Modelling of the physicochemical phenomena in an experiment similar to a gasoline engine

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SUMMARY

Combustion is a very complex field, since it simultaneously involves several disciplines such as heat transfer, chemistry, turbulence, mass transport etc. In this paper we tried to model a combustion chamber with a geometry close to that of the spark ignition engine. The initial and boundary conditions are well-known. The modeling is based on the approach of calculated probability density function (pdf) in case of turbulent combustion. We used a transport equation for the probability density function similar to the modeling case of the physical and chemical species. Indeed, the theoretical study of this pdf is well developed but its applications remain very limited. In the present paper, the pdf is coupled with a simplified chemistry. This model of combustion was introduced into the KIVA II code in order to simulate the combustion process in a rectangular combustion chamber which is very similar to that of the spark ignition engine (SI). The results found by this model of combustion are compared with the experiment at different operating conditions such as the propane/air equivalence ratio, temperature and pressure. The final results and the conclusions are satisfactory. In this paper, we present only the results relating to a given operation condition with a study of the sensitivity of the flame radius on the equivalence ratio. We believe that the results could be implemented on the case of the spark ignition engine.

Key words: *turbulent combustion, chemistry, probability density function.*

1. INTRODUCTION

One of the most important aspects of the combustion theory and its applications is the knowledge of its fundamental mechanisms, i.e. the set of elementary chemical processes, which occur in the course of a chemical reaction. When we use a detailed kinetics mechanism, we can establish the principal stages of a combustion process for any particular conditions. Unfortunately, the use of these detailed mechanisms remains quasi-impossible due to long required computing time. To overcome this problem, one generally uses simplified chemistry whose integration in numerical codes remains feasible. In the present paper, we have chosen a single global reaction for propane (one of the greatest sources of energy). In order to take into account the interactions between

chemistry and turbulence, the method involving a balance equation for the probability density function (pdf) was used. This coupling between the method of calculated pdf and simplified chemistry is used to predict combustion in the case of a rectangular combustion chamber (also called "ARC" combustion chamber). This simulation is validated by comparing the following:

– on the one hand, the pressure profiles (the calculated and the experimental) in the combustion chamber;
– on the other hand, the expansion of the flame starting from its initial position (the ignition is localized in the center of the combustion chamber).

The comparison between the numerical simulation and the experimental result showed a good agreement.

The extension of this study to a complex situation such as a spark ignition engine will be carried on in the future.

2. THE COMBUSTION MODEL USED

In equations governing a reactive flow (conservation of mass, momentum and energy), the source terms $\tilde{\omega}$, representing the chemical production in the turbulent reactive medium, appear either in an implicit or explicit way. The modelling of these terms causes serious problems due to their non-linearity. Under these conditions, the chemical source terms $\tilde{\omega}$ require a representation by the probability density function (pdf). So, the form of Arrhenus which gives the chemical rate by:

$$\omega\left(\tilde{T}\right) = A\tilde{T}^n \, exp\left(\frac{T_a}{\tilde{T}}\right) \qquad (1)$$

is no lounger valid in the case of turbulent combustion. This is because chemistry is greatly influenced by the turbulent flow (presence of fluctuations). We cannot directly introduce this form into the equations governing the reactive flow, such as the transport equations of the chemical species:

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{Y}_i\right) + \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{Y}_i u_j\right) = \frac{\partial}{\partial x_j}\left(\bar{J}_j^i - \bar{\rho}\, u_j' \, Y_i\right) + \bar{\rho}\,\tilde{\omega}_i \quad (2)$$

In fact, $\tilde{\omega}$ and $\omega\left(\tilde{T}\right)$ are two different quantities because of the fluctuations of temperature and concentrations. To take into account these chemistry-turbulence interactions, we use this pdf approach. There are two possible situations, either the approach which uses a presumed pdf (representing the shape by a beta function) with a complex chemistry or the approach using the exact transport equation for the pdf with a chemistry simplified to the extremes.

In the present paper, we have chosen the second approach. This model consists of calculating the pdf starting from a transport equation. It was examined earlier by Hopf [1] then by Lundgren [2]. Later on, O'Brien applied it in the field of turbulent combustion. This introduction of the concept of pdf into the field of combustion contributed to a better understanding of the process of turbulent combustion. Even though the formalism related to the calculation of transport equation of pdf was the subject of several theoretical investigations [3-5], the applications remained limited for the same reasons indicated earlier.

