A Modelling Approach for the Use of Detailed Kinetics in Closed Premixed Flames

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1 Introduction

The purpose of this paper is to present a new method of introducing complex chemical kinetics into enclosed premixed flame systems such as engines and combustion bombs. The flame structure in these types of systems is complex due to flame instabilities and flow turbulence. Numerical simulations of these systems have made tremendous progress, and realistic three-dimensional results have been obtained of important engineering interest. However, the introduction of complex kinetics in a direct fashion will not be possible in the immediate future. In the present we will present an approach that will allow the use of detailed chemical kinetics, and the method can be made to be used in conjunction with CFD, Computation Fluid Dynamic, models, experimental results or semi-empirical models. In the paper we will present an example where the technique has been applied that involves the use of CH4 as a fuel. The reaction mechanism for CH4 is well described by the GRI, Gas Research Institute, mechanism, and this reaction mechanism is of the size of the new reduced reaction mechanism being developed for practical fuels such as n-octane. Therefore, we are confident that in the near future the present methods can be directly applied to a wide variety of hydrocarbon fuels.

2 Methods of Approach

The model consists of three parts and they will now be described. The first sub-model predicts a fuel burning rate, usually from a detailed pressure curve. The pressure curve is directly related to the fuel consumption rates in the system. Of course, this pressure curve could be obtained from CFD results or experimental measurements, and the fuel consumption rate is related to pressure for enclosed flames, Heywood [1].

The second sub-model consists of a “time” accurate flame code that predicts the detailed burning of the fuel mixture at a given pressure and temperature in the system. This time accurate flame code solves the time-dependent equations of continuity, energy, and species transport that are appropriate for the GRI 3.0 reaction mechanism [2]. It should be mentioned that all fluid properties and reaction rates in this paper have been determined with the use of Ref. [3]. In order to model the influences of the compression of the unburned mixture in the bomb, the flame is formed at the local conditions of pressure and temperature of the unburned mixture.

The final sub-model is used to take the flame products that have been created during the local combustion process, and compress them based on the variation of the pressure curve. In order to obtain a complete simulation during the whole combustion, the flame structure was calculated every 5% of the total increase of pressure during fuel burning. Our model assumes that there is no mixing between the various flame products that have been created during different times of the flame life. This assumption is partially justified by the expansion of the gases, as well as the higher temperatures, which tends to substantially reduce turbulent mixing. The

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present model can be considered as a Lagrangian model of typical fluid particles, as they are compressed and burned in the combustion bomb enclosure.

In order to obtain the time evolution of the species in the GRI mechanism with the pressure variation, we have developed an operator splitting technique to separate the temperature changes due to compression from those due to chemical reactions. The procedure consisted of first solving the reacting transport equations without the spatial terms, and this is equivalent to a homogeneous bomb model. Then the gas mixture was compressed based on the multi-component values of Cp and Cv.

The total amount of NOx can be obtained by assembling the different fluid parcels formed during combustion, and we have to weight those fluid parcels with a weighting function which accounts for the amount of fuel burned at the given time. The weighting function is the rate of fuel burned multiplied by a time step associated with the condition of burning. In general, we feel that the present model captures the essence of NOx production in a combustion model. The predicted total value of NO does neglect the effects of the mixing of products, and it also neglects the effects of fluid stretch caused by turbulence

3 Results

The example given in the paper involves a combustion bomb filled with a stoichiometric mixture of methane, and pressure measurements have been made in a spherical vessel of 20 cm of diameter [4]. The vessel is filled with a stoichimetric mixture of methane and air at 568.5 K and 11.20 atm. The mixture is ignited at time t = 0 at the center of the vessel by a spark, therefore the flame is symmetrical. The experimental pressure results can be used to get the temporal evolution of the burnt mass fraction under reasonable assumptions. For a constant volume and closed vessel the burned and unburned gases can be related to the vessel pressure by the following equation, Heywood [1],

$$\frac{pV}{m} = Y_b R_b \overline{T_b} + (1 - Y_b) R_u T_u$$

where the averaged temperature of the burnt gases is determined from

$$\overline{T_b} = \frac{1}{Y_b} \int_0^{Y_b} T_b \, dY$$

In order to account for the different flame conditions that evolve in the bomb we consider different fluid parcels. These fluid parcels can be considered as Lagrangian parcels and they are compressed and burned themselves and further compressed by the combustion of the other fluid parcels. Each fluid parcel has a different combustion history due to the changing pressure in the closed vessel, and the fluid parcels are characterised by a spherical layer of radius r_{bi}, burned temperature T_{bi} and mass fraction Y_{bi}, as well as the parameters of the fresh mixture: temperature T_{uj} and mass fraction Y_{uj}. The i-index defines the number of the parcel and the j-index refers to the time step, Fig. 1.

