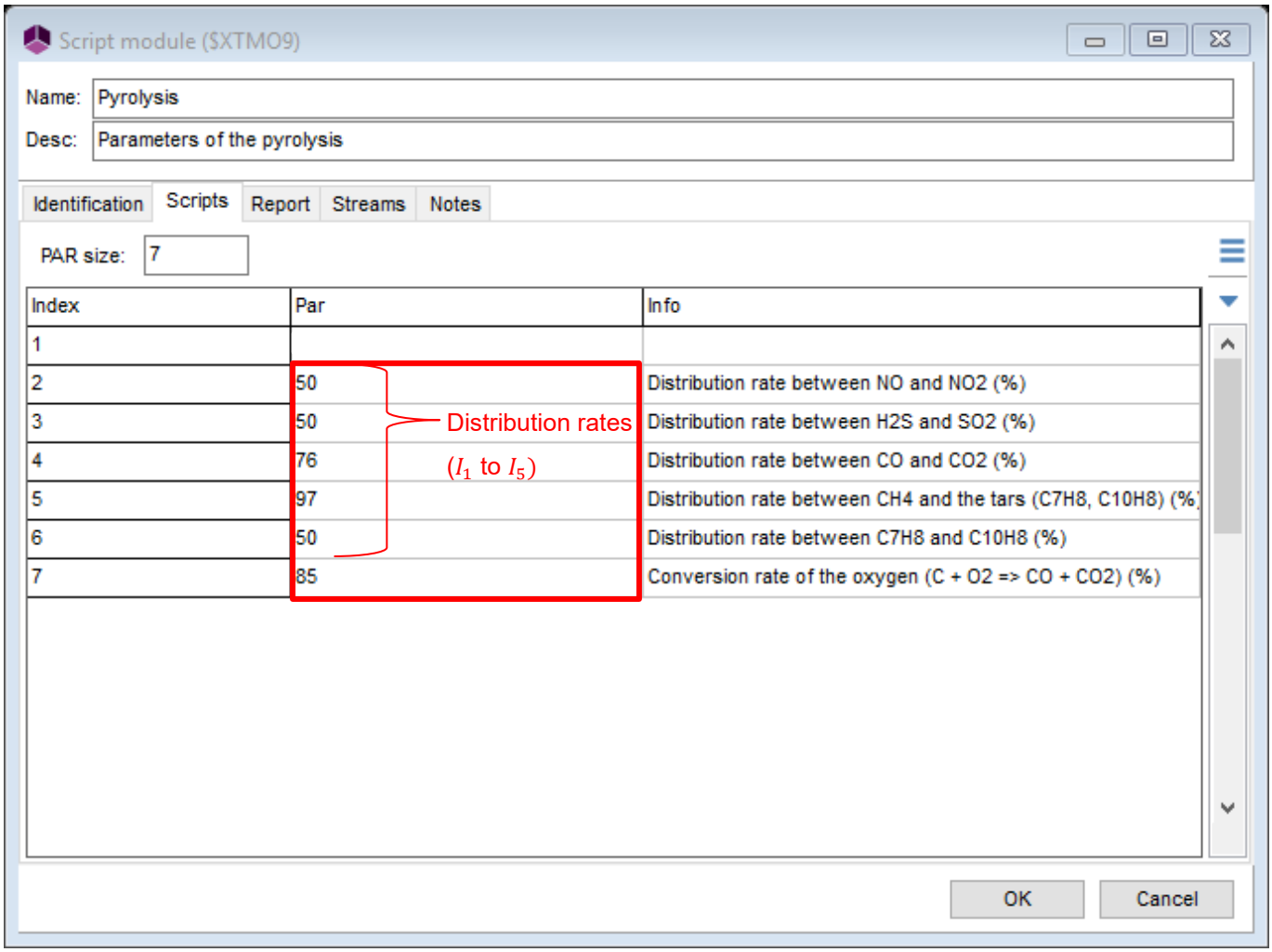
Operating parameters	***Decomposition***
Reaction set	"Decomposition"
Specification type	Reactor with a specified output temperature
Temperature specified (°C)	600
Key component	Waste
Conversion rate of the reaction	1

Operating parameters	***Combustion***
Reaction set	"Combustion"
Specification type	Adiabatic reactor
Key component	Oxygen
Conversion rate of the combustion reaction	1

Operating parameters	***Balancing***
Reaction set	"Balancing"
Specification type	Constant temperature reactor
Key component for reaction n°1	Nitrogen
Conversion rate of the reaction n°1	1
Key component for reaction n°2	Sulfur
Conversion rate of the reaction n°2	1
Key component for reaction n°3	Char
Conversion rate of the reaction n°3	0.85
Key component for reaction n°4	Oxygen
Conversion rate of the reaction n°4	1
Key component for reaction n°5	Char

Conversion rate of the reaction n°5	1

According to the reaction set for the “Balancing” reactor, distribution rates have to be defined (I_1, I_2, I_3, I_4, I_5). These values are provided directly in the “Pyrolysis” script. Moreover, the conversion rate for the reaction n°3 of the “Balancing” set is also supplied in this script (values in the interface of the “Balancing” reactor” are initial values and are modified by the values of the script). This script enables the user to directly change the distribution rates and the conversion rate without opening the chemical reaction windows editor  .



The following script has been used (“Balancing” reactor script):

```
Sub OnCalculationStart()

  ' Indexes calculation
  ' -------------------
  For i = 0 To Project.Compounds.Count-1
    CasN = Project.Compounds.Items(i).CasRegistryNumber
    Select Case casN
    Case "7440-44-0"
      C = Module.GlobalToCalculator(i)
    Case "7782-44-7"
      O2 = Module.GlobalToCalculator(i)
    Case "7727-37-9"
      N2 = Module.GlobalToCalculator(i)
    Case "7732-18-5"
      H2O = Module.GlobalToCalculator(i)
    Case "1333-74-0"
```



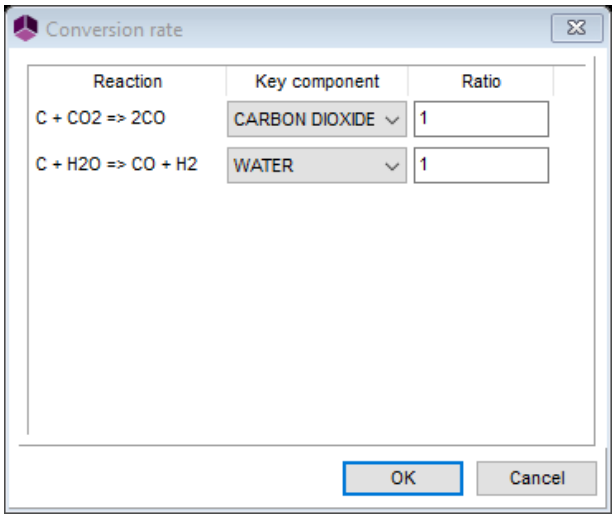
```
    H2 = Module.GlobalToCalculator(i)
  Case "630-08-0"
    CO = Module.GlobalToCalculator(i)
  Case "124-38-9"
    CO2 = Module.GlobalToCalculator(i)
  Case "74-82-8"
    CH4 = Module.GlobalToCalculator(i)
  Case "108-88-3"
    C7H8 = Module.GlobalToCalculator(i)
  Case "91-20-3"
    C10H8 = Module.GlobalToCalculator(i)
  Case "7783-06-4"
    H2S = Module.GlobalToCalculator(i)
  Case "7446-09-5"
    SO2 = Module.GlobalToCalculator(i)
  Case "10102-43-9"
    NO = Module.GlobalToCalculator(i)
  Case "10102-44-0"
    NO2 = Module.GlobalToCalculator(i)
  Case "7704-34-9"
    S = Module.GlobalToCalculator(i)
  End Select
Next

' Calculation of the stoichiometric coefficients
' ----------------------------------------------

' Get the parameters from "Pyrolysis" windows script
With Project.Modules("Pyrolysis")
  L1 = .Parameter(2) / 100.0
  L2 = .Parameter(3) / 100.0
  L3 = .Parameter(4) / 100.0
  L4 = .Parameter(5) / 100.0
  L5 = .Parameter(6) / 100.0
  Tx = .Parameter(7) / 100.0
End With

Dim Reaction

With Module
  'MsgBox .ReactiveCalculator.Reactions.Count
  For i=1 To .ReactiveCalculator.Reactions.Count
    Set Reaction = .ReactiveCalculator.Reactions.Items(i-1)
    'MsgBox Reaction.Name
    If Reaction.Name = "0,5N2 + 0,5(2-l1)O2 => l1NO + (1-l1)NO2" Then
      'MsgBox Reaction.Name
      Reaction.StoichiometricCoefficient(N2) = -0.5
      Reaction.StoichiometricCoefficient(O2) = -(2.0-L1)/2.0
      Reaction.StoichiometricCoefficient(NO) = L1
      Reaction.StoichiometricCoefficient(NO2) = 1.0 - L1
    ElseIf Reaction.Name = "S + (1-l2)O2 +l2H2 => l2H2S + (1-l2)SO2" Then
      'MsgBox Reaction.Name
      Reaction.StoichiometricCoefficient(S) = -1.0
      Reaction.StoichiometricCoefficient(O2) = -(1.0-L2)
      Reaction.StoichiometricCoefficient(H2) = -L2
      Reaction.StoichiometricCoefficient(H2S) = L2
      Reaction.StoichiometricCoefficient(SO2) = 1.0 - L2
    ElseIf Reaction.Name = "C + 0,5(2-l3)O2 => l3CO + (1-l3)CO2" Then
      'MsgBox Reaction.Name
      Reaction.StoichiometricCoefficient(C) = -1.0
      Reaction.StoichiometricCoefficient(O2) = -(2.0-L3)/2.0
      Reaction.StoichiometricCoefficient(CO) = L3
      Reaction.StoichiometricCoefficient(CO2) = 1.0 - L3
    ElseIf Reaction.Name = "H2 + 0,5O2 => H2O" Then
      'MsgBox Reaction.Name
      Reaction.StoichiometricCoefficient(H2) = -1.0
      Reaction.StoichiometricCoefficient(O2) = -0.5
      Reaction.StoichiometricCoefficient(H2O) = 1.0
```



```
      ElseIf Reaction.Name = "(10-9l4-3l5-3l4l5)C + (4-2l4)H2 => l4CH4 + l5(1-l4)C7H8 + (1-l5)(1-
l4)C10H8" Then
        'MsgBox Reaction.Name
        Reaction.StoichiometricCoefficient(C) = -(10.0-9.0*L4-3.0*L5+3.0*L4*L5)
        Reaction.StoichiometricCoefficient(H2) = -(4.0-2.0*L4)
        Reaction.StoichiometricCoefficient(CH4) = L4
        Reaction.StoichiometricCoefficient(C7H8) = L5*(1.0-L4)
        Reaction.StoichiometricCoefficient(C10H8) = (1.0-L5)*(1.0-L4)
      End If
    Next
    Set Reaction = Nothing
    ' Calculation of the conversion rate
    ' ----------------------------------
    ' Reaction C + O2 => CO + CO2
    .ConversionRatios(3) = Tx
  End With

End Sub
```

