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Teaching combustion thermochemistry with an interactive Matlab application

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Abstract

Computer-aided-learning has been found to improve notably the learning efficiency as compared with classical teaching. In this study, an interactive Matlab application has been developed to be used when teaching combustion thermochemistry in engineering degrees. The use of this tool in practical sessions allows the students to concentrate on understanding the links between the boundary conditions of a combustion process and the corresponding outputs in terms of species composition and temperature. Moreover, the students can check the differences between the results obtained from a complex calculation (with the interactive tool) and those obtained by means of the simplified calculations performed during the theoretical lessons and written exams. The analysis of the outcomes after several years using this tool revealed that the students are generally satisfied with the practical session, and the analysis of the marks confirms the robustness of the methodology proposed.

KEYWORDS

combustion, educational tool, engineering teaching, practical Session, thermochemistry

1 | INTRODUCTION

Combustion science is essential for engineering purposes worldwide. The current lifestyle of the majority of the societies around the world requires using combustion processes to cover fundamental requirements, such as electricity generation, people mobility, and freight transport.[1,2] As a counterpart, the massive use of combustion processes has a negative impact on the environment, worsening the global warming problem due to the increased CO_2 emissions.[3] Considering this context, it is clear that teaching engineering students the fundamentals of combustion science becomes necessary,[4] so that the future professionals will be prepared to fight against global warming and improve air quality in cities.[5]

In fundamental combustion courses of engineering degrees, calculations of combustion reactions during the theoretical lessons, and exams must be simplified considering the course-level and time constraints. The simplified method for calculating combustion reactions for lean and stoichiometric mixtures assumes that combustion products are a simple mixture of few species (CO_2, H_2O, N_2, and O_2).[6] With this single-step reaction approach, the combustion stoichiometry can be resolved by means of a simple atom balance.[7] After that, some parameters defining

Abbreviations: CAL, computer-aided learning; CBI, computer-based Instruction; CMI, computer-managed instruction; EGR, exhaust gas recirculation; Tad, adiabatic temperature.

the combustion process, such as species composition or adiabatic flame temperature can be estimated.[8] The main assumption within this simplified approach is to neglect dissociation reactions occurring for several species. In real conditions, however, major species dissociate producing large quantities of minor species. Thus, the dissociation of ideal products promotes the appearance of H_2, OH, CO, H, O, N, NO, and some others.[9] The energy consumption by dissociation reactions leads to a reduction in adiabatic flame temperature, which at the end is a magnitude used for predicting NOx emissions during combustion.[10] To take into account such phenomena, chemical equilibrium calculations must be performed. Chemical equilibrium is a condition where the reaction rates of species are the same in both forward and backward directions, hence at this condition no net change in species composition results. Chemical equilibrium is usually described by two equivalent formulations, namely the equilibrium constants and the minimization of free energy. Both methods entail working with highly nonlinear equations, requiring the use of mathematical methods to resolve the problem by an iterative approach. This fact makes the analytical solution of the problem too difficult when no computer is used. For this reason, performing a dedicated activity on a computer lab seems to be appropriate for the students to learn the main effects of dissociation in combustion compared with the simple stoichiometry approach.

Computers are very useful tools for both research and teaching purposes.[11] The role of the computers in the teaching-learning process has been widely studied in the literature. In 1972, Luehrmann[12] expressed as five roles of computer: learning about the computer, learning with the computer, learning from the computer, learning about thinking with computers and managing learning with computers. Most recently, any application of computer for instruction is known as Computer-Based Instruction (CBI).[13] CBI is a teaching approach that integrates computer software programs with other teaching materials in the classroom. CBI includes different approaches as computer-aided learning (CAL),[14] computer-managed instruction (CMI)[15] and computer-assisted instruction.[16]

CAL, where a computer is treated as an aid to an overall teaching learning strategy with other methods, has been found to be a suitable method to improve the motivation and promote different learning abilities to the students.[17] With CAL, the learning efficiency has been found to improve notably as compared to classical teaching.[18] In this sense, it has been demonstrated that the students are better able to pick up concepts or skills faster and with less effort, and also retain what they have learned longer.[19] Consequently, they would require less teacher time. The basic objectives of CAL material are:

- To facilitate transition from the teacher-centered classroom to a more interactive one.
- To make the class more interactive and engaging.
- To ensure conceptual clarity and better application.
- To create a self-learning provision for both teachers and students. In this study, a virtual tool developed to be used in practical sessions for teaching combustion thermochemistry in engineering degrees is described. The main objective with this approach is that the student does not need to solve on his own the complex equations needed to derive a result, and instead they can concentrate on understanding the links between the boundary conditions of a combustion process and corresponding outputs in terms of species composition and temperature. The outcomes in terms of numerical assessment and opinion from the students of several years using the virtual tool are reported. The learning objectives of the practical session are:
- Formulate the equations that control the chemical equilibrium applied to combustion systems.
- Justify the differences between the calculations with a one-step reaction and the chemical equilibrium.
- Acquire orders of magnitude of dependencies of the adiabatic flame temperature with respect to its controlling parameters.
- Apply the methodology of the parametric study to analyze a system.

2 | MATERIALS AND METHODS

2.1 | Description of the chemical model

This subsection describes how the composition of the equilibrium products is calculated, and how the kinetic NO scheme is coupled within the resolution of the combustion reactions.

