Numerical study of the three-folded effect of steam dilution on hydrogen ignition in a RCM with detailed kinetics

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Introduction

Moderate or Intense Low-oxygen Dilution (MILD) regime is a promising candidate for combustion future, since it meets the nowadays requested criteria for fuel flexibility, efficiency and inhibition of pollutant formation, such as NOx and soot [1]. This regime is obtained through preheating of the oxidizer flow, and a specific internal aerodynamic of the burner in conjunction with high velocity inlet, which is responsible for flue gases recirculation and turbulent mixing [2]. This results in a localized reduction of O_2, and a strongly diluted fuel mixture, leading to delayed ignition and to a homogeneous as well as distributed reaction zone. In the last years, hydrogen has attracted great attention as Energy Carrier for its storage opportunity and the absence of the pollutant (CO_2, SO_x and UHC) among its products. Its importance will increase within the next years [3]. Its usage as an enrichment for methane, has been investigated for MILD condition in a Jet in hot coflow burner [4, 5]. In particular, A. Parente et al. [4] concluded that the hydrogen addition leads to complex oxidation behaviors, which requests detailed kinetics for a full phenomenon description. In fact, MILD combustion is characterized by a low Damköhler numbers regime, and the presence of a relevant amount of diluent make the mixing and the chemistry time scales overlap. For this reason, the kinetic mechanism, which were validated using conventional combustion data, usually accomplish a non-accurate estimation for these, conditions [6]. According to Koroglu et al. [7], diluents like CO_2, and H_2O exert a three-folded effect on the system, namely thermal (like N_2 does), indirect and direct participation to single kinetic steps, as a collider and a reactant, respectively. However, we are far away from having a clear insight into the role of such species in MILD combustion, especially for Ignition delay time, one of the most important kinetic parameters in MILD combustion, along with the maximum temperature [1]. Different experimental studies faced the *H₂/Oxidizer/Steam* mixtures combustion in canonical reactors, namely: Wang et al. [8] and Vasu et al. [9] using a shock tube reactor, while Das et al. [10], and Donohoe et al. [11]. Recently, Shareh et al. [12] studied the three-folded effect of CO_2 dilution on methane flame speed for oxyfule combustion performing a fake species analysis (FSA). The aim of this work is to understand what is the steam dilution driving effect, for hydrogen ignition using the latter FSA approach for high Temperatures.

Experimental data

The experimental data, which guide this numerical study come from A. K. Das et al. [10], who studied the ignition delay time of a stoichiometric mixture of hydrogen, highly diluted in nitrogen and steam (H₂/ O₂ /diluent = 0.125/0.625/0.8125), in a Rapid compression machine. The water content into the starting mixture is varied from 0% up to 40%, for three different compressed pressure values, namely, 10, 30, 70 bar. The end of compression temperature varies between 900- 1050 K, which are generally higher than the auto-ignition temperature of the mixture, so relevant for MILD oxidation.

Fake Species Analysis

The simulations were carried out using the 0-D reactors solver in OpenSMOKE++ [13]. The RCM is numerically approximated through a Batch reactor adopting the adiabatic core hypothesis, where the compression stroke and the heat losses after compression are taken in account specifying a user-defined volume history. Different kinetic mechanisms' predictions were compared with the experimental data, and the Aramco2.0 [14], was found to show the best predictions. Figure 1shows the results obtained for a pressure of 70 bar, using the aforementioned mixtures. Even though, the mechanism shows good agreement with the experimental set in absence of water vapor it clearly overestimates the ignition delay times for higher steam contents.
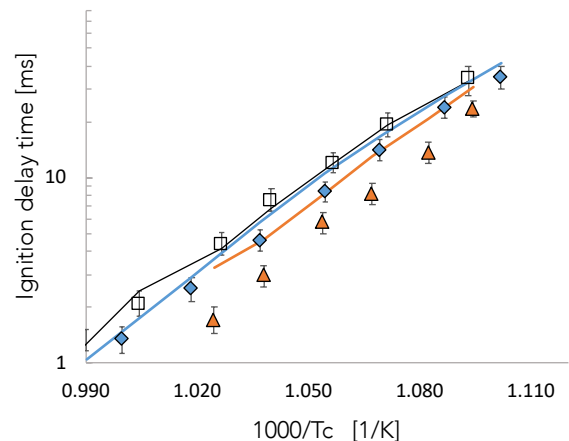

Figure 1: RCM Ignition delay time for H2/H2O in a RCM. Three different dilution degrees are adopted: 0% (□), 10% (◇), and 40%(△). Experimental data from [10].

In order to better understand on which kinetic parameters to act for mechanism improvements 3 fake species where added to the mechanisms for isolating the three different effects of steam on the oxidation process. Their properties are listed in Table 1.

Table 1: Fake species properties for FSA.

Species	Thermal Properties	Indirect (collider)	Direct (reactant)	Isolated effect
A	H_2O	-	-	*Thermal*
B	N_2	$(H_2O)_I$	-	*3rd Body*
D	H_2O	$(H_2O)_I$	-	*Both*
H_2O	H_2O	$(H_2O)_I$	*Yes*	-

The great advantage of FSA is the capability of highlighting differences between the way different isolated effects impact on the model's outputs. Figure 2 displays the results of the FSA for one combination of steam dilution and pressure. The model predictions show that when water doesn't participate to any reaction the ignition is delayed. What is actually speeding up the chemistry is the balance with the reactivity of the diluent, this appears clear when looking at the difference between H_2O and the species D, which embodies both thermal and third body characteristics of steam. From here, the influence of direct participation to reactions can be deduced, and it's nearly null. The picture clearly shows that the fake species B, which only act as a collider through third body reactions, is capable of reproducing the same ignition delay time of the mixture where real water is present. For all the simulations, similar ignition delay time behaviours were individuated, leading to the conclusion that the driving force for hydrogen ignition in diluted conditions is the participation of water to re- actions as a collider. In fact, its enhanced third body efficiencies strengthen the competition between the main kinetic path $H_2 \rightarrow OH \rightarrow H_2O$, and the alternative $H_2 \rightarrow HO_2 \rightarrow H_2O_2 \rightarrow OH \rightarrow H_2O$, involving hydroperoxy radical and hydrogen peroxide. The latter path is governed by third body reactions.
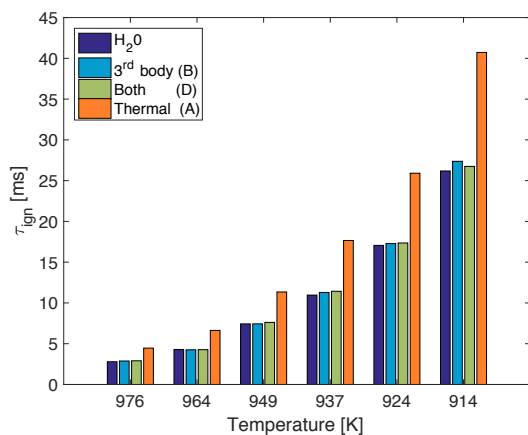

Figure 2: Fake Species analysis for Ignition delay time of H2/H2O diluted mixtures in a RCM, H2O (%)= 40 and P=70 bar.

Conclusions

The third body efficiency of steam in different reactions was found to drive the ignition behavior of hydrogen in steam diluted conditions, relevant for MILD combustion. These observations give a hint for mechanisms improvements, in particular it would be interesting

to optimize the mechanism's performarce trying to act only on steam third body efficiencies of the sensitive reactions.

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