✓ *Reaction tank*

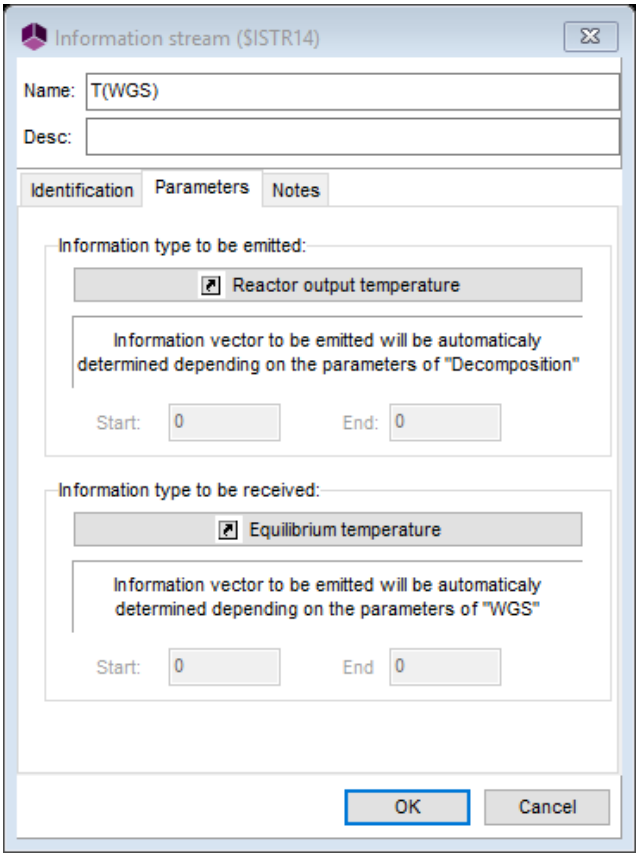
Operating parameters	***Gasification***
Reaction set	“Gasification”
Specification type	Adiabatic reactor
Temperature specified (°C)	600
Key component of reaction n°1	Carbon dioxide
Conversion rate of the reaction n°1	1
Key component of reaction n°2	Water
Conversion rate of the reaction n°2	1



✓ *Equilibrium reactor*

Operating parameters	***WGS***
Reaction set	"WGS"
Method	Equilibrium constants
Specification type	Equilibrium temperature
Temperature specified (°C)	700

In the gasifier, the WGS and the pyrolysis take place at the same temperature. To take into account this additional specification, an information stream is added from the "Decomposition" reaction to the "WGS" reactor.
The temperature specification from the "Decomposition" is sent to the "WGS" reactor:



✓ *Windows script*

The "DHR_Pyro" is used to compute the heat of reaction of the "Pyrolysis" reaction.

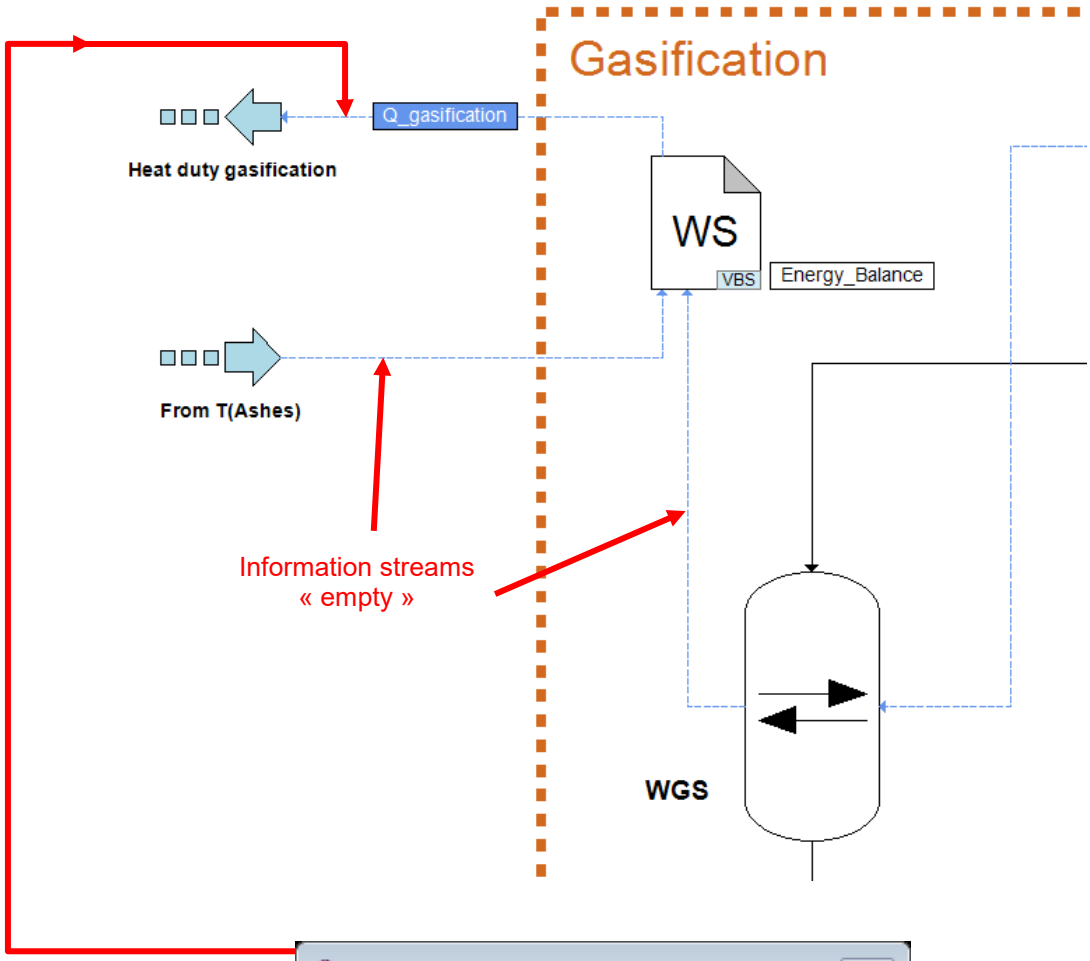
The following script has been used ("DHR_Pyro" windows script):

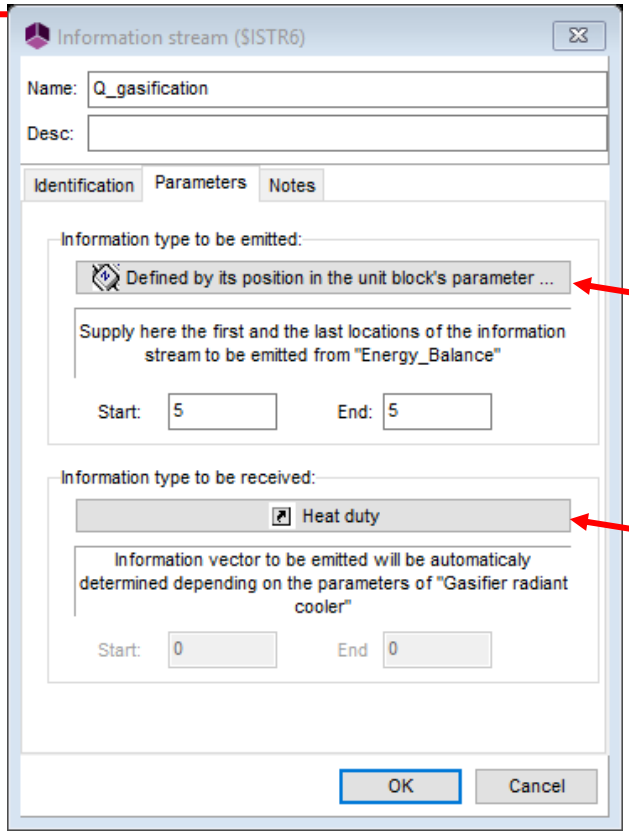
```
'-------------------------------------------------------------------------'
' CALL OF "UNIT CONVERSION" SCRIPT
'-------------------------------------------------------------------------'
with CreateObject("Scripting.FileSystemObject")
  ExecuteGlobal .OpenTextFile(Project.ApplicationPath & "Scripts\UnitConversion.vbs",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


'-------------------------------------------------------------------------
```



```
' Calculation of the enthalpy of the pyrolysis reaction
'-------------------------------------------------------------------------------
Function OnCalculation()
' Statement
' ---------
  Dim DH0f()
  With Project

'   Get enthalpy of formation DH0f
'   ------------------------------
    NC = .Compounds.Count
    ReDim DH0f(NC)
    For i = 1 To NC
        DH0f(i-1) = Convert("Molar enthalpy", .Compounds.Items(i-1).DeltaH0v.Value,
       .Compounds.Items(i-1).DeltaH0v.UnitName, "kcal/kmol")

        CasN = Project.Compounds.Items(i-1).CasRegistryNumber
        If Casn = "55000-01-6" Then
              MwDIB     = Convert("Molar mass", .Compounds.Items(i-1).Mw.Value, .Compounds.Items(i-
              1).Mw.UnitName, "kg/kmol")
           DIBDebMol = .Streams("Dry_Solid").PartialMolarFlowRate(i)
        End If
    Next

'   Calculation of the reaction heat
'   --------------------------------
    DHR = 0.0
    For i = 1 To NC
       DHR = DHR + (.Streams("Pyrolysis_Solid").PartialMolarFlowRate(i) +
       .Streams("Pyrolysis_Gas").PartialMolarFlowRate(i) -
       .Streams("Dry_Solid").PartialMolarFlowRate(i) -
       .Streams("Pyrolysis_Air").PartialMolarFlowRate(i)) * DH0f(i-1)
    Next

  End With

  Module.Parameter(3) = DHR
  Module.Parameter(1) = DHR / DIBDebMol
  Module.Parameter(2) = (DHR / DIBDebMol) / MwDIB

' Validation of the module
'-------------------------------------------------------------------------------
  OnCalculation = True

End Function

'-------------------------------------------------------------------------------
' Print results
'-------------------------------------------------------------------------------
Sub OnPrintResults()
  MolarEnthalpy_Unit = ReportUnit("Molar enthalpy")
  MassEnthalpy_Unit  = ReportUnit("Mass enthalpy")
  EnthalpicFlow_Unit = ReportUnit("Enthalpic flow")

  With Module
    .PrintReport(" ")
    .PrintReport(" PYROLYSIS HEAT OF REACTION")
    .PrintReport(" -------------------------------------------------" & vbLf)

    .PrintReport("      - Molar     : " & FormatNumber(Convert("Molar enthalpy", .Parameter(1),
       "kcal/kmol",  MolarEnthalpy_Unit),1)  & " " & MolarEnthalpy_Unit)
    .PrintReport("      - Mass      : " & FormatNumber(Convert("Mass enthalpy",  .Parameter(2),
       "kcal/kg",    MassEnthalpy_Unit) ,1)  & " " & MassEnthalpy_Unit)
    .PrintReport("      - Heat duty : " & FormatNumber(Convert("Enthalpic flow", .Parameter(3),
       "kcal/h",     EnthalpicFlow_Unit) ,1) & " " & EnthalpicFlow_Unit)
  End with

End Sub
```


