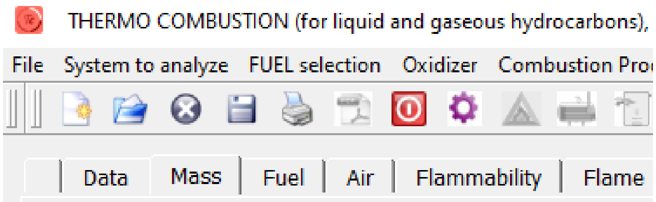
ThermoCombustion
Hidrocarbon Fuels Edition

SéNeCa(+) Agencia de Ciencia y Tecnología Región de Murcia

Universidad Politécnica de Cartagena

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).

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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
- Combustion diagrams
- Sensitivity analysis
- Pollutant emissions control

Applications

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

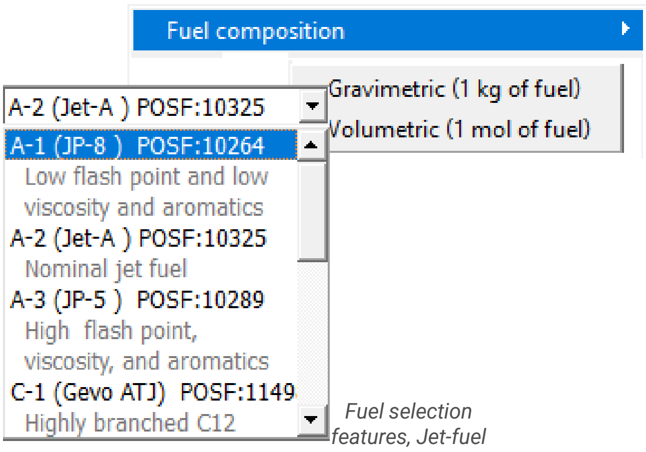
Main application in industry for process optimization or in academia (technical studios).

Characteristics

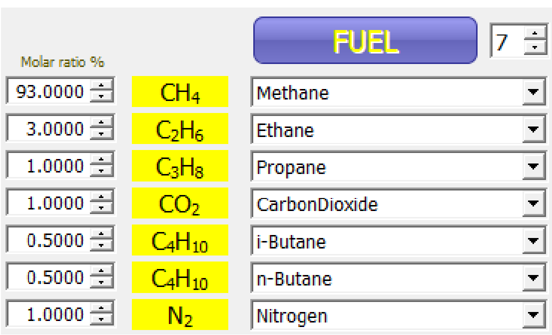
Software algorithms are based on up-to-date bibliography and the latest mathematical models, which in conjunction result in a **well-defined** and **solid technology**. The software has been set up with an **intuitive interface** that allows **easy handling**.

Input variability

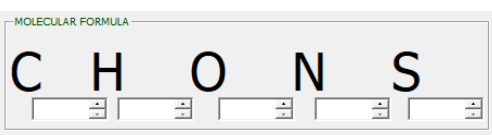
Allow the user to choose the **composition**: mixture of hydrocarbons, aviation fuel, by empirical formula, etc.



