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Thermodynamic Analysis of Combustion Processes Using a New Educational Software

Jose S. Garcia[1], Guillermo E. Valencia[1] and Luis G. Obregón[2]

[1] Research Group on Efficient Energy Management, Facultad de Ingeniería
Universidad del Atlántico, km 7 antigua vía Puerto, Atlantico, Colombia

[2] Research Group on Sustainable Chemical and Biochemical Processes
Facultad de Ingeniería, Universidad del Atlántico
km 7 antigua vía Puerto, Atlántico Colombia

Abstract

This article presents the use of a graphical user interface in MATLAB® language called CombustionUA v1.0, for the thermodynamic study of the behavior of excess air, relative humidity, and air temperature in complete and incomplete combustion processes. The tool developed allows comparing the performance of different fuels under different operating conditions, since stoichiometry of different combustion reactions, calculation of thermochemical properties of fuels and energy balances have been programmed, so that the user can develop parametric case studies. The work shows the methodology and results of the application of three case studies, which were analyzed using the new educational software. In addition, the fundamental equations used in the development of the software algorithm are presented, as well as the maximum error rates obtained when validating the software in a group of mechanical engineering students at the Universidad del Atlántico. With the help of the software, it was concluded that the fuels with the best air fuel ratio and the highest heat transfer were determined, as well as the differences between the dew point temperatures of a complete combustion and an incomplete combustion.

Keywords: MATLAB®, computational tool, thermodynamic, combustion process, dew point temperature

1. Introduction

Combustion is one of the most interesting processes worldwide, due to the variety of its applications, which range from passenger compartment heating, energy production, propulsion, waste disposal, among others [1]. Although work is currently underway to develop new energy sources to reduce their use, they remain the most widely used energy production processes globally. Because of this, combustion processes have been extensively researched, with the aim of improving their efficiency and reducing their environmental impact, to specific applications such as reducing the arsenic emission rate in combustion processes, which causes a negative effect on the environment and human health [2]. In addition, experiments have been carried out to demonstrate the feasibility of reducing the temperature of coal processing waste to 750 °C - 800 °C in order to achieve sustainable combustion and reduce CO_2 and CO emissions by 1.2 to 1.7 times [3], and the dual-fuel process has been proposed as a solution for reducing emissions of nitrogen dioxide and particulate matter in diesel compression ignition engines [4].

In the quest to improve the efficiency of combustion processes, the development of programmed interfaces has had a fundamental performance, due to the fact that much of the research has been carried out by means of simulation. In order to increase the efficiency of a boiler through proper control of the combustion process, an optimization software was developed, integrated with the distributed control system and the temperature profile measurement system in the furnace [5]. Similarly, software has been developed for the calculation and optimization of diesel operating processes and fuel injection [6], which have been complemented by the development of multiple numerical models for the simulation of different hydrogen combustion applications, synthesis of sustainable processes, process of combustion of chemical loops in fluidized bed with iron-based oxygen carrier, process of combustion of a pellet fall boiler, pyridine combustion, among others [7,8], however, these software are focused on research and lack a pedagogical component. Therefore, the main contribution of this work is to present the software CombustionUA v1.0, as a user-friendly graphic interface focused on the learning of combustion processes for undergraduate engineering students, allowing them to analyze important parameters such as dew point temperature, air fuel ratio [9,10], adiabatic flame temperature, heat transfer, and excess air.

2. Methodology

2.1 Software presentation

CombustionUA v1.0 is a MATLAB-based software that facilitates the study of chemical reactions in combustion processes. The software allows the user to select between fifteen different fuels, where the complete and incomplete combustion processes, as well as the effects of excess air and relative air humidity on the process can be analyzed. In addition, importance parameter in the combustion process can be calculated, such as the air fuel ratio, the dew point temperature of the products, the heat transferred during the process or the adiabatic flame temperature. The application was designed to become a support tool for both students and professors of mechanical engineering at the Universidad del Atlantico, easy to use and easy to work with, as shown in Figure 1. The application allows to raise the levels of compression in the study of combustion processes in the subject of Thermodynamics in a practical and interactive way, allowing students to understand the effect of different variables in the process, through a parametric variation, changing one or more initial conditions.