The “Energy_Balance” script is used to compute the heat duty released in the gasifier. This amount of heat duty is used to heat the HP (high pressure) condensed water to generate HP steam.





Heat duty computed in the « Energy_Balance » windows script

Heat duty of the « Gasifier radiant cooler » unit operation

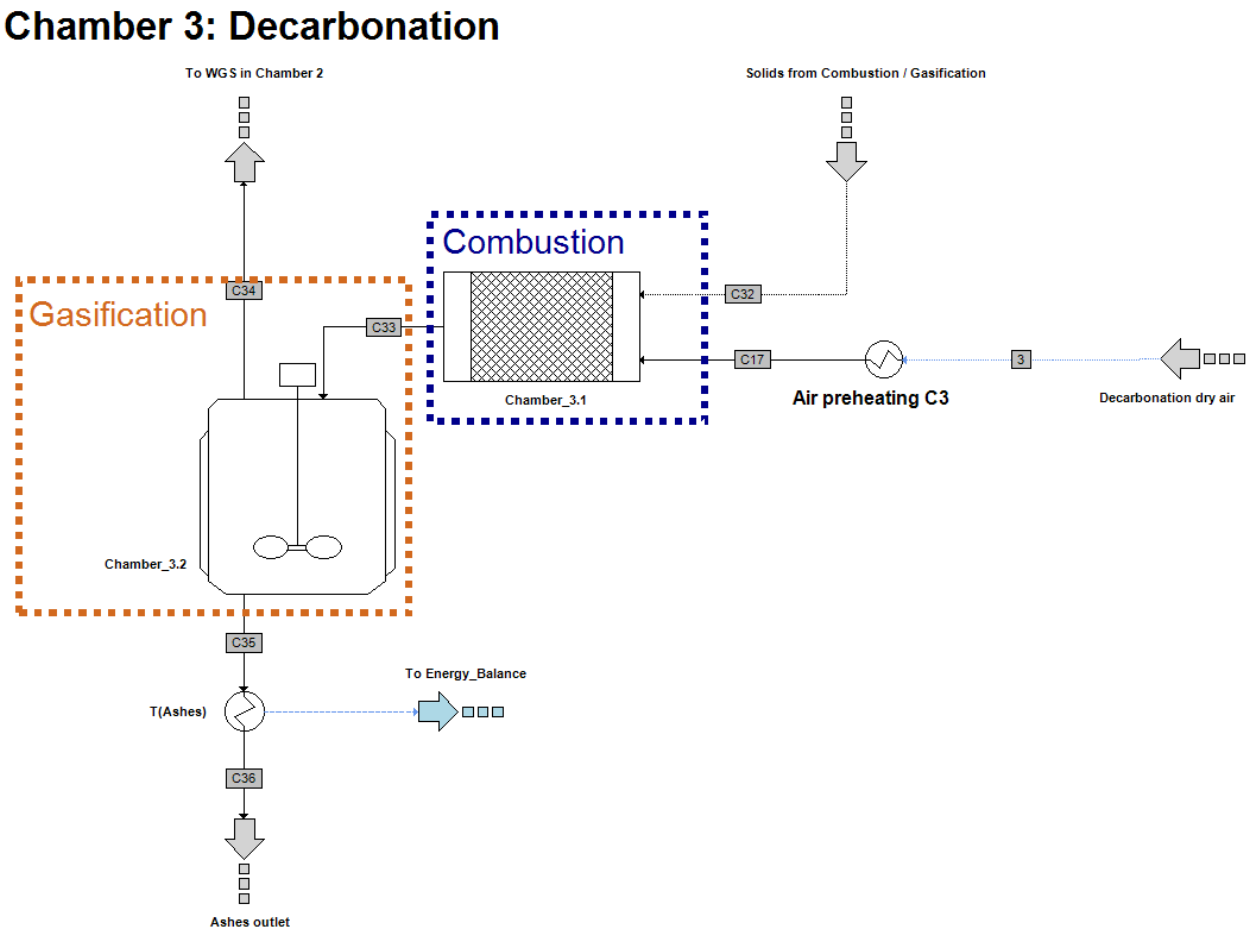
The following script has been used (“Energy_Balance” windows script):

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


'-------------------------------------------------------------------------------
' Energy balance on the component splitter "Devolatization"
'-------------------------------------------------------------------------------
Function OnCalculation()

' Heat duty recovery
' ------------------
  With Project
    Hin            = .Streams("Elements").EnthalpyFlux
    Hout_Solides   = .Streams("Devola_Solid").EnthalpyFlux
    Hout_Gaz       = .Streams("Devola_Gas").EnthalpyFlux

    Q_Decomposition  = .Modules("Decomposition").HeatDuty
    Q_SolidePyrolyse = .Modules("T_Solid_Pyrolysis"). HeatDuty
    Q_Equilibrage    = .Modules("Balancing"). HeatDuty

    Q_Ciel_Gazeux = .Modules("WGS"). HeatDutySpecValue

    Q_Cendres = .Modules("T(Ashes)"). HeatDuty
  End With

' Calculation
' -----------
' Balance on conversion
  Q_Devolatilisation = (Hout_Solides + Hout_Gaz) - Hin

' Balance on pyrolysis
  Q_Pyrolyse = Q_Decomposition + Q_Devolatilisation + Q_Equilibrage + Q_SolidePyrolyse

' Balance on the gasifier
  Q_calc = Q_Pyrolyse + Q_Ciel_Gazeux + Q_Cendres

' Gap
  Q_Consigne = Module.Parameter(1)
  Ecart      = Q_calc - Q_Consigne

' Save results
' ------------
  With Module
    .Parameter(2) = Q_Pyrolyse
    .Parameter(3) = Q_Ciel_Gazeux
    .Parameter(4) = Q_Cendres
    .Parameter(5) = Q_calc
    .Parameter(6) = Ecart
  End With

' Validation of the module
'-------------------------
  OnCalculation = True

End Function


'-------------------------------------------------------------------------------'
' Print results
'-------------------------------------------------------------------------------'
Sub OnPrintResults()
  With Module
```



```
    .PrintReport(" Energy balance on the gasification process" & vbLf )
    .PrintReport("      - Q(Pyrolysis)              : " & FormatNumber(ProSimToReport("Enthalpic
    flow", .Parameter(2)),2) & " " & ReportUnit("Enthalpic flow"))
    .PrintReport("      - Q(Gas overhead)           : " & FormatNumber(ProSimToReport("Enthalpic
    flow", .Parameter(3)),2) & " " & ReportUnit("Enthalpic flow"))
    .PrintReport("      - Q(Ashes)                  : " & FormatNumber(ProSimToReport("Enthalpic flow",
    .Parameter(4)),2) & " " & ReportUnit("Enthalpic flow"))
    .PrintReport("      - Energy balance            : " & FormatNumber(ProSimToReport("Enthalpic flow",
    .Parameter(5)),2) & " " & ReportUnit("Enthalpic flow") & vbLf)

    .PrintReport("      - Thermal losses specified  : " & FormatNumber(ProSimToReport("Enthalpic flow",
    .Parameter(1)),2) & " " & ReportUnit("Enthalpic flow") & vbLf)

    .PrintReport("      - Absolute difference       : " & FormatNumber(ProSimToReport("Enthalpic flow",
    .Parameter(6)),2) & "  " & ReportUnit("Enthalpic flow"))

  End with
End Sub
```

1.6.2.3. Chamber 3: Decarbonation



Decarbonation modeling

✓ Coolers/Heaters

Name	*Outlet temperature (°C)*	*Pressure drop (bar)*
Air preheating C3	600	0
T(Ashes)	1200	0

✓ *Simple reactor*

Operating parameters	***Chamber_3.1***
Reaction set	"Combustion"
Specification type	Adiabatic reactor
Key component	Oxygen
Conversion rate of the reaction	1

✓ *Reaction tank*

Operating parameters	***Chamber_3.2***
Reaction set	"Gasification"
Specification type	Adiabatic reactor
Temperature specified (°C)	600
Key component of reaction n°1	Carbon dioxide
Conversion rate of the reaction n°1	1
Key component of reaction n°2	Water
Conversion rate of the reaction n°2	1

1.6.2.1. Air preheating

The syngas produced at 600°C preheats the oxygen or air for the 3 chambers. The simple heat exchanger "Air Preheating Balancing" is added on the syngas outlet from the gasifier and cools the syngas from 600°C to ≈ 360°C.

✓ Simple heat exchanger

Name	***Heat duty (W)***	***Pressure drop (bar)***
Air Preheating Balancing	0	0

The following script is coded in the "Script" tab of the "Air Preheating Balancing" unit operation to extract the heat duties from the 3 preheating exchangers:

```
Sub OnCalculationStart()
    Q1 = Project.Modules("Air preheating C1").HeatDuty
    Q2 = Project.Modules("Air preheating C2").HeatDuty
    Q3 = Project.Modules("Air preheating C3").HeatDuty
    Module.HeatDutySpecValue = Q1 + Q2 + Q3
End Sub
```

1.6.3. H2S Removal and Heat Recovery

The syngas produced from the gasifier goes through successive purification steps. The main objective of the purification is to remove the sulfur, the chlorine, the ammonia and the carbon dioxide from the syngas. The syngas traditionally crosses filters (fly ash particles removal), water wash column (part of H_2S, HCl, HF and ammonia).

The acid gas resulting from desulfuration, with a high H_2S content, is sent to a Claus unit for recovering sulfur, obtaining pure solid sulfur ready to be sold. The Claus tail gas is recirculated into the process, enabling 99.8% of the sulfur content of the gas to be recovered.

Note: A number of different sulfur removal and recovery systems have been studied in IGCC and coal-to-SNG plant designs. Another most common configuration is the Selexol process for sulfur removal from the raw syngas, a two-stage Claus plant for recovery of elemental sulfur, and the Shell Claus off-gas treating (SCOT) process for treatment of the tail gas from the Claus plant.

In this example, the Claus unit is not modeled. This part of the process is dealt in the “PSPS_EX_EN-Claus-Process” application example. Moreover, the successive purification steps are simulated with a simple component splitter.

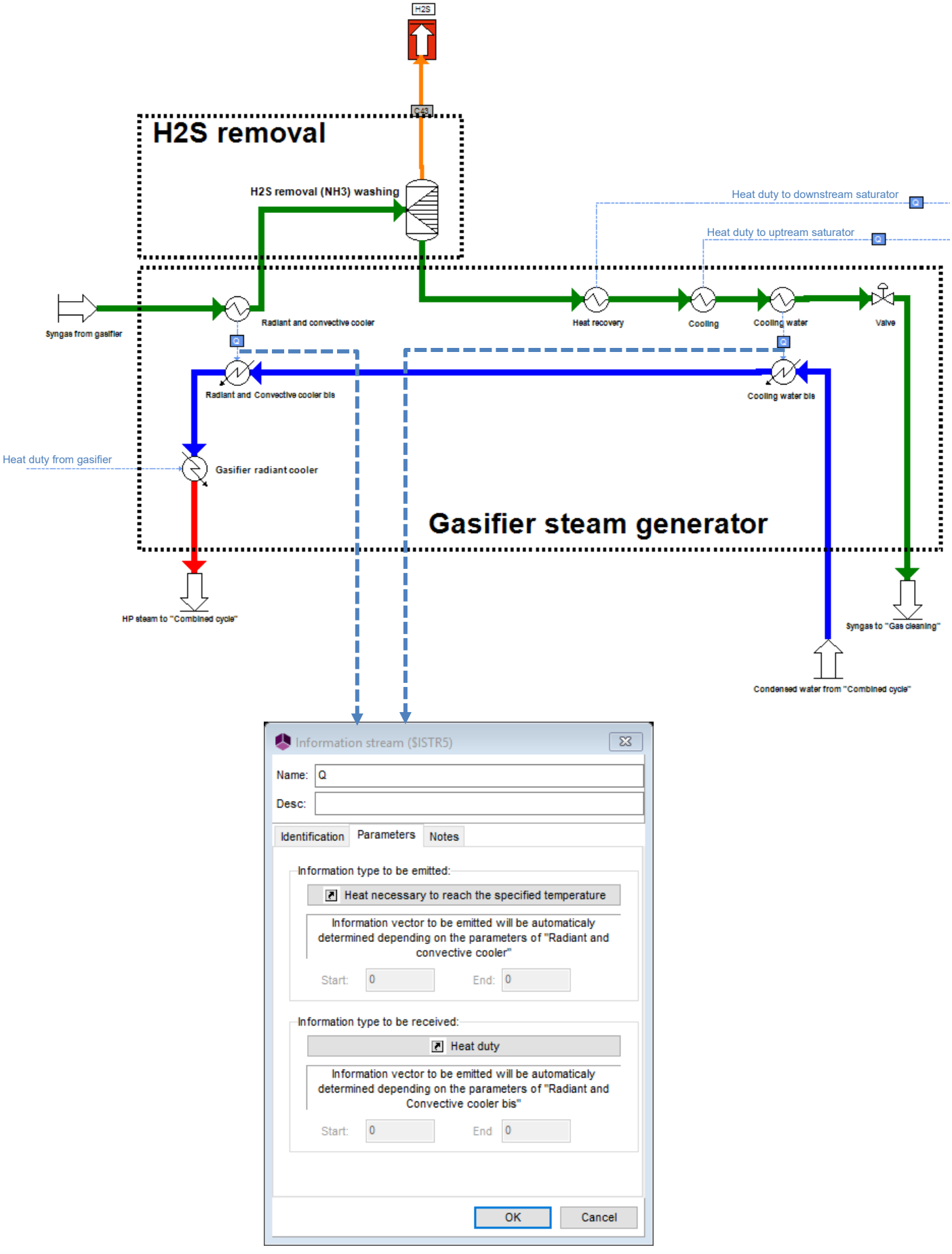
The syngas is cooled before and after the “H2S Removal” to recover a maximum of energy.

- ✓ Coolers/Heaters

Name	***Outlet temperature (°C)***	***Pressure drop (bar)***
Radiant and convective cooler	250	0
Heat recovery	180	0
Cooling	120	0
Cooling water	50	0

- ✓ *Component splitter*

Operating parameters	***H2S removal (NH3) washing***
Recovery ratios on the overhead stream	Overhead stream goes to the “Cleaning gas” process
Hydrogen sulfide	0.99
Sulfur dioxide	0.9

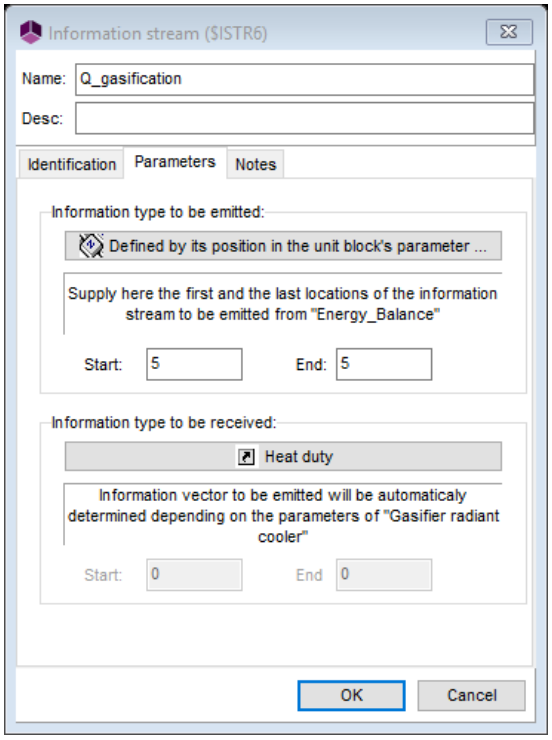


Cooler/Heater and simple heat exchanger basic connection

✓ Simple heat exchangers

Name	*Heat duty (W)*	*Pressure drop (bar)*
Radiant and convective cooler bis	0	0
Cooling water bis	0	0
Gasifier radiant cooler	0	0

The simple heat exchangers duties of “Radiant and convective cooler bis” and “Cooling water bis” are fixed by information streams from coolers on the syngas pipe. The heat duty of “Gasifier radiant cooler” is provided by the “Energy_balance” windows script:



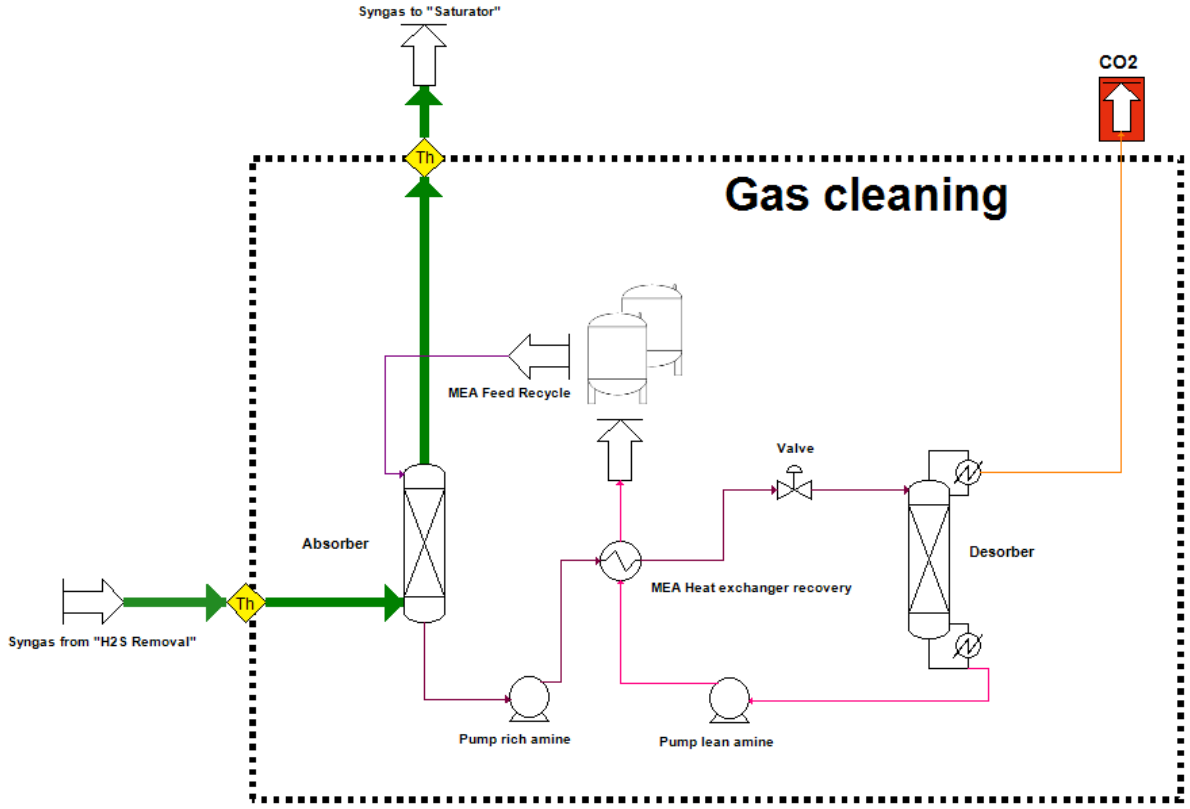
Information stream windows editor (between “Gasifier radiant cooler” and “Energy_balance”)

✓ Expansion valve

Operating parameters	*Valve*
Constraint type	Pressure specification
Pressure supplied (atm)	1

1.6.4. Gas Cleaning

As the final gas cleaning process, the remaining sulfur compounds and the carbon dioxide CO_2 are separated in an absorber using an amine solvent.



"Gas cleaning" process

✓ "MEA Feed Recycle" feed

		MEA Feed Recycle
Mass percentage	**H_2O**	80
	MEA	20
Total mass flowrate (t/h)		100
Temperature (°C)		40
Pressure (atm)		1

✓ *Pumps*

Operating parameters	***Pump rich amine***
Exhaust pressure (kPa)	750
Isentropic efficiency	0.75
Mechanical efficiency	1
Electrical efficiency	1

Operating parameters	Pump lean amine
Exhaust pressure (kPa)	700
Isentropic efficiency	0.75
Mechanical efficiency	1
Electrical efficiency	1

✓ Expansion valve

Operating parameters	***Amine valve***
Constraint type	Pressure specification
Pressure supplied (kPa)	200

✓ Absorber

Operating parameters	***Absorber***
Number of theoretical stages	2

