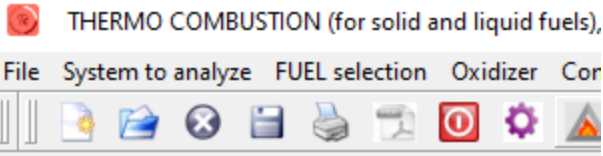


## THERMO COMBUSTION | Technical & Educational Software

Software developed for combustion processes' characterization. Major application to industrial combustion processes, such as combustion heat or electricity generation processes; whether they take place in steam generators, gas turbines or stationary engines, and in industrial furnaces (with or without fire contact).



### INDEX

#### 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
- Combustion diagrams
- Sensitivity analysis
- Pollutant emissions control

#### Applications

Improvement of combustion process design, comprehensive study of main variables effect in the combustion, whether reducing irreversibilities or pollutant emissions; or performing several sensitivity analysis that **Thermocombustion** facilitates by default.

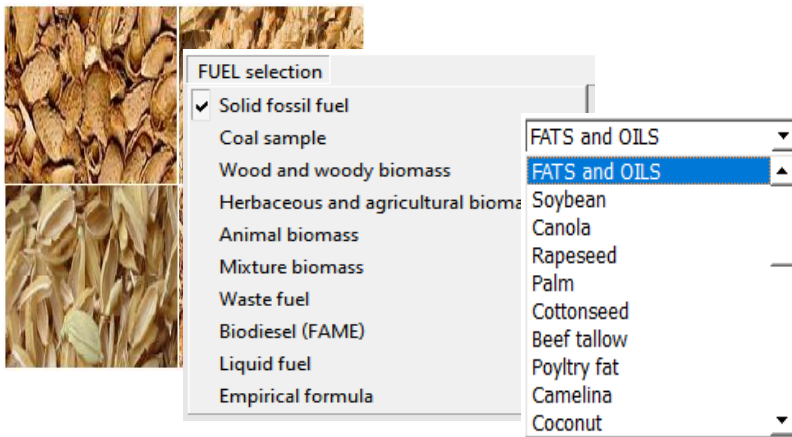
Main application in industry for process optimization or in academia (technical studios).

### 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 variability

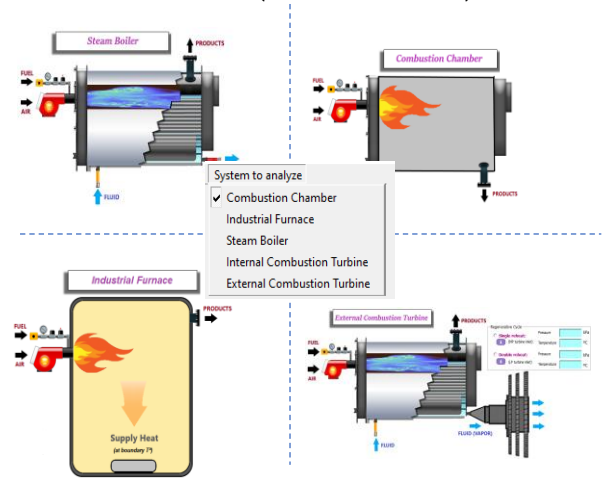
Available calculations with solid (including coals, biomass and biodiesel) and liquid fuel.



Fuel selection features

#### Application in several industrial systems

Combustion chamber, industrial furnace, steam boiler or combustion turbine (internal or external).