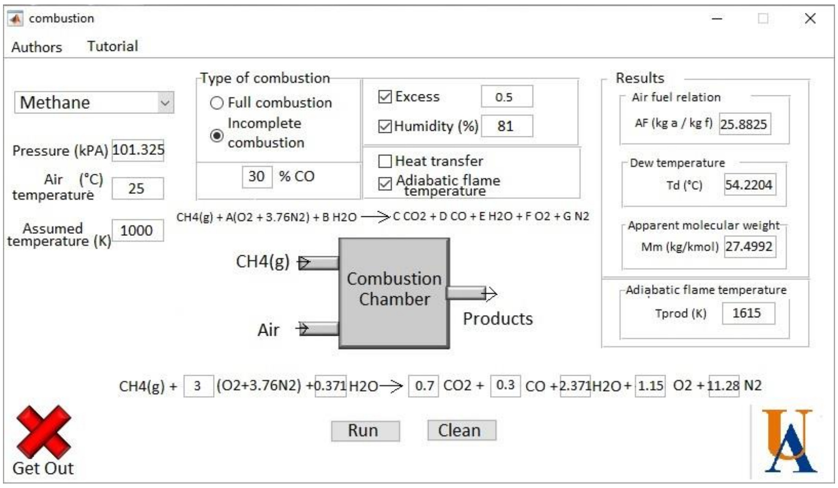

Figure 1. View of the CombustionUA software.

2.2 Fundamental Equations

The equations used in the development of the software algorithm are presented in detail below, which are taken from the classical thermodynamics books. The algorithm balances the chemical equation to calculate each of the available parameters, which depends entirely on the molecular formula of the fuel selected and the type of combustion to be carried out. When incomplete combustion is selected, the amount of CO_2 produced is calculated using equation (1).

$$CO_2 = 1 - \left({}^{CO}\!/_{100} \right), \tag{1}$$

where CO is the percentage of carbon monoxide entered by the user in the software. When there is relative humidity in the air, the user must enter the air inlet temperature into the combustion chamber to determine the saturation pressure ($P_{sat@T_{air}}$), this pressure is multiplied by the percentage of relative humidity ($\varnothing_{air}$) to calculate the partial pressure of the humidity in the air ($P_{v,air}$), as shown in equation (2).

$$P_{v,air} = \o_{air} P_{sat@T_{air}} \tag{2}$$

The number of moles of moisture in the air is then determined by equation (3).

$$N_{v,air} = \left(\frac{P_{v,air}}{P_{total}}\right) N_{total} \tag{3}$$

With the balanced chemical equation, the air-fuel ratio (AF) is calculated using equation (4), in addition to the dew point temperature of the products and the apparent molecular weight of the products.

$$AF = \frac{m_{air}}{m_{fuel}} = \frac{(NM)_{air}}{(NM)_C + (NM)_{H_2}} \tag{4}$$

where N is the number of moles and M is the molar mass. To calculate the dew point temperature of the products, the partial pressure of the water vapour in the flue gases ($P_{v,prod}$) must first be calculated using equation (5).

$$P_{v,prod} = \left(\frac{N_{v,prod}}{N_{prod}}\right) P_{total} \tag{5}$$

The saturation temperature of the partial pressure of the water vapour is then calculated, which is the dew point temperature of the products. To apply the first law of thermodynamics to combustion processes, the combustion chamber is considered a stationary flow system, which is a function of the enthalpy of each component of the reaction, which is calculated using equation (6).

$$Enthalpy = \bar{h}°_f + \left(\bar{h} - \bar{h}°\right), \tag{6}$$

where $\bar{h}°_f$ is the formation enthalpy in the reference state at 25°C temperature and 1 atm pressure, $\bar{h}$ is the sensitive enthalpy in the specified state and $\bar{h}°$ is the sensitive enthalpy in the reference state. When the kinetic and potential energies are insignificant, the energy balance for a chemically reactive stationary system to calculate the heat delivery (Q_{out}) is expressed as shown in equation (7).

$$Q_{out} = \sum N_r \left(\bar{h}°_f + \bar{h} - \bar{h}°\right)_r - \sum N_p \left(\bar{h}°_f + \bar{h} - \bar{h}°\right)_p \tag{7}$$

3. Results and Discussion

Initially, the validation of the CombustionUA v1.0 software was presented, which was carried out through a comparative study between the results obtained by the undergraduate students in Mechanical Engineering using the software and in a manual way using the texts of literature in classical Thermodynamics. Below are the results of three case studies developed to understand the behavior of excess air, relative humidity, and air temperature.

