Analysis of hydrogen non-premixed auto-ignition in mixture fraction space using detailed mechanisms

I. Stanković*[1], A. Triantafyllidis[2], E. Mastorakos[2], B. Merci[1,3]
[1]*Ghent University - UGent, Belgium;* [2]*Cambridge University, UK*
[3]*Postdoctoral Fellow of the Fund of Scientific Research - Flanders (Belgium) (FWO-Vlaanderen)*
*Ivana.Stankovic@UGent.be

1 Introduction

Auto-ignition is a problem of great fundamental importance and practical interest. In many combustion devices it involves complex interaction between chemistry and turbulence. Our research objective is the performance of Large-Eddy Simulation (LES) with first order Conditional Moment Closure (CMC) of the test case experimentally studied by Markides and Mastorakos [1]. The experiment concerns auto-ignition of hydrogen, diluted with nitrogen, in a co-flow of heated air. In order to better understand auto-ignition phenomena, use of detailed chemical mechanisms is important. Therefore, we focus here on the low temperature non-premixed auto-ignition behaviour of different chemical mechanisms: Li et al [2], O'Conaire et al [3], Konnov [4] and Yetter et al [5]. The temperature of the air stream is much higher than temperature of fuel stream. The effect of the co-flow temperature, conditional scalar dissipation rate and resolution in mixture fraction space is investigated. With respect to the conditional scalar dissipation rate, we discuss the Amplitude Mapping Closure (AMC) model [6] with imposed maximal scalar dissipation rate (at mixture fraction equal 0.5). Combustion is only considered at atmospheric pressure.

2 Equations

The CMC transport equations concern the conditional mean of reactive scalars, Q. Conditioning is performed on mixture fraction: $Q(\eta; x, t) \equiv \langle Y(x,t) \mid \xi(x,t) = \eta \rangle \equiv \langle Y(x,t) \mid \eta \rangle$, at location x and time t, with η the sample space variable for the mixture fraction. The governing equations for conditional moment closure of species and temperature are:

$$\frac{\partial Q}{\partial t} = \langle N \mid \eta \rangle \frac{\partial^2 Q}{\partial \eta^2} + \langle W \mid \eta \rangle \tag{1}$$

$$\frac{\partial Q_T}{\partial t} = \langle N \mid \eta \rangle \left[\frac{1}{c_{p_\eta}} \left(\frac{\partial c_{p_\eta}}{\partial \eta} + \sum_{i=1}^{n} c_{p,i_\eta} \frac{\partial Q_i}{\partial \eta} \right) \frac{\partial Q_T}{\partial \eta} + \frac{\partial^2 Q_T}{\partial \eta^2} \right] - \frac{1}{c_{p_\eta}} \left\langle \sum_{i=1}^{n} h_i W_i \middle| \eta \right\rangle \tag{2}$$

The source terms are given by: $\langle W_i \mid \eta \rangle \approx W_i(Q, Q_T)$, where W_i is coming from the chemical mechanism in which n species appear. Conditional scalar dissipation rate is modeled with Amplitude Mapping Closure model (AMC). The AMC model is parametrized on its maximum value at $\eta = 0.5$. The expression for conditional scalar dissipation rate is:

$$\langle N \mid \eta \rangle = \frac{G(\eta)}{\int_0^1 G(\eta) \widetilde{P}(\eta) d\eta} N_{max}, \quad G(\eta) = exp(-2(erf^{-1}(2\eta - 1))^2) \tag{3}$$

The CMC PDEs system is stiff due to the chemical reactions. The system size depends on the number of nodes in mixture fraction space and the number of scalars. The PDEs are transferred into a number of ODEs using Method of Lines. In the present work, the VODPK solver is used, based on a linear multistep method using the Backward Differentiation Formula (BDF).