Fuel selection features, Jet-fuel



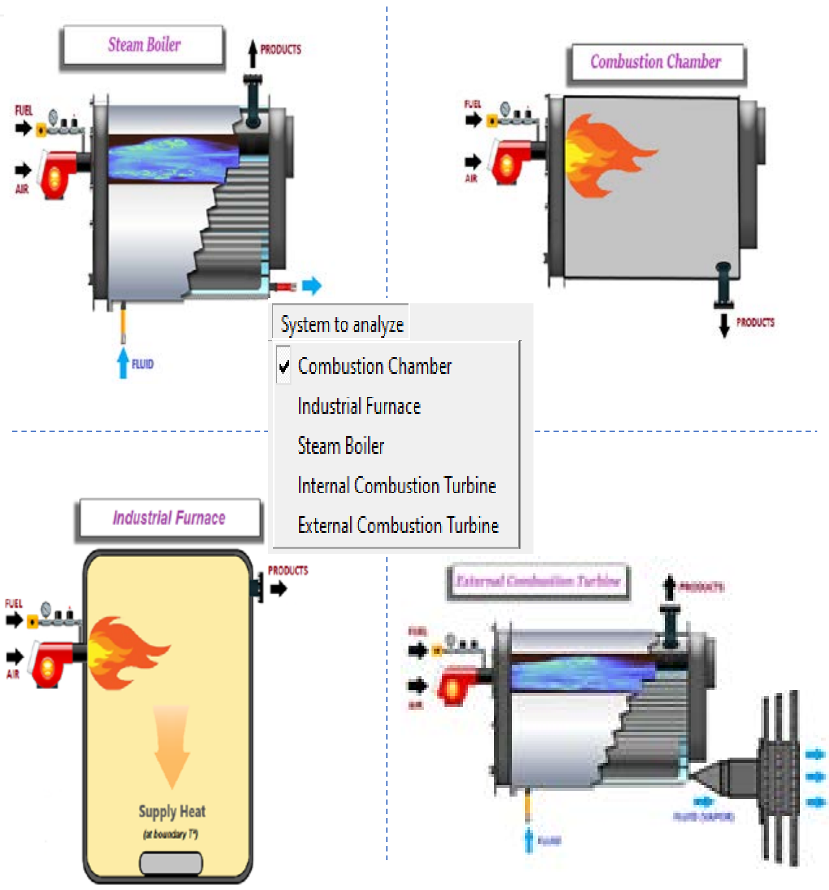
Fuel selection features, Natural gas



Fuel selection features, Molecular formula

Application in several industrial systems

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

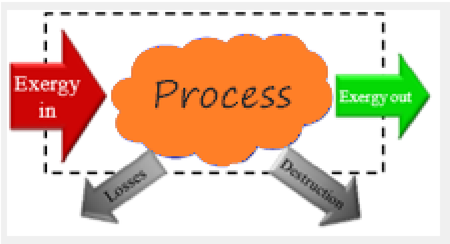


Industrial combustion systems available to analyse

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 exergy, entropy, including the flammability diagram.



Combustion Products Composition

☑ On wet basis ☐ On dry basis

	☐ mol/kg fuel	☐ kg/kg fuel	Mole %	Mass %
CO_2	1.0766549	2.5656038	6.7279286	10.5443677
CO	0.0043451	0.0065898	0.0271522	0.0270834
H_2O	2.0281479	1.9783577	12.6737309	8.13085
N_2	11.8112316	17.9153883	73.8074221	73.6304040
O_2	1.0165737	1.7613777	6.3524859	7.2390813
H_2	0.0018519	0.0002021	0.0115724	0.0008306
NO	0.0638865	0.1037987	0.3992215	0.4266020
NO_2	0.0000776	0.0001932	0.0004849	0.0007940
TOTAL	16.0027695	24.3315086	100.000 %	100.000 %

