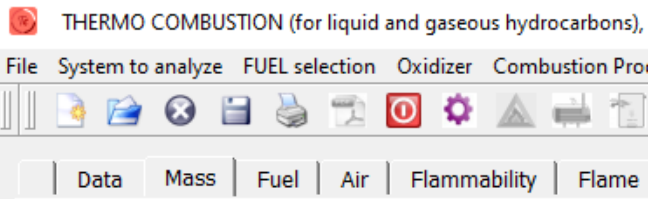




THERMO COMBUSTION | Technical & Educational Software



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.

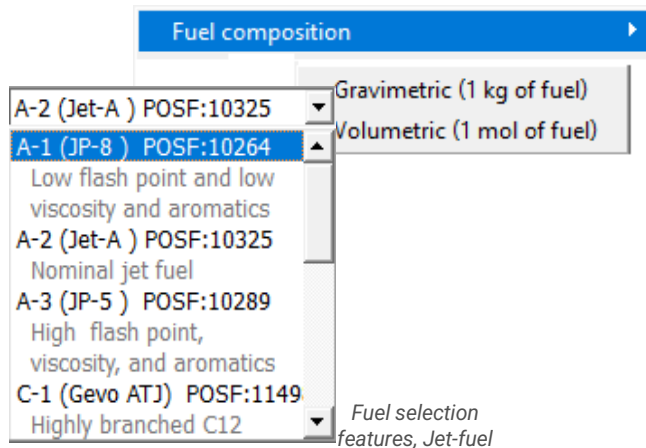
Main application in industry for process optimization or in academia (technical studies).

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**.

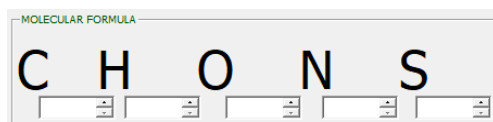
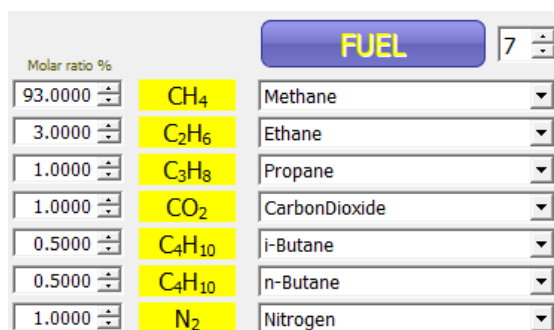
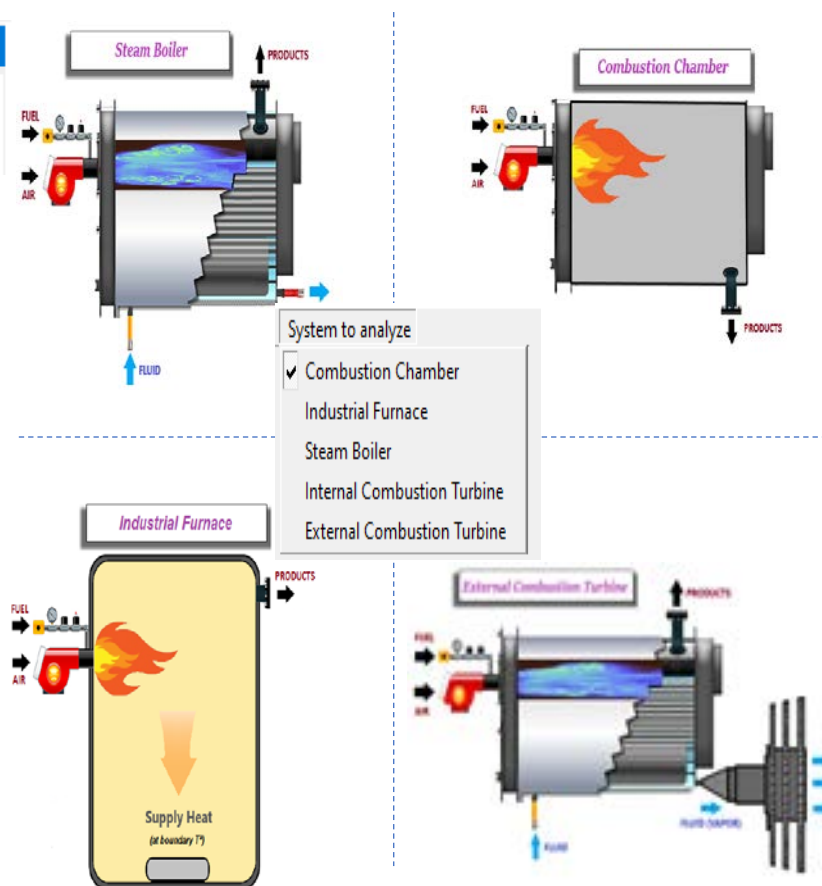
Input variability