2.1.1 | Calculus of equilibrium products of combustion

In this step, a procedure to calculate the combustion products in chemical equilibrium is presented. The whole procedure is based upon Equation 1, which starts from the ideal reaction between n_f fuel moles and n_a air moles:

$$\begin{aligned} n_f C_n H_m \; + \; n_a \, (X_{N2} N_2 + X_{O2} O_2 + X_{H_2O} H_2O \\ + \; X_{CO2} CO2 + X_{Ar} Ar) \rightarrow n_1 N_2 + n_2 O_2 + n_3 CO_2 \\ + n_4 H_2O + \; n_5 CO + n_6 H_2 + n_7 NO + n_8 OH + n_9 N \\ + \; n_{10} H + \; n_{11} O + \; n_{12} Ar \end{aligned} \quad (1)$$

where n_i corresponds to the moles of each specie in the products and X_i to the wet mole fraction of each

component in the air. It is interesting to remark that the air composition is defined to take into account the possible use of exhaust gas recirculation (EGR), which is a typical strategy to reduce NOx emissions in combustion systems.

The terms of the equation that are known are those on the left hand side, the terms on the right hand side are the unknowns. The fuel type (C_nH_m) is chosen from the user. The fuel mass (m_f or n_f in terms of moles) for which we want to calculate its equilibrium products is an input for the model. The air mass (m_a or n_a in terms of moles) is calculated as the air mass needed for a stoichiometric A/F ratio for the aforementioned fuel mass.

Twelve combustion products are unknown, so twelve equations are needed to solve the system. Five equations are obtained from the atom balances:

$$\text{Nitrogen:} \quad 2\,n_a XN_2 = 2\,n_1 + n_7 + n_9 \tag{2}$$

$$\text{Oxygen:} \quad 2\,n_a XO_2 + n_a XH_2O + 2\,n_a XCO_2 = 2\,n_2 + 2\,n_3 + n_4 + n_5 + n_7 + n_8 + n_{11} \tag{3}$$

$$\text{Carbon:} \quad n\,n_f + n_a XCO_2 = n_3 + n_5 \tag{4}$$

$$\text{Hydrogen:} \quad m\,n_f + 2\,n_a XH_2O = 2\,n_4 + 2\,n_6 + n_8 + n_{10} \tag{5}$$

$$\text{Argon:} \quad n_a X_{ar} = n_{12} \tag{6}$$

The remaining seven equations are given by the seven equilibrium constants of the combustion reactions:

$$N_2 + O_2 \leftrightarrow 2\,NO \qquad K_e(1) = \frac{n_7^2}{n_1 n_2} \qquad K_e(1) n_1 n_2 - n_7^2 = 0 \tag{7}$$

$$2H_2O + O_2 \leftrightarrow 4OH \qquad K_e(2) = \frac{n_8^4}{n_4^2 n_2} \qquad n_4^2 n_2 - n_8^4 = 0 \tag{8}$$

$$2CO + O_2 \leftrightarrow 2CO_2 \qquad K_e(3) = \frac{n_3^2}{n_5^2 n_2} \qquad K_e(3) n_5^2 n_2 - n_3^2 = 0 \tag{9}$$

$$2H_2 + O_2 \leftrightarrow 2H_2O \qquad K_e(4) = \frac{n_4^2}{n_6^2 n_2} \qquad K_e(4) n_6^2 n_2 - n_4^2 = 0 \tag{10}$$

$$N_2 \leftrightarrow 2N \qquad K_5(5) = \frac{n_9^2}{n_1} \qquad K_e(5) n_1 - n_9^2 = 0 \tag{11}$$

$$H_2 \leftrightarrow 2\,H \qquad K_e(6) = \frac{n_{10}^2}{n_6} \qquad K_e(6) n_6 - n_{10}^2 = 0 \tag{12}$$

$$O_2 \leftrightarrow 2\,O \qquad K_e(7) = \frac{n_{11}^2}{n_2} \qquad K_e(7) n_2 - n_{11}^2 = 0 \tag{13}$$

To obtain the equilibrium constants referred to moles (K_e) we start from the data of equilibrium constants referred to partial pressures ($K_{p,\text{reacc}}$), which are tabulated in terms of temperature. The relation between $K_{p,\text{reacc}}$ and K_e is:

$$K_e = K_{p,reacc} R_{transf}^{\left(\sum n_{\text{products}} - \sum n_{\text{reactives}}\right)} \tag{14}$$

where R_{transf} is the transformation coefficient:

$$R_{transf} = \left(\frac{P_{ref} f_{Vf}}{R\ T_{eq}}\right) \tag{15}$$

where P_{ref} is the reference pressure (1 atm = 1.013 bar = 101325.02 Pa), V_b the total volume occupied for the burnt gases, R universal gas constant (8314.3 J/Kmol K), and T_{eq} the equilibrium temperature.

For a chemical equation of the following type:

$$a\ A + b\ B \leftrightarrow c\ C \quad \rightarrow K_{p,\text{reacc}} = \frac{\left(\frac{P_C}{P_{ref}}\right)^c}{\left(\frac{P_A}{P_{ref}}\right)^a \left(\frac{P_B}{P_{ref}}\right)^b} \tag{16}$$

where P_A, P_B, and P_C are the partial pressures of the species of the chemical reaction.