Mass balance interface

Exergy analysis

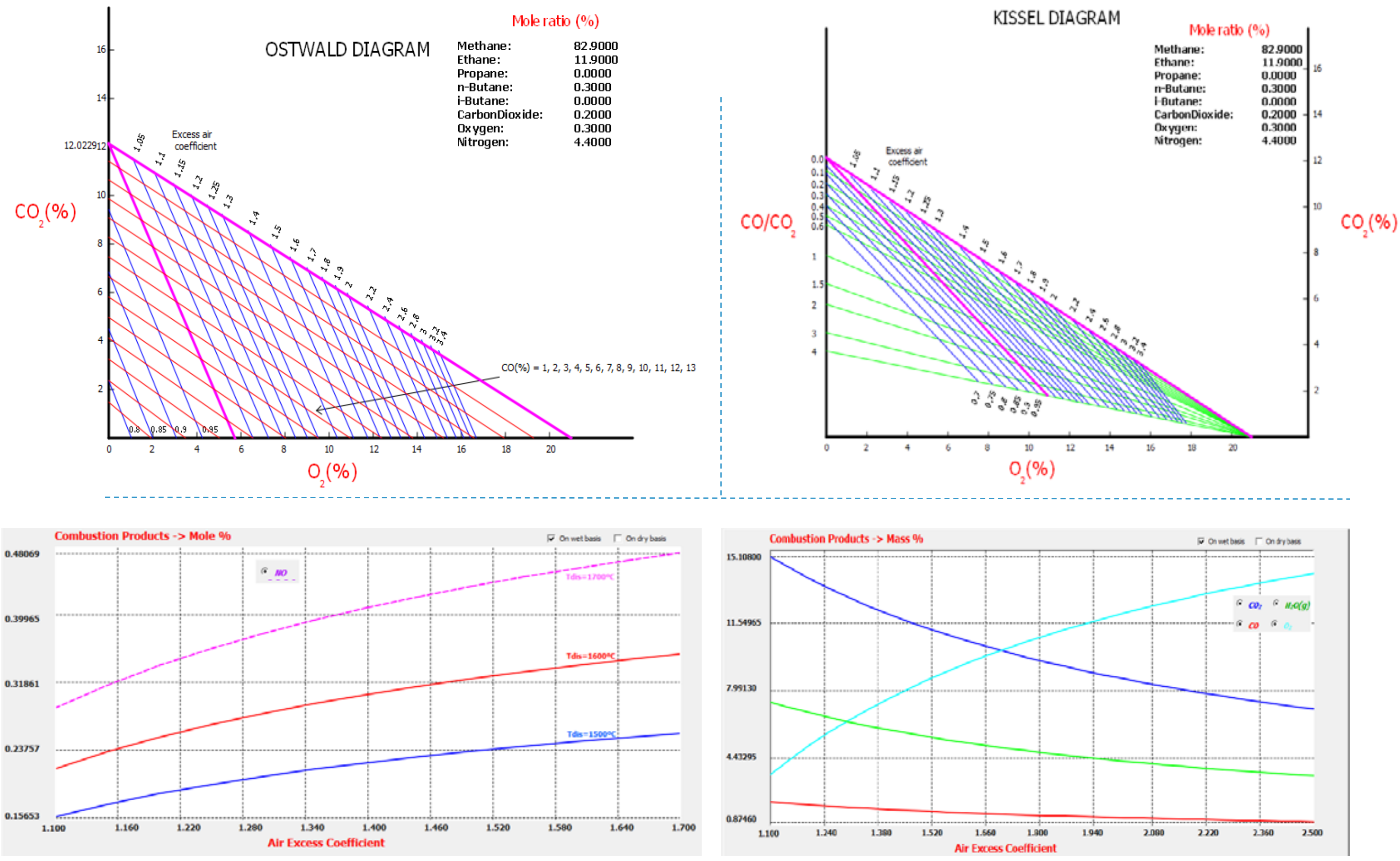
From second law evaluations (entropy or exergy evaluations) it is generally known that thermodynamic losses of boilers and furnaces are much higher than the thermal efficiencies do suggest.

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.

In order to get an analysis closer to reality, it is possible to work in '**dissociation' mode**; it facilitates the combination of the most common chemical reactions in this processes.



Graphic representations of sensitivity analysis

Pollutant emissions control / Sulfuric acid dew point

Includes critical pollutants as carbon monoxide (**CO**), nitrogen oxides (**NO, NO2**) or sulfur dioxide (**SO2**) among others.

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.

