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Combustion Modelling for Training Power Plant Simulators

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1. Introduction

In 2013, the Comisión Federal de Electricidad (CFE¹), the Mexican Utility Company, had a production capacity of about 41.1 GW with a brute generation of 174.4 TW-h and transmits, distributes and commercialises electric energy for about 37 millions of clients that represent almost 105 millions of people [1]. In that same year, external energy producers generated about 32% of total energy consumed in Mexico.

Between others, like modernisation, an important factor of economical and performance results of a power plant, including those based on gas turbines, is the training of their operators. It is not easy to quantify the impact of training but there exists some feedback from plant's directors about improvement in operation skills. A classical study [2] demonstrated the importance of training power plants operators.

The Simulation and Advanced Training Systems Department (GSACS) is part of the Electrical Research Institute (IIE) and it is formed by a specialised group in training simulators that designs and implements tools and methodologies to support the simulators development, exploiting and maintenance.

Modelling the process of power plants for training is not an easy task and involves multidisciplinary work. In this chapter a general review of training simulator modelling is addressed with special emphasis on the combustion process.

¹ Some acronyms are written after their name or phrase spelling in Spanish. A full definition of the used acronyms in this chapter is listed in Section 8.

The main attribute of a combustion model for training is to reproduce the behaviour of the phenomenon in order to report the variables in the control station of a power plant operator. The measurement of NO_x present in the exhaust gases is a very important variable. The major part of the sulphur, NO_x , and dust emissions from stationary installations result from fuel combustion to produce heat and power [3]. How to simulate these variables in a real time training simulator in a relatively easy approach is the goal of this chapter.

2. Mathematical modelling previous works

Depending on the application, a phenomenon may be represented by a mathematical model formulated by different techniques. Some examples of models applications are: design, analysis, optimisation, education, training, general tendencies, *etc.* Thus, modelling approach may vary from very detailed physical models (governing principles) like finite differences or finite elements, to empirical models like curves fitting, in the extremes. In fact, there is a vast task trying to classify all possibilities a model may be designed.

Some authors detail the general formulation of the combustion process considering the different conditions where the phenomenon is achieved. The model must be solved together with continuity, momentum and transport equations but any possible numerical method is not mentioned [4].

CFD methods model the phenomenon based on Navier–Stokes equations considering a finite volume partitioned normally into millions of cells considering the detailed geometry of the simulated space. Interaction with the solid boundaries is taken in account. A 3-D visualisation is normally achieved but accuracy depends on the detailed models used and, in the case of combustion, serious errors would arise. In fact, for example, it has been claimed that the design and development of combustors, until recent past, was more an art than science [5]. Although the author applies a CFD by using prePDF combustion model (it took nearly 2000 h of CPU time in a 4 node sun server with main memory of 128 GB) he states that validation must be attempted in future studies.

Studies consider different phenomenology like supersonic combustion [6], chilling of the combustor liner by film cooling [7], micro-turbine engine with annular combustion chamber design [8], comparison of several turbulence models [9], swirling air flow [10,11], and many others. In spite of the promise of having good results, this approach is far enough to be used in real time applications.

Models with less spatial details are intended for design. A “simplified” methodology has been developed where different fuels and inlet conditions were studied for steady state conditions [12]. Direct fuel injection and diffusion flames, together with numerical methods like Newton-Raphson, LU Factorization and Lagrange Polynomials, are used for the calculations. Diesel, ethanol and methanol fuels were chosen for the numerical study. Finally, a computer code sequentially calculates the main geometry of the combustor. Design modes are not suitable for real time simulators.

A model was presented to study the influence of different air cooling systems validated against real plant data [13]. Gas composition was not included and an ideal gas model was considered. The input data were the air cooling system configuration and the ambient conditions. The combustion was simulated just increasing the gas temperature as a function of the mass flowrate and the fuel high heating value.

A model for desktop for excel was elaborated for a standard air Brayton cycle [14]. A total of five components and the combustion reaction stoichiometric with possibilities of excess of oxygen were considered. The output temperatures of the turbine were simulated as a second degree equation in function of the enthalpy instead using well known thermodynamic properties. The inputs variables are efficiencies, some pressure drops, temperatures, *etc.*

In other approach, the ideal gas assumption was adopted even when other aspects were modelled in detail like the flow through the equipment, the heat transfer phenomena and basing the process on a temperature-entropy diagram [15]. In this case the gas composition and the combustion process were ignored (considering only an increase of the temperature of gas) and the model, designed for optimisation, runs around the full load point.

A model based on Simulink was used to analyse the dynamical behaviour of an industrial electrical power system [16]. An ideal gas approach was used. The model was validated against real data but not details of the combustor model are mentioned.

The most important feature of a combustion model for training is the capacity of reproducing the behaviour of, at least, the variables reported in the control station of a power plant operator in such a way he cannot distinguish between the real plant and the simulator. Nowadays, the measurement of NO_x present in the exhaust gases is a very important factor to consider in an operator training program. However, the authors did not find a single paper where this theme is developed for real time training simulation.

Combustion models used specifically for training simulators are those created by companies that develop real time simulators, so the information is proprietary and the formulation is not available [17], in [18] an excellent explanation of the uses of training simulators is explained but presents not a single equation of the process model.

For a real time simulator application, the variables affecting the operation of a plant, including the combustion process, may be taken in account. The model is not developed to design a combustion chamber or burners, but to reproduce the plant operation data with the capacity to predict the plant behaviour during the transients occurred during all the normal and emergency operational scenarios. The real time execution characteristics required by a training simulator is accomplished by the present model.

3. Power plant simulation for training

High-performance computing help engineers and scientists apply modelling and simulation. One of the most useful applications is the use of software to make environments for training

in different technological areas. In a power plant, for example, it is important to train personnel in risk and unusual actions; a tool which has been widely tested is training simulators.

The IIE has developed several power plant simulators for Thermal-Electric Units, Nuclear, Geo-Thermal, Dual (Coal and liquid fuel), Gas Turbine, Combined Cycle, VU-60 Boiler and simulators with new web technologies.

The simulators must accomplish the ANSI norm [19] and are tested in the whole operation range; including malfunctions and transients according the operation procedures designed by the clients who are the final users of the simulator.

A simulator is designed to recreate a particular control room where operators may practise the plant procedures. An instructor coordinates and guides the simulator sessions (practical lessons).

3.1. Typical software configuration

The simulation environment is called MAS a trade mark software of the IIE; designed as a general tool to support simulators. MAS is both: a development tool and a man-machine interface for instructors; basically consists of three independent and coordinated tasks: *The Real Time Executive*, *The Operator Module*, and *The Instructor Module*.

The *Real Time Executive* is a function to manage the execution sequence of each mathematical model with all tasks performed by the simulator. These models may be executed in a parallel scheme, with a distributed architecture of PCs or with multi-core equipment or sequentially.

The Operator Module coordinates the interactive process diagrams (IPD) execution (IPD conforms the operation consoles). This module manages command messages of the operation consoles, controls the alarms system, the historical trends and the control of each IPD component (valve, pump, controllers, etc.). It refreshes each IPD periodically, and coordinates the sequence of events in the operation consoles.

The Instructor Module executes the instructor actions in a synchronized way during simulation; receives and responds the commands from-to the instructor console actions as start, stop and freeze a simulation session, actives malfunctions, modifies external conditions, etc. Figure 1 represents the standard instructor console.

The instructor console has icons for fast access; also has the possibility to modify the simulation velocity of the simulator to be increased up to ten times or to be decreased up to 10 times respect to real time. Another function is to simulate step by step, it means to run the whole simulation cycle on the minimum unit time in which simulator models are executed; it is equivalent to 0.1 s.

Most of first level instructor console menus are shown in Figure 2.

3.1.1. Control menu

The main functions of this menu are *Run/Freeze Simulation*, *Backtrack* and *Automatic function*. *Run/Freeze Simulation*: with this function the instructor may run or stop a simulation session.

This is an alternating button, which means that if simulator is in stop mode, clicking the button, simulation runs, and *vice versa*. *Backtrack*: allows reproducing automatically all instructor and operator actions that were made in a simulation session. *Automatic function*: allows the instructor to design training sceneries by pre-programming automatic actions during a simulation session as introduce malfunctions or modifying variables as ambient, temperature, humidity, *etc.* in pre-established times.