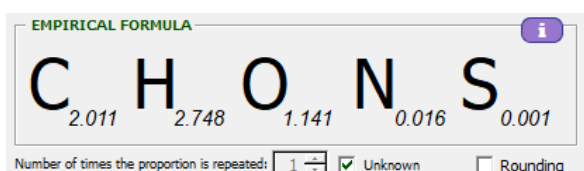


Industrial combustion systems available to analyse

### 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 energy and entropy.



Molar Analysis		Ultimate Analysis		FUEL	
mol/kg fuel	Molar ratio %	Mass ratio %			
20.10890	29.21354	24.1528	C	CARBON	
13.73779	19.95780	2.7694	H <sub>2</sub>	HYDROGEN	
0.08103	0.11772	0.2270	N <sub>2</sub>	NITROGEN	
5.70337	8.28567	18.2508	O <sub>2</sub>	OXYGEN	
0.00568	0.00825	0.0182	S	SULPHUR	
29.19740	42.41702	52.6000	H <sub>2</sub> O	MOISTURE	
14.52767	g/mol (as AF)	2.0000	ASH	ASH	
25.22910	g/mol (as DAF)	0.0091	Cl	CHLORINE	
		100.0273	Total (%)		

Composition of the fuel (ultimate analysis)



## Sulphuric Acid Dew Point

When flue gas reaches a temperature below the acid dew point, acidic elements will condense. This could cause heat exchanger corrosion. Knowing the acid dew point of your flue gas enables you to select the appropriate materials for your heat recovery installation. Most of the solid fuels contain sulphur, which get readily converted to  $SO_x$  in the combustion chamber. Mainly  $SO_2$  is formed, but part of this  $SO_2$  (about 2-4%) oxidizes further to  $SO_3$ . The formed  $SO_3$  subsequently reacts with  $H_2O$  to form sulphuric acid, when the flue gas cools below the Acid Dew Point. The sulphuric acid is highly corrosive and affects susceptible equipment surfaces.

**[SO<sub>3</sub>] / [SO<sub>2</sub>]** SO<sub>3</sub> from SO<sub>2</sub>

Calculated, CHEMICAL EQUILIBRIUM (by volume)  
1.2331 %

Chosen by user (by volume)  
1.2498 % (by weight)

1.00 % In boiler i

0.00 % In SCR, Selective Catalytic Reduction

1.00 % TOTAL

### Experimental correlations:

#### Recommended (Thermocombustion)

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

Recommended (Thermocombustion)

Sulphuric Acid Dew Temperature

122.32 °C

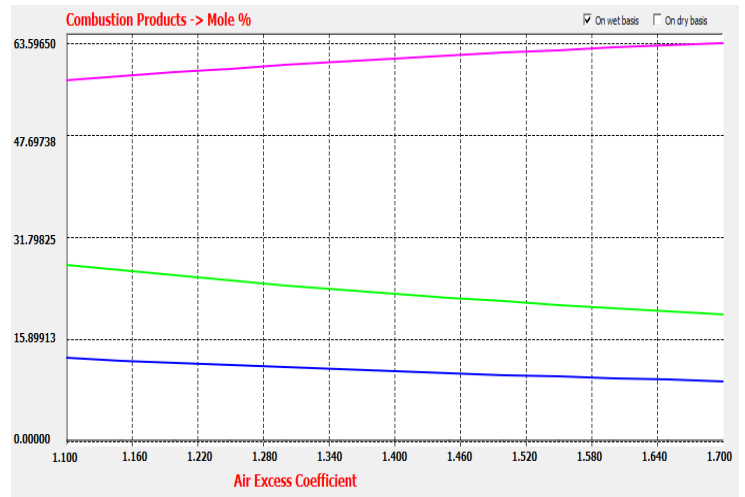
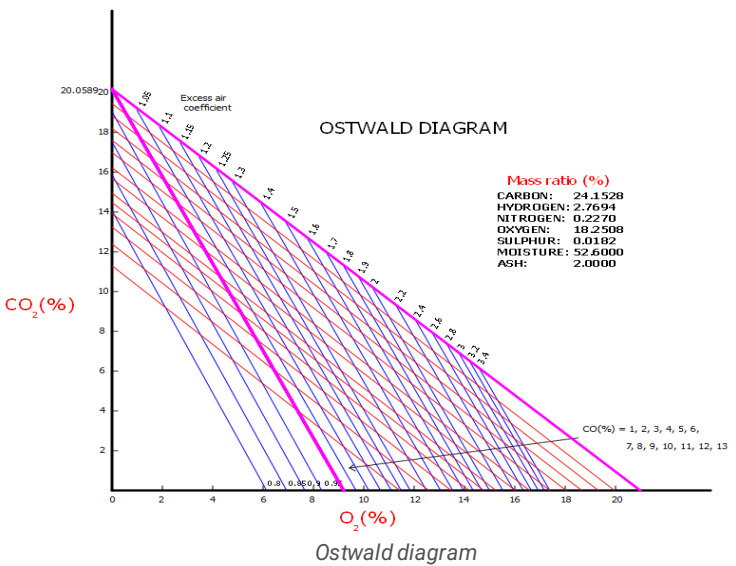
#### Requirement:

