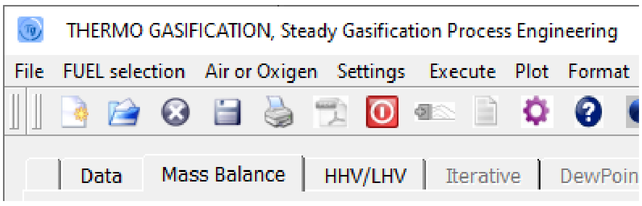
ThermoGasification

THERMO GASIFICATION | Technical & Educational Software



THERMOGasification is a software for the thermodynamic analysis of the thermochemical process in which the reactions between fuel and the gasification agent take place and syngas (product gas, synthetic gas, or synthesis gas) is produced. THERMOGasification is at the forefront of thermal technology, offering innovative and efficient thermal energy solutions applied to the gasifier.

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Characteristics

- **Solid technology**
- **Precision**
- **Easy handling**
- **Intuitive interface**
- **Input variability**
- **Application in several industrial systems**

Software capabilities

- Thermo-chemical analysis
- Mass, energy and exergetic balance
- Energetic flow and *Grassmann* diagram
- Thermal and exergetic efficiency
- Sensitivity analysis
- Pollutant emissions control

Applications

i) Production of fuel for use in electric power generation units.

ii) Manufacturing synthetic or substitute natural gas for use as pipeline gas supplies.

iii) Producing hydrogen for fuel cell applications.

iv) Production of synthesis gas for use as a chemical feedstock.

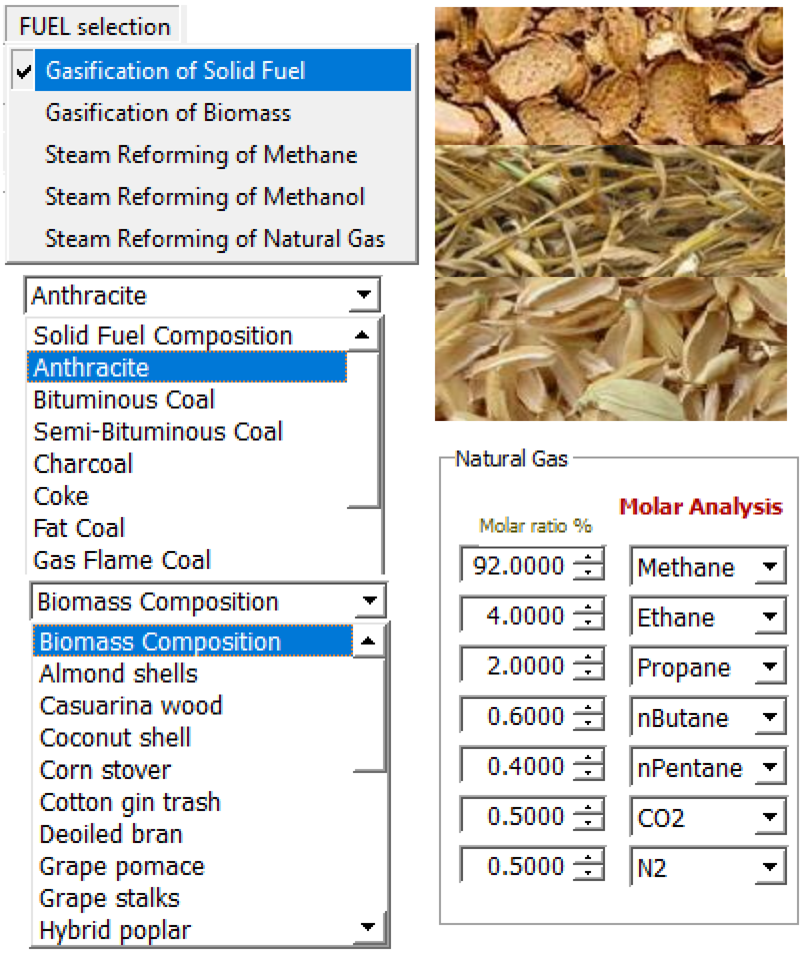
v) Generation of fuel gas (low-Btu or medium-Btu gas) for industrial purposes.