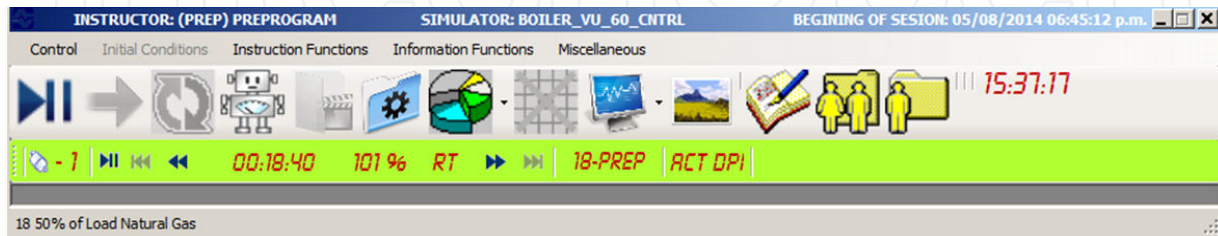


Figure 1. Instructor console

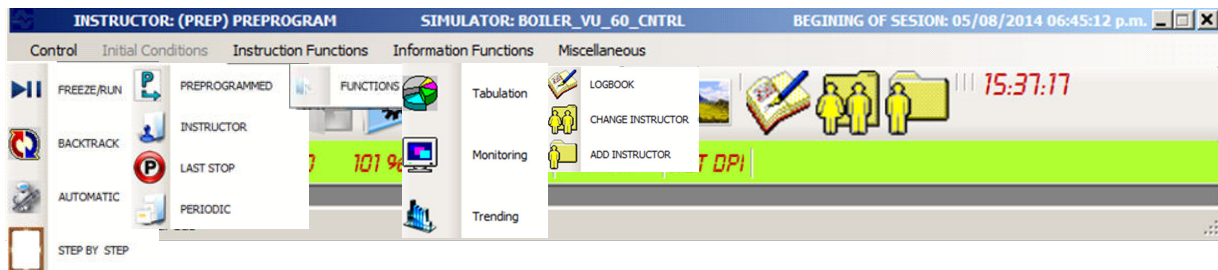


Figure 2. Menus of the instructor console

3.1.2. Initial conditions menu

An initial condition (IC) contains the necessary information to start-up a simulation session in any predefined plant condition (from cold condition up to nominal operation point). In the simulator are four IC options, namely *Preprogramed*, *Instructor*, *Periodic*, and *From Last Stop*. *Preprogramed*: are those IC with the whole information from cold condition up to nominal operation point and all the instructors may establish it. The *Instructor* IC is defined by one particular user and only he may access it. *Periodic* are IC automatically created when the simulator is running; default period is established in 2 minutes; this function is useful if instructor desires to get back to a previous condition within simulation session to explain some effect. *Last Stop* IC is automatically created, when the simulation session is freeze.

3.1.3. Instruction functions menu

There are three set of functions in this menu: *External Parameters*, *Malfunctions* and *Remote Functions*. *External Parameters*: permit simulates changes on external conditions of the plant that operator cannot control like environment pressure or temperature, gas fuel composition, etc. *Malfunctions*: modifies the behaviour of the system by simulating an abnormal event as broken pipes, fouling filters, loss of pilots, trip of pumps, etc. *Remote Functions*: represents actions that in a plant would be realized by a worker through manual actions because they cannot be made from the control room, for example: opening and closing valves; in the simulator, these actions are achieved by the instructor (requested by the operator). Malfunctions and remote functions are organized in groups related with the plant modelled systems. They may be modified according to some options like delay, evolution time and severity percentage.

3.1.4. Information functions menu

These functions are: *Tabulation*, *Monitoring*, and *Trending*. *Tabulation*: this function permits to select some variables from a predefined variables group and register them in a file during a simulation period defined by the user. *Monitoring*: this function permits to select a group of variable for its supervision during a simulation session, normally used while a simulator is being developed. *Trending*: this tool permits to create variables groups on line to be displayed graphically during a simulation session. Trending is available for the operators too.

3.1.5. Miscellaneous functions menu

This menu is formed by *Logbook*, *Change of instructor* and *Create a user account*. *Logbook*: is a function than can save and display the operator and/or the instructor actions during a simulation session. *Change of Instructor*: It permits to establish another instructor account to guide a simulation session. *Create a User Account*: permits to create new instructors.

3.2. Hardware configuration

The standard hardware configuration consists in a PC network and several monitors for the Instructor and operation consoles; normally the instructor console is installed in a different room than the operation console separated by a glass wall; in the first area the simulation sessions are initiated and guided by the instruction consoles and in the second area the hardware looks as a replica of the real plant control stations and it is here where the operator is trained. Figure 3 shows a typical hardware configuration of a simulator.

An example of an IPD where the operator may monitor the whole process and act on the plant is presented in Figure 4. In this case is the main screen of a gas turbine power plant with the summary of the plant conditions.



Figure 3. Hardware configuration (instructor and operation consoles)

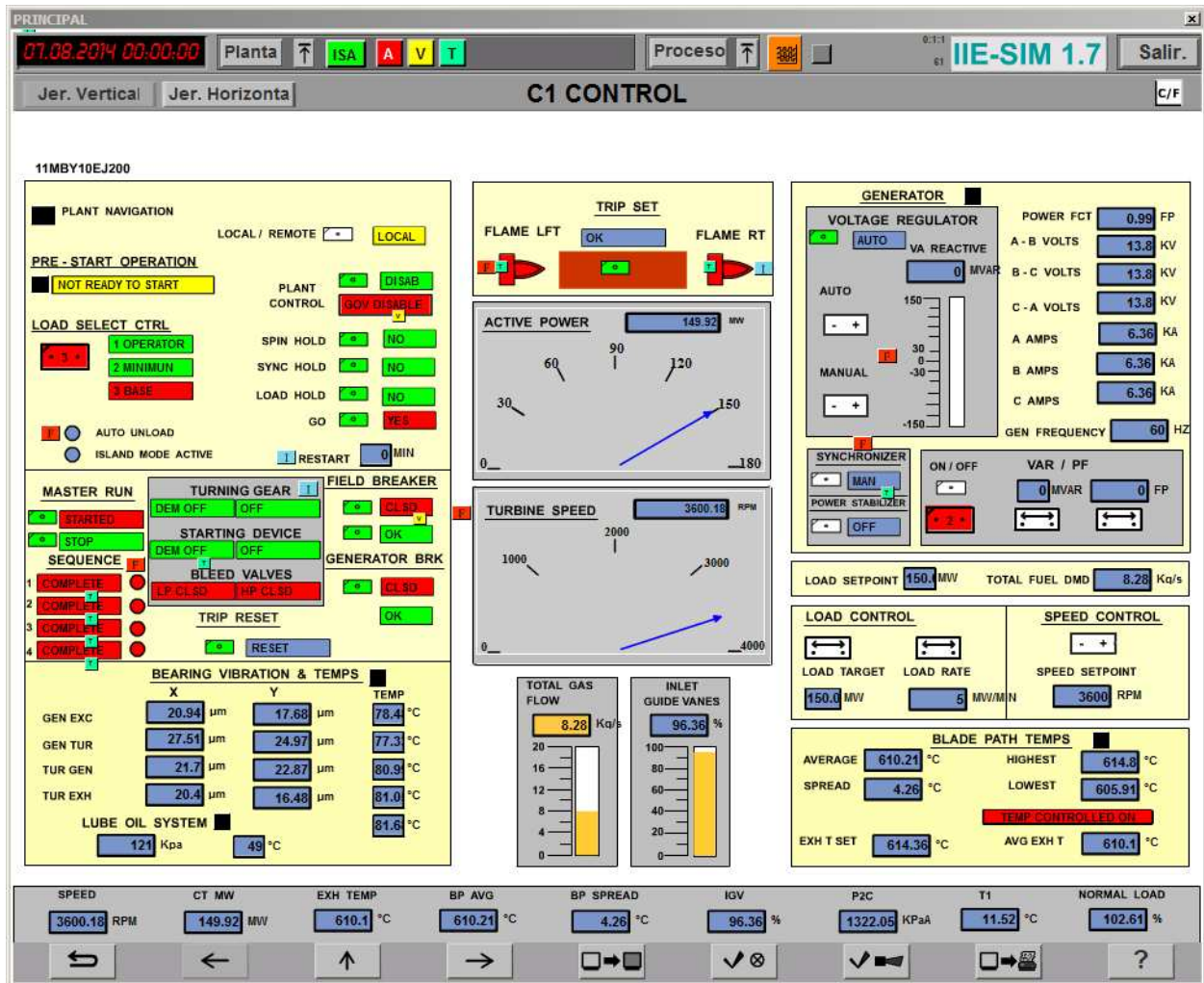


Figure 4. Example of an IPD in the operation consoles

4. Modelling of combustion surrounding systems

The models of any simulated plant were divided in two groups: process and control models.

4.1.1. Process models

Traditional methods of modelling and simulation considered approaches often using empirical relations and approximated procedures in model development. The models of a modern training simulator are a set of algebraic and differential equations obtained from the application of basic principles (energy, momentum, mass balances and constitutive equations). The models are designed to work under a full range of operational conditions, from 0% to 100% of load including all possible transients that may exist during operational manoeuvres, including malfunctions and changes of external parameters, always replicating the real plant comportment. The simulator was developed applying a methodology developed by the IIE [20].

Process models may be divided in electrical, mechanical, and fluid phenomena. All are important but in this chapter only a brief summary on thermal fluid modelling is revised.

Changes in the state of a fluid are not instantaneous. When a system is perturbed to change the steady state conditions of a system (a fluid in this case) takes a minimal time. Time of getting a new steady state is a function of the perturbation magnitude and the inertia of the system (which normally depends on the mass of the system).

In the IIE, the fluid mechanics phenomena are modelled with algebraic equations. A generic model that automatically solves the mass and moment balances and constitutive equations for pressure drops in valves, pipelines and other fittings like elbows, pumps, compressors, fans, turbines, *etc.*, has been developed by the GSACS [21]. This program (flupre) is configured with the plant networks of pipelines and fittings and it automatically detects the “active” topology of a network. This is the arrangement of the grid, in a given instant, formed only by the elements allowing flow through them. The active topology may change, for instance, a stream is “eliminated” of the network when a valve is closed or pumps are turned off. The full topology is that theoretically formed if all streams allow flow through them. During a session of dynamic simulation a system may change its active topology depending on the operator’s actions. This means that the order of matrix associated to the equations that represent the system changes. Flupre assumes that mass accumulation is not hold in the network.

