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ANALYSIS OF AUTO-IGNITION OF TURBULENT HYDROGEN JETS WITH DIFFERENT DETAILED REACTION MECHANISMS

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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, the Large-Eddy Simulation (LES) approach has recently received attention, while for the turbulence-chemistry interaction, the Conditional Moment Closure (CMC) can be used.

Large-Eddy Simulation (LES) results with first-order Conditional Moment Closure (CMC) are presented for a hydrogen jet, diluted with nitrogen, issuing into a turbulent co-flowing hot air stream [2]. We focus here 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. The LES are performed using the VUB in-house CFD code [3], while an in-house code developed in Cambridge [4] is used to solve CMC equations. The full three-dimensional CMC equations are solved on a coarser grid than the LES. The solution domain ($67.5\text{mm} \times 25\text{mm} \times 25\text{mm}$) contains $192 \times 48 \times 48$ CFD cells and we compare to the results obtained on a CFD mesh with $192 \times 48 \times 48$ cells. The basic CMC mesh, covering the same physical space domain as the CFD mesh, consists of $80 \times 8 \times 8$ cells. The mixture fraction space is discretized into 50 bins, clustered at the lean side in mixture fraction space. The inflow turbulence generator is based on a digital filter [5]. The chosen length and time scales are 4.5mm and 1ms, with turbulence intensity 12.5% [2].

Focus is on assessing the impact of different detailed chemical mechanisms on the auto-ignition predictions. At relatively low temperatures, where there is more uncertainty in the reaction rate constants, the choice of the detailed chemical mechanism can be of great importance. Crucial are intermediate 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. [6], Mueller et al. [7] and Yetter et al. [8]. The Li mechanism results in earlier auto-ignition and hence gives shorter lift-off heights than the Mueller and Yetter mechanisms over the entire test range.

The fuel mixes with the air co-flow, ignites, and forms a lifted-like flame. The evolution of HO_2 and OH from inert to burning conditions in mixture fraction space is discussed (Figure 1). Radially averaged and time averaged conditional species mass fractions are shown in Fig. 1. Each line in Fig. 1 corresponds to one CMC cell. Time averaging for the LES and CMC results was performed with data being collected over 10ms. During the auto-ignition process, H_2 and O_2 are also slowly consumed while the concentrations of H, OH, H_2O increase at the ignition location. The highest values of the H radical are found in the rich region, after ignition, while H_2O corresponds to the high temperature region. The hot regions, corresponding to high OH mass fraction, are convected downstream out of the domain. Auto-ignition of hydrogen is characterized by destruction of the pre-ignition species (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 HO_2 radical. Build-up of 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 HO_2 is a key intermediate species. The other species have low concentration at the ignition point.

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. With increasing co-flow temperature, the differences between the mechanisms considered diminish. In the statistically steady-state condition of the flow, reaction is balanced by convection at the flame base, showing that auto-ignition is the stabilization mechanism, with scalar dissipation rate and diffusion in physical space being relatively unimportant there.

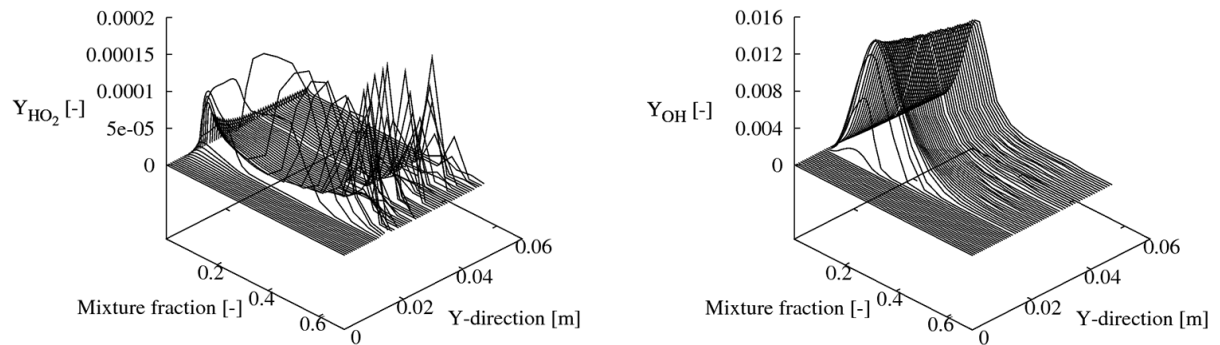


Figure 1: Evolution in the axial direction of time averaged conditional HO_2 and OH mass fractions as a function of mixture fraction (co-flow temperature: 960K, fuel temperature: 691K, mechanism of [6]).

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