Characteristics

Software algorithms are based on up-to-date bibliography and the latest mathematical models, which in conjunction result in a **well-defined** and **solid technology**. The software has been set up with an **intuitive interface** that allows **easy handling**.

Input data (fuel)

The demand for energy sources to satisfy human energy consumption continues to increase. Prior to the use of fossil fuels, biomass was the primary source of energy for heat via combustion.

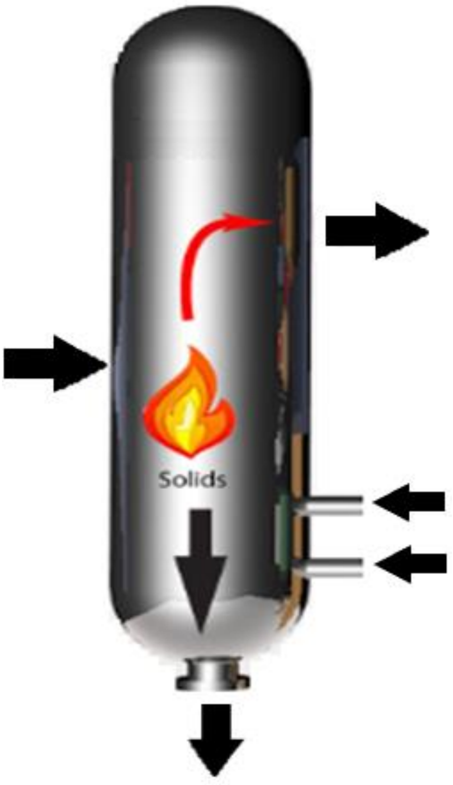


Molar ratio %	Molar Analysis
92.0000	Methane
4.0000	Ethane
2.0000	Propane
0.6000	nButane
0.4000	nPentane
0.5000	CO2
0.5000	N2

Fuel selection features

Application in industrial systems

The main operating parameters of the gasifier include type and design of gasifier, gasification temperature, flow rates of biomass and oxidizing agents (air or steam), type and amount of catalysts, and biomass type and properties.
Gasification takes place at high temperature in the presence of an oxidizing agent. Char and tar are the result of incomplete conversion of biomass.

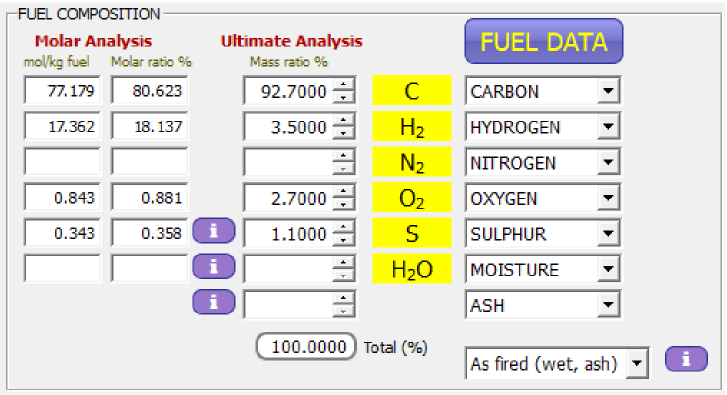


Gasifier (for biomass or coal)

Software capabilities

Thermo-chemical analysis

As a first step, a **mass balance** of combustion products can be obtained. Strict analysis on whole range of **fuel properties**: calorific powers, specific heat, enthalpy of formation, chemical exergy and entropy.