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



Application in several industrial systems

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

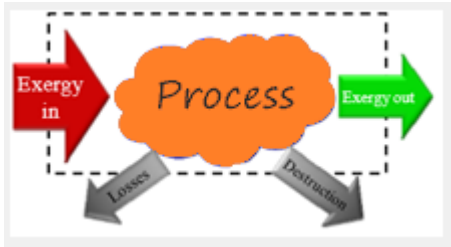


Fuel selection features, Molecular formula

Industrial combustion systems available to analyse

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.



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.

	<input type="checkbox"/> mol/kg fuel	<input type="checkbox"/> kg/kg fuel	<input checked="" type="checkbox"/> On wet basis	<input type="checkbox"/> On dry basis
CO ₂	1.0766549	2.5656038	6.7279286	10.5443677
CO	0.0043451	0.0065898	0.0271522	0.0270834
H ₂ O	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 %

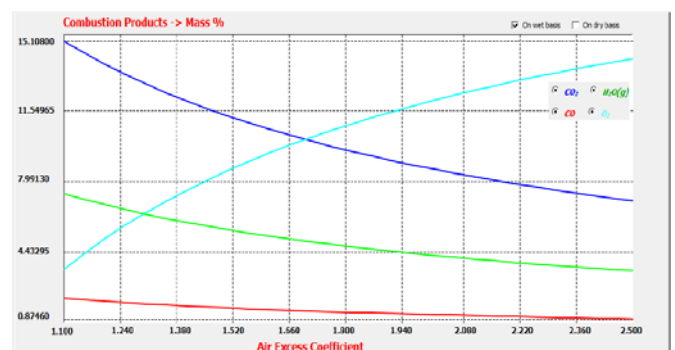
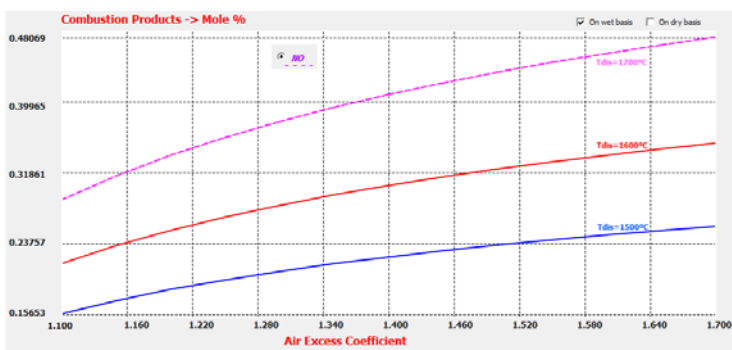
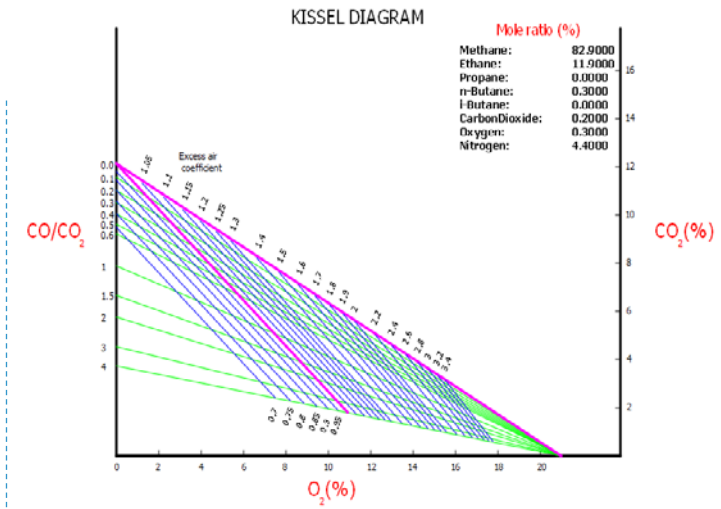
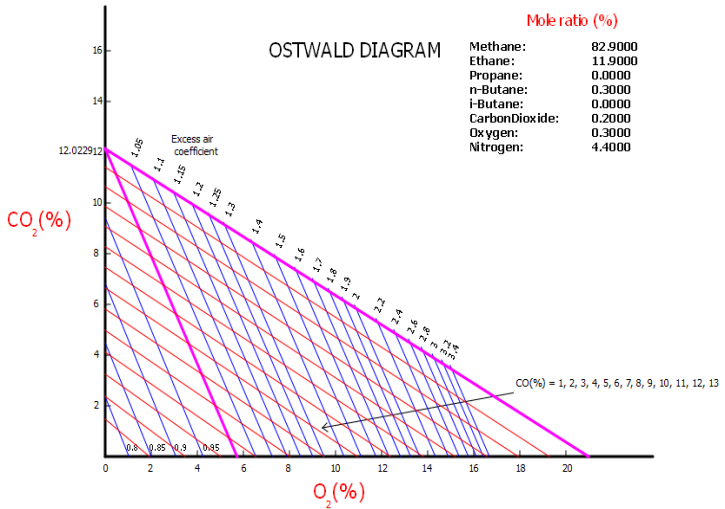
Mass balance interface