3.1 Validation of the software CombustionUA v1.0

To validate the computer application developed, a comparative analysis was made between the average results obtained by a group of 33 students as shown in Table 1, when the case studies were solved both manually and the application, obtaining an absolute maximum error of 0.8816% for the calculation of thermal energy transfer.

Table 1. CombustionUA software validation results.

Case Study	Parameter	GUI	Manual	Error (%)
Excess air	AF (kg air/kg fuel)	19.9096	19.9096	0
Excess air	Mm (kg/kmol)	29.4714	29.4713	3.39×10^{-4}
Relative humidity	Td full combustion (°C)	45.2443	45.1476	0.214
Relative humidity	Td incomplete combustion (°C)	44.7451	44.406	0.087
Air temperature	Thermal energy transfer (kJ/kg)	12853.9	12968.22	0.8816
Air temperature	Dew point temperature (°C)	52.4393	52.4359	6.48×10^{-3}

3.2 Case study Excess air

The behavior of a complete combustion process was analyzed to view the influence of the excess air parameter on the air-fuel ratio and the apparent molecular weight of the products for acetylene, methyl alcohol gas, and propane gas, varying the excess air every 0.5 from 0 to 4. From the results of the analysis of the influence of excess air and for an operating condition of 101.325 kPa of pressure in the combustion chamber, it can be observed that as the excess air increases, the air-fuel ratio increases linearly independently of the fuel used, while the apparent mass of the products presents a parabolic behaviour, being concave for methyl alcohol and propane gas, and convex for acetylene, i.e. for methyl alcohol and propane gas the apparent molecular weight of the products increases gradually as the excess air increases, while for acetylene it decreases, as shown in Figure 2a.

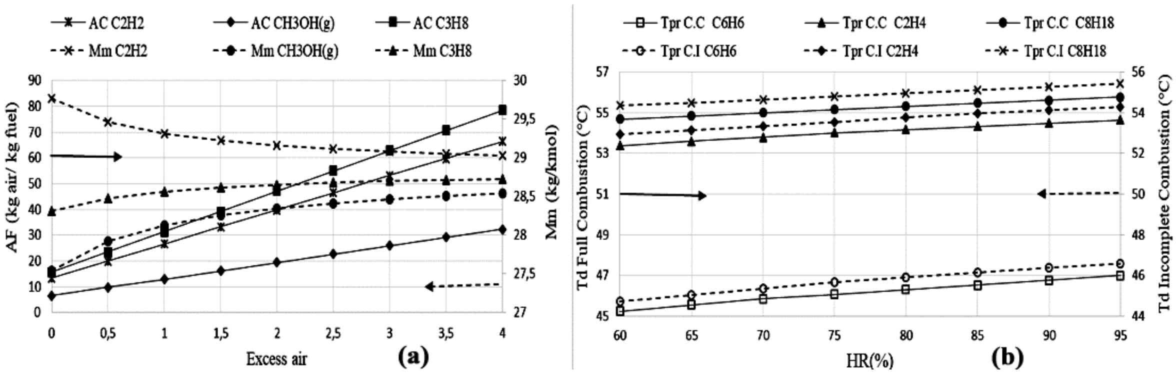

Figure 2. a) Results of the Excess Air Analysis, b) Results of the Relative Humidity Analysis.