A flows and pressures network is constituted of nodes and streams. A node is a point where two or more streams converge in or divert from. A stream transports a fluid and has fittings that arise or drop pressure through them. If not mass accumulation is assumed and a simplified expression relating mass flowrate and pressure drop is used, an equation system may be stated with a continuity equation for each node and a flow-pressure drop expression for each stream:

$$\sum w'_{in} - \sum w'_{o} = 0 \quad (1)$$

$$w^2 = k_1 \Delta P + k_2 \quad (2)$$

The equations are solved simultaneously and the flowrate of each stream and the pressure of each node are then known. Initial values for these variables have to be established as initial value for iterations.

There exist other nodes not being part of the flows and pressures networks. Normally, they are considered to accumulate mass (like a steam header or a pressurised air tank), so, a proper mass balance should be stated, one equation for each stream component j :

$$\frac{dm_j}{dt} = \sum w_{in} c_{in,j} - \sum w_o c_j \quad (3)$$

Commonly, elements simulated with differential equations, like Equation (3), are denominated capacitive nodes. The variables associated with derivatives are “state variables” and their values define the condition of a system. These variables have an initial condition to start any simulation session.

For these nodes normally the pressure is also a state variable. The more simple case is when the node is assumed to behave like an ideal gas:

$$\frac{dP}{dt} = \frac{R T}{V} \left(\frac{dm}{dt} \right) + \frac{R m}{C_p V} \left(\frac{dh}{dt} \right) \quad (4)$$

In this case, m represents moles.

Also enthalpy is a variable associated with a derivative:

$$\frac{dh}{dt} = \frac{\sum w_{in} h_{in} - w_o h - q_o}{m} \quad (5)$$

More complex cases exist by considering other phenomena like phases' equilibrium, separation process, chemical reactions, evaporation and condensation situations, *etc.* However these models are not considered now, except the combustion developed later.

Numerical methods to solve algebraic and differential equations are employed. For algebraic equation the most used method is Newton-Raphson either, with analytical or numerical derivatives calculations. For differential equations, the Euler method is enough for training simulator models. As an example of this method, let's considered the integration of the pressure of any node:

$$P_{t+\Delta t} = P_t + \frac{dP}{dt} \Delta t \quad (6)$$

Normally, the integration step Δt is assigned to a value of 0.1 s.

Capacitive nodes intrinsically have an inertia affecting the derivative calculation.

Algebraic equations, by definition, are assumed to reach instantaneously its final value (an instant, numerically, is a time period with a value of Δt). So, a lag may be defined for these variables. For example, for a calculated flowrate w there exists a flowrate w' :

$$w' = w + (w - w') \Delta t_{lag} \quad (7)$$

that may be reported in an operation consoles. Note that if Δt_{lag} has a value of 1, no lag exists.

4.1. Control models

The control models acquire and process the actions realised by the operator in the control room by actions on the operation consoles. These models generate, *via* digital and analogic programs, changes on some simulated elements, depending on any particular condition of the simulated plant. For example, the control adjusts demand of valves to regulate some process variables around a set point fixed by the operator (levels of tanks, pressures, temperatures, *etc.*).

For the development of the plant control models, generally two approaches are followed:

- a. To develop in a graphic environment a copy of the control diagrams provided by the client or control developer. Once the diagrams have been drawn, this environment is embedding into the simulator to be sequenced and executed in real time. These diagrams are drawn in the format defined by the Scientific Apparatus Makers Association (SAMA).
- b. To translate the control algorithms as well as the IPD of the operation consoles, obtained from the control station of the real plant. The control is an exact copy of the functioning control system (both, logical and analogical), including PID constants.

4.2. Combustion chamber surrounding systems

By using the proper equations as that presented in section 4.1, the systems that feed or extract flow or energy from a combustion chamber may be simulated.

A couple of examples of systems around the combustion chamber are shown in Table 1. There are included both, process and control models.

5. Combustion modelling

5.1. General approach

For the so called thermal NO_x , *i.e.* nitrogen oxides, formed from the oxidation of the free nitrogen in the combustion air or fuel, the main factor affecting the formed NO_x in combustion reaction is the stoichiometric adiabatic flame temperature of the fuel, which is the temperature reached by burning a theoretically correct mixture of fuel and air in an insulated vessel. The main factors affecting this flame temperature are [22]:

- NO_x increases strongly with fuel-to-air ratio or with firing temperature.

- NO_x increases exponentially with combustor inlet air temperature.
- NO_x increases with the square root of the combustor inlet pressure.
- NO_x increases with increasing residence time in the flame zone.
- NO_x decreases exponentially with increasing water or steam injection or increasing specific humidity.

	Gas Turbine Combustor		Boiler Furnace
Air System:	IGV Control Compressor Air Heater	Air System:	Induced Fan Draft Forced Fan Draft Air/Vapour Pre-Heater Ljunström Heater BMS Control
Fuel Systems:	Gas Combustion Control	Fuel Systems:	Gas Liquid Fuels Atomising Steam BMS Control
Water Injection System		Soot Blowers System	
Gas Turbine		Convective Heat Zone	

Table 1. Typical combustion chamber surrounding systems

The formation of NO_x due to oxidation of organically bound nitrogen in the fuel (fuel-bound nitrogen), called “organic NO_x” is important only for crude or residual oils and it is not included in this model.

A generic model for the combustion process was developed by the IIE. The stated objective was to calculate flame temperature and composition of the burned gases including the simulated heat transfer phenomena. It is possible simulate a mixture up to twenty components, all displayed in Table 2.

Thermodynamic properties were calculated using cubic state and corresponding states equations for non-polar substances. The application range is for low pressure up to 80 bars.

Cubic equations properties are in next general form [23]:

$$P = \frac{RT}{\hat{v} - b} - \frac{a}{\hat{v}^2 + u\hat{v}b + wb^2} \quad (8)$$

where R is the ideal gas constant, \hat{v} molar volume, and a, b, u and w , are constants that in fact determine the precise cubic equation that may be used: Van der Waals, Redlich-Kwong, Soave, Peng-Robinson, Lee-Kesler, Racket (for saturated liquid only), Hankinson-Brobst-Thompson (for liquid only), and Ideal Gas. Also may be used the corresponding states equation Lee Kesler:

No.	Component	No.	Component
1	N ₂ Nitrogen	11	C ₆ H ₁₄ n-Hexane
2	O ₂ Oxygen	12	C ₇ H ₁₆ n-Heptane
3	H ₂ S Hydrogen Sulphide	13	C ₈ H ₁₈ n-Octane
4	CO ₂ Carbon Dioxide	14	C ₉ H ₂₀ n-Nonane
5	CH ₄ Methane	15	C ₁₀ H ₂₂ n-Decane
6	C ₂ H ₆ Ethane	16	H ₂ O Water
7	C ₃ H ₈ Propane	17	CO Carbon Monoxide
8	C ₄ H ₁₀ n-Butane	18	NO Nitrogen Monoxide
9	iC ₄ H ₁₀ i-Butane	19	NO ₂ Nitrogen Dioxide
10	C ₅ H ₁₂ n-Pentane	20	SO ₂ Sulphur Dioxide

Table 2. Possible combustion components

$$Z^{(0)} = 1 + \frac{B}{V_r^{(0)}} + \frac{C}{(V_r^{(0)})^2} + \frac{D}{(V_r^{(0)})^5} + \frac{C_4}{T_r^3 (V_r^{(0)})^2} \left(\beta + \frac{\gamma}{(V_r^{(0)})^2} \right) e^{\frac{-\gamma}{(V_r^{(0)})^2}} \quad (9)$$

$$Z^{(0)} = \frac{P_r V_r^{(0)}}{T_r}; \quad Z^{(R)} = \frac{P_r V_r^{(R)}}{T_r}; \quad Z = Z^{(0)} + \frac{\Omega}{\Omega_r} (Z^{(R)} - Z^{(0)}) \quad (10)$$

where B , C , D , C_4 , β , and γ are characteristics (constants) Ω is Pitzer's acentric factor.

For the solution of any of the equations for a gas mixture, the Newton-Raphson method is used.

For the water, thermodynamic properties data [24] were adjusted as a function of pressure and enthalpy or temperature. Functions were adjusted by least squares method. The application range is between 0.1 and 4520 *psia* for pressure, and -10 and 720 °C (equivalent to 0.18 and 1635 *BTU/lb* of enthalpy).

5.2. Definition of efficiencies

To calculate the products of the reaction as a function of the inlet reactants moles, the stoichiometric coefficients are needed. However, in the approach proposed by the authors, a couple of efficiencies are defined to be used in these calculations.

Total combustion efficiency $\alpha_{j,1}$ for component j is the fraction of the amount of oxygen that is consumed for a total combustion. It is 1 if a complete combustion reaction is hold, for example production of CO₂. It is 0 if the product (for example CO₂) is not at all produced.

Partial combustion efficiency $\alpha_{i,2}$ for component j is defined as the fraction of the amount of oxygen that is consumed for a partial combustion. It is 1 if partial oxidised products are generated, for example production of CO. It is 0 if the product (for example CO) is not at all produced.

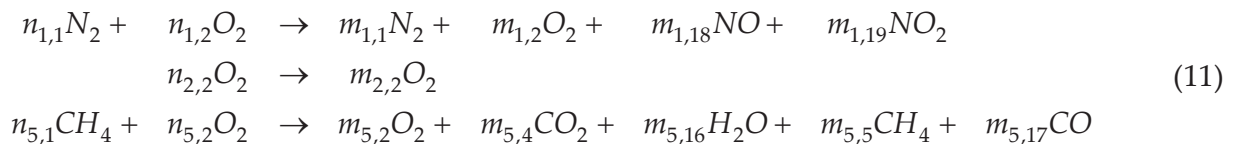
A special case is the production of NO and NO_2 . The values of efficiencies are represented on basis of the moles quantity of N_2 instead O_2 .