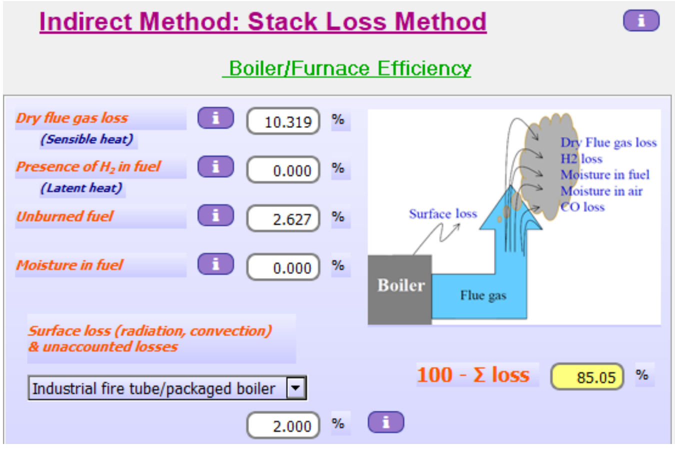
Gaseous air pollutants

	CO_2 Global Warming	SO_2 Acid Rain	NO Smog and Acid Rain	NO_2 Smog and Acid Rain
kg/kWh fuel	160.796	0.0000	16.8509	0.0316543
kg/GJ fuel	44665.546	0.0000	4680.81	8.79286
kg/kWh electricity	459.417	0.0000	48.1454	0.0904408
kg/GJ electricity	127615.845	0.0000	13373.7	25.1224
ppm (mass)	144457	0	4179.58	7.851

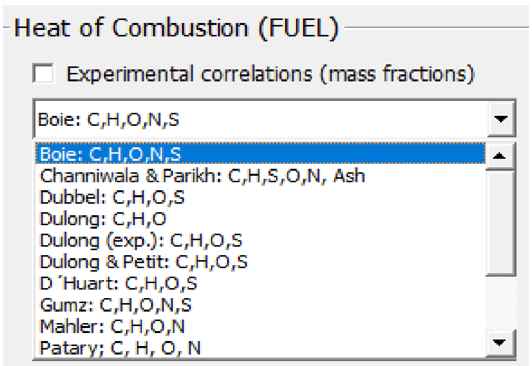
Pollutant emissions

Energetic analysis

Includes flow diagram with **energetic efficiency** obtained by different methods.



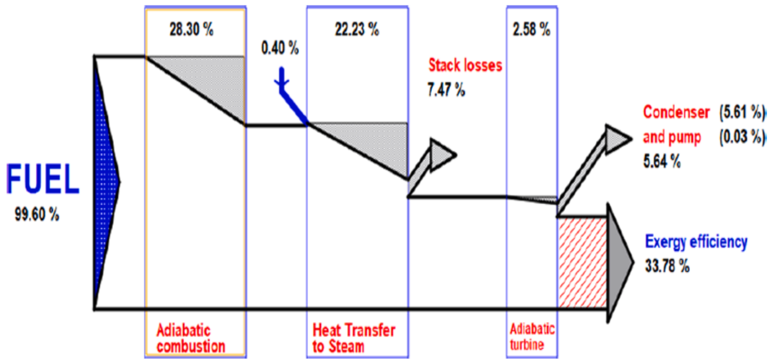
Energetic analysis interface by indirect method



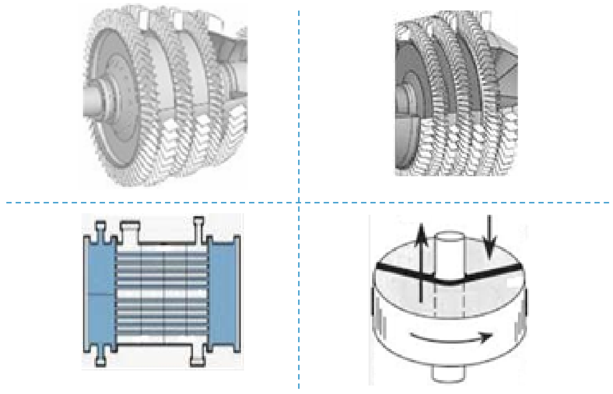
Heat of combustion of the fuel by means of experimental correlations

Exergy analysis

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



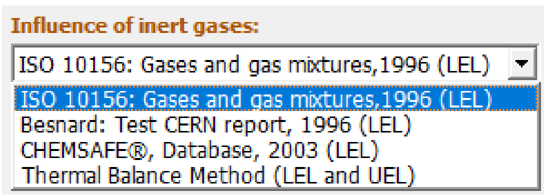
Results visualization using a Grassmann combustion diagram