Stack Temperature > Dew Temperature

## Sensitivity analysis

Analysis of main variables involved in the combustion processes' study. Graphical display of results and calculation of Ostwald and Kissel combustion diagrams.

Ostwald and Kissel combustion diagrams allow fast and accurate combustion calculations.



## ASH

Solid fuel: exhaustive thermodynamic study related to the composition of ashes: molecular weight, enthalpy of formation, entropy, exergy, melting temperatures and fouling tendency among others.

**Ash constituents & Properties of the ash** Coal  Lignitic ash  Bituminous ash

	Mass ratio %	Molar ratio %	Molecular weight (kg/kmol)	Standard enthalpy (kJ/kmol)	Standard entropy (kJ/kmol)	Standard chemical exergy (kJ/mol)
SiO <sub>2</sub>	37.5300	47.0632	60.0	-911300	41.9	1.6400
Al <sub>2</sub> O <sub>3</sub>	20.1400	14.8564	102.0	-1674400	51.1	4.4800
Fe <sub>2</sub> O <sub>3</sub>	13.8300	6.5036	160.0	-825900	87.0	17.6600
CaO	9.9700	13.3956	56.0	-634600	38.8	129.8800
MgO	2.1400	4.0254	40.0	-601500	26.8	62.4200
TiO <sub>2</sub>	0.3100	0.2916	80.0	-945200	50.2	21.2200
Na <sub>2</sub> O	0.1000	0.1214	62.0	-418200 *	75.0	296.3200
K <sub>2</sub> O	1.1200	0.8965	94.0	-418200 *	102.0	412.5400
SO <sub>3</sub>	12.1100	11.3896	80.0	-437900	257.0	242.0000
P <sub>2</sub> O <sub>5</sub>	2.7500	1.4571	142.0	-1505900	117.0	377.1200
Others	0.0000	0.0000	44.0	-393520	214.0	20.1400

High-temperature ash analysis (815 °C)

Total: 100.000 (kg/kmol), 100.000 (kg/kmol), 75.241 (kg/kmol), -1025027 (kJ/kmol), 71.374 (kJ/kmol ash °C), 55.731 (kJ/mol ash)

Enthalpy of formation: -12346.834 (kJ/kg ash), 0.949 (kJ/kg ash °C), 740.701 (kJ/kg ash)

Ratio of bottom ash to fly ash: 15 %

\* Na<sub>2</sub>O + K<sub>2</sub>O

Fusion temperatures

	Oxidising	Reducing
Initial deformation T <sup>a</sup>	1235.88 °C	1193.93 °C
Softening T <sup>a</sup>	1252.98 °C	1211.08 °C
Hemisphere T <sup>a</sup>	1263.76 °C	1223.61 °C
Flow T <sup>a</sup>	1283.94 °C	1249.72 °C

FOULING AND SLAGGING PROPENSITY OF COAL ASH

Attig & Duzy (U.S.), Rb/a %Na<sub>2</sub>O in coal

Fouling index: 1.624 **SEVERE**

Attig & Duzy U.S. (for bituminous ashes)

Slagging index: 0.016 **LOW**

Viscosity (at 1426 °C): 12.338 Poise

Multi-Viscosity Index: 1.898

Reid & Cohen, 1944

Critical viscosity T<sup>a</sup>: 1380.42 °C

Liquidus T<sup>a</sup>: 1406.79 °C

Silica/alumina ratio SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub>: 3.065