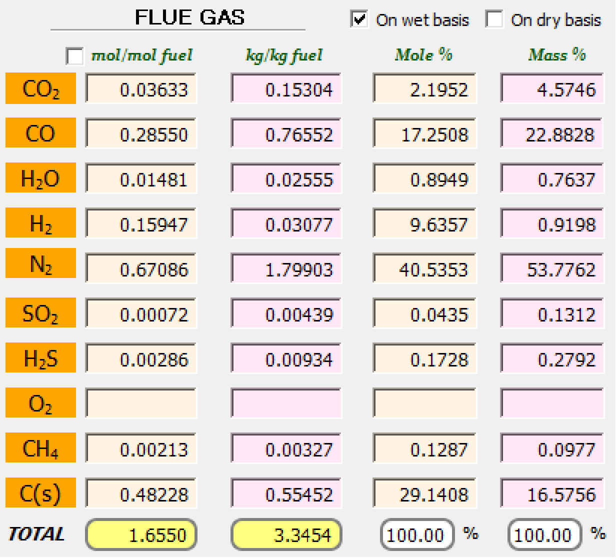


FUEL COMPOSITION

Molar Analysis mol/kg fuel	Molar ratio %	**Ultimate Analysis** Mass ratio %		
77.179	80.623	92.7000	C	CARBON
17.362	18.137	3.5000	H_2	HYDROGEN
			N_2	NITROGEN
0.843	0.881	2.7000	O_2	OXYGEN
0.343	0.358	1.1000	S	SULPHUR
			H_2O	MOISTURE
				ASH

Total (%): 100.0000

As fired (wet, ash)



FLUE GAS ☑ On wet basis ☐ On dry basis

	☐ mol/mol fuel	kg/kg fuel	Mole %	Mass %
CO_2	0.03633	0.15304	2.1952	4.5746
CO	0.28550	0.76552	17.2508	22.8828
H_2O	0.01481	0.02555	0.8949	0.7637
H_2	0.15947	0.03077	9.6357	0.9198
N_2	0.67086	1.79903	40.5353	53.7762
SO_2	0.00072	0.00439	0.0435	0.1312
H_2S	0.00286	0.00934	0.1728	0.2792
O_2				
CH_4	0.00213	0.00327	0.1287	0.0977
C(s)	0.48228	0.55452	29.1408	16.5756
TOTAL	1.6550	3.3454	100.00 %	100.00 %

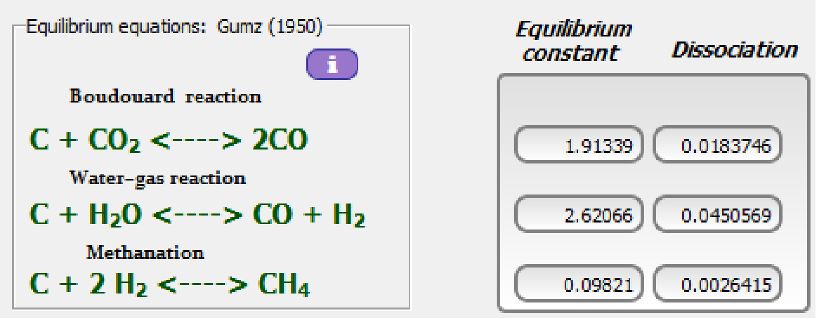
Mass balance interface

With the definition of fuel composition by means of an ultimate analysis, or the carbon, hydrogen, oxygen, nitrogen, sulphur, ash and water is possible the modelling for different types of fuel. It is also possible to define a mixture of hydrocarbons for a natural gas.

Mathematical model

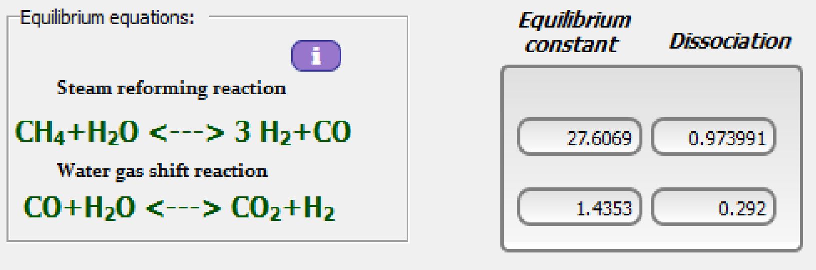
The chemistry of gasification is quite complex and is accomplished through a series of physical transformations and chemical reactions within the gasifier: Water-gas, steam reforming, combustion, Boudouard, water-gas-shift and methanation.