In this approach, by now, the value of efficiencies is proposed by the programmer in order to fit the results of the reference plant.

5.3. Simple example

In order to explain the model used for the combustion in a clear way, a simple reaction will be contemplated.

Let's assume the ideal case where CH_4 is the only fuel component. No inlet water is considered. The possible reactions are presented here (the subscripts nomenclature maintains the numbering of the global equations presented later):



Coefficients of Equations (11) represent moles, no mass. Up to now, the stoichiometric is not included.

In general, the O_2/N_2 ratio of atmospheric air is taken as 21/78 whereas 1% other gases as inert [25].

Considering the stoichiometric coefficients and the efficiencies of each reaction, by knowing the reactants feed streams, it is possible to calculate the moles reactions (considering also the possible reactant that appears also as a product, for example the CH_4 that is not consumed).

Let's assume next arbitrary definition of efficiencies just for this example (efficiency values for production of NO , NO_2 and CO are too high compared with actual expected values but works good for this example):

$$\begin{aligned}
 N_2 \quad \text{If } O_2 \text{ excess} \geq 200\% & \quad \alpha_{1,1} = 0.0046 ; \quad \alpha_{1,2} = 0.0000 \\
 \quad \text{If } O_2 \text{ excess} = 100\% & \quad \alpha_{1,1} = 0.0000 ; \quad \alpha_{1,2} = 0.0040 \\
 \quad \text{If } O_2 \text{ excess} \leq 50\% & \quad \alpha_{1,1} = 0.0000 ; \quad \alpha_{1,2} = 0.0000 \\
 CH_4 \quad \text{If } O_2 \text{ excess} \geq 200\% & \quad \alpha_{5,1} = 1.0000 ; \quad \alpha_{5,2} = 0.0000 \\
 \quad \text{If } O_2 \text{ excess} = 130\% & \quad \alpha_{5,2} = 0.4500 \\
 \quad \text{If } O_2 \text{ excess} \geq 100\% & \quad \alpha_{5,1} = 0.0000 ; \\
 \quad \text{If } O_2 \text{ excess} \leq 50\% & \quad \alpha_{5,1} = 0.0000 ; \quad \alpha_{5,2} = 0.0000
 \end{aligned} \tag{12}$$

Considering stoichiometric of reactions:

$$\begin{aligned}
 N_2 \quad n_{1,1} &= \text{input data } 78 / 21 n_{1,1} \\
 m_{1,19} &= 2\alpha_{1,1} n_{1,1} \\
 m_{1,18} &= 2\alpha_{1,2} n_{1,1} \\
 m_{1,1} &= 0.5(2n_{1,1} - m_{1,18} - m_{1,19}) \\
 n_{1,2} &= 0.5m_{1,18} + 1m_{1,19} \\
 O_2 \quad n_{2,2} &= \text{input data} \\
 m_{2,2} &= n_{2,2} - \sum n_{i,2} \text{ for } i = 1, 3, 4, \dots, 20 \\
 CH_4 \quad n_{5,1} &= \text{input data} = 1.0 \\
 m_{5,4} &= \alpha_{5,1} n_{5,1} \\
 m_{5,17} &= \alpha_{5,2} n_{5,1} \\
 m_{5,5} &= n_{5,1} - m_{5,4} - m_{5,17} \\
 m_{5,16} &= 2n_{5,1} - 2m_{5,5} \\
 n_{5,2} &= m_{5,4} + 0.5m_{5,16} + 0.5m_{5,17}
 \end{aligned} \tag{13}$$

Tables 3, 4, and 5 present three different cases for this example. The difference is the inlet moles of air feed to the combustion chamber. The inlet mole flowrates is a function of the oxygen excess (O_e), namely: 2.5, 1.5 and 0.45.

In Tables 3, 4, and 5 the way to verify that calculated mole flowrates of products are correct is that sum of moles of elements must be equal in reactants and products.

Inlet mole flowrate of reactants				Exit mole flowrate of products			
O_2	$n_{2,2}$	2.5885	moles of elements	O_2	$m_{2,2}$	0.5000	moles of elements
N_2	$n_{1,1}$	9.6142	O	5.1769	N_2	$m_{1,1}$	9.5700 O
				5.1769			
CH_4	$n_{5,1}$	1.0000	N	19.2285	O_2	$m_{1,2}$	0.0000 N
				19.2285			19.2285
O_2	$n_{1,2}$	9.5700	C	1.0000	NO_2	$m_{1,19}$	0.0885 C
				1.0000			1.0000
O_2	$n_{5,2}$	2.0000	H	4.0000	NO	$m_{1,18}$	0.0000 H
				4.0000			4.0000
					CO_2	$m_{5,4}$	1.0000
					CH_4	$m_{5,5}$	0.0000
					CO	$m_{5,17}$	0.0000
					H_2O	$m_{5,16}$	2.0000
Total		13.2027		29.4054	Total		10.7268
							29.4054
$\alpha_{1,1} = 0.0046 ; \alpha_{1,2} = 0.0000 ; \alpha_{5,1} = 1.0000 ; \alpha_{5,2} = 0.0000$							

Table 3. Example of moles balance; oxygen excess=2.5

Inlet mole flowrate of reactants				Exit mole flowrate of products					
O_2	$n_{2,2}$	1.3460	moles of elements	O_2	$m_{2,2}$	0.0572	moles of elements		
N_2	$n_{1,1}$	4.9994	O	2.6920	N_2	$m_{1,1}$	4.9925	O	2.6920
CH_4	$n_{5,1}$	1.0000	N	9.9988	O_2	$m_{1,2}$	0.0000	N	9.9988
O_2	$n_{1,2}$	0.0138	C	1.0000	NO_2	$m_{1,19}$	0.0138	C	1.0000
O_2	$n_{5,2}$	1.2750	H	4.0000	NO	$m_{1,18}$	0.0000	H	4.0000
					CO_2	$m_{5,4}$	0.3000		
					CH_4	$m_{5,5}$	0.2500		
					CO	$m_{5,17}$	0.4500		
					H_2O	$m_{5,16}$	1.5000		
Total		7.3454		17.6908	Total		7.5635		17.6908
$\alpha_{1,1} = 0.0014 ; \alpha_{1,2} = 0.0000 ; \alpha_{5,1} = 0.3000 ; \alpha_{5,2} = 0.4500$									

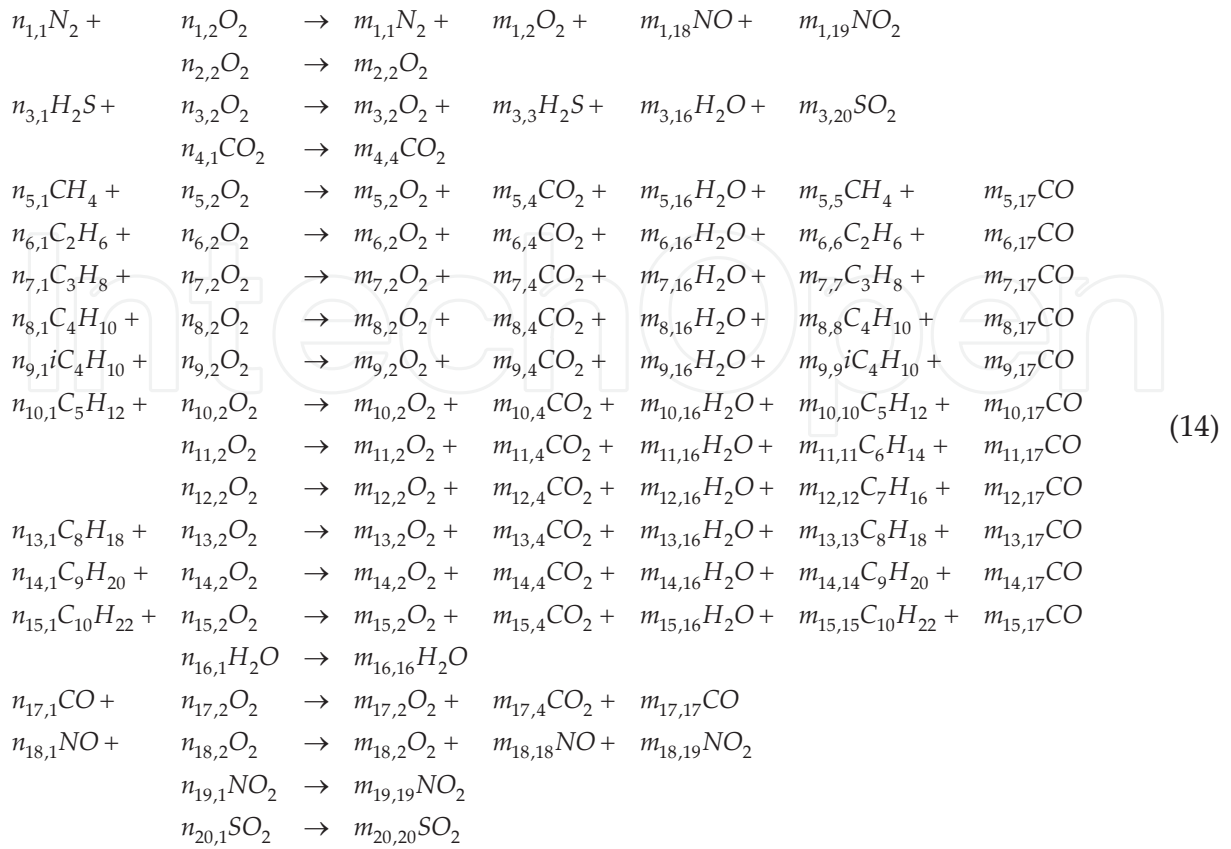
Table 4. Example of moles balance; oxygen excess=1.5