In the present simulation twenty one fluid parcels have been created and these parcels are burned every 5% of the total increase of pressure in the constant volume bomb. The specific heat of every parcel is calculated by using the local multicomponent composition and its corresponding local thermodynamic state. The combustion of the fluid parcels is treated locally as a constant pressure process and the combustion products are determined from the flame structure code. Temperature changes in the fresh mixture and each burned parcels due to pressure changes are calculated with the following locally time dependent relations:

$$T_{u,j} = T_{u,j-1} \left(\frac{P_j}{P_{j-1}} \right)^{\frac{\gamma_u - 1}{\gamma_u}} \qquad T_{b,j} = \left(T_{b,j-1} \right) \left(\frac{P_j}{P_{j-1}} \right)^{\frac{\gamma_b - 1}{\gamma_b}}$$

The averaged temperature, $\overline{T_b}$, and the finite rate burnt mass fractions are implicitly solved by an iterative procedure. Based on the pressure measurements, the mass of unburned fuel and the rate of fuel burning can be obtained as shown in Fig. 2.

Typical results of the simulation of the local flame structure are shown in Fig. 3, and this figure contains three axes, which are time, space and temperature, while the contour surface displays the levels of nitrous oxide, NO. In order to obtain a steady flame, a thin transition region is formed between the incoming mixture and the hot mixture. As the flame forms the gases used for the ignition process are convected out of the computation region, and the steep flame zone is captured with the use of an adaptive mesh procedure near the midpoint of the computational zone.

The detailed predictions of temperature and NOx are shown in Figs. 4 for different fluid parcels that evolve during the combustion process in the bomb. These predictions are qualitatively expected, since the first fluid parcels to burn reach the highest temperature and have the largest values of NO. It is clearly seen from the figures that the average values of temperature and species are much different than the local fluid particles, however the final values agree well with the equilibrium prediction.

The experimental results that were used in the present work are shown in Fig. 5, along with pressure predictions from a zero dimensional equilibrium bomb model, as well as a pressure prediction from a 2D model using a commercial CFD code.

It should be pointed out that our commercial CFD code simulation has significant limitations in resolving flame structure due to fine spatial scale of the methane flame. Even a fine mesh of 0.4 mm/cell is not enough to resolve the real flame structure, and this limitation is shown in Fig. 6. Also shown in Fig. 6 is the predicted distribution of fuel mass fraction and temperature in the flame as a function distance at the same conditions in time for the bomb. It is quite clear from Fig. 6 that the flame structure is more than two orders of magnitude thicker for the commercial code, and this can lead to significant errors in some of the pollutant predictions.

4 Conclusions

In the present paper we have applied detailed kinetics to predict the production of pollutants, such as NO, in a combustion bomb. The method developed in the paper can be used simultaneously with CFD results, experimental results, or semi-empirical correlations which predict pressure and fuel burning rate. The method can be used parametric to study variations in stoichiometry. The key components of the model and the conclusions are the following:

- For homogeneous closed systems such as IC engines and combustion bombs, pressure changes lead to good predictions of fuel burning rate, and the burning rate can be used to predict local flame structure.
- A time accurate flame structure code has been developed and used to predict the local flame structure for closed combustion systems.
- The use of the GRI chemical kinetic mechanism for methane leads to good predictions of NO.

Acknowledgements

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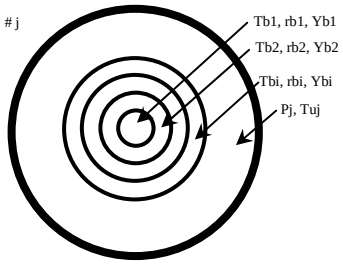


Fig. 1. Scheme of the fluid parcels during combustion in the bomb.