✓ Distillation column

Operating parameters	***Desorber***
Number of theoretical stages	12
Feed stage	2
Specification type for operating conditions	Vapor distillate and reflux ratio
Vapor distillate flowrate (t/h)	10
Molar reflux ratio	1
Initialization of vapor distillate recovery ratios	-
Water	0.1
Carbon dioxide	0.6
Monoethanolamine	0.001

✓ Generalized heat exchanger

Operating parameters	***MEA Heat exchanger recovery***
Constraint type : "Other"	Minimal internal temperature approach
Temperature deviation (°C)	10

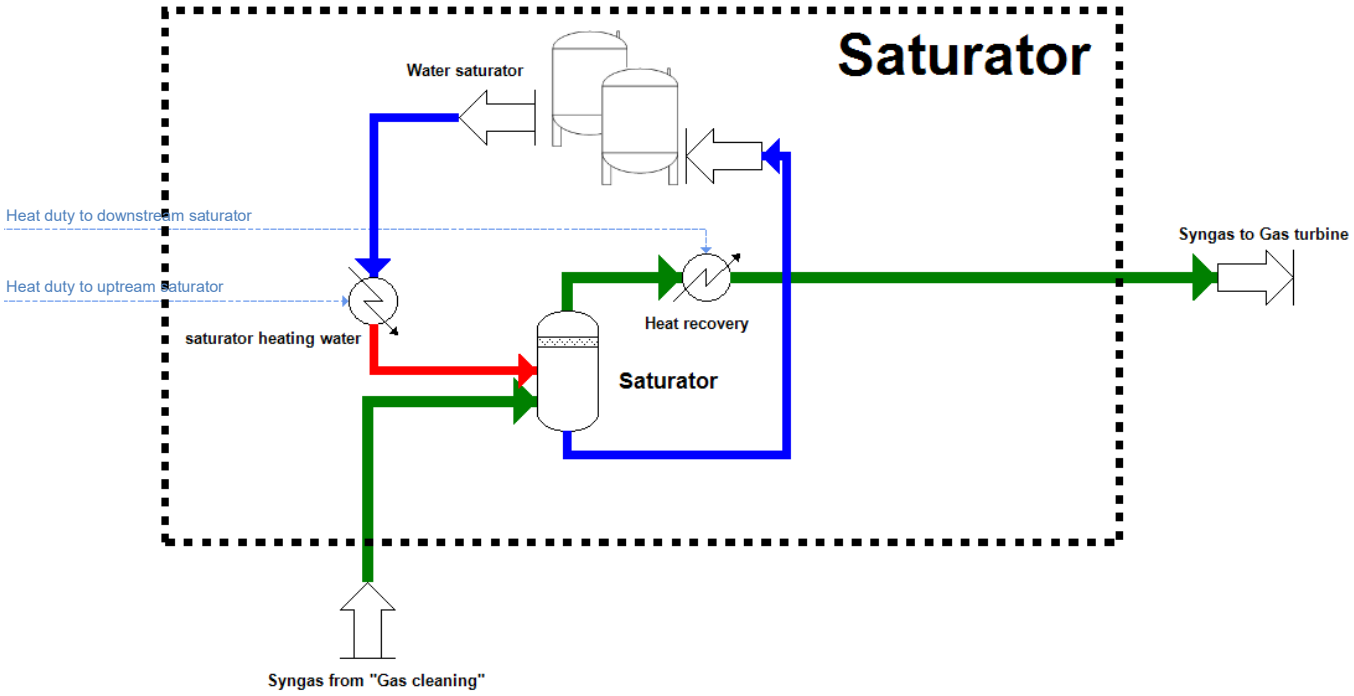
✓ Calculator Switch

Name	***MEA Heat exchanger recovery***
Calculator Switch (input syngas)	"Syngas cleaning"
Calculator Switch 1 (output syngas)	Global model ("Global calculator")

Note: The add-in and the recycle of the MEA (connection between the feed and the outlet of MEA mixture) is not modelled in this example. Refer to the "PSPS_EX_EN – Simple Example" or "PSPS_EX_EN – Cyclohexane Plant" application examples to deal with recycle in process.
Note: A more detailed example of gas sweetening with alkanol amine is available in the "PSPS_EX_EN_CO2 capture with amine process" application example.

1.6.5. Saturator

The cleaned gas obtained is saturated with water and sent to the combined cycle.



"Saturator" process

✓ "Water saturator" feed

		Water saturator
Mass percentage	**H_2O**	100
Total mass flowrate (t/h)		2
Temperature (°C)		45
Pressure (atm)		15

Note: The calculator used for water streams is the "Pure water" calculator.

Note: The add-in and the recycle of the water (connection between the feed and the outlet of water) are not modelled in this example.

✓ Separator

Operating parameters	*Saturator*
Separator type	Constant pressure and enthalpy flash
Pressure (bar)	The lowest of the feed streams
Heat duty (W)	Adiabatic

✓ Simple heat exchangers

Name	*Heat duty (W)*	*Pressure drop (bar)*
Saturator heating water	0	0
Heat recovery	0	0

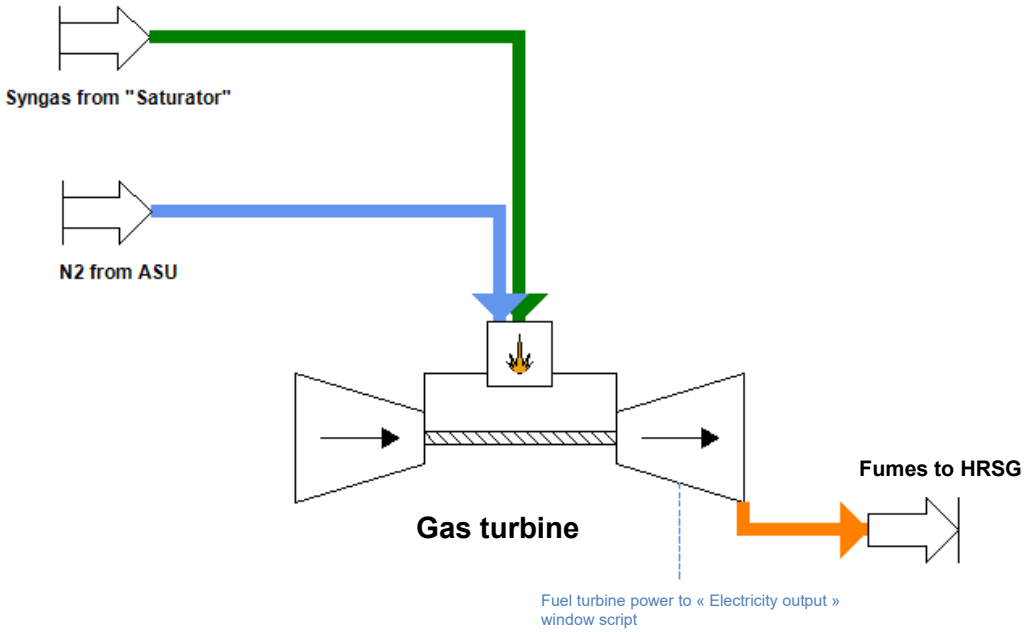
The simple heat exchangers duties are fixed by incoming information streams from coolers on the syngas pipe (cf. 1.6.3 H2S Removal and Heat Recovery).

1.7. Operating conditions of the “Combined cycle” block

1.7.1. Gas turbine

The syngas exits from the saturator and comes in the gas turbine.

Note: the “Fuel turbine” unit operation uses conventional combustion reaction. It is not necessary to add combustion reactions concerning the syngas. This step is performed automatically in the “Reactions” tab of the combustion definition.



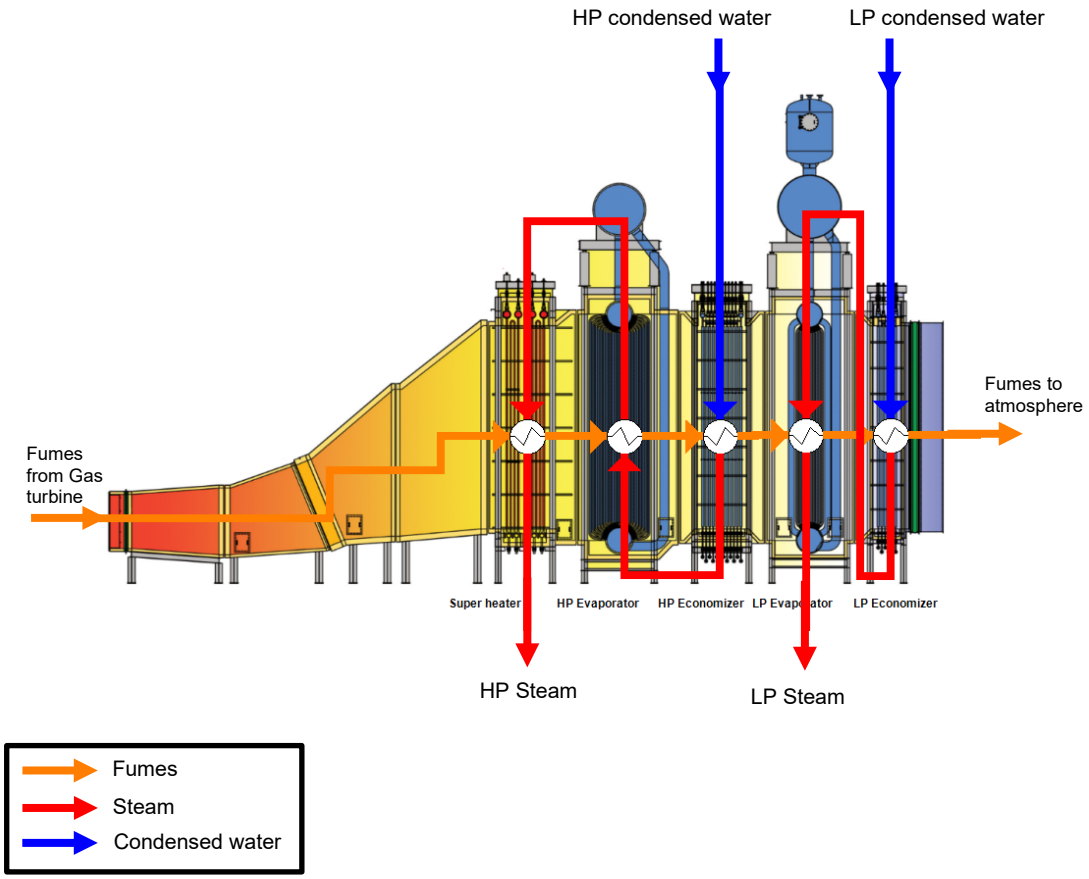
✓ Fuel Turbine

Operating parameters	*Gas turbine*
Compressor constraint	Compression ratio
Ratio of the compressor	21
Mechanical yield of the compressor (%)	98
Isentropic yield of the compressor (%)	75
Turbine constraint	Outlet pressure
Pressure (atm)	1
Mechanical yield of the turbine (%)	98
Electrical yield of the turbine (%)	99
Isentropic yield of the turbine (%)	80
Combustive type	Air
% mass content of O_2 in fumes	2
LHV of the fuel	Calculated from compounds data

1.7.2. Heat Recovery Steam Generator (HRSG)

The heat recovery steam generator (HRSG) is a set of heat exchangers in which heat is removed from the gas turbine exhaust gas (fumes) to generate steam. Typically, steam is generated at two or three different pressures, and associated with the HRSG is one steam drum for each steam pressure level. High pressure superheated steam is generated for use in the steam turbine, and typically the exhaust from the steam turbine first stage is reheated. The input streams to the HRSG section include the gas turbine exhaust and the water feed. The major output streams are the high and low-pressure steams to the steam turbines. Several parts of the HRSG must be sized to accommodate the high-pressure steam flow, including the superheater, reheater, high pressure steam drum, high pressure evaporator, and the economizers.