Inlet mole flowrate of reactants				Exit mole flowrate of products					
O_2	$n_{2,2}$	0.4659	moles of elements	O_2	$m_{2,2}$	0.4659	moles of elements		
N_2	$n_{1,1}$	1.7306	O	0.9318	N_2	$m_{1,1}$	1.7306	O	0.9318
CH_4	$n_{5,1}$	1.0000	N	3.4611	O_2	$m_{1,2}$	0.0000	N	3.4611
O_2	$n_{1,2}$	0.0000	C	1.0000	NO_2	$m_{1,19}$	0.0000	C	1.0000
O_2	$n_{5,2}$	0.0000	H	4.0000	NO	$m_{1,18}$	0.0000	H	4.0000
					CO_2	$m_{5,4}$	0.0000		
					CH_4	$m_{5,5}$	1.0000		
					CO	$m_{5,17}$	0.0000		
					H_2O	$m_{5,16}$	0.0000		
Total		3.1965		4.0000	Total		3.1965		4.0000
$\alpha_{1,1} = 0.0000 ; \alpha_{1,2} = 0.0000 ; \alpha_{5,1} = 0.0000 ; \alpha_{5,2} = 0.0000$									

Table 5. Example of moles balance; oxygen excess=0.45

5.4. Full combustion reactions

The whole model considers up to twenty reactants. Full components possible reaction may be stated as:



The reactions that have an associated efficiency are shown in Table 6:

Component	Partial Combustion		Full Combustion	
	Component	Efficiency	Component	Efficiency
N_2	NO	$\alpha_{1,2}$	NO_2	$\alpha_{1,1}$
H_2S	-	-	SO_2	$\alpha_{3,1}$
CH_4	CO	$\alpha_{5,2}$	CO_2	$\alpha_{5,1}$
C_2H_6	CO	$\alpha_{6,2}$	CO_2	$\alpha_{6,1}$
C_3H_8	CO	$\alpha_{7,2}$	CO_2	$\alpha_{7,1}$
C_4H_{10}	CO	$\alpha_{8,2}$	CO_2	$\alpha_{8,1}$
iC_4H_{10}	CO	$\alpha_{9,2}$	CO_2	$\alpha_{9,1}$
C_5H_{12}	CO	$\alpha_{10,2}$	CO_2	$\alpha_{10,1}$
C_6H_{14}	CO	$\alpha_{11,2}$	CO_2	$\alpha_{11,1}$
C_7H_{16}	CO	$\alpha_{12,2}$	CO_2	$\alpha_{12,1}$
C_8H_{18}	CO	$\alpha_{13,2}$	CO_2	$\alpha_{13,1}$
C_9H_{20}	CO	$\alpha_{14,2}$	CO_2	$\alpha_{14,1}$
$C_{10}H_{22}$	CO	$\alpha_{15,2}$	CO_2	$\alpha_{15,1}$
CO	CO	$\alpha_{17,2}$	CO_2	$\alpha_{17,1}$
NO	NO	$\alpha_{18,2}$	NO_2	$\alpha_{18,1}$

Table 6. Full combustion reactions

Considering basically the same general assumptions that those presented in the simple example explained above, including the linear interpolation between the efficiency definitions as a function of O_2 excess. Efficiencies adjusted for a gas turbine simulator [26] are:

N_2	If O_2 excess $\geq 200\%$	$\alpha_{1,1} = 1.3 \times 10^{-5}$;	$\alpha_{1,2} = 0.0000$
	If O_2 excess = 100%	$\alpha_{1,1} = 0.0000$;	$\alpha_{1,2} = 1.9 \times 10^{-5}$
	If O_2 excess $\leq 50\%$	$\alpha_{1,1} = 0.0000$;	$\alpha_{1,2} = 0.0000$
H_2S	If O_2 excess $\geq 200\%$	$\alpha_{3,1} = 7.3 \times 10^{-5}$	
	If O_2 excess = 100%	$\alpha_{3,1} = 1.1 \times 10^{-5}$	
	If O_2 excess $\leq 50\%$	$\alpha_{3,1} = 0.0000$	
CH_4	If O_2 excess $\geq 200\%$	$\alpha_{5,1} = 1.0000$;	$\alpha_{5,2} = 0.0000$
	If O_2 excess = 100%	$\alpha_{5,1} = 0.0000$;	$\alpha_{5,2} = 2.3 \times 10^{-4}$
	If O_2 excess $\leq 50\%$	$\alpha_{5,1} = 0.0000$;	$\alpha_{5,2} = 0.0000$
C_2H_6	If O_2 excess $\geq 200\%$	$\alpha_{6,1} = 1.0000$;	$\alpha_{6,2} = 0.0000$
	If O_2 excess = 100%	$\alpha_{6,1} = 0.0000$;	$\alpha_{6,2} = 2.3 \times 10^{-4}$
	If O_2 excess $\leq 50\%$	$\alpha_{6,1} = 0.0000$;	$\alpha_{6,2} = 0.0000$
C_3H_8	If O_2 excess $\geq 200\%$	$\alpha_{7,1} = 1.0000$;	$\alpha_{7,2} = 0.0000$
	If O_2 excess = 100%	$\alpha_{7,1} = 0.0000$;	$\alpha_{7,2} = 2.3 \times 10^{-4}$
	If O_2 excess $\leq 50\%$	$\alpha_{7,1} = 0.0000$;	$\alpha_{7,2} = 0.0000$
C_4H_{10}	If O_2 excess $\geq 200\%$	$\alpha_{8,1} = 1.0000$;	$\alpha_{8,2} = 0.0000$
	If O_2 excess = 100%	$\alpha_{8,1} = 0.0000$;	$\alpha_{8,2} = 2.3 \times 10^{-4}$
	If O_2 excess $\leq 50\%$	$\alpha_{8,1} = 0.0000$;	$\alpha_{8,2} = 0.0000$
iC_4H_{10}	If O_2 excess $\geq 200\%$	$\alpha_{9,1} = 1.0000$;	$\alpha_{9,2} = 0.0000$
	If O_2 excess = 100%	$\alpha_{9,1} = 0.0000$;	$\alpha_{9,2} = 2.3 \times 10^{-4}$
	If O_2 excess $\leq 50\%$	$\alpha_{9,1} = 0.0000$;	$\alpha_{9,2} = 0.0000$
C_5H_{12}	If O_2 excess $\geq 200\%$	$\alpha_{10,1} = 1.0000$;	$\alpha_{10,2} = 0.0000$
	If O_2 excess = 100%	$\alpha_{10,1} = 0.0000$;	$\alpha_{10,2} = 2.3 \times 10^{-4}$
	If O_2 excess $\leq 50\%$	$\alpha_{10,1} = 0.0000$;	$\alpha_{10,2} = 0.0000$
C_6H_{14}	If O_2 excess $\geq 200\%$	$\alpha_{11,1} = 1.0000$;	$\alpha_{11,2} = 0.0000$
	If O_2 excess = 100%	$\alpha_{11,1} = 0.0000$;	$\alpha_{11,2} = 2.3 \times 10^{-4}$
	If O_2 excess $\leq 50\%$	$\alpha_{11,1} = 0.0000$;	$\alpha_{11,2} = 0.0000$

C_7H_{16}	If O_2 excess $\geq 200\%$	$\alpha_{12,1} = 1.0000;$	$\alpha_{12,2} = 0.0000$	(15)
	If O_2 excess = 100%	$\alpha_{12,1} = 0.0000;$	$\alpha_{12,2} = 2.3 \times 10^{-4}$	
	If O_2 excess $\leq 50\%$	$\alpha_{12,1} = 0.0000;$	$\alpha_{12,2} = 0.0000$	
C_8H_{18}	If O_2 excess $\geq 200\%$	$\alpha_{13,1} = 1.0000;$	$\alpha_{13,2} = 0.0000$	
	If O_2 excess = 100%	$\alpha_{13,1} = 0.0000;$	$\alpha_{13,2} = 2.3 \times 10^{-4}$	
	If O_2 excess $\leq 50\%$	$\alpha_{13,1} = 0.0000;$	$\alpha_{13,2} = 0.0000$	
C_9H_{20}	If O_2 excess $\geq 200\%$	$\alpha_{14,1} = 1.0000;$	$\alpha_{14,2} = 0.0000$	
	If O_2 excess = 100%	$\alpha_{14,1} = 0.0000;$	$\alpha_{14,2} = 2.3 \times 10^{-4}$	
	If O_2 excess $\leq 50\%$	$\alpha_{14,1} = 0.0000;$	$\alpha_{14,2} = 0.0000$	
$C_{10}H_{22}$	If O_2 excess $\geq 200\%$	$\alpha_{15,1} = 1.0000;$	$\alpha_{15,2} = 0.0000$	
	If O_2 excess = 100%	$\alpha_{15,1} = 0.0000;$	$\alpha_{15,2} = 2.3 \times 10^{-4}$	
	If O_2 excess $\leq 50\%$	$\alpha_{15,1} = 0.0000;$	$\alpha_{15,2} = 0.0000$	
CO	If O_2 excess $\geq 200\%$	$\alpha_{17,1} = 1.0000;$	$\alpha_{17,2} = 0.0000$	
	If O_2 excess $\leq 100\%$	$\alpha_{17,1} = 0.0000;$	$\alpha_{17,2} = 1.0000$	
NO	If O_2 excess $\geq 200\%$	$\alpha_{18,1} = 1.0000;$	$\alpha_{18,2} = 0.0000$	
	If O_2 excess $\leq 100\%$	$\alpha_{18,1} = 0.0000;$	$\alpha_{18,2} = 1.0000$	

In order to avoid imbalances in the reactions, next restriction must be addressed at any moment:

$$0 \leq \alpha_{i,1} + \alpha_{i,2} \leq ul \quad (16)$$

Upper limit ul usually may have a value of 1, but some off-line tests should be carried on in order to be sure that not negative mole flowrate are calculated as result of Equations (17).