Within the gasification process, the chemical reactions of gasification can progress to different extents depending on the gasification conditions and the feedstock used. The main steps involved in the gasification process can be categorized as upstream processing, gasification and downstream processing.



Equilibrium equations: Gumz (1950)

	Equilibrium constant	Dissociation
Boudouard reaction $C + CO_2 <----> 2CO$	1.91339	0.0183746
Water-gas reaction $C + H_2O <----> CO + H_2$	2.62066	0.0450569
Methanation $C + 2\ H_2 <----> CH_4$	0.09821	0.0026415

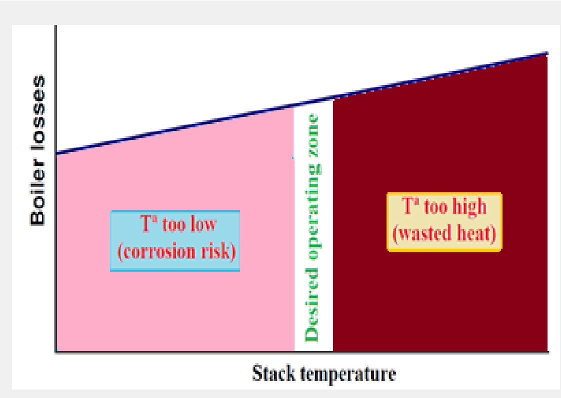


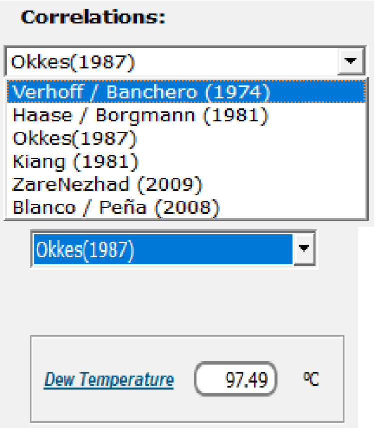
Equilibrium equations:

	Equilibrium constant	Dissociation
Steam reforming reaction $CH_4+H_2O <---> 3\ H_2+CO$	27.6069	0.973991
Water gas shift reaction $CO+H_2O <---> CO_2+H_2$	1.4353	0.292

Sulfuric acid dew point

To prevent sulfuric acid condensation problems in industrial facilities that burn fuels with the presence of sulfur, it is necessary to know the dew point temperature of the sulfuric acid. An exhaustive analysis of the chemical reactions involved until reaching the formation of sulfuric acid is carried out.





Correlations:

Okkes(1987)

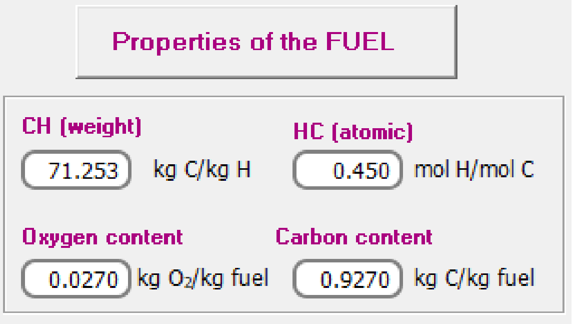
- Verhoff / Banchero (1974)
- Haase / Borgmann (1981)
- Okkes(1987)
- Kiang (1981)
- ZareNezhad (2009)
- Blanco / Peña (2008)

Okkes(1987)

Dew Temperature: 97.49 ºC

Fuel characterization

Includes different properties of the fuel for each type of fuel: biomass, coal, natural gas, methane, methanol, etc.