In this example, the HRSG is simplified with 2 stages (high and low pressure) for which fumes crosses the super heater, the HP evaporator, the HP economizer, the LP Evaporator and finally the LP economizer before being released in the atmosphere:



Schematics of the HRSG

✓ Generalized heat exchangers

Operating parameters	***Super heater***
Constraint type: "Cold stream"	Superheated over its dew point temperature
Temperature difference (°C)	200

Operating parameters	***HP Evaporator***
Constraint type : "Cold stream"	Superheated over its dew point temperature
Temperature difference (°C)	1

Operating parameters	***HP Economizer***
Constraint type : "Cold stream"	Superheated over its dew point temperature
Temperature difference (°C)	-1

Operating parameters	*LP Evaporator*
Constraint type: "Cold stream"	Superheated over its dew point temperature
Temperature difference (°C)	150

Operating parameters	*LP Economizer*
Constraint type: "Cold stream"	Superheated over its dew point temperature
Temperature difference (°C)	-1

1.7.3. Steam turbines

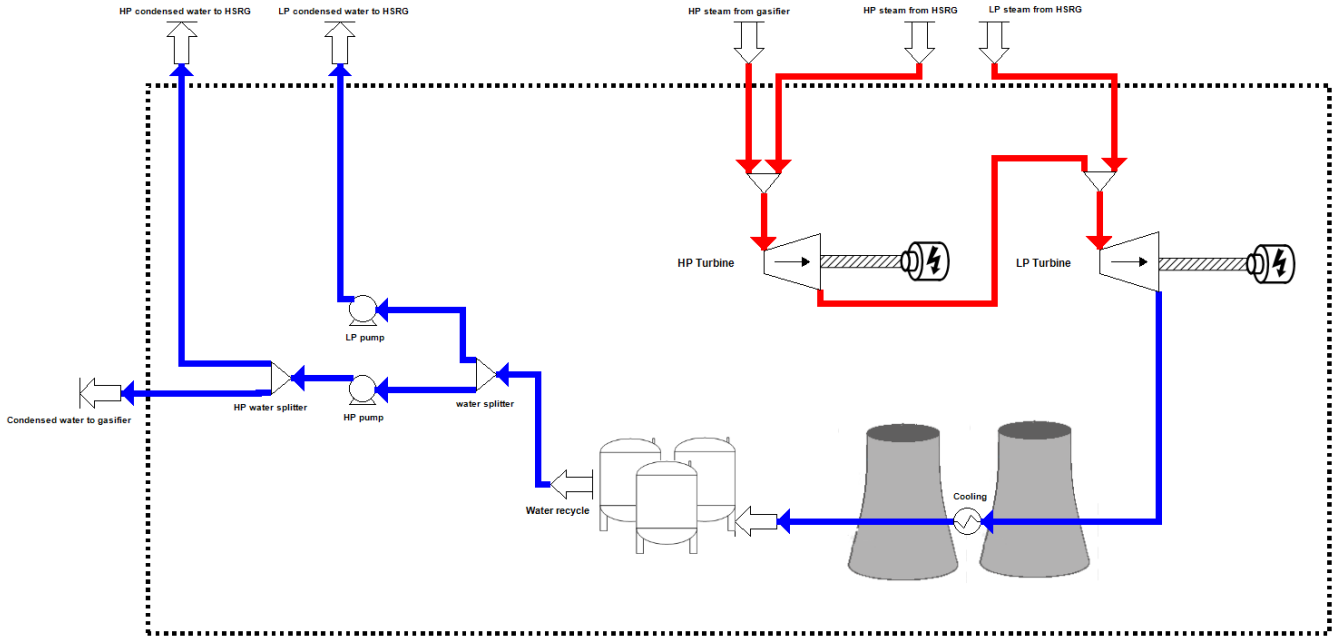
A typical steam turbine system for an IGCC plant consists of high-pressure, intermediate pressure, and low-pressure turbine stages, a generator, and an exhaust steam condenser. The high-pressure stage receives high pressure superheated steam from the HRSG. The outlet steam from the high-pressure stage returns to the HRSG for reheat, after which it enters the intermediate pressure stage. The outlet from the intermediate pressure stage goes to the low-pressure stage.

In this example, the steam turbine system is simplified with a 2 stages steam turbine.

- ✓ "Water saturator" feed

		Water recycle
Mass percentage	**H_2O**	100
Total mass flowrate (t/h)		33
Temperature (°C)		25
Pressure (atm)		1

Note: The calculator used for water streams is the "Pure water" calculator.



"Steam turbine" process

✓ *Pumps*

Operating parameters	*LP pump*
Exhaust pressure (bar)	50
Volumetric efficiency	0.65
Mechanical efficiency	1
Electrical efficiency	1

Operating parameters	*HP pump*
Exhaust pressure (bar)	120
Volumetric efficiency	0.65
Mechanical efficiency	1
Electrical efficiency	1

✓ *Expanders*

Operating parameters	*LP Turbine*
Exhaust pressure (bar)	0.07
Isentropic efficiency	0.85
Mechanical efficiency	0.98
Electrical efficiency	0.99

Operating parameters	*HP Turbine*
Exhaust pressure (atm)	50
Isentropic efficiency	0.85
Mechanical efficiency	0.98
Electrical efficiency	0.99

- ✓ *Stream splitter*s

Operating parameters	*Water splitter*
Specification type	Mass flowrates
Mass flowrate of the HP water (to "HP pump") (t/h)	25

Operating parameters	*HP water splitter*
Specification type	Mass flowrates
Mass flowrate of water to the gasifier (t/h)	16

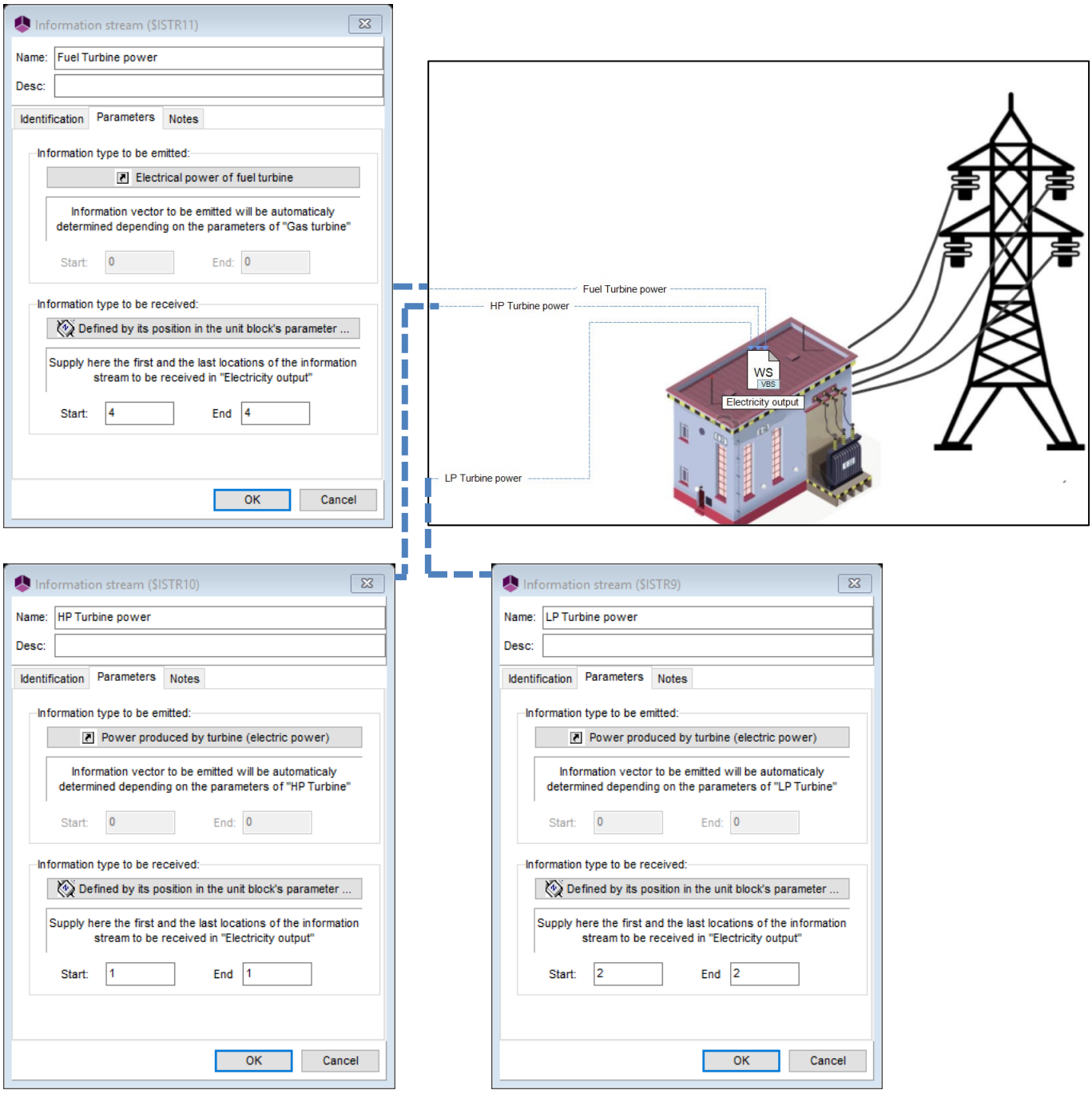
Note: The mixers are defined with default values (outlet pressure is the lowest pressure of the feeds).

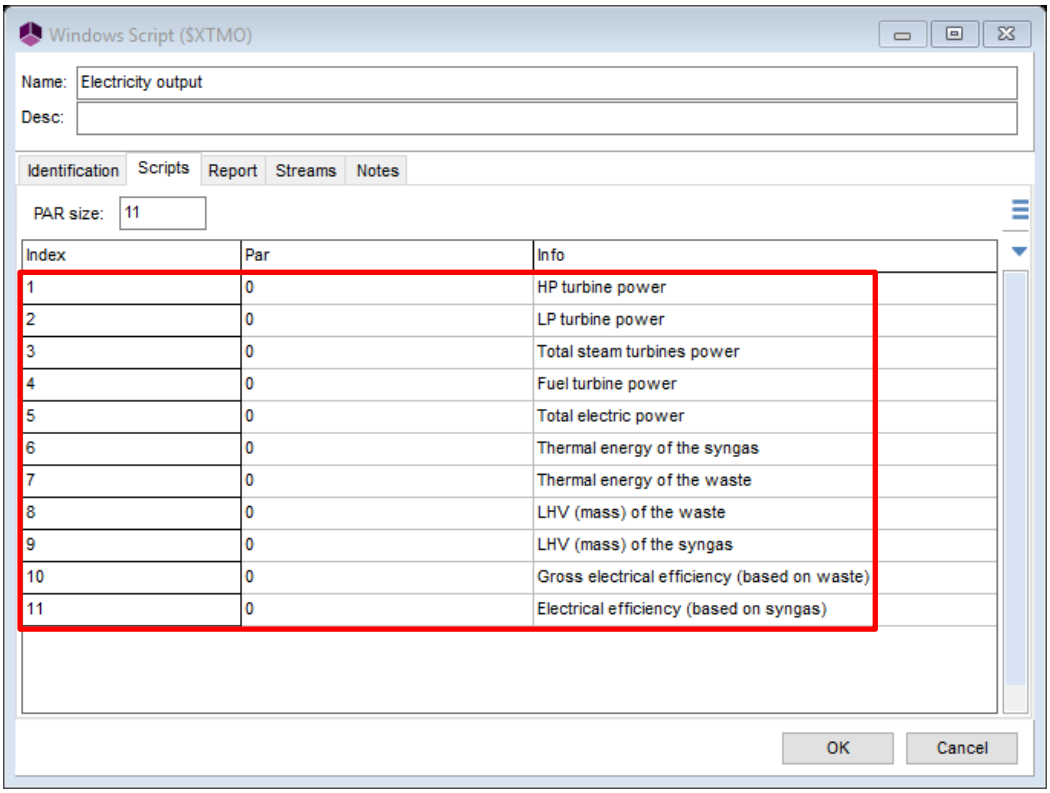
Note: The add-in and the recycle of the water (connection between the feed and the outlet of water) are not modelled in this example.

2. SIMULATION RESULTS

2.1. Results summary

In the same way the “Pyrolysis” windows script allows the user to provide and define input parameters, the “Electricty output” windows script aims to summarize the global performance of the IGCC plant.

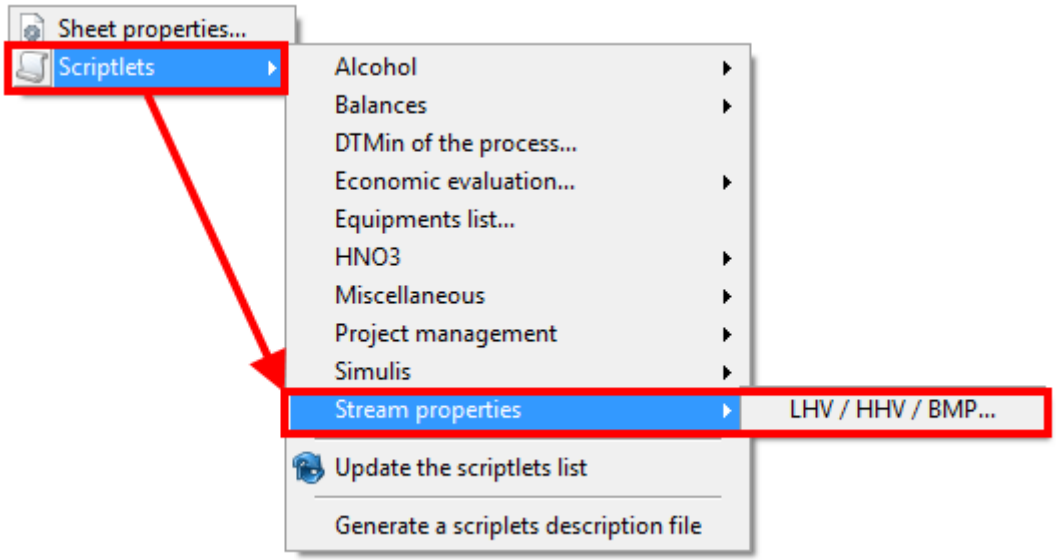





