Modelling of hydrogen flame in perfectly clean combustion regimes using LES-CMC

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Abstract. The LES coupled with the first-order CMC method and detailed chemical mechanism is used for the calculations of hydrogen jet burning in the atmosphere of water vapour and oxygen mixture. The flame is initiated by a spark, then it spreads and propagates through the domain and eventually stabilises as a lifted or attached one. Three dimensional calculations were proceeded with analysis of the flame in the mixture fraction space. The main focus of the paper is on the effect of oxidizer composition on the flame characteristics and stabilization mechanisms. The flame structure during the propagation phase is represented based on the so-called pre-ignition species. Time-averaged results show the flame lift-off distance, shape and radial size. It is found that these factors may be effectively controlled by the amount of water vapour in the co-flowing oxidizer.

1. Introduction
Recently, the hydrogen power engineering has been getting attention, mostly in developing countries, which want to reduce the greenhouse gasses and pollutions emission. Even with disadvantages such the large cost of production or difficult transport and storage the hydrogen is considered as an attractive fuel option. This is because of its tendency to zero emission if combustion is carried out in pure oxygen. The oxy-combustion technology [1] is also currently one of the most important direction in the field of searching for clean combustion technologies. It assumes the removal of nitrogen from oxidizer and the use of oxygen mixed with recycled flue gases to enhance the combustion process.

In this paper, the analysis of oxy-combustion of pure hydrogen jet is presented. We proposed the environmental friendly conditions in which the mixture composed of oxygen and water vapour is used as the co-flowing oxidizer. Hence the hydrogen burning process yields only the water vapour. The goal of the study was to find out how to control the process of flame stabilisation through the composition of the oxidizing atmosphere. We focused on the flame shape and radial size. The effect of the presence of the water vapour on ignition and extinction phenomena in counterflow configuration was studied experimentally and numerically in [2]. It was shown that for the water mass fraction above 20% the flames were harder to ignite and easier to extinguish. In the recent work devoted to self-ignition process in similar atmosphere [3] we found that the flames ignited only below 50% of water vapour in the oxidizer stream. Additionally, an interesting finding was that the predicted flame lift-off distance directly depended on the co-flow parameters and applied chemical kinetics [4].

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| Item                  | Fuel jet | Co-flow |
|----------------------|----------|---------|
| Diameter ($D$) [mm]  | 4.57     | -       |
| Velocity [m/s]       | 107      | 16.5    |
| Temperature [K]      | 305      | 1045    |
| $Y_{H_2}$ [-]        | 1        | -       |
| $Y_{H_2O}$ [-]       | -        | 0.2-0.85|
| $Y_{O_2}$ [-]        | -        | 1-2$Y_{H_2O}$ |

2. Mathematical model

2.1. LES-CMC equations

The ignition, propagation and stabilisation of the flame are strongly unsteady phenomena, whose correct prediction requires the use of accurate numerical methods and combustion models. In this research, the computations were carried out applying the Large Eddy Simulation (LES) approach [5], enabling thorough analysis of the flow field, and an advanced Conditional Moment Closure (CMC) method [6] that attempts to close the turbulence-chemistry interactions. The LES-CMC equations are derived applying the density-weighted conditional filtering operation to the transport equations for the reactive scalars (species mass fraction and enthalpy) [7]. For the non-premixed combustion the conditioning is done on the quantity called mixture fraction ($0 \leq \xi \leq 1$, $\xi = 0 \rightarrow$ oxidizer, $\xi = 1 \rightarrow$ fuel). Hence, the CMC model is defined in the four dimensional space, physical space $\vec{x}$ and $\xi$-space, and its application along with the detailed chemical mechanism is very expensive from the computational point of view. Typically, in order to reduce the computational costs, without reducing the accuracy of the solution, dual mesh approach is used. On the LES mesh the physical flow field is computed and the much coarser mesh is used to resolved the CMC equations. In the present work the 1st order closure is applied where the conditional fluctuations are expected to be small compared to the unconditional fluctuations and therefore they might be neglected. In the oxy-combustion modelling the LES-CMC approach was used by Garmory and Mastorakos [8] and Kim et al. [9]. Both papers showed that the CMC predictions with 1st order closure enable capturing complex combustion phenomena.