For a certain reaction, the $K_{p,\text{reacc}}$ is calculated from the values of the formation K_p ($K_{p,\text{for}}$) of the species that are included in the chemical equation:

$$\log K_{p,\text{reacc}} = \sum \nu_j \log K_{p,\text{for}}(\text{products}) - \sum \nu_i \log K_{p,\text{for}}(\text{reactants}) \tag{17}$$

where ν_i and ν_j are the stoichiometric coefficients of each specie in the reaction.

$K_{p,\text{for}}$ values for all species are retrieved from the Thermodynamic JANAF Tables, tabulated in terms of the absolute temperature within the range of 298 K and 6000 K, from which the corresponding $K_{p,\text{reacc}}$ and K_e for each of the seven combustion reactions are calculated. That implies knowing the seven unknowns that we needed to solve the equation system.

Because equilibrium constants in the end depend on temperature, the temperature of the products has to be calculated. To do so, an adiabatic flame temperature is included, which is based upon the following equation:

$$\begin{aligned} &n_f h_f(T_0) + n_a\,(X_{N2} h_{N2}(T_0) + X_{O2} h_{O2}(T_0) \\ &+ X_{H_2O} h_{H2O}(T_0) + X_{CO2} h_{H2O}(T_0) \\ &+ X_{Ar} h_{Ar}(T_0)) \rightarrow n_1 h_{N2}(T_{AD}) + n_2 h_{O2}(T_{AD}) \\ &+ n_3 h_{CO2}(T_{AD}) + n_4 h_{H2O}(T_{AD}) + n_5 h_{CO}(T_{AD}) \\ &+ n_6 h_{H2}(T_{AD}) + n_7 h_{NO}(T_{AD}) + n_8 h_{OH}(T_{AD}) \\ &+ n_9 h_N(T_{AD}) + n_{10} h_H(T_{AD}) + n_{11} h_O(T_{AD}) \\ &+ n_{12} h_{Ar}(T_{AD}) \end{aligned} \tag{18}$$

Where again the left hand-side terms are known while the right hand side ones are to be solved.

After formulating the problem in terms of thirteen equations and the corresponding unknowns, the system is solved with an iterative method that searches for the solution.[20]

From a point of view of user inputs, the equilibrium composition of the combustion products will depend on the following factors:

- Initial temperature for which it is calculated
- Pressure (constant-pressure combustion is assumed)
- Initial air composition (depending on the EGR addition)
- Fuel selected
- Air/fuel mass ratio (A/F) (in principle stoichiometric A/F ratio is selected)

2.2 | Approach of the practical session

The typical number of students enrolled on the present course within an engineering degree is around 180 per year, which are divided in several groups for the theoretical lessons (three in this case). The practical sessions have a typical share of around one-third of the total time of the course, what gives higher flexibility to create more working groups to boost the development of transversal competences.[21] In this case, 8 different groups of 24 people maximum are proposed. This is intended to create a more collaborative ambient that enables the interaction among students.[22] Even if the computer laboratory in which the practical session is carried out has more than 24 computers, two persons per group has been determined to be ideal for active participation of all students and to stimulate their work-in-group capabilities with both participants being fully active in the assignment.[23]

The allocated time for the practical session is 3 hours maximum. First of all, an introduction of around 30 minutes is made by the teacher to summarize the theoretical concepts related to the practical session. At this time, the objective of the work proposed to the students is justified. The next 10 minutes are used to explain how to use the Matlab application into which the previously described solver is embedded, as well as the different study cases proposed in the assignment that the students are asked to solve. The rest of the time is given to the students to solve the different cases using the Matlab application and fill the assignment document, which typically takes around 60 minutes.

The evaluation of the practical session takes into account two inputs from the students. The first one is the actual document that they fill in, which must be delivered by each pair of students at the end of the practical session. The second item is a test exam that is carried out through the institutional virtual learning environment) so-called PoliformaT. The approach of the practical session is sketched in Figure 1. Both items accounts for 50% of the practical session mark.

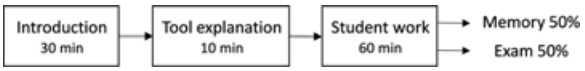

FIGURE 1 Approach of the practical session

3 | RESULTS OBTAINED FROM INDIVIDUAL GROUPS

Each working group of two students is asked to solve four cases. The first case highlights the main differences between the simplified combustion reaction and equilibrium calculations. The other three cases are intended to remark the main effects of different parameters on the dissociation phenomenon and their implications on other variables that characterize the combustion process.

3.1 | Case 1: Atmospheric burner

The objective of this case is to compare the results obtained with the simplified calculation approach used in the theoretical lessons versus those obtained from the chemical equilibrium. For this purpose, a constant pressure combustion at a temperature of 30°C is considered. The students are asked to perform a parametric sweep with the conditions summarized in Table 1 to compare the adiabatic flame temperature (T_{ad}) and the mass fraction of fuel, CO_2, CO, and O_2 obtained with both calculation methods.