The description of turbulent combustion by this approach requires a pdf as a function of several variables depending on the number of unknowns in the physical problem. For example, in the case of the flow containing N species, the pdf is a function of the fractions Y_k $(k=1...N)$, the velocity of flow (three components), the enthalpy, the space and time coordinates. Obviously, the difficulty to determine and calculate this joined pdf depends on the number of parameters used. To simplify the shape of this pdf, one generally considers this pdf to be only the function of the concentrations of the various chemical species and the space and time coordinates. Thus, the modelling of combustion consists of calculating the pdf and choosing the chemistry. In this work, we used the following equation obtained with the Lundgren-Dopazo-O'Brien closures and previously tested by Borghi [6]:

$$\frac{\partial}{\partial t}\left[\bar{\rho}\,\tilde{P}(Y_1,Y_2,h)\right] = \frac{\bar{\rho}}{\tau}\left(\tilde{P}_e - \tilde{P}\right) - \frac{\partial}{\partial Y_1}\left[\bar{\rho}\omega(Y_1,Y_2,h)\tilde{P}\right] -$$

$$- \bar{\rho}\frac{D}{2\tau}\left\{\frac{\partial}{\partial Y_1}\left[\left(Y_1 - \tilde{Y}_1\right)\tilde{P}\right] + \frac{\partial}{\partial Y_2}\left[\left(Y_2 - \tilde{Y}_2\right)\tilde{P}\right] + \frac{\partial}{\partial Y_3}\left[\left(h - \tilde{h}\right)\tilde{P}\right]\right\} \quad (3)$$

where:
   Y_1 - the molar fraction of the oxidizer,
   $Y_2 = Y_1 - 5Y_K$ - a species without chemical
        production,
   Y_K - the molar fraction of propane,
   h - the enthalpy,
   $\bar{\rho}$ - the mean mixture density,
   $\tilde{P}$ - the pdf,
   D - a Damkohler number,
   τ - dimensioned as time.

The advantage of the use of this pdf transport equation is that we do not need to model the chemical term of the production but it is given directly by the chemical mechanism used. Here, the chemistry was represented by a single chemical reaction, and the rate of the chemical reaction is given by the following formula:

$$\omega = -A\rho\, Y_1 Y_K \, exp\left(-\frac{T_a}{T}\right) \qquad (4)$$

This formula has two constants T_a and A which will be adjusted to give a good agreement with the experiment. In fact, these constants will be determined by making comparisons with the experimental data obtained in a machine with fast compression.

Once the pdf is known, we can calculate the average rate of the chemical production $\tilde{\omega}$ relating to a given chemical species which appears in the equations governing the flow reactive, in particular, in Eq. (2).

After this formulation, the model of combustion was introduced into the numerical computer code KIVA II [7] which allows us to do the simulation of the reactive flows. This code was modified to adapt it to simulation of combustion in an ARC combustion chamber as described in the following paragraph.

3. THE MODELED EXPERIMENT: ARC COMBUSTION CHAMBER

The numerical results are validated by using those obtained in the ARC combustion chamber. Indeed, for this case one has all the initial conditions (measured by Floch [8]), as opposed to the case of a spark ignition engine, where these same conditions are not perfectly known. All measurements were made with a premixed propane-air mixture. The comparison between our calculations and the experimental results is performed on the level of the flame radius and pressure in the combustion chamber. The calculated average radius corresponds to the position of the isotherm *600 K*, which corresponds to the evaporation temperature of the droplets of the silicone oil. These droplets were also used in an experiment by Mouqallid [9] to sow the propane-air mixture in order to detect this isotherm. The combustion device is composed of two main parts: a combustion chamber of *60x60 mm* square cross section and a *100 mm* length, and an axisymmetrical, pneumatic driven, single shot piston mounted in a cylinder. Both parts are connected by means of interchangeable perforated blocs. The initial turbulence is generated in the combustion chamber by the interaction of the jets due to the piston movement towards its top dead center. The energy and scales of turbulence can be modified by varying the number and the diameter of the holes in the interchangeable turbulence generator, by adjusting the piston velocity, and by igniting the mixture at different times after the piston arrival.

4. DISCUSSION OF THE RESULTS

The results presented in this paper are obtained under the following operating conditions:
- equivalence ratio is *1*
- the compression ratio produced is *3*
- initial pressure is *3 bars*
- turbulence level is *1 m/s*
- dilution level is *0*
- sparks have duration of *1 ms*
- ignition energy deposed is *3 mj*