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.

Indirect Method: Stack Loss Method

Boiler/Furnace Efficiency

Dry flue gas loss (Sensible heat): 10.319 %

Presence of H₂ in fuel (Latent heat): 0.000 %

Unburned fuel: 2.627 %

Moisture in fuel: 0.000 %

Surface loss (radiation, convection) & unaccounted losses: 2.000 %

100 - Σ loss: **85.05 %**

Industrial fire tube/package boiler

Energetic analysis interface by indirect method

Heat of Combustion (FUEL)

Experimental correlations (mass fractions)

Boie: C, H, O, N, S

Boie: C, H, O, N, S

Channiwala & Parikh: C, H, S, O, N, Ash

Dubbel: C, H, O, S

Dulong: C, H, O

Dulong (exp.): C, H, O, S

Dulong & Petit: C, H, O, S

D'Huart: C, H, O, S

Gumz: C, H, O, N, S

Mahler: C, H, O, N

Patary: C, H, O, N

Heat of combustion of the fuel by means of experimental correlations

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.

Influence of inert gases:

ISO 10156: Gases and gas mixtures, 1996 (LEL)

ISO 10156: Gases and gas mixtures, 1996 (LEL)

Besnard: Test CERN report, 1996 (LEL)

CHEMSAFE®, Database, 2003 (LEL)

Thermal Balance Method (LEL and UEL)

Estimation of the flammable limits: Thermocombustion database

Temperature Dependence: Zabetakis et al. (1958)

25,00 °C

50,00 °C

5.0000 % LEL (lean)

4.9099 %

15.0000 % UEL (rich)

15.2704 %

10.0000 % Limiting Oxygen Concentration

9.8197 %

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.