Properties of the FUEL

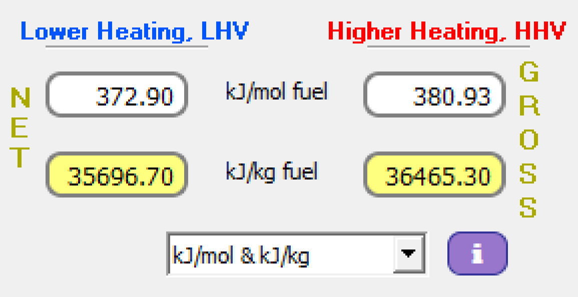
CH (weight): 71.253 kg C/kg H

HC (atomic): 0.450 mol H/mol C

Oxygen content: 0.0270 kg O_2/kg fuel

Carbon content: 0.9270 kg C/kg fuel

Properties of the fuel (biomass, coal, natural gas, methane, methanol, etc)

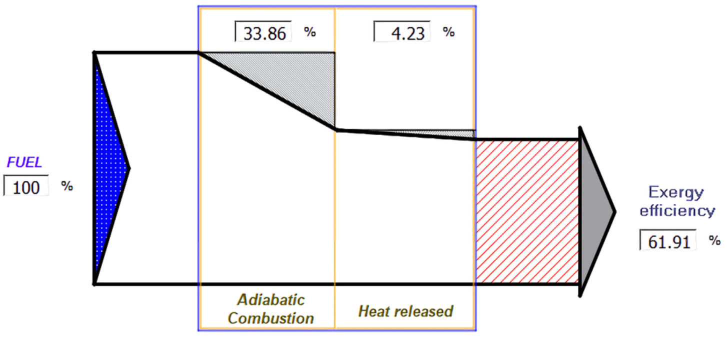


	Lower Heating, LHV		Higher Heating, HHV
NET	372.90	kJ/mol fuel	380.93
	35696.70	kJ/kg fuel	36465.30

Heat of combustion of the fuel

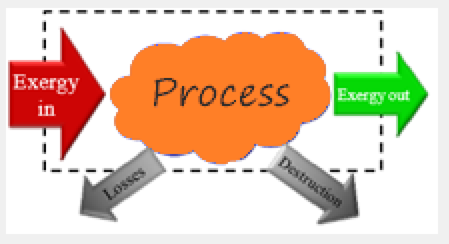
Exergy analysis

Based on Second Principle, it provides information about **irreversibilities** generated in each device of the installation, including the internal of the all the process.



Results visualization using a Grassmann combustion diagram

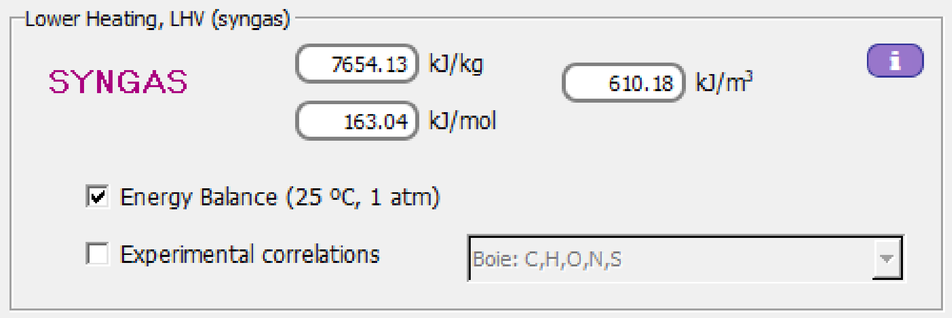
From second law evaluations (entropy or exergy evaluations) it is generally known that thermodynamic losses of boilers and furnaces are much higher than the thermal efficiencies do suggest.



Exergy flow diagram

Syngas production

It provides the different categories of gasification reactors as they apply to various types of feedstocks. In terms of feedstock variability, several different types of feedstocks that vary widely in composition are available for gasification and include crude oil residues, coal, wood, wood waste as well as a multitude of agricultural residues, domestic waste, and industrial waste.