If efficiencies values are known, moles flow of products may be calculated as a function of moles flow of reactants. In next equations, input data ($n_{i,1}$ for $i=1,20$) are known defined by air, injection water and fuel composition. Mole flowrates of oxygen ($n_{i,2}$) are calculated as the required O_2 considering the calculated efficiencies defined by Equations (15):

All reactantes :

$$\begin{aligned}
 n_{i,1} &= \text{input data for } i = 1, 20 \\
 N_2 \quad m_{1,19} &= 2\alpha_{1,1}n_{1,1} \\
 m_{1,18} &= 2\alpha_{1,2}n_{1,1} \\
 m_{1,1} &= 0.5(2n_{1,1} - m_{1,18} - m_{1,19}) \\
 n_{1,2} &= 0.5m_{1,18} + 1m_{1,19} \\
 O_2 \quad m_{2,2} &= n_{2,2} - \sum n_{i,2} \text{ for } i = 1, 3, 4, \dots, 20 \\
 H_2S \quad m_{3,20} &= \alpha_{3,1}n_{3,1} \\
 m_{3,3} &= n_{3,1} - m_{3,20} \\
 m_{3,16} &= n_{3,1} - m_{3,3} \\
 n_{3,2} &= 0.5m_{3,16} + m_{3,20} \\
 CO_2 \quad m_{4,4} &= n_{4,1} \\
 CH_4 \quad m_{5,4} &= \alpha_{5,1}n_{5,1} \\
 m_{5,17} &= \alpha_{5,2}n_{5,1} \\
 m_{5,5} &= n_{5,1} - m_{5,4} - m_{5,17} \\
 m_{5,16} &= 2n_{5,1} - 2m_{5,5} \\
 n_{5,2} &= m_{5,4} + 0.5m_{5,16} + 0.5m_{5,17} \\
 C_2H_6 \quad m_{6,4} &= 2\alpha_{6,1}n_{6,1} \\
 m_{6,17} &= 2\alpha_{6,2}n_{6,1} \\
 m_{6,6} &= n_{6,1} - 0.5m_{6,4} - 0.5m_{6,17} \\
 m_{6,16} &= 3n_{6,1} - 3m_{6,6} \\
 n_{6,2} &= m_{6,4} + 0.5m_{6,16} + 0.5m_{6,17} \\
 C_3H_8 \quad m_{7,4} &= 3\alpha_{7,1}n_{7,1} \\
 m_{7,17} &= 3\alpha_{7,2}n_{7,1} \\
 m_{7,7} &= n_{7,1} - 1/3m_{7,4} - 1/3m_{7,17} \\
 m_{7,16} &= 4n_{7,1} - 4m_{7,7} \\
 n_{7,2} &= m_{7,4} + 0.5m_{7,16} + 0.5m_{7,17} \\
 C_4H_{10} \quad m_{8,4} &= 4\alpha_{8,1}n_{8,1} \\
 m_{8,17} &= 4\alpha_{8,2}n_{8,1} \\
 m_{8,8} &= n_{8,1} - 1/4m_{8,4} - 1/4m_{8,17} \\
 m_{8,16} &= 5n_{8,1} - 5m_{8,8} \\
 n_{8,2} &= m_{8,4} + 0.5m_{8,16} + 0.5m_{8,17}
 \end{aligned}$$

$$\begin{aligned}
iC_4H_{10} \quad m_{9,4} &= 4\alpha_{9,1}n_{9,1} \\
m_{9,17} &= 4\alpha_{9,2}n_{9,1} \\
m_{9,9} &= n_{9,1} - 1/4m_{9,4} - 1/4m_{9,17} \\
m_{9,16} &= 5n_{9,1} - 5m_{9,9} \\
n_{9,2} &= m_{9,4} + 0.5m_{9,16} + 0.5m_{9,17} \\
C_5H_{12} \quad m_{10,4} &= 5\alpha_{10,1}n_{10,1} \\
m_{10,17} &= 5\alpha_{10,2}n_{10,1} \\
m_{10,10} &= n_{10,1} - 1/5m_{10,4} - 1/5m_{10,17} \\
m_{10,16} &= 6n_{10,1} - 6m_{10,10} \\
n_{10,2} &= m_{10,4} + 0.5m_{10,16} + 0.5m_{10,17} \\
C_6H_{14} \quad m_{11,4} &= 6\alpha_{11,1}n_{11,1} \\
m_{11,17} &= 6\alpha_{11,2}n_{11,1} \\
m_{11,11} &= n_{11,1} - 1/6m_{11,4} - 1/6m_{11,17} \\
m_{11,16} &= 7n_{11,1} - 7m_{11,11} \\
n_{11,2} &= m_{11,4} + 0.5m_{11,16} + 0.5m_{11,17} \\
C_7H_{16} \quad m_{12,4} &= 7\alpha_{12,1}n_{12,1} \\
m_{12,17} &= 7\alpha_{12,2}n_{12,1} \\
m_{12,12} &= n_{12,1} - 1/7m_{12,4} - 1/7m_{12,17} \\
m_{12,16} &= 8n_{12,1} - 8m_{12,12} \\
n_{12,2} &= m_{12,4} + 0.5m_{12,16} + 0.5m_{12,17} \\
C_8H_{18} \quad m_{13,4} &= 8\alpha_{13,1}n_{13,1} \\
m_{13,17} &= 8\alpha_{13,2}n_{13,1} \\
m_{13,13} &= n_{13,1} - 1/8m_{13,4} - 1/8m_{13,17} \\
m_{13,16} &= 9n_{13,1} - 9m_{13,13} \\
n_{13,2} &= m_{13,4} + 0.5m_{13,16} + 0.5m_{13,17} \\
C_9H_{20} \quad m_{14,4} &= 9\alpha_{14,1}n_{14,1} \\
m_{14,17} &= 9\alpha_{14,2}n_{14,1} \\
m_{14,14} &= n_{14,1} - 1/9m_{14,4} - 1/9m_{14,17} \\
m_{14,16} &= 10n_{14,1} - 10m_{14,14} \\
n_{14,2} &= m_{14,4} + 0.5m_{14,16} + 0.5m_{14,17}
\end{aligned} \tag{17}$$

$$\begin{aligned}
 C_{10}H_{22} \quad m_{15,4} &= 10\alpha_{15,1}n_{15,1} \\
 m_{15,17} &= 10\alpha_{15,2}n_{15,1} \\
 m_{15,15} &= n_{15,1} - 1/10m_{15,4} - 1/10m_{15,17} \\
 m_{15,16} &= 11n_{15,1} - 11m_{15,15} \\
 n_{15,2} &= m_{15,4} + 0.5m_{15,16} + 0.5m_{15,17} \\
 H_2O \quad m_{16,16} &= n_{16,1} \\
 CO \quad m_{17,4} &= \alpha_{17,1}n_{17,1} \\
 m_{17,17} &= \alpha_{17,2}n_{17,1} \\
 n_{17,2} &= -0.5n_{17,1} + m_{17,4} + 0.5m_{17,17} \\
 NO \quad m_{18,19} &= \alpha_{18,1}n_{18,1} \\
 m_{18,18} &= \alpha_{18,2}n_{18,1} \\
 n_{18,2} &= -0.5n_{18,1} + m_{18,19} + 0.5m_{18,18} \\
 NO_2 \quad m_{19,19} &= n_{19,1} \\
 SO_2 \quad m_{20,20} &= n_{20,1}
 \end{aligned}$$

A proper sequence must be addressed in the calculations. Components present in more than one reaction must be calculated at the end of sequence. Total flow of products in more than one reaction is the results of the sum of the products of all reactions.

The efficiencies could be substituted for any function, according the available plant data. A very important factor not used in this work is the actual flame temperature.

Although no kinetics is taken into account, this approach considering these original two efficiencies, allows simulate the behaviour of a combustion chamber for training purposes (whatever, a combustor of a gas turbine or the furnace zone of a boiler).

So, the combustion chamber simulation should be able to predict the amount of heat generated by the reactions, the products temperature leaving and the products flowrates and compositions.

The transferred heat toward the combustion chamber surroundings depends on the desired design. For example, for a combustor, the designer wants the heat not to be transferred in order to have more potential work to be done in the gas turbine (of course a compromise with the NO_x production must be considered). For a furnace, the heat transfer depends on the boiler type (radiant, convective, once-through, *etc.*) and the desired pattern of the heat absorption in all different elements of the boiler (waterwalls, superheaters, economisers, *etc.*).

In any case the heat transference phenomenon it is not treated in detail in this chapter but a couple of general expressions are used. A representative surrounding walls temperature T_{sw} is assumed to be known at any time.

5.5. Calculation sequence

With the mass flowrate of each reactant, their mass composition and the molecular weight of the components, mass flowrates are converted into mole flowrates and mass compositions into mole compositions.