Silica ratio SR: 49.309 %

Total base oxide: 45.470 %

Total acid oxides: 50.700 %

Base/acid ratio Rb/a: 0.897

Base-to-acid ratio Rb/a+P: 0.956

Dolomite ratio: 65.554

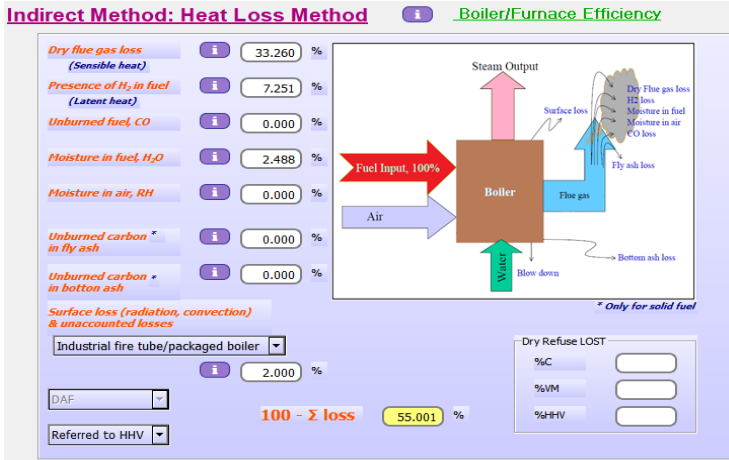
Detrital/authigenic index: 1.489

Alkali: 0.078

Thermal conductivity: 0.658 W/m K

## Energetic analysis

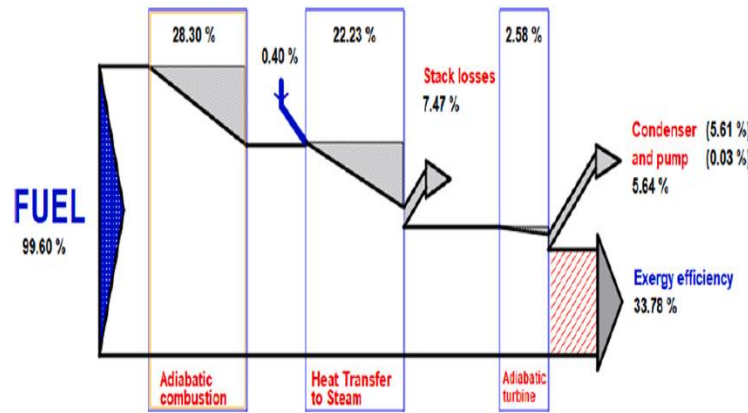
Includes flow diagram with **energetic efficiency** obtained by different methods, including indirect method on solid fuel.



Energetic analysis interface by indirect method

## Exergy analysis

Based on Second Principle, it provides information about **irreversibilities** generated in combustion process. The combustion process is responsible for a significant part of these losses.



Results visualization using a Grassmann combustion diagram

## Energy, Entropy, Exergy and Gibbs analysis

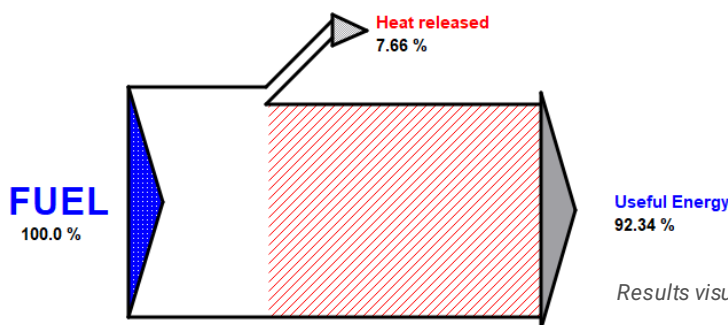
The results of the analysis of energy and availability balance show that the first and second laws efficiency for biomass, carbon and biodiesel fuel are useful tools to obtain the total availability, indicated work availability, the heat loss availability, burned fuel availability, other irreversibilities, etc.