```
'-------------------------------------------------------------------------------'
' CALL OF "UNIT CONVERSION" SCRIPT
'-------------------------------------------------------------------------------'
with CreateObject("Scripting.FileSystemObject")
  ExecuteGlobal .OpenTextFile(Project.ApplicationPath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


'-------------------------------------------------------------------------------'
' Calculation of the total electric power and efficiencies
'-------------------------------------------------------------------------------'
Function OnCalculation()
   '
   ' Total electric power of steam turbines and gas turbine
   Module.Parameter(3) = abs(Module.Parameter(1)) + abs(Module.Parameter(2))
   Module.Parameter(5) = abs(Module.Parameter(3)) + abs(Module.Parameter(4))
   '
   ' LHV calculation of syngas and waste
   Module.Parameter(9) = Project.Modules("Gas turbine").FuelLHVCalculated/Project.Modules("Gas
     turbine").FuelMolecularWeightCalculated
   Module.Parameter(8) = ConvertToProSim("Mass enthalpy", LHV_Mol = ConvertToProSim("Molar
     enthalpy", LHVStream(Project.Modules("Waste_Feed").OutputStream(1), 0), ReportUnit("Molar
     enthalpy"))
   Module.Parameter(8) = LHV_Mol/Project.Modules("Waste_Feed").OutputStream(1).MolarWeight
   '
   ' Thermal energy power
  Module.Parameter(6) = Project.Modules("Gas turbine").FuelMassFlowrateCalculated *
     Module.Parameter(9)
  Module.Parameter(7) = Project.Modules("Waste_Feed").OutputStream(1).MassFlowrate *
  Module.Parameter(8)
   '
   ' Efficiencies
   Module.Parameter(10) = (Module.Parameter(5) / Module.Parameter(7))*100
   Module.Parameter(11) = (Module.Parameter(5) / Module.Parameter(6))*100
   '
```