2.2. Numerical set-up

The solver used in the simulations is based on the low Mach number approach and the half-staggered arrangements for the pressure nodes [10]. The Navier-Stokes and continuity equations are discretized using 6th order compact difference method and the 5th order WENO scheme is applied for the mixture fraction. The time integration is performed with a predictor-corrector approach (second-order Adams-Bashforth/Adams-Moulton methods). The operator splitting approach is applied to the CMC equations which means that the transport in physical space, transport in mixture fraction space and chemistry are solved separately. For the chemical reactions modelling we used detailed mechanism of Li et al. [11] (13 species, 25 reactions) and the CHEMKIN interpreter. The numerical code was verified in previous LES-CMC studies [12] as well as it was used in other works concentrating on reacting and non-reacting flows [13, 14].

The flame studied in this paper is a turbulent hydrogen jet flame issuing into a co-flow of O$_2$/H$_2$O mixture. The present configuration is similar to the so-called Cabra flame [15]. In the present case we modified the fuel and oxidizer compositions. Also the co-flow velocity is higher than in case of [15]. It was motivated by the fact that for similar conditions, the observed flame
lift-off distance was about ten nozzle diameters [3]. We consider various oxidizer compositions that differ in mass fractions of water vapour ($Y_{H_2O}$). Table 1 summarizes the boundary conditions for the simulations. The computational domain extends axially $30D$ downstream from the jet inlet ($y$ coordinates the stream axis) and radially up to $14D$. The LES grid consists of $128 \times 160 \times 128$ nodes stretched smoothly in the axial and radial directions toward the jet region. The CMC mesh comprising of $15 \times 80 \times 15$ cells is uniform. The mesh in mixture fraction space has 51 nodes compacted around the stoichiometric value. The most reactive mixture fraction ($\xi_{MR}$) as a function of $Y_{H_2O}$ was determined in [4].

![Figure 1.](image-url) 0D-CMC results: the temperature and species mass fraction profiles for various oxidizer compositions.

3. Results

3.1. Analysis of zero-dimensional CMC results

First we discuss the quantitative description of the oxy-hydrogen flames and analyse the results of zero-dimensional calculations of CMC equations (OD-CMC). In 0D model the effect of convective and diffusive transport in physical space is not considered. Figure 1 gives the profiles of temperature, fuel and radicals mass fractions in mixture fraction space for different oxidizer compositions. Initially the solution corresponding to inert mixing between the fuel and oxidizer is assumed. It is clear that due to differences in oxidizer composition the stoichiometric ($\xi_{ST}$) mixture fractions are also strongly different. As the $H_2O$ mass fraction increases the maximum temperature is lower and shifts towards leaner side around $\xi = \xi_{ST}$. Similarly behaves the peak value of the $Y_{H_2O}$. The $HO_2$ and OH radicals are the key intermediate species playing...
the important role in self-ignition process. It is known that during the ignition phase, there is a substantial growth in the OH mass fraction. However prior to generation of the OH, the HO$_2$ radical appears in the locations where $\xi = \xi_{MR}$. Hence this species is considered as a self-ignition precursor. As combustion proceeds the peak of HO$_2$ travels across the entire $\xi$-space (note the second local maximum in Fig 1c) and large amount of the OH is simultaneously formed. Figure 1d reveals that $Y_{OH}$ is about four order of magnitude larger compared to the HO$_2$ mass fraction. Finally, note that the radical concentration significantly depends on the $Y_{H_2O}$ in the oxidizer stream.

3.2. Turbulent hydrogen flame in O$_2$/H$_2$O co-flow

Full three dimensional CMC calculations of forced ignition are started from a developed flow field. The flame is initiated by placing the OD-CMC solution presented in Fig. 1 in the CMC cells belonging to a sphere with the diameter 5mm and holding for a time period $\Delta t_{spark} = 0.1$ms. In order to ensure the successful ignition the spark overlaps the shear layer region where the stoichiometric and most reactive composition can be found. After the flame develops the statistics are collected over 35ms.