The students are asked to answer the next questions:

- What is the dependency of the adiabatic flame temperature with the equivalence ratio? Is there a maximum in the T_{ad} profile? At which equivalence ratio does it appear?
- Summarize the differences observed between the simplified calculation and the chemical equilibrium results

TABLE 1 Conditions to perform the parametric sweep of the Case 1

Fuel [-]	Dodecane ($C_{12}H_{26}$)
m_a/m_f [-]	Corresponding to an equivalence ratio of 0.5 to 3 (20 points)
EGR [%]	0
P_{ini} [bar]	1
T_{ini} [K]	303

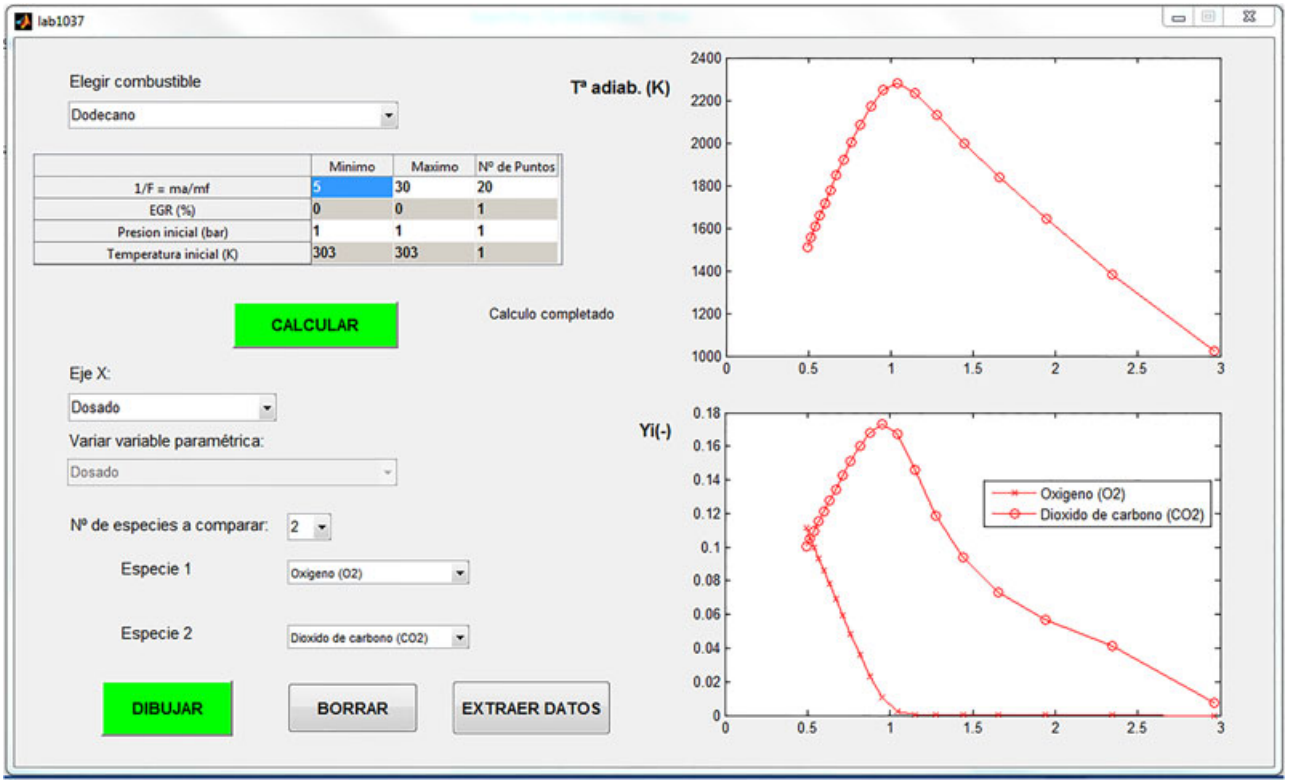

FIGURE 2 Graphical interface of the Matlab tool after calculating the case 1

To calculate the ma/mf range to perform the parametric sweep, the stoichiometric air-fuel ratio must be calculated first. The stoichiometry for a combustion reaction in stoichiometric conditions must be solved, as shown in Equation 19:

$$C_{12}H_{26} + a\,(O_2 + 3.76N_2) \rightarrow b\ CO_2 + c\ H_2O + d\ N_2 \quad (19)$$

To solve the stoichiometry for the combustion reaction shown in Equation 19, the equations for the atom balances (20-23) are used:

$$C:\ \ 12 = b \quad (20)$$

$$H:\ 26 = 2c \quad (21)$$

$$O:\ 2a = 2b + c \quad (22)$$

$$N:\ 2*3.76a = 2d \quad (23)$$

The four unknowns (a, b, c, and d) can be obtained solving the simple four-equation system. The values for the unknowns are $b = 12$, $c = 13$, $a = 18.5$, and $d = 69.56$. The fuel mass can be calculated considering the atomic weight of carbon (12 g/mol) and hydrogen (1 g/mol), being $m_{fuel} = 12*12 + 26*1 = 170$ grams. The air mass can be calculated considering the atomic weight of the nitrogen (14 g/mol) and oxygen (16 g/mol), being the $m_{air} = 18.5*(2*16 + 3.76*2*14) = 592 + 1947.68 = 2539.68$ grams. With this, the mass-based stoichiometric air-fuel ratio for $C_{12}H_{26}$ is $(m_a/m_f)_{est} = 2539.68/170 = 14.94$. Thus, for the Fr range proposed in Table 1, the values for the ma/mf sweep range from 5 to 30.

Figure 2 shows the Graphical User Interface (GUI) of the Matlab tool after calculating the Case 1. The left-upper region is used to introduce the data of the parametric sweep. It is interesting to remark that different fuels are available to perform the calculations, dodecane ($C_{12}H_{26}$), methane (CH_4), and propane (C_3H_8). The left-lower region is used for selecting the variables to be represented. In the right hand side, the plots of the different parameters are shown. After each calculation, the Matlab tool exports a data file containing all the results.