ENERGY BALANCE: FLUE GAS

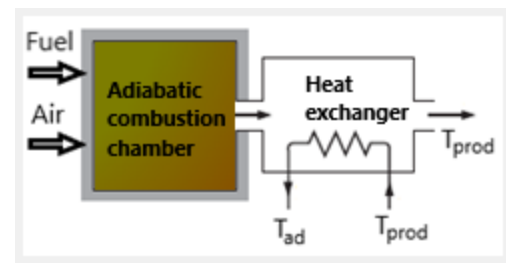
	<i>kJ/mol</i>	<i>kJ/kg fuel</i>
CO <sub>2</sub>	-360.1150	-7241.5278
CO	0.0000	0.0000
H <sub>2</sub> O	-215.8420	-9266.9404
O <sub>2</sub>	22.7070	289.9259
N <sub>2</sub>	21.4600	2750.4668
H <sub>2</sub>	0.0000	0.0000
SO <sub>2</sub>	-262.7260	-1.4923
HCl	-88.1093	-0.2176
Ar	0.0000	0.0000
<b>TOTAL</b>	<b>-882.6253</b>	<b>-13469.7861</b>

ENTROPY BALANCE: FLUE GAS

	<i>kJ/mol K</i>	<i>J/mol fuel K</i>
CO <sub>2</sub>	288.5716	346.2859
CO	262.9121	105.1648
H <sub>2</sub> O	253.4695	253.4695
O <sub>2</sub>	273.3625	92.3957
N <sub>2</sub>	230.5037	2114.0701
H <sub>2</sub>	0.0000	0.0000
SO <sub>2</sub>	316.7540	63.3508
Ar	0.0000	0.0000
He	316.7540	63.3508
unburned	0.0000	0.0000
<b>TOTAL</b>	<b>1625.5732</b>	<b>2974.7368</b>



Results visualization using a Sankey combustion diagram



## Pollutant emissions control

Includes critical pollutants as carbon monoxide (CO), nitrogen oxides (NO, NO<sub>2</sub>) or sulfur dioxide (SO<sub>2</sub>), ash, among others.

To reduce the amount of hazardous air pollutants emitted by commercial and industrial boilers, it is necessary to know exactly and completely the behavior of a certain fuel when it is subjected to a reactive process, in order to act effectively through a control mechanism.

For example, while replacing a significant amount of coal with wood would reduce sulfur emissions, the effect on other pollutants is not straightforward.

Gaseous air pollutants

CO <sub>2</sub> <i>Global Warming</i>	SO <sub>2</sub> <i>Acid Rain</i>	NO <i>Smog and Acid Rain</i>
NO <sub>2</sub> <i>Smog and Acid Rain</i>	N <sub>2</sub> O <i>Global Warming</i>	N <sub>2</sub> O <sub>4</sub> <i>Smog and Acid Rain</i>
CO <i>Health Effects</i>	Particulate matter, fly ash <i>Smog</i>	

Pollutant emissions



## Applications

In summary, **Thermocombustion (for biomass and biodiesel)** provides a complete solution of combustion processes; analysing the effect of the main variables that participate in the process, through the possibility of performing a graphical sensitivity analysis.

Whole range of software capabilities facilitates an improvement in combustion process design, an exhaustive study of main variables effects, and the possibility to reduce irreversibilities or pollutant emissions. A final report (set up by the user) can be submitted, containing graphs and predictions.

Major application for process optimization in **industry** or combustion processes study in **academia**.

### Application specifications

This software's capabilities are appropriate for combustion studies in academia. The features explained above are highly useful. Moreover, a prediction of **thermodynamic properties** of combustion products and **equilibrium composition** can be obtained.