With the inlet temperature of each reactant (water, air and gas fuel), using the thermodynamic properties, the enthalpy of each inlet stream is calculated. And the total reactants enthalpy may be known:

$$h_r = \frac{w_w h_w + w_a h_a + w_{fg} h_{fg}}{w_w + w_a + w_{fg}} \quad (18)$$

According to the present reactants they may be predicted the possible combustion products.

Reactants enthalpy (Δh_r^{298}) and formation heat (Δh_r^f) are calculated, both at 298 K.

$$\Delta h_r^f = w_r \Delta h_r^f ; \Delta h_r^{298} = w_r \Delta h_r^{298} \quad (19)$$

Flame temperature T_f is assumed with an initial value (normally the last instant value). In this point begins an iterative process called Level 1.

Theoretical O_2 flowrate w_{fc} for a complete combustion is calculated applying Equations (17) with efficiencies values calculated considering an Oe equal to 9 (to assure a complete combustion).

Oxygen excess Oe is assumed with an initial value. In this point begins an iterative process called Level 2.

Efficiencies are calculated with Equations (15) and restrictions shown in Equation (16). These variables are a function of Oe and also could be a function of other variables as T_f , burners tilt, etc.

O_2 flowrate w_{O_2} is calculated with Equations (17) with the estimated efficiencies.

Oxygen excess is calculated as:

$$Oe = \frac{w_{fc}}{w_{O_2}} \quad (20)$$

If Oe has practically same value than that calculated in the beginning of iterative process Level 2, the calculation process continues, otherwise, a Newton-Raphson with numerical derivatives is used to converge Oe from the point where Level 2 initiates.

Actual products flowrates and composition are calculated with Equations (17).

Formation heat and enthalpies at 298 K and T_f are calculated.

$$\Delta h_p^f = w_p \Delta h_p^f; \Delta h_p^{298} = w_p \Delta h_p^{298}; \Delta h_p^{Tf} = w_p \Delta h_p^{Tf} \quad (21)$$

Sensible heat of reactants q_{s-r} from reactants temperature to 298 K, sensible heat of products q_{s-p} and combustion heat q_{com} are calculated as (consider that products are the sum of the results of reactions and the reactants going through combustion chamber being not burned):

$$q_{s-r} = \sum w_r (h_r - h_r^{298}) \quad (22)$$

$$q_{s-p} = \sum w_p (h_p - h_p^{298}) \quad (23)$$

$$q_{com} = \Delta h_p^f - \Delta h_r^f \quad (24)$$

Radiant and convective heat flowing to surrounding metal walls are calculated using known heat transfer coefficients that depends on the geometry and exposed area (these coefficients correlations and calculations are beyond the subject of this chapter):

$$q_{rad} = hA_{rad} (T_f^4 - T_{sw}^4) \quad (25)$$

$$q_{con} = hA_{con} (T_f - T_{sw}) \quad (26)$$

The process is complete if the sum of the heat flowrates is balanced *i.e.* are equal to zero:

$$f = q_{s-r} - q_{s-p} + q_{com} - q_{rad} - q_{con} \quad (27)$$

If f is enough near zero, the process is finished; otherwise a numerical Newton-Raphson is used to converge to the proper flame temperature from the point where Level 1 initiates.

The conceptual combustor chamber model is presented in Figure 5. The reaction node represents the reactions procedure explained above to get reaction products and flame temperature. The capacitive node is solved with Equations (4) and (5). Combustion chamber temperature and density are calculated with the proper cubic equations properties.

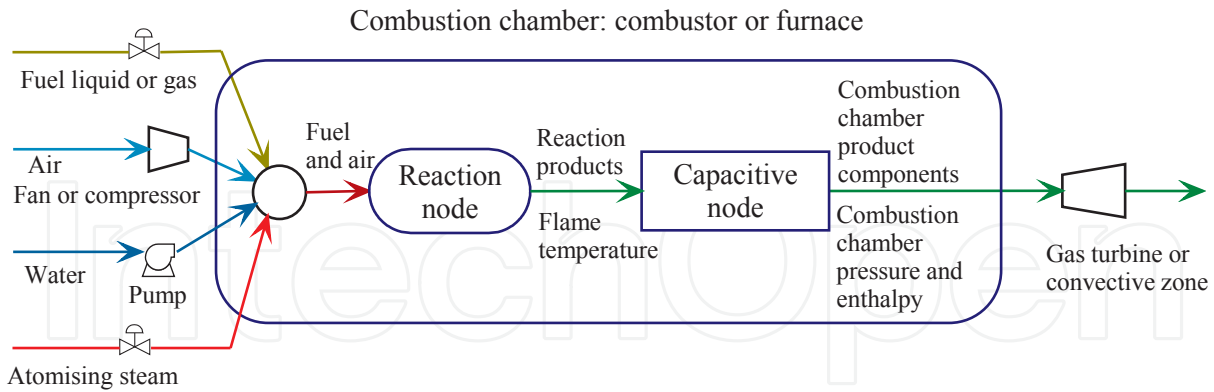


Figure 5. Conceptual model of the combustion chamber.

Although there are not mentioned in the above calculations, there are taken into account possible malfunctions or events as trip of burners, sudden turning off of flame, low efficiency of combustion (simulated as a factor less than one on the combustion heat), change in fuel composition, *etc.*

6. Application examples

More than a validation of the model, in this section one application example is presented. The basis for this example is a model installed in a simulator of a gas turbine power plant developed for CFE by the GSACS [26]. The reference plant produces nominally 150 MW. For this particular application of the combustion model, a linear function was used to represent each efficiency as shown in Equations (15), based only on the oxygen excess. Several real plant data were available and some of them were included in the graphics presented in this section.

The natural gas fuel and air composition of the presented test are shown in Table 7.

Component	N_2	O_2	CO_2	CH_4	C_2H_6	C_3H_8	C_4H_{10}	iC_4H_{10}	C_5H_{12}	C_6H_{14}	H_2O
Air	78.51	20.88	-	-	-	-	-	-	-	-	0.01
Gas Fuel	1.69	-	0.05	88.81	8.89	0.45	0.04	0.02	0.02	0.03	-

Table 7. Mole per cent composition of combustion chamber inlet flowrates

Selected results are presented here simulating an automatic start-up of the gas turbine power plant (Figures 6 to 9).

Figure 6 presents, as a reference, the simulated gas turbine speed and the generated power. Five seconds after the simulation is initiated, the start button is press and the automatic start-up procedure begins.

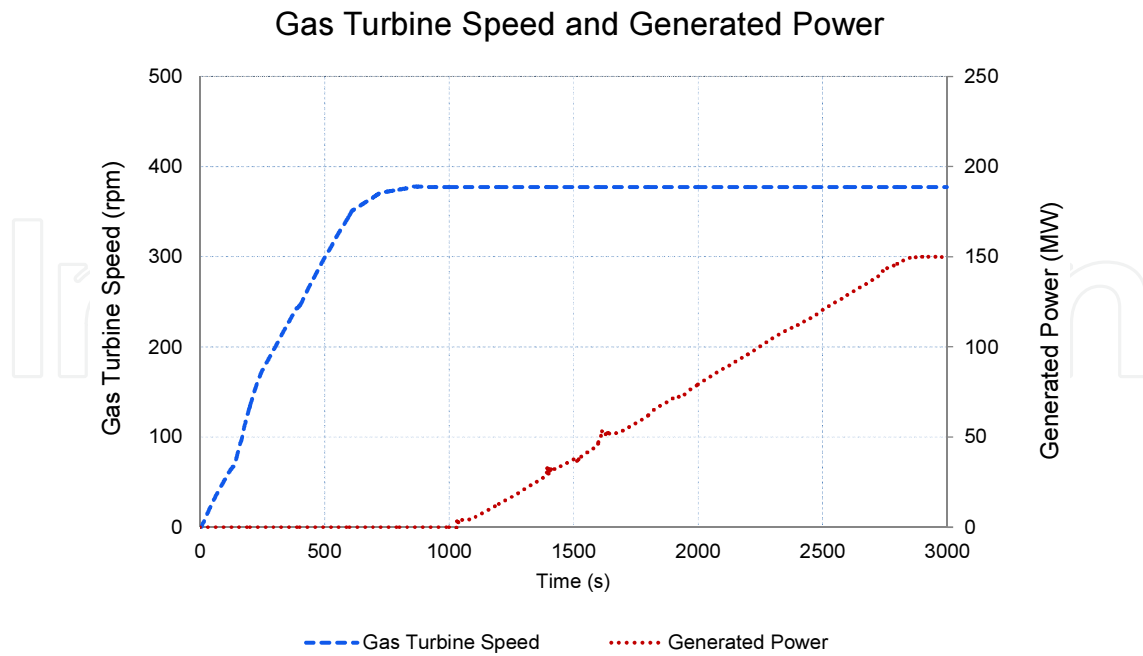


Figure 6. Automatic start-up gas turbine speed and generated power.

Figure 7 has the simulated mole flowrates of gas fuel and air feed to the combustor.