Lower Heating, LHV (syngas)

SYNGAS

7654.13 kJ/kg

163.04 kJ/mol

610.18 kJ/m³

☑ Energy Balance (25 ºC, 1 atm)

☐ Experimental correlations — Boie: C,H,O,N,S

Heat of combustion of the syngas

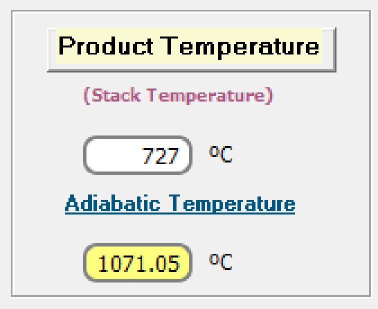
Syngas production efficiency

$$\eta = \frac{N_{H2} LHV_{H2} + N_{CO} LHV_{CO}}{Q_{reactor} + N_{coal} LHV_{coal}}$$

25.0 ºC

100.0 kPa

4.38621 %



Product Temperature

(Stack Temperature)

727 ºC

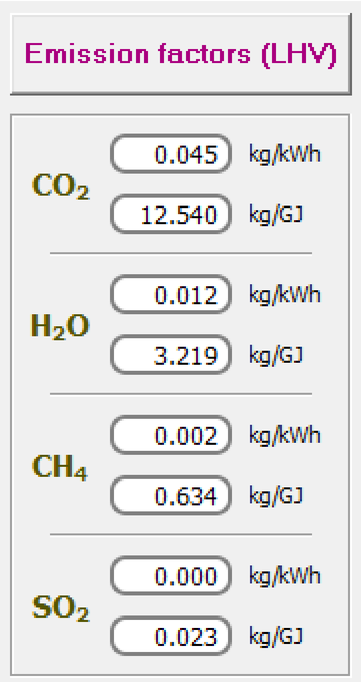
Adiabatic Temperature

1071.05 ºC

The increase in gasification temperature gives rise to an increase in gas formation and a subsequent decrease in tar and char yields. Temperature also has an effect on the gas composition. The rise in temperature usually gives rise to an increase in H_2 and a decreased in CO and light hydrocarbons. Nevertheless, thermodynamic models have shown that a smooth decrease in H_2 yield occurs at very high reaction temperatures.

Pollutant emissions control

Includes critical pollutants as carbon monoxide (**CO**), methane (**CH_4**) or sulfur dioxide (**SO_2**) among others (**CO_2**),



Emission factors (LHV)

CO_2	0.045	kg/kWh
	12.540	kg/GJ
H_2O	0.012	kg/kWh
	3.219	kg/GJ
CH_4	0.002	kg/kWh
	0.634	kg/GJ
SO_2	0.000	kg/kWh
	0.023	kg/GJ