```
    OnCalculation = true
End Function

'-------------------------------------------------------------------------------
' Print results
'-------------------------------------------------------------------------------
Sub OnPrintResults()
    Module.PrintReport("ELECTRIC POWER")
    Module.PrintReport("HP Turbine power              : " &
     FormatNumber(ProSimToReport("Power",abs(Module.Parameter(1))),3) & " " & ReportUnit("Power"))
    Module.PrintReport("LP Turbine power              : " &
     FormatNumber(ProSimToReport("Power",abs(Module.Parameter(2))),3) & " " & ReportUnit("Power"))
    Module.PrintReport("-----------------------------------------------------------")
    Module.PrintReport("Steam Turbines power          : " &
     FormatNumber(ProSimToReport("Power",abs(Module.Parameter(3))),3) & " " & ReportUnit("Power"))
    Module.PrintReport("")
    Module.PrintReport("Fuel Turbine power            : " &
     FormatNumber(ProSimToReport("Power",abs(Module.Parameter(4))),3) & " " & ReportUnit("Power"))
    Module.PrintReport("-----------------------------------------------------------")
    Module.PrintReport("Total power produced          : " &
     FormatNumber(ProSimToReport("Power",abs(Module.Parameter(5))),3) & " " & ReportUnit("Power"))
    Module.PrintReport("")
    Module.PrintReport("")
    Module.PrintReport("THERMAL ENERGY POWER (LHV)")
    Module.PrintReport("LHV of the waste              : " & FormatNumber(ProSimToReport("Mass
     enthalpy",abs(Module.Parameter(8))),3) & " " & ReportUnit("Mass enthalpy"))
    Module.PrintReport("LHV of the syngas             : " & FormatNumber(ProSimToReport("Mass
     enthalpy",abs(Module.Parameter(9))),3) & " " & ReportUnit("Mass enthalpy"))
    Module.PrintReport("")
    Module.PrintReport("Thermal energy of the waste   : " &
     FormatNumber(ProSimToReport("Power",abs(Module.Parameter(7))),3) & " " & ReportUnit("Power"))
    Module.PrintReport("Thermal energy of the syngas  : " &
     FormatNumber(ProSimToReport("Power",abs(Module.Parameter(6))),3) & " " & ReportUnit("Power"))
    Module.PrintReport("")
    Module.PrintReport("")
    Module.PrintReport("EFFICIENCIES")
    Module.PrintReport("Gross electrical efficiency (based on LHV waste)  : " &
     FormatNumber(abs(Module.Parameter(10)),3) & " (%)")
    'Module.PrintReport("Electrical efficiency (based on LHV syngas)       : " &
     FormatNumber(abs(Module.Parameter(11)),3) & " (%)")
End Sub
```

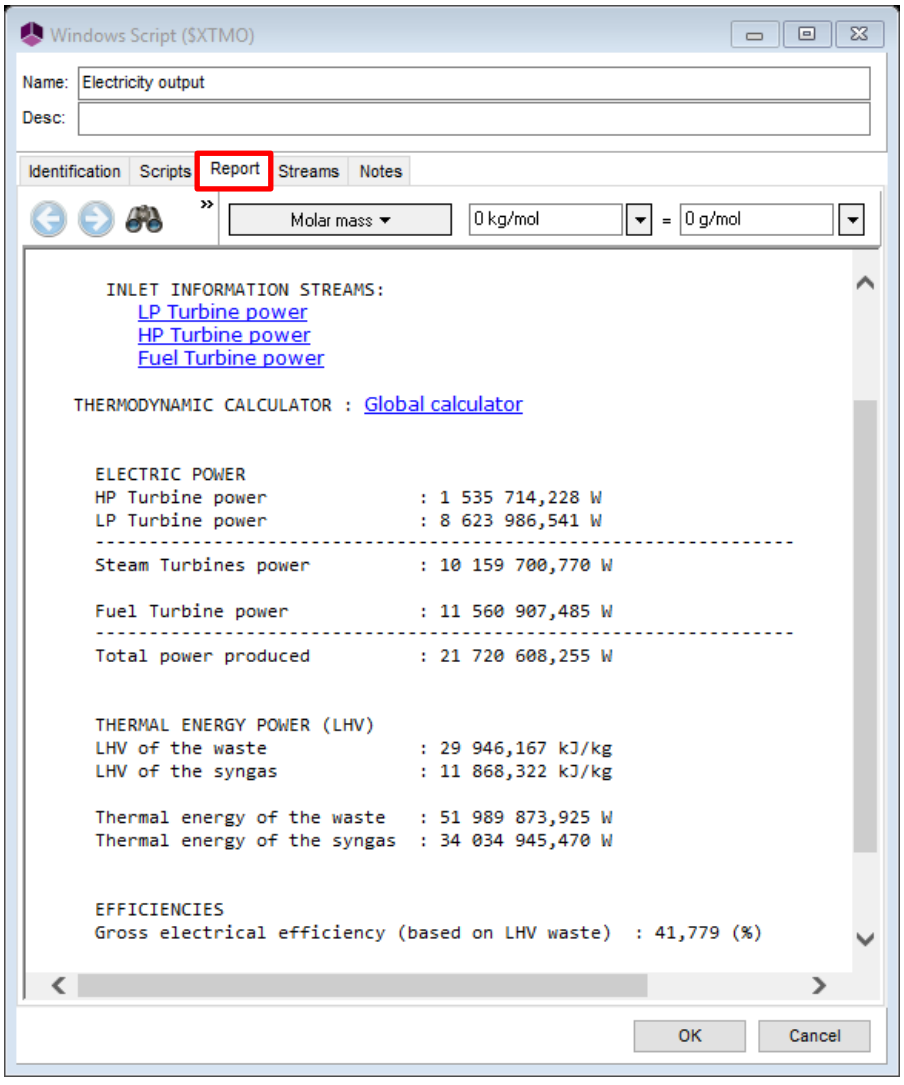
Note: the LHV of a stream can be calculated using the "LHV / HHV / BMP" scriptlet as follows (the right click to access to the scriptlets can be done on the project, on a group of selected unit operations or on a specific stream):



2.2. Net Power Output and Plant Efficiency

The main results are summarized in the following table:

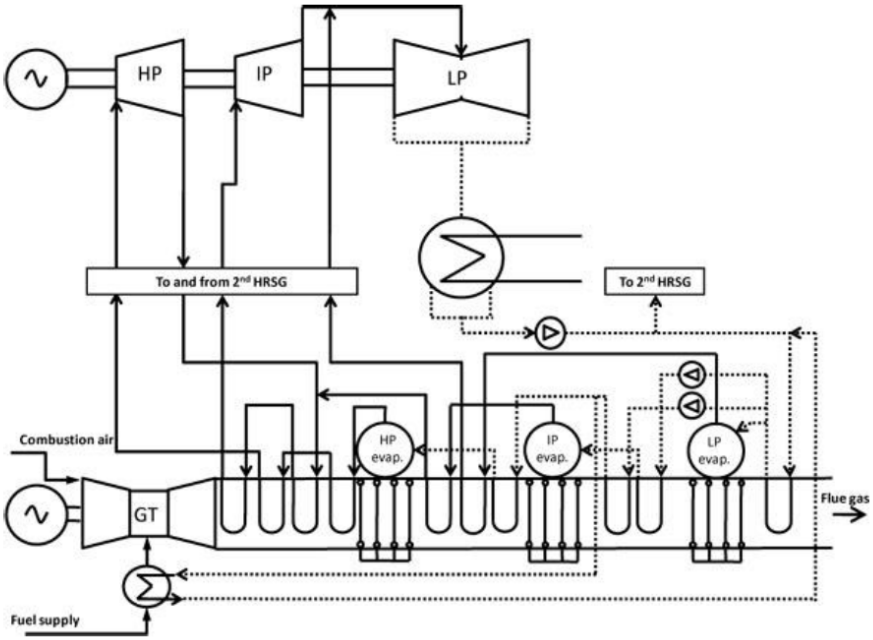
Simulation results	Notation	Value
HP Turbine power (MW)	A	1.5
LP Turbine power (MW)	B	8.6
Total Turbine power (MW)	C (A+B)	10.1
Gas Turbine power (MW)	D	11.6
Total electric power produced (MW)	E (C+D)	21.7
LHV of the coal (MJ/kg)	F	30
LHV of the syngas (MJ/kg)	G	11.9
Coal mass flowrate (t/h)	H	6.25
Syngas mass flowrate (t/h)	I	10.3
Thermal energy of the coal (MW)	J (H*F)	52
Gross electrical efficiency (%)	K (E/J)	41.8



Results displayed in the "Electricity ouput" windows script

In this example, the gross efficiency is of 42%. In order to compute the net efficiency, the input power consumed for the ASU (compressors consumption), pumps and other supplies have to be taken into account. These electrical consumptions reach up to 10-15% of the total power produced by the plant. Conventional IGCC plants reach between 35 and 45% of net efficiency.

Note: The IGCC plant modelled in this example was simplified which explains the relative "low" gross efficiency. Indeed, the HRSG efficiency, the gasifier efficiency and especially the "Combined cycle" of the IGCC are improvable to reach typical net efficiency up to 40%.



Schematics of an advanced "Combined cycle" of IGCC plant

3. REFERENCES

[NT172] Technical note NT172 : Scriptlet « Solid compound ».

[EDW07] Edward S.Rubin, “Technical Documentation: Integrated Gasification Combined Cycle Systems (IGCC) with Carbon Capture and Storage (CCS)”, Carnegie Mellon University, 5-2007.

[ENE17] Manuel Trevino Coca, “Integrated gasification combined cycle technology: IGCC”, ELCOGAS, Puertollano, ENERCLUB (Club espanol de la energia).

[NAY11] Rajul Nayak, Raju K. Mewada, “Simulation of Coal Gasification Process using ASPEN PLUS”, INSTITUTE OF TECHNOLOGY, NIRMA UNIVERSITY, AHMEDABAD – 382 481, 08-10 DECEMBER, 2011.

[ROW17] R.L. Rowley, W.V. Wilding, J.L. Oscarson, N.F. Giles, DIPPR® Data Compilation of Pure Chemical Properties, Design Institute for Physical Properties, AIChE, New York, NY (2017)