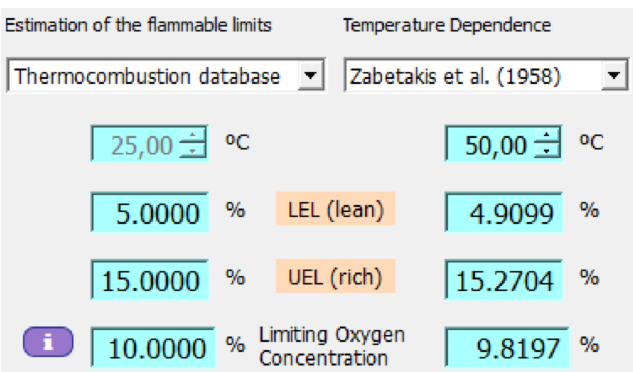


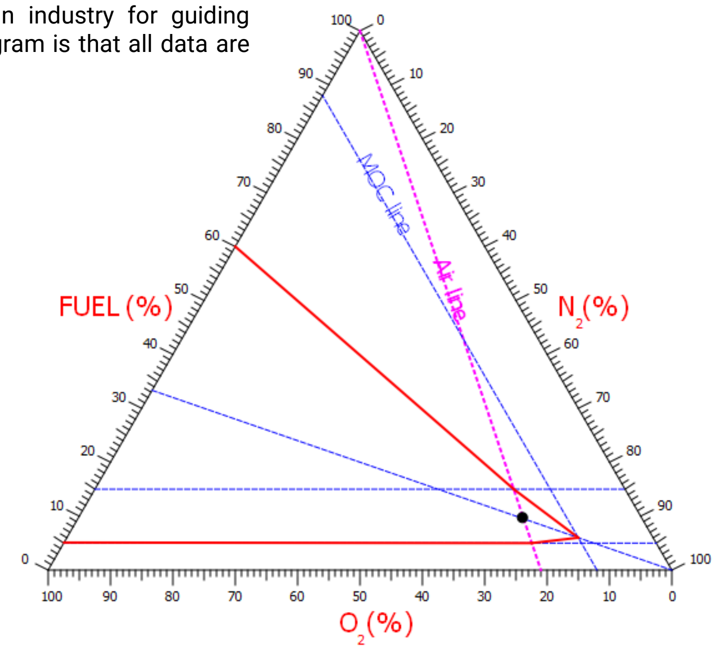
Devices

Flammability

A ternary flammability diagram gained a popular position in industry for guiding dilution and purge operations. The advantage of a ternary diagram is that all data are directly readable and oxygen enriched atmosphere is allowed.



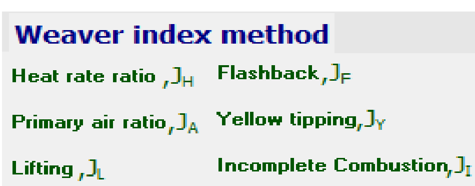


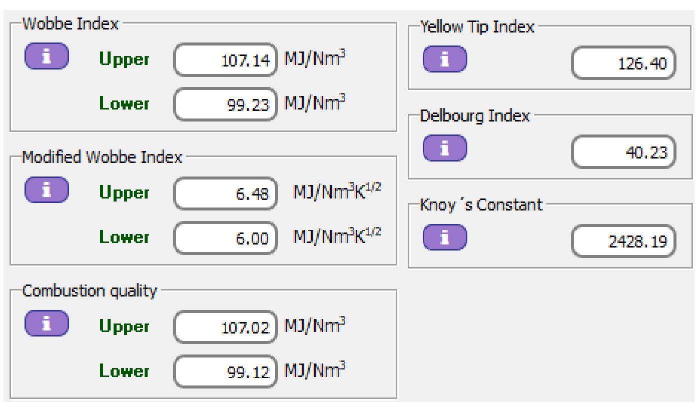


Ternary flammability diagram

Specifications according to fuel type

Fuel gas: availability to predict **interchangeability** of a fuel gas for another gas or a gas mixture. Use of *Yellow Tip*, *Wobbe, AGA* and *Weaver* indexes.