In parallel, the simplified combustion calculations are performed in a Microsoft Excel spreadsheet, over which the results from the Matlab tool can be imported for comparison. The results from both methods are directly compared in Microsoft Excel, as shown in Figure 3. As it can be seen, the CO_2 calculated with the simplified method (legend "1p") is underestimated compared with that calculated in equilibrium. This is because the

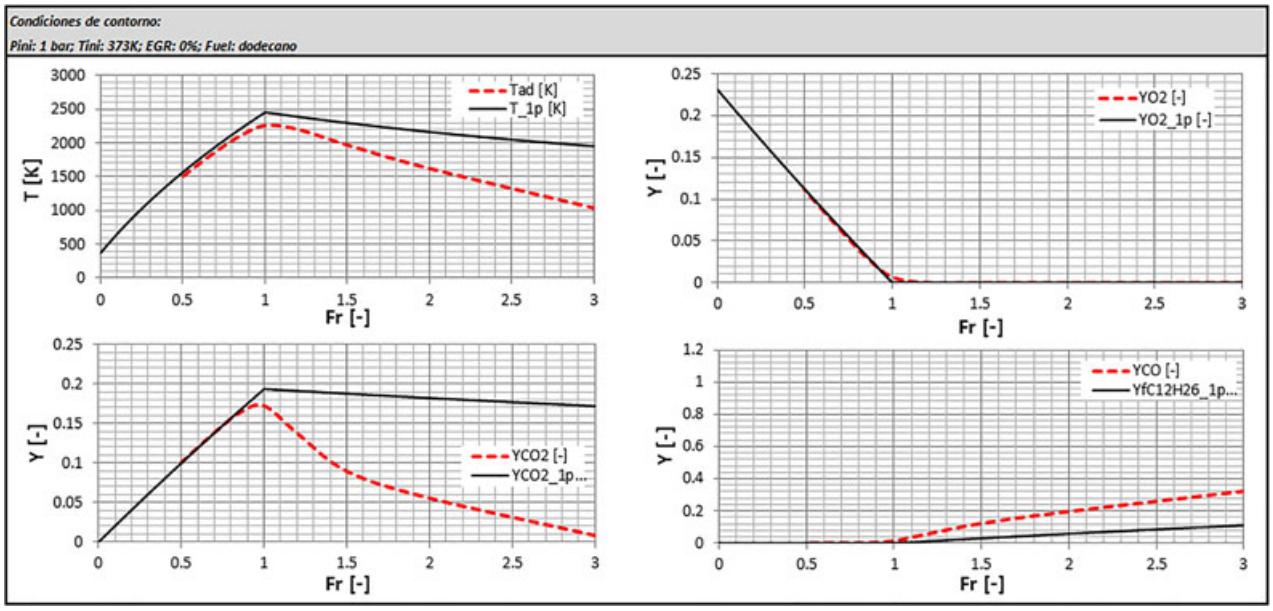

FIGURE 3 Comparison of the results simplified versus equilibrium calculation

dissociation phenomenon, which at high temperatures leads to convert part of the CO_2 into CO and O_2. This phenomenon consumes part of the energy in the combustion chamber, leading to a lower adiabatic flame temperature than the one estimated with the simplified method. The dissociation phenomenon also influences the relationship between the adiabatic flame temperature and the equivalence ratio. As Figure 3 shows, the adiabatic flame temperature peak in equilibrium is shifted to an equivalence ratio value slightly higher than 1, due to the dissociation effect.

3.2 | Case 2: Atmospheric burner with preheated air

The aim of this case is to analyze the effect of the initial temperature of the mixture on the adiabatic flame temperature and the mass fraction of CO_2, CO, O_2, and NO. For this purpose, the students are asked to perform a parametric sweep with the conditions summarized in Table 2.

The students must answer the next questions in the memory document:

TABLE 2 Conditions to perform the parametric sweep of the case 2

Fuel [-]	Dodecane ($C_{12}H_{26}$)
m_a/m_f [-]	15.0199 (Fr = 1)
EGR [%]	0
P_{ini} [bar]	1
T_{ini} [K]	300-900 (20 points)

- What is the dependency of the adiabatic flame temperature with the initial temperature?
- What does it occur with the CO_2 and CO when increasing the initial temperature? Why? What is its influence on T_{ad}?
- Analyze the changes observed in the NO when the initial temperature is modified.

The results provided by the model are shown in Figure 4, which shows the adiabatic flame temperature and mass fraction of CO_2 and CO, as a function of the initial temperature. The figure shows a linear increase of the adiabatic flame temperature with the initial pressure. Moreover, the CO_2 mass fraction decreases as the initial temperature increases with the same slope than CO decreases. This is due to the dissociation phenomenon, which is more pronounced at high temperatures.

3.3 | Case 3: Internal combustion engine with ambient air

The objective of this case is to highlight the effects of the ambient pressure on the adiabatic flame temperature and the mass fraction of CO_2, CO, and O_2. To do this, similar conditions to those found during the combustion process in internal combustion engines are proposed. In Table 3, a stoichiometric combustion with no EGR and initial temperature of 900 K is proposed. In this case, the pressure is varied in the range of 1 to 100 bar.