3.3 Case study Relative humidity

In a combustion chamber, the influence of the percentage of relative humidity of the air (ø) on the dew point temperature of the products was analyzed, both for complete combustion and for incomplete combustion, when different fuels were burned, varying the percentage of relative humidity every 5% from 60% to 95%, for benzene, ethylene and n-octane gaseous. The operating conditions established to developed the case was 100 kPa in pressure, 25°C in temperature of the combustion chamber, and 30% CO for incomplete combustion. It can be seen in Figure 2b as the relative humidity percentage of the air increases as the dew point temperature increases, both for complete and incomplete combustion, regardless of the fuel used. Detailing the behavior of the fuels used during the study, it was observed that benzene is the fuel with the lowest dew point temperatures for both complete and incomplete combustion and octane has the highest dew point temperatures. The study showed that there is no difference between the dew point temperatures of complete and incomplete combustion. However, as the percentage of carbon monoxide in the products increases, this difference between the dew point temperatures would tend to increase. It is important to know the spray temperature because studies have shown that the condensation of vapours present in the exhaust gases significantly accelerates the fouling of the surfaces of some areas of the boiler [1].

3.4 Case study Air temperature

In the combustion chamber, the influence of the air inlet temperature on the thermal energy transfer and the dew point temperature of the products for incomplete combustion was analyzed, varying the air temperature every 5°C between 15°C and 60°C, when different fuels are burned, which were propylene, ethyl alcohol, gaseous and methane gas. From the results of the study, it can be seen in Figure 3 that as the air temperature increases, the heat transfer decreases parabolically, while the spray temperature increases. Ethyl alcohol gas is the fuel with the lowest heat transfer, showing a great difference concerning the other fuels studied, this difference is higher when the air temperature is lower, being more than 6500kJ/kg with respect to propylene when the air temperature is 15°C.

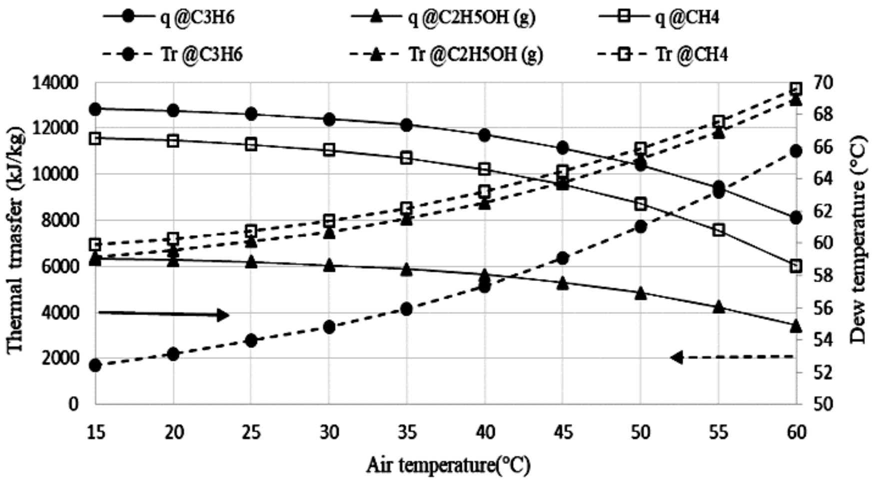

Figure 3. Air temperature analysis results.

Analyzing the behavior of the dew point temperature in the different fuels studied, it can be observed that propylene has the lowest temperatures, with a considerable difference with respect to the other two fuels studied, while methane gas is the fuel with the highest temperatures, however, it does not present great differences with respect to the temperature obtained by ethyl alcohol gas.

4. Conclusions

CombustionUA v1.0 was presented as a graphical user interface to study the under a thermodynamics focus the combustion processes, capable to analyze complete and incomplete combustion processes, which allows the integration of the effects of the relative humidity and excess air on parameters such as the air-fuel ratio, dew point temperature, adiabatic flame temperature and the thermal energy transfer.

Similarly, the performance of three fuels in a complete combustion process was compared when varying the excess air, where methyl alcohol had a better air-fuel ratio. The dew point temperatures of three other fuels were also analyzed, comparing them to complete combustion and incomplete combustion with a percentage of 30% of carbon monoxide in the products, varying the relative humidity of the air, where there was not a great difference between the temperatures under different combustion processes.

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