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# LARGE EDDY SIMULATIONS OF HYDROGEN AUTO-IGNITION IN A TURBULENT CO-FLOW OF HEATED AIR WITH CONDITIONAL MOMENT CLOSURE

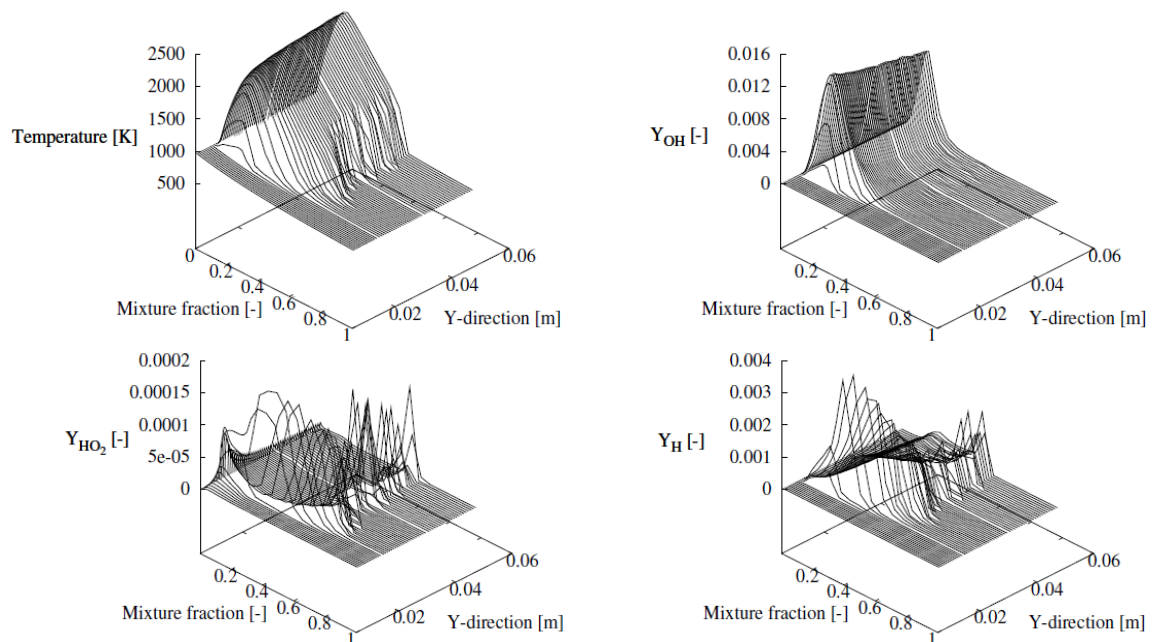
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Auto-ignition in turbulent non-premixed flows has significant practical applications and quite subtle fundamental aspects [1]. In numerical studies of auto-ignition phenomena, turbulence and unsteady chemistry must be modelled accurately. In order to obtain accurate simulation results for the turbulence, Large-Eddy Simulation (LES) approach has recently received attention, while for the turbulence-chemistry interactions, the Conditional Moment Closure (CMC) can be used.

Large-Eddy Simulation (LES) results with the first-order Conditional Moment Closure (CMC) are presented for a hydrogen jet, diluted with nitrogen, in a turbulent co-flowing hot air stream [2]. The fuel, with mass fractions  $Y(\text{H}_2) = 0.13$  and  $Y(\text{N}_2) = 0.87$ , is injected into a heated air co-flow through a 2.25mm internal diameter pipe at ambient pressure. In the experiments, air velocities ( $u_{\text{cf}}$ ) up to 35m/s, with air temperature ( $T_{\text{cf}}$ ) up to 1015K, have been applied. The fuel velocity ranged from 20 to 120m/s, with fuel temperature ( $T_{\text{fuel}}$ ) between 650K and 930K. For the given composition, the stoichiometric mixture fraction  $\xi_{\text{ST}}$  is 0.184. We focus on the case where  $T_{\text{fuel}} = 691\text{K}$  and  $T_{\text{cf}} = 935, 945, 960, 980\text{K}$ . The fuel velocity is 120m/s while the co-flow velocity ranges from 20 to 35m/s.