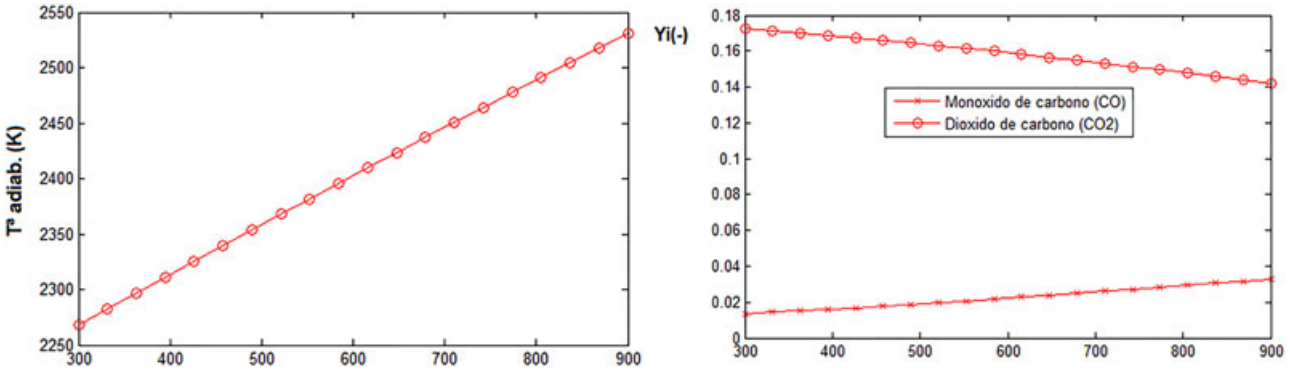

FIGURE 4 Adiabatic flame temperature and mass fraction of CO2 and CO as a function of the initial temperature

TABLE 3 Conditions to perform the parametric sweep of the case 3

Fuel [-]	Dodecane ($C_{12}H_{26}$)
ma/mf [-]	15.0199 (Fr = 1)
EGR [%]	0
Pressure [bar]	1-100 (20 points)
T_{ini} [K]	900

The students must be able to answer the next questions:

- Describe the effect of the pressure on the T_{ad}
- What does it occur with the different species when the pressure is increased? Why?

The results provided by the model are shown in Figure 5, which shows the adiabatic flame temperature and mass fraction of CO_2, CO, O_2, and NO as a function of the initial pressure. As it can be seen, the adiabatic flame temperature increases exponentially with the initial pressure. On the other hand, higher pressures inhibit the dissociation phenomenon, so that CO_2 mass fraction increases while that of CO decreases.

3.4 | Case 4: Internal combustion engine with EGR

This case proposes to study the effect of the EGR on the combustion thermochemistry. The conditions to run the Matlab application are summarized in Table 4. The students are asked to evaluate the effect of the EGR on

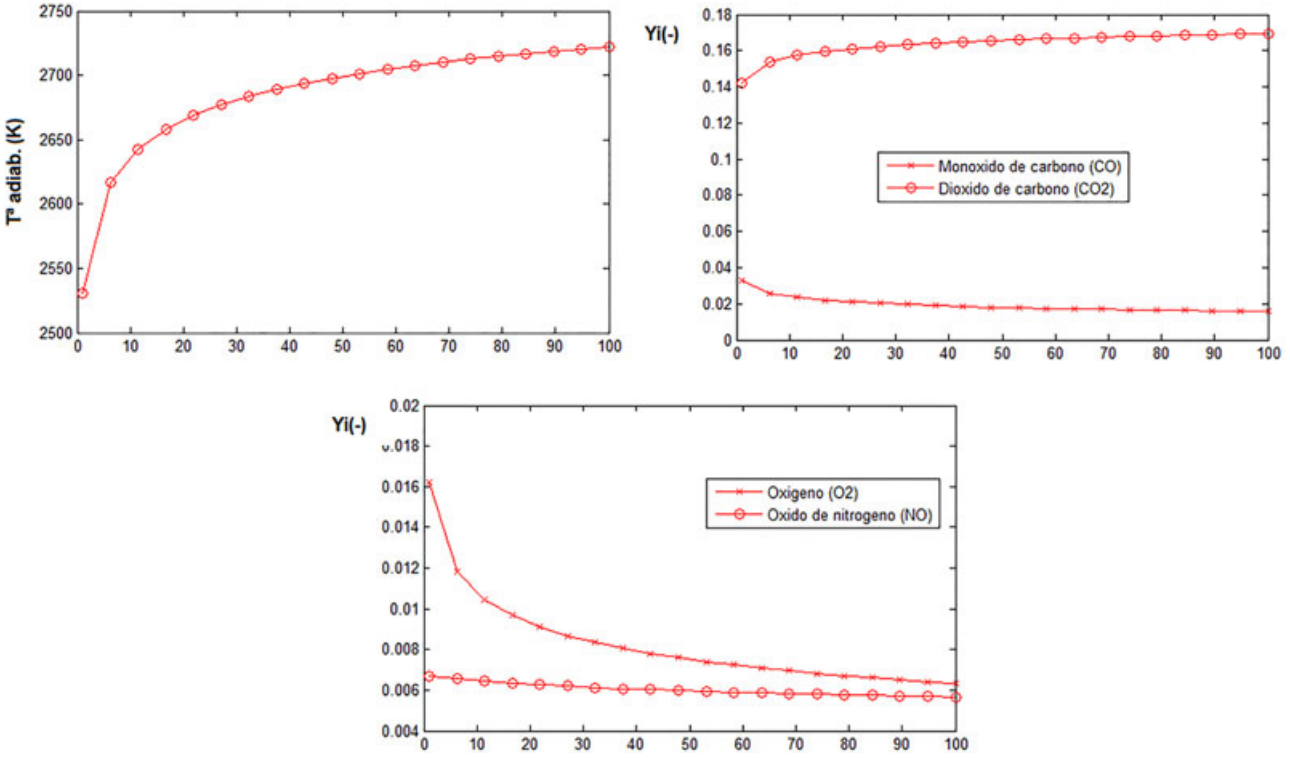

FIGURE 5 Adiabatic flame temperature and mass fraction of CO2, CO, O_2, and NO as a function of the initial pressure