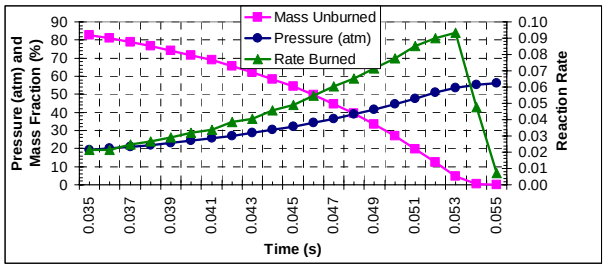


Fig. 2. Combustion bomb graph of pressure, mass fraction of unburnt mixture and fuel burn rate as a function of time. Stoichimetric CH4/Air mixture with initial conditions of 568.5 K and 11.20 atm.

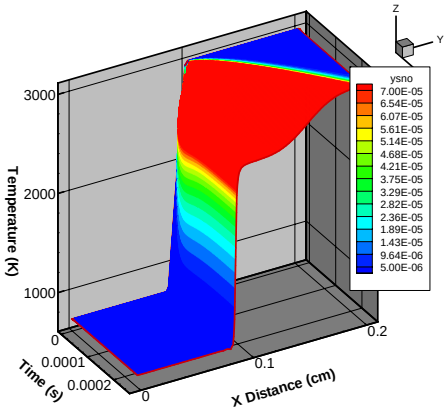
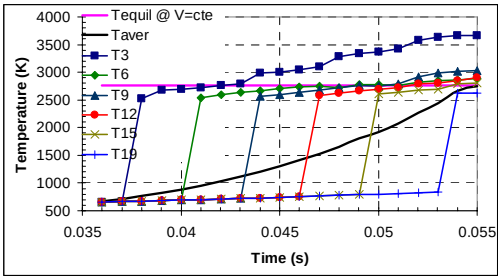


Fig. 3. Time accurate simulation of instantaneous flame structure. Stoichimetric CH4/Air mixture at bomb conditions of 730.6 K and 30.3 atm

a)



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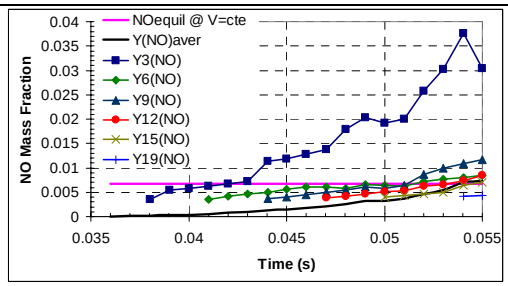

c)

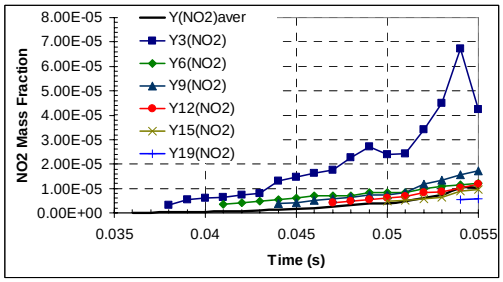

Fig. 4 Variation with time of different particles during combustion a) Temperature, b) Mass fraction of NO and c) Mass fraction of NO2

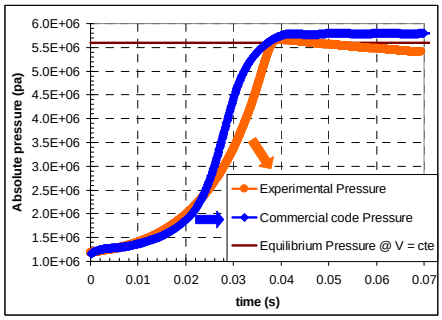

Fig. 5. Temporal evolution of the pressure in the combustion bomb.

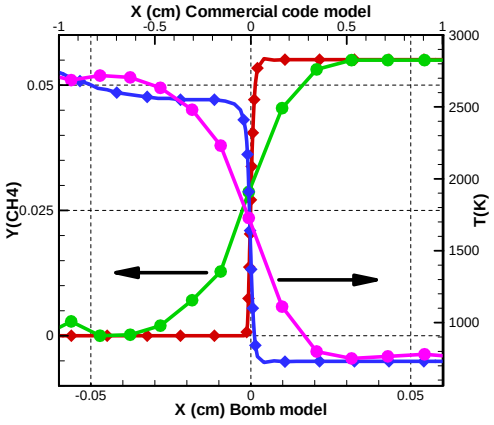

Fig. 6. Spatial distribution of methane and temperature using a multipurpose commercial code (circles) and the combustion bomb model (diamonds).