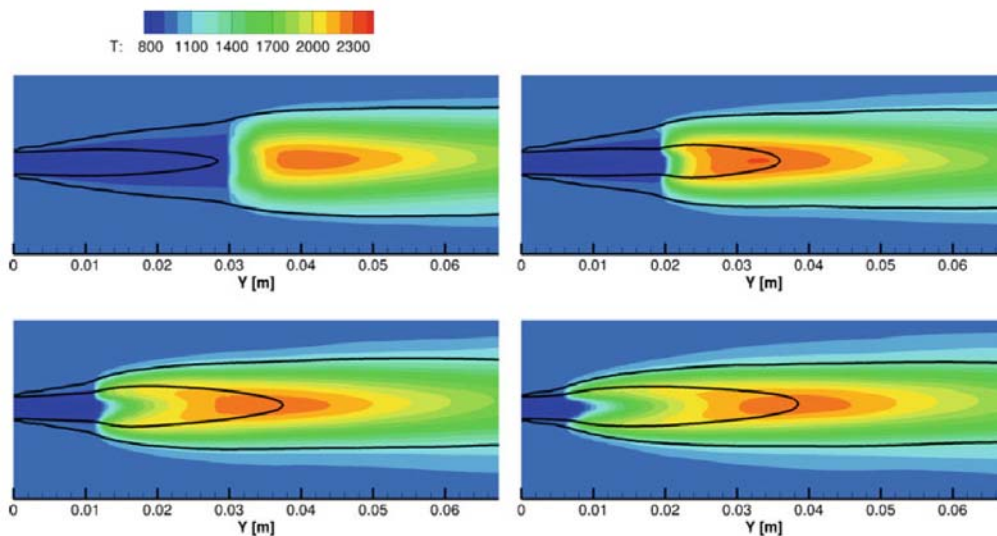
**Figure 1:** Evolution in the axial direction of the time averaged conditional temperature, OH, HO<sub>2</sub> and H mass fractions as a function of mixture fraction (mechanism of [3],  $T_{\text{cf}} = 960\text{K}$  and  $u_{\text{cf}} = 26\text{m/s}$ ).

The fuel mixes with the air co-flow, ignites, and forms a lifted-like flame. The evolution of the time averaged conditional temperature, OH, HO<sub>2</sub> and H mass fractions, from inert to burning conditions in mixture fraction space, is discussed (Figure 1). Each line in Fig. 1 corresponds to one CMC cell. Time averaging for the LES and CMC results was performed with data collected over 10ms. The flame

structure evolves gradually from the inert (“frozen”) distribution at the inlet to fully “burning” distribution. At first, a small amount of fuel and oxygen is consumed and temperature and OH mass fraction increase only by a small amount, while intermediate species ( $\text{HO}_2$ ) increase faster. The maximum temperature (2400K) and OH mass fraction (0.0136) are reached near stoichiometry. The region of high OH concentration corresponds to the high temperature region. The creation of H first occurs at the lean side and, when combustion proceeds, it slowly shifts to the rich mixture fractions.

Auto-ignition of hydrogen is characterized by destruction of the pre-ignition species ( $\text{HO}_2$ ) and rapid generation of OH [1]. Consistently, just upstream of the auto-ignition point (i.e. at the flame base), there is a build-up of  $\text{HO}_2$  radical. Build-up of  $\text{HO}_2$  ahead of the flame edge, prior to creation of H and OH, shows that base of the flame is stabilized by auto-ignition. Therefore  $\text{HO}_2$  is a key intermediate species. The other species have low concentrations at the ignition point. In the statistically steady-state condition of the flow, reaction is balanced by convection at the flame base, confirming that auto-ignition is the stabilization mechanism, with scalar dissipation rate and diffusion in physical space being relatively unimportant there.