The constants A and T_a were adjusted by comparing the calculated pressure profile with that obtained in the experiment. One notices in Figure 1 that the values $ln(A)=10.5$ and $T_a=7200 K$ give a good estimate of the evolution of the pressure in the combustion chamber. The pressure rises to its peak value and then drops to its lower level in a short period of time. The difference noted on the levels of both profiles (the curve of the calculated pressure compared to that obtained in the experiments) could be accounted for by the heat exchange on the walls of the combustion chamber and at the level of initial turbulence. The difference in the burning velocities (calculated and experimental) can contribute also to this difference between the profiles.
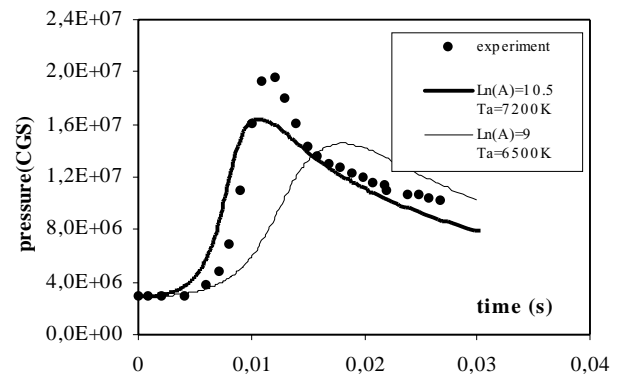

Fig. 1 Pressure in the combustion chamber

The validation of the present combustion model is confirmed by a comparison of the volumes of the burned gases (volumetric expansion or flame radius). The results are presented in Figure 2 showing a comparison between the calculations and the experiment. The flame radius begins to grow due to flame propagation and thermal expansion. This comparison shows a good prediction of the flame radius by the combustion model used. Indeed, the flame radius obtained numerically is well within the values obtained experimentally for various cycles having the same conditions. According to the same figure, the flame arrives at the combustion chamber wall after a *6ms* duration. So, the flame has a mean velocity of *5m/s*. The flame radius is affected by different factors such as the fuel/air equivalence ratio, the dilution, the temperature, the pressure and the turbulence level.
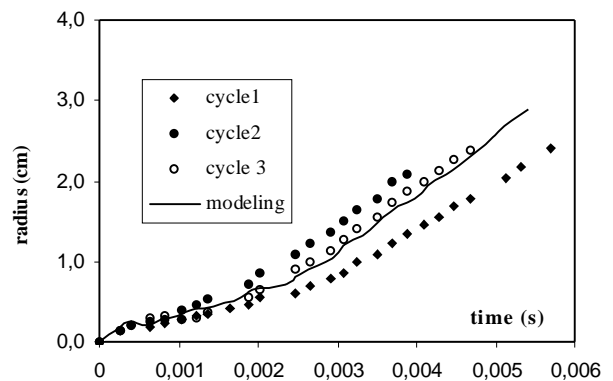

Fig. 2 The evolution of the flame radius

Concerning the dependence on the equivalence ratio of propane-air mixture Figure 3 represents the evolution of the flame radius for different values of this parameter. One can, thus, notice in this figure that the expansion of the flame is not the same if the mixture is poor or rich. Therefore, the model of combustion used has a good sensitivity to the equivalence ratio of the mixture. Figure 4 presents the fractions of the burned and unburned gases. As shown in this figure, all the fresh gases are transformed into the product of combustion or into the burned gases after a *12 ms* duration.
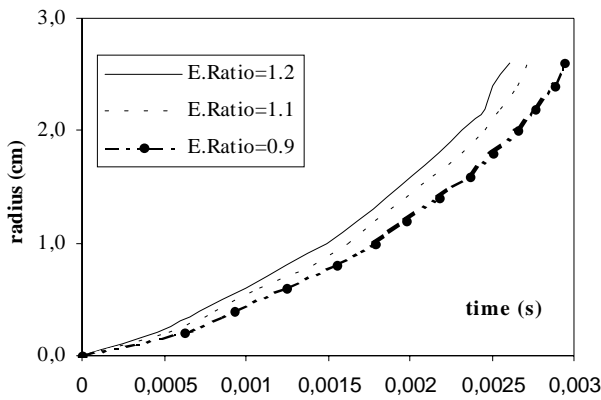
Fig. 3 The effect of equivalence ratio on the flame radius
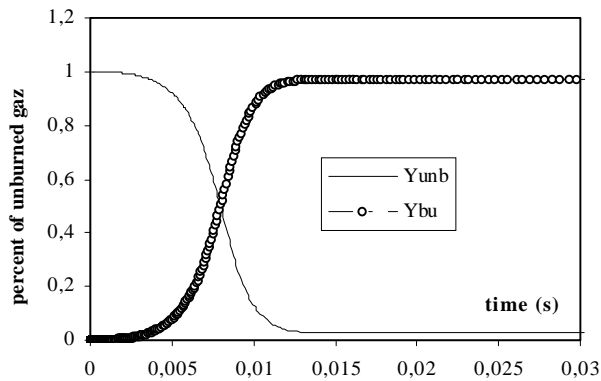