Weaver index method

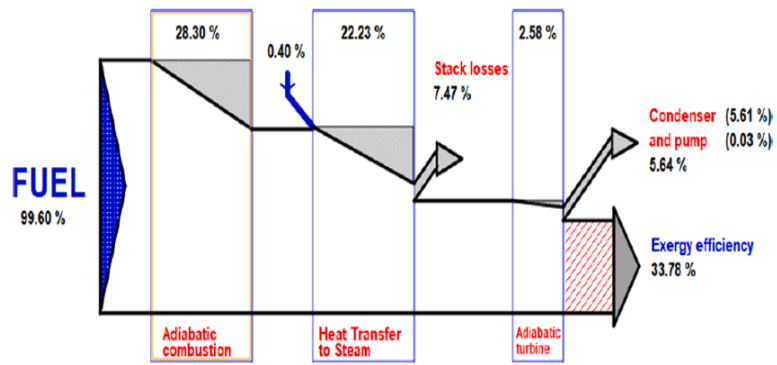
Heat rate ratio, J_H Flashback, J_F

Primary air ratio, J_A Yellow tipping, J_Y

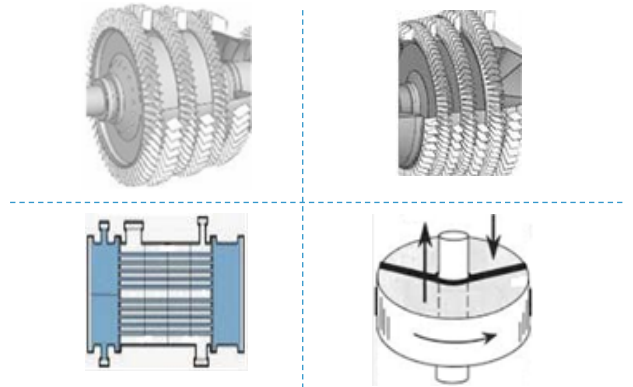
Lifting, J_L Incomplete Combustion, J_I

Exergy analysis

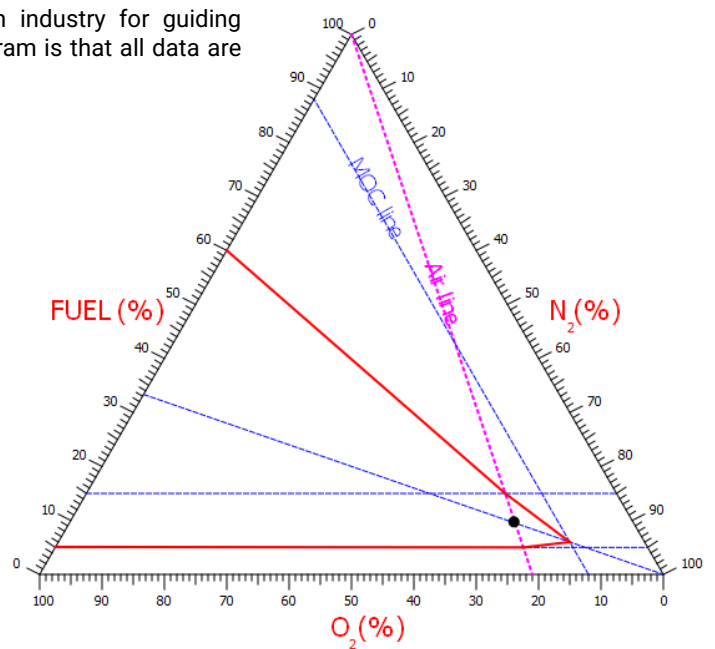
Based on Second Principle, it provides information about **irreversibilities** generated in each device of the installation, including the internal of the combustion process.



Results visualization using a Grassmann combustion diagram



Devices



Ternary flammability diagram

Wobbe Index: Upper 107.14 MJ/Nm³, Lower 99.23 MJ/Nm³

Yellow Tip Index: 126.40

Modified Wobbe Index: Upper 6.48 MJ/Nm³K^{1/2}, Lower 6.00 MJ/Nm³K^{1/2}

Delbourg Index: 40.23

Knoy's Constant: 2428.19

Combustion quality: Upper 107.02 MJ/Nm³, Lower 99.12 MJ/Nm³

Interchangeability analysis interface on fuel gas

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.

EDIT VALUES

Thermodynamic state
 Liquid Gas

Cas number:

Molecular Weight	58.0791	kg/kmol
Enthalpy of Formation	-218500	kJ/kmol
Internal Energy of Formation	-212303	kJ/kmol
Standard Gibbs Free Energy of Formation	-156.6	kJ/mol
Helmholtz Free Energy of Formation	-150.403	kJ/mol
Standard Entropy at 1atm	295.3	kJ/kmol K
Standard Chemical Exergy	1798.44	kJ/mol

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.



CHEMICAL EQUILIBRIUM REACTIONS

Temperature (400°C < T < 5000°C)
 Adiabatic T^a 1700.0 °C Products T^a

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

	IAEI	Degree of dissociation	Equilibrium constant, K _p	ΔG	ΔH	ΔS
	kJ/mol fuel			kJ/mol	kJ/mol	kJ/mol 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:

Polytechnic University of Cartagena (UPCT), Cronista Isidoro Valverde sq., 30202 Cartagena (Murcia), Spain.

Joaquín Zueco Jordán | joaquin.zueco@upct.es

+34 968 325 989