TABLE 4 Conditions to perform the parametric sweep of the case 4

Fuel [-]	Dodecane ($C_{12}H_{26}$)
ma/mf [-]	15.0199 (Fr = 1)
EGR [%]	0%-50% (20 points)
P_{ini} [bar]	100
T_{ini} [K]	900

the adiabatic flame temperature and the mass fraction of CO_2, CO, O_2, and NO.

The students are must be able to answer the next questions:

- What is the effect of the EGR on T_{ad}? What is the explanation of this effect?
- What does it occur with the different species when the pressure is increased?

The results provided by the model are shown in Figure 6, which shows the adiabatic flame temperature and mass fraction of CO_2, CO, O_2, and NO as a function of the EGR rate. The reason for the adiabatic flame temperature decrease with the EGR rate increase is two-fold: on the one hand, the substitution of the fresh air by the EGR gas reduces the intake oxygen concentration, which limits the combustion reaction. On the other hand, the addition of the inert exhaust gas into the intake increases the heat capacity of the nonreacting matter present during the combustion process. The increased heat capacity promotes lowering the peak combustion temperature. The NO formation through the thermal mechanism requires high temperatures and oxygen availability, so that the NO mass fraction decreases as the EGR increases. Finally, the CO and CO_2 trend is explained by the effect of the temperature on the CO_2 dissociation reaction: when increasing EGR, the lower temperature achieved implies that dissociation is less prone to happen, inducing higher levels of CO_2 in the exhaust gases.

The last table to be fulfilled in the memory document by the students is aimed at summarizing the effects of the different parameters studied on the adiabatic flame temperature and the mass fraction of the different species. The students are asked to fill in Table 5 with arrow symbols to denote the sensitivity of to each parameter as very sensitive (↑↑↑ or ↓↓↓), sensitive (↑↑ or ↓↓), or little sensitive (↑ or ↓).

4 | OUTCOMES

This section reports the outcomes, in terms of marks and opinion from the students, of several years using the virtual tool.

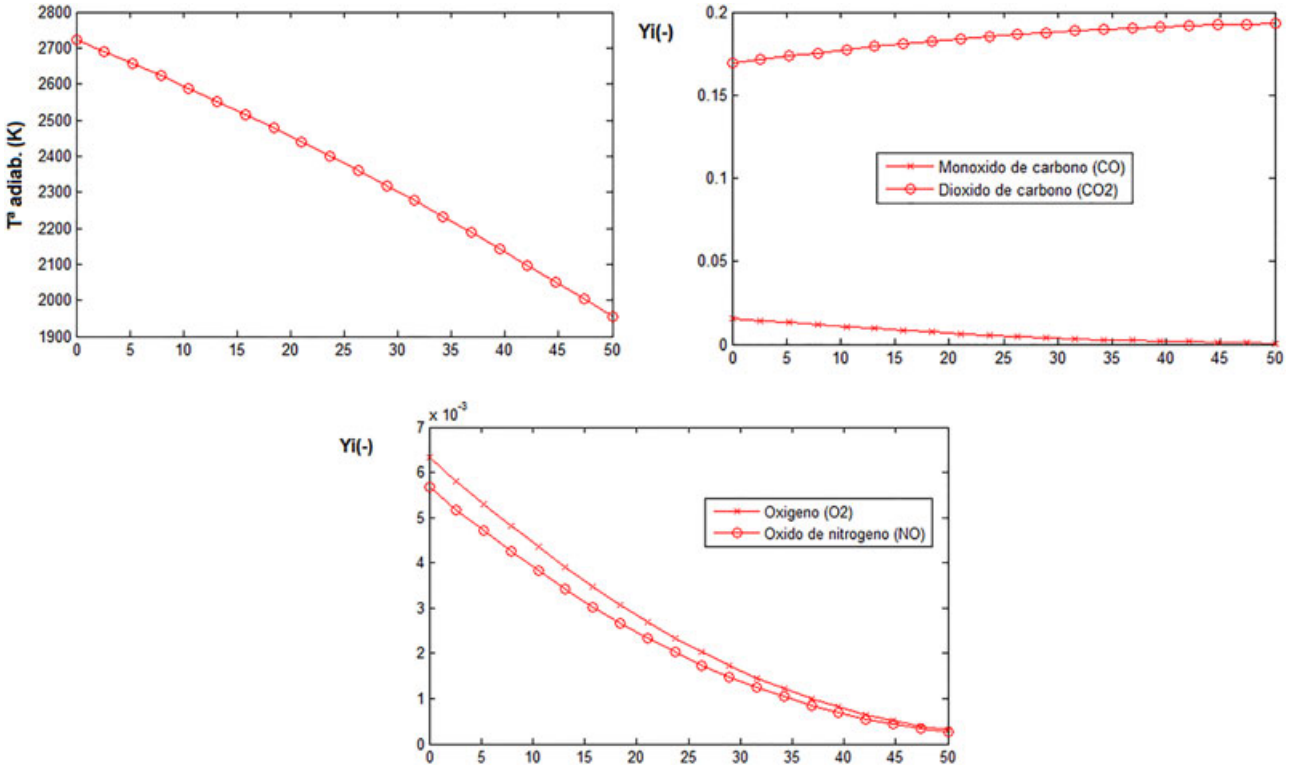

FIGURE 6 Adiabatic flame temperature and mass fraction of CO2, CO, O_2, and NO as a function of the EGR rate