3.2.1. Flame structure

The process of ignition and flame propagation for the case with $Y_{H_2O} = 0.6$ is presented in Fig. 2 showing the results in a central plane of the computational domain. The temporal evolution of HO$_2$ mass fraction, as it is generated just before the reaction zone, is used to illustrate the flame front propagation. As we can observe, the heat released as a result of proceeding chemical reactions does not extend over the border of pre-ignition species HO$_2$. Firstly, the burning gases are convected downstream and the flame grows in the radial direction. As mentioned, the first reactions occur at the most reactive conditions (red line). These self-ignition spots cause subsequently the ignition of the richer mixture. Shortly after the flame starts to expand along the stoichiometric composition (blue line). At the next time instances it moves towards the outlet plane faster than in the upstream direction. Finally, the reaction front propagates towards the jet inlet. Worth noticing is the process of consumption of the HO$_2$ radical during the ignition process. At the end of the propagation phase the high values of $Y_{HO_2}$ are found only in the region close to the flame stabilization point. This structure of the flame is consistent with previous findings [12].
Figure 3. Contours of instantaneous and time averaged temperature and the fuel mass fraction for different co-flow compositions.

Figure 4. Radial distribution of time-averaged temperature and species mass fraction at various axial positions.
3.2.2. Effect of the co-flow composition

For the cases with $Y_{\text{H}_2\text{O}} \leq 0.6$ the flames stabilised very close to the inlet, the flame lift-off distance was equal to $L_f = 1D$. With a higher $Y_{\text{H}_2\text{O}}$ the influence of the co-flow composition was much more pronounced and the flames stabilised further downstream. The $L_f$ changed in strongly non-linear manner and for $Y_{\text{H}_2\text{O}} = 0.85$ it was approximately equal to $7D$. The flame position for various cases is nicely visualised in Fig. 3 presenting the contours of instantaneous (left side) and mean (right side) temperature along with the fuel mass fraction fields. The effect of water vapour addition manifests in changes of size and shape of the flames. Increasing $Y_{\text{H}_2\text{O}}$ results in smoother and narrower flames. In Fig. 4 the radial profiles of time-averaged temperature, H$_2$O, HO$_2$ and OH mass fraction at various axial locations are compared for different oxidizer compositions. Selected positions were marked in the contour plots in Fig. 2. The profiles show that depending on $Y_{\text{H}_2\text{O}}$ the ignition zone is located at different radial positions. In principle, the temperature profile at $y/D=10$ reveals that the flame extends radially up to approximately $2.2D$ for $Y_{\text{H}_2\text{O}} = 0.6$, whereas for $Y_{\text{H}_2\text{O}} = 0.4$ it covers the region of $1.9D$ despite the flames positions are similar for both cases. Regarding the HO$_2$ mass fraction, Fig. 4c shows that after the flame stabilizes only the small amount of this radical occur in the narrow region near the flame stabilization point and further downstream close to the axis, while the concentration of OH remains at the significant level (Fig. 4d). The peaks of $Y_{\text{OH}}$ are mainly found in the high temperature region.

4. Conclusions

The LES-CMC method has been applied to analyse hydrogen flame in oxy-combustion regimes. In order to properly reflect the phenomena like ignition, flame propagation and stabilization process the detailed chemical kinetics was involved. The simple spatial configuration used in the study allowed us to formulate the general findings. The problem analysed constitutes the new configuration in which the perfectly clean conditions are ensured. The only product of the combustion process, the water vapour, can be recycled and used for the controlling of the combustion process. This idea seems to be tempting in the context of the practical applications. The performed investigation showed that the flames size and shape is sensitive to H$_2$O mass fraction in the co-flowing oxidizer. However this dependency was not so pronounced compared to the effect on the flame lift-off distance.

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