Fig. 4 Burned and unberned fraction as function of time

Our numerical results related to the concentrations of chemical species and temperature in the combustion chamber are represented by the profiles in Figures 5 and 6. This is an important result since it predicts the temperature and concentrations behaviour.
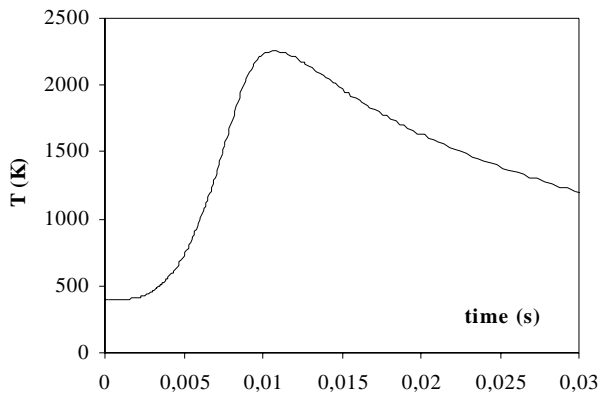

Fig. 5 Mean temperature in the combbustion chamber
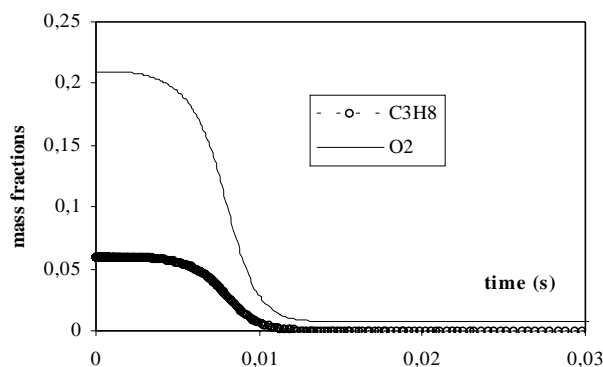

Fig. 6 Mass fractions of the propane and oxygen

Unfortunately, there are no experimental data available which could be used for comparisons. According to these curves, the temperature which dominates in the combustion chamber can reach *2260 K*. This is a completely reasonable temperature. Indeed, the geometry of the combustion chamber and the operating conditions are very similar to those of the spark ignition engine where the temperature can even exceed *2500 K*. According to Figures 4 and 6 the temperature reaches its maximum value at the time when the burned fraction reached *100 %*. As for profiles of reactive species (O_2 and C_3H_8), they are represented by normal evolution curves. In fact, as we can note in Figure 6 propane and oxygen are consumed in a regular way until the end of combustion.

5. CONCLUSION

The combustion model presented in this paper yields encouraging results concerning the pressure evolution in the combustion chamber, the flame expansion and the flame radius sensitivity to the fuel/air equivalence ratio. As for the necessary computing time, it remains relatively moderate. This is due to two mail reasons: the first reason is the regularity of the geometry of the combustion chamber used in this work and the second reason is the simplified chemistry adopted. It would be interesting to attempt to apply these calculations to the case of the spark ignition engine with a complex chemistry (four or five reactions). In this case, we will need to compare these results to those, already obtained using the presumed pdf model coupled to the reduced chemistry of nine reactions [10].

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MODELIRANJE FIZIOKEMIJSKIH POJAVA U EKSPERIMENTU SLIČNOM BENZINSKOM MOTORU

SAŽETAK

Sagorijevanje je vrlo složeno područje budući da istovremeno obuhvaća nekoliko disciplina kao što su prijenos topline, kemija, turbulencija, prijenos mase, itd. U ovom radu pokušali smo modelirati komoru za sagorijevanje s geometrijom koja je slična geometriji motora s paljenjem svjećicom. Početni i rubni uvjeti su dobro poznati. Modeliranje se temelji na pristupu proračuna funkcije gustoće vjerojatnosti (pdf) u slučaju turbulentnog sagorijevanja. Koristili smo jednadžbu prijenosa za funkciju gustoće vjerojatnosti koja je slična slučaju modeliranja fizičkih i kemijskih vrsta. Teorijsko proučavanje ove funkcije je zaista dobro razvijeno, ali je primjena još uvijek prilično ograničena. U ovom radu, funkcija gustoće vjerojatnosti se povezuje s pojednostavljenom kemijom. Ovaj model sagorijevanja uveden je u KIVA II kodu kako bi se simulirao proces sagorijevanja u komori za sagorijevanje, oblika pravokutnika, koja je vrlo slična komori motora s paljenjem svjećicom. Rezultati dobiveni ovim modelom sagorijevanja uspoređuju se s eksperimentom pri različitim uvjetima rada kao što su odnos ekvivalencije propan/zrak, temperatura i pritisak. Konačni rezultati i zaključci su zadovoljavajući. U ovom radu prikazujemo samo rezultate koji se odnose na date uvjete rada uz proučavanje osjetljivosti promjera plamena na odnos ekvivalencije. Vjerujemo da se rezultati ovog rada mogu primijeniti na motor s paljenjem svjećicom.

Ključne riječi: turbulentno sagorijevanje, kemija, funkcija gustoće vjerojatnosti.