TABLE 5 Summary of the effects of the different parameters studied on the adiabatic flame temperature and the mass fraction of the different species

Parameter	Tad	YCO_2	YCO	YO_2
↑Fr	↑↓	↑↓	↑↑	↓↓
↑T_{ini}	↑↑↑	↓	↑	↓
↑ P_{ini}	↑↑	↑	↓	↓↓
↑EGR	↓↓↓	↑	↓	↓↓↓

4.1 | Student opinion

During the last 10 minutes of the practical session, the students are asked to give their feedback about the practical session by means of a survey consisting of rating 12 different items from 0 (worst) to 5 (best) to evaluate the professor, contents, resources, and organization of the session. Later, six of these items are analyzed to measure the satisfaction degree of the students with the practical session:

- Q1: Overall assessment of the practice
- Contents
  - **a.** Q2: It is interesting
  - **b.** Q3: It is related to the theoretical concepts of the course
  - **c.** Q4: Applies the theoretical knowledge of the course
- Resources
  - **a.** Q8: The material is adequate
  - **b.** Q9: There is enough material
  - **c.** Q10: The laboratory is comfortable
- Comments, observations, and suggestions

Figure 7 shows the mean results of the survey for 5 consecutive years. The results shown in the figure correspond to Q1 and the sections contents and resources, since they are directly related to the methodology and development of the practical session. As it can be seen, all the mean rates are between 4 and 5. Therefore, it can be concluded that the students are generally satisfied with the session and the methodology used. This is particularly encouraging considering that chemistry is not typically among the most preferred subjects among mechanical engineering students.

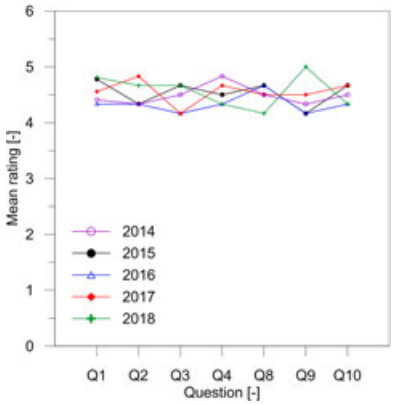

FIGURE 7 Results of the survey about the practical session for 5 consecutive years

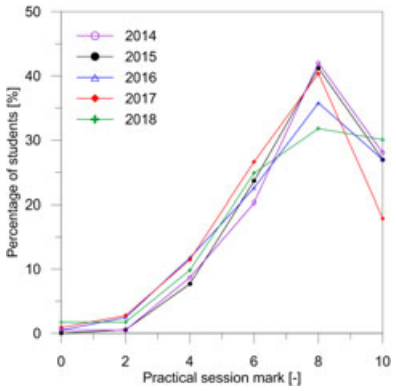

FIGURE 8 Marks of the practical session for 5 consecutive years

4.2 | Practical session marks

As explained in subsection 2.2, the evaluation of the practical session takes into account two inputs from the students, the test examination and the assignment document. Figure 8 shows the final marks of the practical session for five consecutive years. As seen in the figure, the trend of the percentage of students falling in each mark is quite repetitive for the different years, which confirms the robustness of the methodology proposed. The most common mark is 8 out of 10, which means that the students properly acquire the concepts explained in the practical session. In addition, it has to be noted that only around 10% of the students fail the test (ie reach a mark lower than 5).

5 | CONCLUSIONS

A Matlab application for teaching combustion thermochemistry in engineering degrees has been presented. The computer application has been created to highlight the effects of neglecting the dissociation phenomenon occurring during a real combustion process, which

complements the simplified combustion calculations performed during the theoretical lessons and exams.

For this purpose, an open-source code developed in the department is used. This code combines the main combustion reaction with seven dissociation reactions, solved under equilibrium assumption. The students use this software to perform several parametric studies, including the effect of equivalence ratio, initial pressure and temperature, and air composition, characterized by a certain level of EGR. The purpose is to analyze the main effects of these variables on dissociation reactions, and the differences compared with the simple stoichiometry solution performed during theoretical classes.

The outcomes of the session were analyzed from two points of view. On the one hand, surveys from students show that the overall satisfaction with the practical session and the methodology used has been quite high (average around 4.5, with a maximum of 5) during the 5 years that the practical session has been run. A great satisfaction of the students with respect to the interactive/virtual application was expected considering the results reported in literature reported by other authors.[24,25] On the other hand, test results prove that the main theoretical concepts related to the session have been well understood by most of the students, since around 70% of them have achieved a mark higher than 8 out of a maximum of 10. The improvement observed in learning efficiency agrees with the experience reported in literature about using virtual laboratories.[26,27]

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