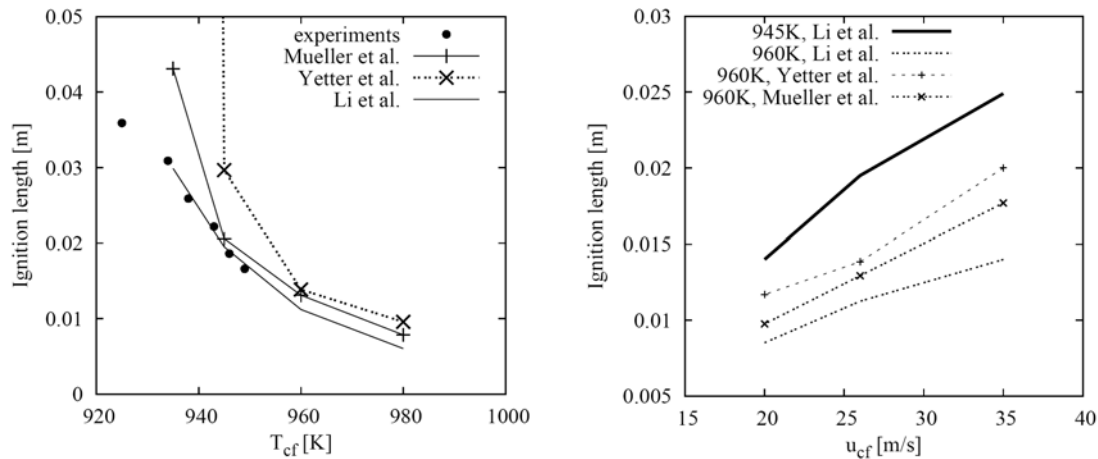
In order to show the sensitivity of the system to the co-flow temperature, four simulations were carried out with different co-flow temperatures: 935 K, 945 K, 960 K and 980 K and mechanism of [3] (Figure 2). At low temperature (935K), the ignition kernels are formed at a certain distance from the nozzle and convected downstream. This is consistent with experimental observations where flame kernels extinguish and re-ignite continuously (random spots regime). Further increase in the co-flow temperature (960K, 980K), results in flashback, where flame kernels ignite at locations downstream and stabilize closer to the nozzle where the scalar dissipation rate is high. In this case, the temperature is high enough to allow chemistry to develop and overcome the influence of the scalar dissipation rate and convection.



**Figure 2:** Contours of the time averaged temperature in a symmetry plane with different co-flow temperatures: 935 K (*top left*), 945 K (*top right*), 960 K (*down left*) and 980 K (*down right*). Inner isoline: stoichiometric mixture fraction; outer isoline: most reactive mixture fraction.

Figure 3 shows comparison of auto-ignition length from experiments (shifted by 60K) and present calculations for  $u_{cf} = 26\text{m/s}$ . The trends in the experimental observations are in general well reproduced: the auto-ignition length decreases with an increase in co-flow temperature and increases with increase in co-flow velocity. The discrepancy can be attributed to uncertainties in the chemical mechanism,

resolution in physical space (CFD and CMC mesh) and in the determination of the temperature in the experiment. The random experimental error associated with  $T_{cf}$ ,  $T_{fuel}$  and  $L_{ign}$  was  $\pm 4\%$ . However, the results are in qualitative agreement with experiments.



**Figure 3:** Comparison of auto-ignition length from experiments (shifted by 60K) and present calculations (*left*). Influence of the co-flow velocity on the flame lift-off height (*right*).

The flame is stabilized by auto-ignition and therefore sensitive to chemical kinetics. At relatively low temperatures, where there is more uncertainty in the reaction rate constants, the choice of the detailed chemical mechanism can be important. Crucial are intermediates and slow reactions, which increase the pool of reactants. Therefore, we investigate the low temperature non-premixed auto-ignition behavior with different chemical mechanisms: Li et al. [3], Mueller et al. [4] and Yetter et al. [5]. With increasing co-flow temperature, the differences between the mechanisms considered diminish (Figure 3). It is apparent that each mechanism requires a different co-flow temperature in order to achieve the same lift-off height. All mechanisms perform in a similar way following ignition. For mechanism of [5] no-ignition was observed for the co-flow temperature 935K.

## References

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