Interchangeability analysis interface on fuel gas

Applications

In summary, ***Thermocombustion*** 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.

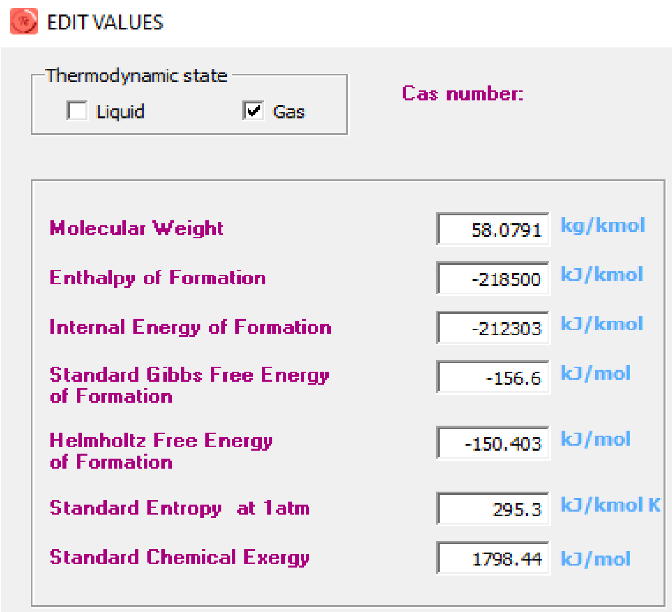
Whole range of software capabilities facilitates an improvement in combustion process design, an exhaustive study of main variables effects, and the possibility to reduce irreversibilities or pollutant emissions. A final report (set up by the user) can be submitted, containing graphs and predictions.

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

Application specifications

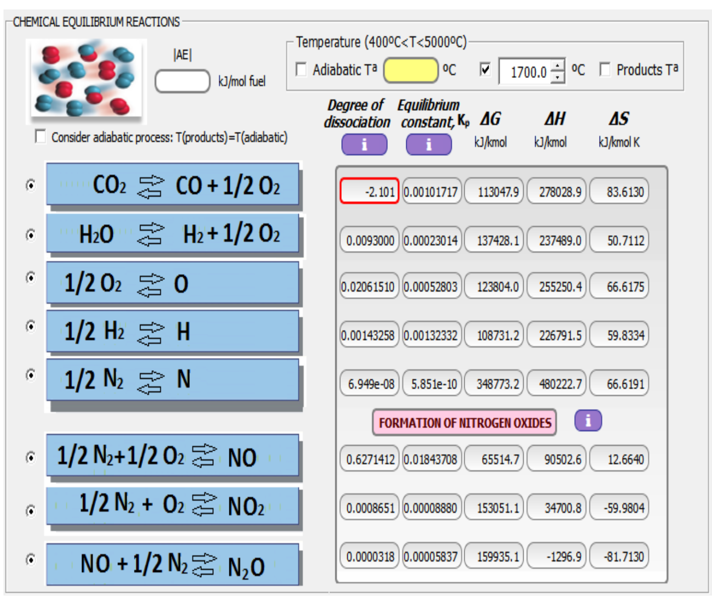
This software's capabilities are appropriate for combustion studies in academia. The features explained above are highly useful; however, some additional ones should be taken into consideration. ***Thermocombustion*** include an **integrated database** with thermo-physic properties annotated from a wide range of chemical compounds. Moreover, a prediction of **thermodynamic properties** of combustion products and **equilibrium composition** can be obtained.

An **integrated database** on software with more than 100 chemical compounds with thermo-physic properties annotated. Available to **combine at least 24 compounds as an input mixture** to analyse.



Thermodynamic properties annotated on software database for methane

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.



Composition analysis of combustion products on chemical equilibrium

ThermoSuite
Technical Software Suite

For product-related and techical questions:

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