Pollutant emissions

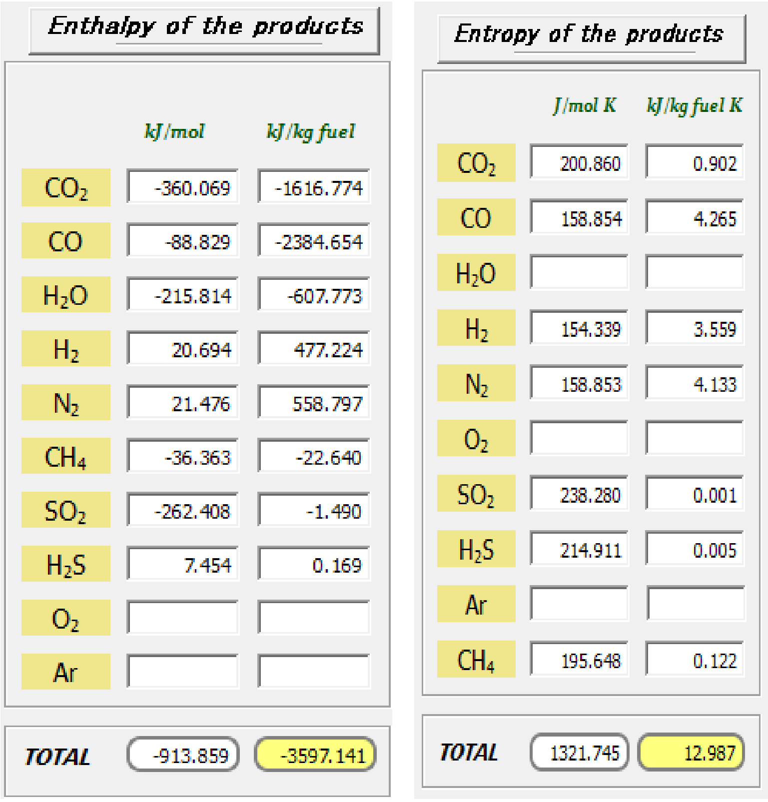
Applications

The gasification of the biomass implies an incomplete combustion that results in the production of combustible gases (syngas) consisting of carbon monoxide (CO), hydrogen (H_2) and traces of methane (CH_4). This mixture is called producer gas. The producer gas can be used to run internal combustion engines (both compression and spark ignition), can be used to power furnaces in direct heat applications and can be used to produce, in an economically viable manner, methanol, which is useful both as fuel for thermal engines and for chemical raw materials for industries.

Since any biomass material can undergo gasification, this process is much more attractive than the production of ethanol or biogas, where only selected biomass can produce these fuels. In addition, since solid waste is seldom in a form that can be easily used economically, it is advantageous to convert this waste into a more easily usable fuel from a similar producer gas. Hence the attraction of gasification.

Academia application specifications

This software's capabilities are appropriate for gasification studies in academia. Major application for process optimization in industry or equilibrium-chemical processes study in **academia**.



Enthalpy of the products

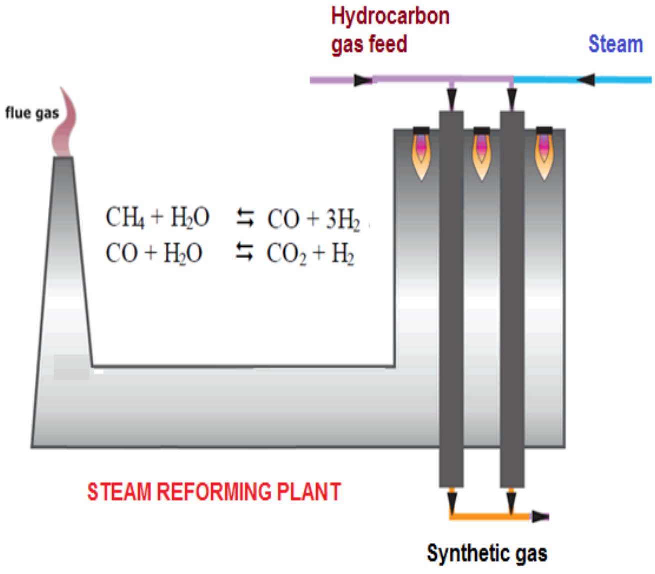
	kJ/mol	kJ/kg fuel
CO_2	-360.069	-1616.774
CO	-88.829	-2384.654
H_2O	-215.814	-607.773
H_2	20.694	477.224
N_2	21.476	558.797
CH_4	-36.363	-22.640
SO_2	-262.408	-1.490
H_2S	7.454	0.169
O_2		
Ar		
TOTAL	-913.859	-3597.141

Entropy of the products

	J/mol K	kJ/kg fuel K
CO_2	200.860	0.902
CO	158.854	4.265
H_2O		
H_2	154.339	3.559
N_2	158.853	4.133
O_2		
SO_2	238.280	0.001
H_2S	214.911	0.005
Ar		
CH_4	195.648	0.122
TOTAL	1321.745	12.987

Thermodynamic properties for each specie of the syngas

Methane steam reforming is the most common and cost-effective method for hydrogen production, and it contributes about 50% of the world's hydrogen production. First stage is the steam reforming of methane. Second stage is the water–gas shift process. Steam methane reforming is a process requiring high temperature and pressure. During the process, hydrogen is generated in reactions and with methane/CO and water participation under pressure.



Methane steam reforming installation

ThermoSuite
Technical Software Suite

For product-related and techical questions:

https://thermosuite.com/thermogasification

Email: info@thermosuite.com