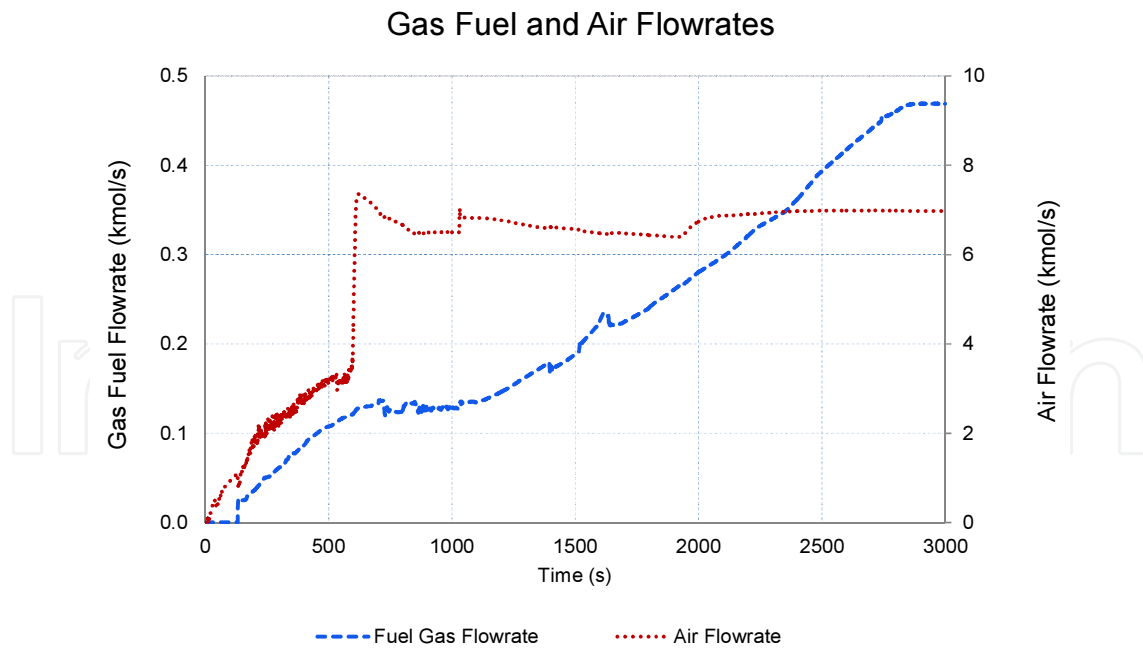


Figure 7. Automatic start-up mole gas fuel and air flowrates.

In Figure 8, real exhaust gases temperature and the result of simulation are compared. Simulation results of oxygen excess and CO₂ concentration are also included in Figure 8.

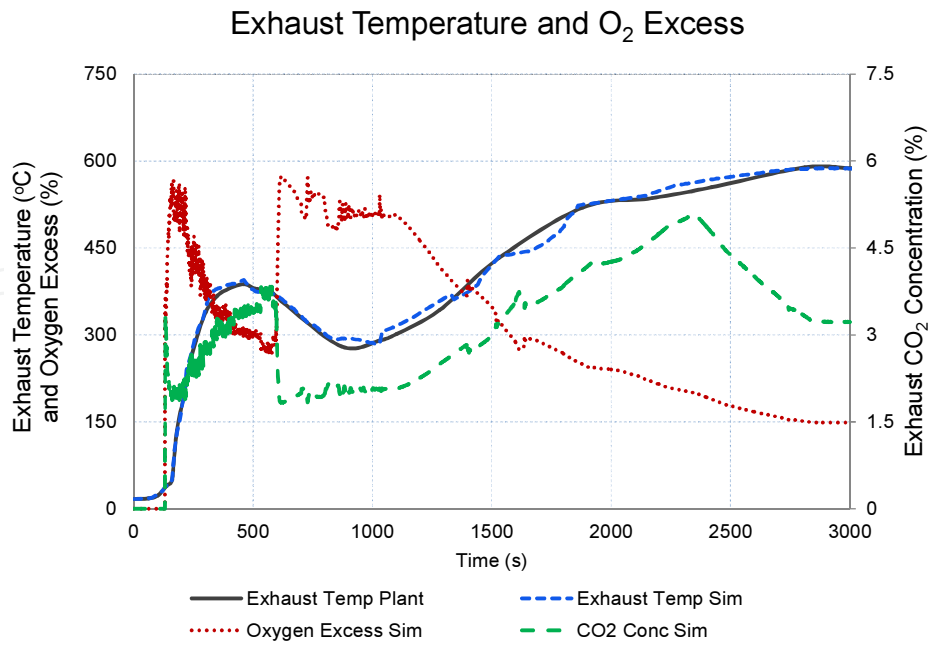


Figure 8. Automatic start-up exhaust temperatures and oxygen excess.

In Figure 9, simulated exhaust concentration of oxygen and nitrogen oxides are compared against real plant data.

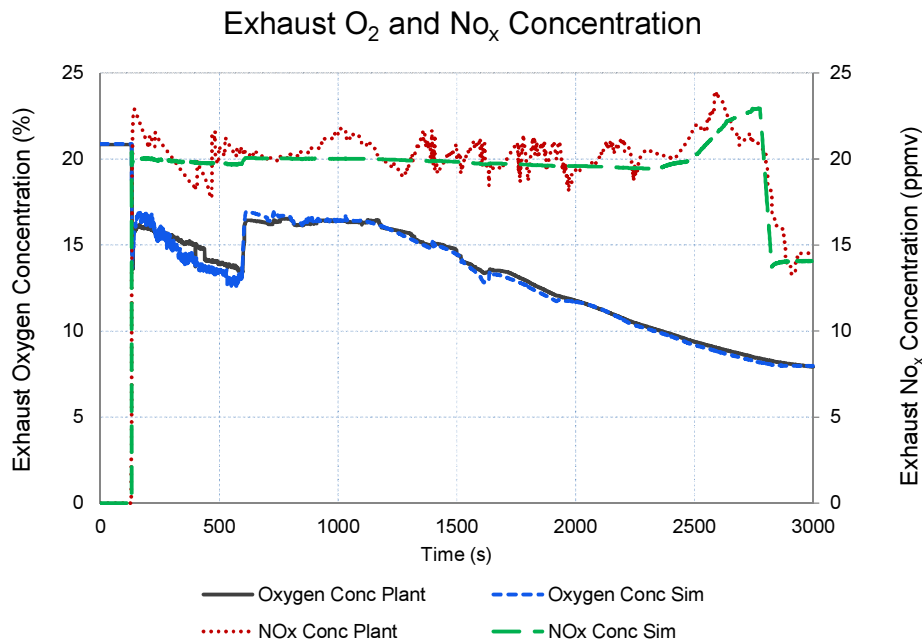


Figure 9. Automatic start-up exhaust oxygen and nitrogen oxides concentrations.

No SO_2 results exist because the natural gas considered in this simulator does not have any sulphur component.

All results are enough to satisfy the ANSI norm for fossil power plants simulators [19]. However, it is clear, according to Figure 9, that efficiencies should have an extra factor besides the oxygen excess to behave not so smooth as the curve presented by simulation results. This factor is an open issue to be studied.

No plant data are presently available for emission concentration during other transients, including malfunctions, but the qualitative simulation results are acceptable for training purposes.

7. Conclusion

7.1. Remarks

From the literature review, it may be concluded that few works on simple handled combustion models for training purposes have been reported. This work intends to cover the particular needs of the GSACS. A generic model of such a combustion process designed to work in any operators' training simulator has been presented.

Validation of the model has been intrinsically demonstrated with the inclusion of the model in a gas turbine and a combined cycle power plants simulators for operators' training. In the proper date, CENAC endorsed and accepted as correct the results of the tests in accordance with the testing acceptance procedures and the ANSI norm.

Some other off-line examples have been presented with the objective to explain the model principles and potential.

7.2. Future work

The combustion model is established and it is a relatively easy task to add new components to the possible set of reactions. Presence of other combustion sub-products such as free radicals or carbon should be studied and eventually considered.

There were mentioned different factors affecting the efficiency of reactions but not yet studied or included as part of the calculations like burner's tilt, ball fire position, gases recirculation, turbulent flow, bad mixing of reactants, level of pressure, kinetics, *etc.*

An automatized procedure should be devised to avoid the manual withdrawal of this model, the manual adjustment of efficiencies. This process should include factors as oxygen excess, the ul values and some other factors influencing the efficiencies like the mentioned above.

8. Nomenclature

Indices

c - Mass or mole concentration	P - Pressure
C_p - Specific heat at constant pressure	q - Heat flowrate
f - Function sum of heat flowrates	R - Ideal gas constant
h - Enthalpy	T - Temperature
hA - Product of transfer area and heat transfer coefficient	t - Time
k - Constant	ul - Upper limit for sum of efficiencies
m - Mass or moles; Mole flowrate of products	V - Volume
n - Mole flowrate of reactants	w - Mole or mass flowrate
O_e - Oxygen excess	

Subscripts

a - air	o - output
com - combustion	p - products
con - convection	r - reactants
f - formation or flame	rad - radiation
fc - full combustion	s - sensible
fg - gas fuel	sw - surrounding walls
i - number of consecutive reaction	T_f - flame temperature
in - input	w - water
j - number of consecutive component	

Acronyms

ANSI- American National Standards Institute	IGV- Inlet Guide Vane
BMS- Burner Management System	IIE- Electrical Research Institute
CENAC- National Centre of Training Ixtapantongo	IPD - Interactive Process Diagrams
CFD- Computational Fluid Dynamics	MAS- Simulation Environment
CFE- Mexican National Utility Company	O _e - Oxygen Excess
EGTEI- Expert Group on Techo-Economic Issues	PDF- Probability Density Function
FLUPRE- Generic Model to Solve Flows and Pressures Networks	PID - Proportional-Integral-Derivative Controller
GSACS- Simulation and Advanced Training Systems Department	SAMA- Scientific Apparatus Makers Association
IC- Initial Condition	

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