Theoretical determination of the **equilibrium composition** and **thermodynamic properties** of combustion products, related to temperature and pressure, as well as the dosage used or the fuel gas mixture, according to chemical balance and dissociation.

CHEMICAL EQUILIBRIUM REACTIONS

Temperature (400°C < T < 5000°C)

Adiabatic T<sup>a</sup> °C  1700.0 °C  Products T<sup>a</sup>

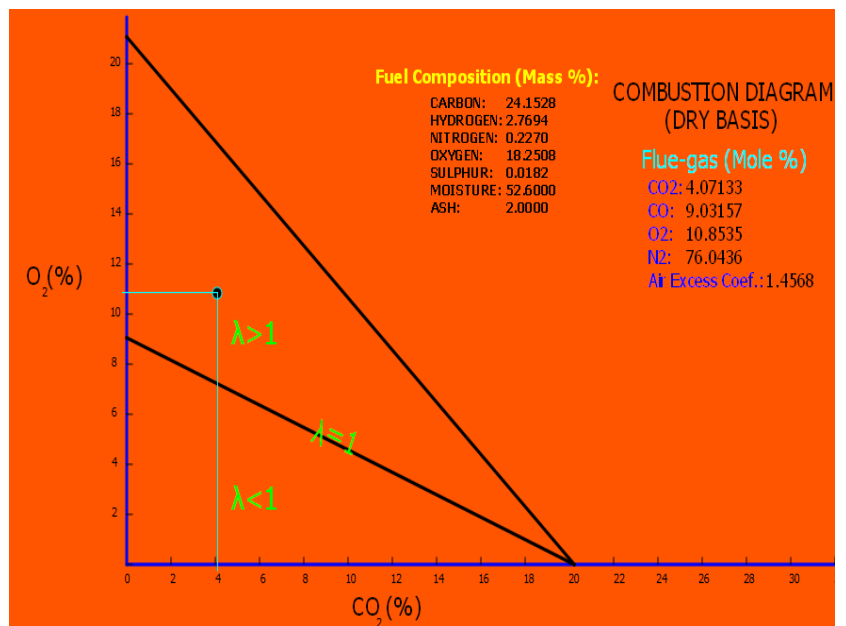
kJ/mol fuel

Consider adiabatic process: T(products)=T(adiabatic)

	Degree of dissociation	Equilibrium constant, K <sub>p</sub>	ΔG	ΔH	ΔS
			kJ/kmol	kJ/kmol	kJ/kmol K
$\text{CO}_2 \rightleftharpoons \text{CO} + 1/2 \text{O}_2$	-2.101	0.00101717	113047.9	278028.9	83.6130
$\text{H}_2\text{O} \rightleftharpoons \text{H}_2 + 1/2 \text{O}_2$	0.0093000	0.00023014	137428.1	237489.0	50.7112
$1/2 \text{O}_2 \rightleftharpoons \text{O}$	0.02061510	0.00052803	123804.0	255250.4	66.6175
$1/2 \text{H}_2 \rightleftharpoons \text{H}$	0.00143258	0.00132332	108731.2	226791.5	59.8334
$1/2 \text{N}_2 \rightleftharpoons \text{N}$	6.949e-08	5.851e-10	348773.2	480222.7	66.6191
FORMATION OF NITROGEN OXIDES					
$1/2 \text{N}_2 + 1/2 \text{O}_2 \rightleftharpoons \text{NO}$	0.6271412	0.01843708	65514.7	90502.6	12.6640
$1/2 \text{N}_2 + \text{O}_2 \rightleftharpoons \text{NO}_2$	0.0008651	0.00008880	153051.1	34700.8	-59.9804
$\text{NO} + 1/2 \text{N}_2 \rightleftharpoons \text{N}_2\text{O}$	0.0000318	0.00005837	159935.1	-1296.9	-81.7130



Composition analysis of combustion products on chemical equilibrium



For product-related and technical questions:

<https://thermosuite.com/thermocombustion-bb>

Email: [info@thermosuite.com](mailto:info@thermosuite.com)