3 Results and conclusions

In the experimental set-up of Markides et al [1], the hydrogen mass fraction (Y_{H_2}) is 0.13, while Y_{N_2} is 0.87. The stoichiometric mixture fraction (Z_{ST}) is 0.184. Air temperatures up to 1015K have been achieved, with fuel temperature range between 650K and 930K. Because of the available experimental data, we focus on the case $T_{fuel} = 691K$, and consider a range of air temperatures. Number of nodes used in the simulations is 101 (IGRID). The results are compared for four different chemical mechanisms. Figure 1 shows OH mass fraction evolution for the studied chemical mechanisms. The Konnov mechanism is the fastest and yields the highest OH mass fractions, while the Yetter mechanism is the slowest with the lower OH mass fractions. Maximal scalar dissipation rate in the AMC model is varied as follows: N_{max} =0.1, 0.5, 1.0, 5.0, 10.0, 20.0, 30.0, 40.0, 50.0, 200.0 s^{-1}. For inhomogeneous mixtures, different auto-ignition criteria can be defined. In this study, we compare two auto-ignition criteria: 1. increase of temperature of 1% over the nominal co-flow temperature [7]; 2. mass fraction of OH reaches 2×10^{-4} [8]. Figure 2 shows the effect of N_{max} for the two criteria. Co-flow temperatures, $T_{cf} = 945, 960, 985, 994, 1003, 1009, 1016, 1100K$ are used. The influence of T_{cf} on the auto-ignition delay time (τ_{ign}) is shown in Figure 3. With increase of temperature, ignition delay time becomes shorter, and ignition moves towards the rich mixture fractions.

As shown in Figure 4, ignition occurs at the lean side. Figure 4 shows the effect of the clustering of the nodes in η-space on the temperature evolution for the mechanism of Li et al [2]. Under-resolved lean side of mixture fraction space leads to an inaccurate prediction of ignition delay times (Figure 5).

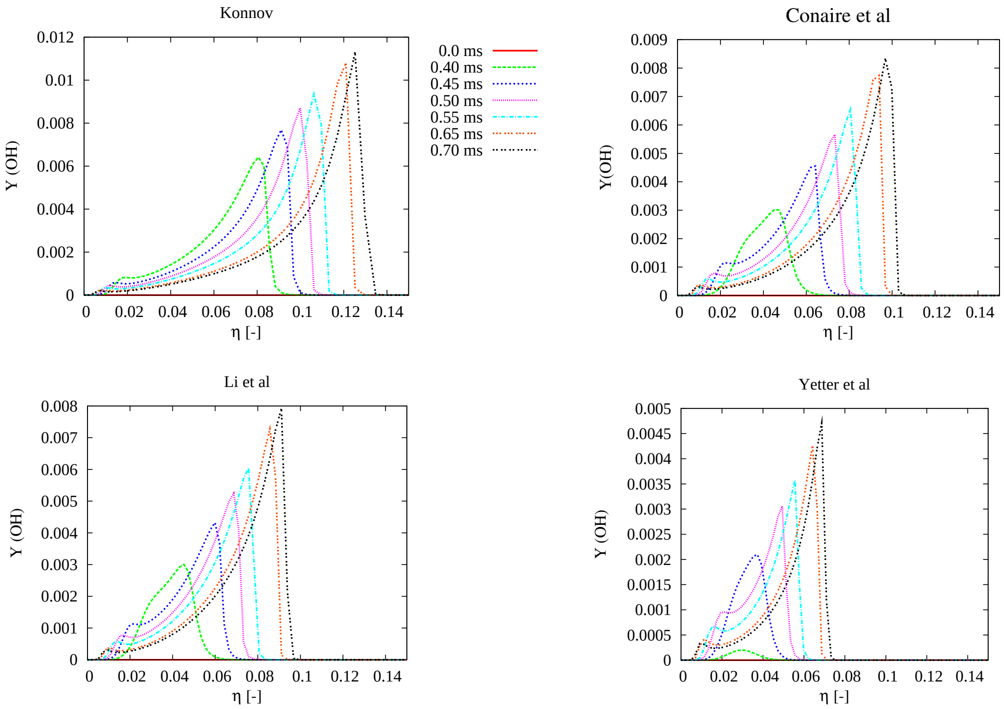

Figure 1: OH mass fraction evolution during initial stages of ignition ($T_{cf} = 1009K$ and $N_{max} = 0.1s^{-1}$)

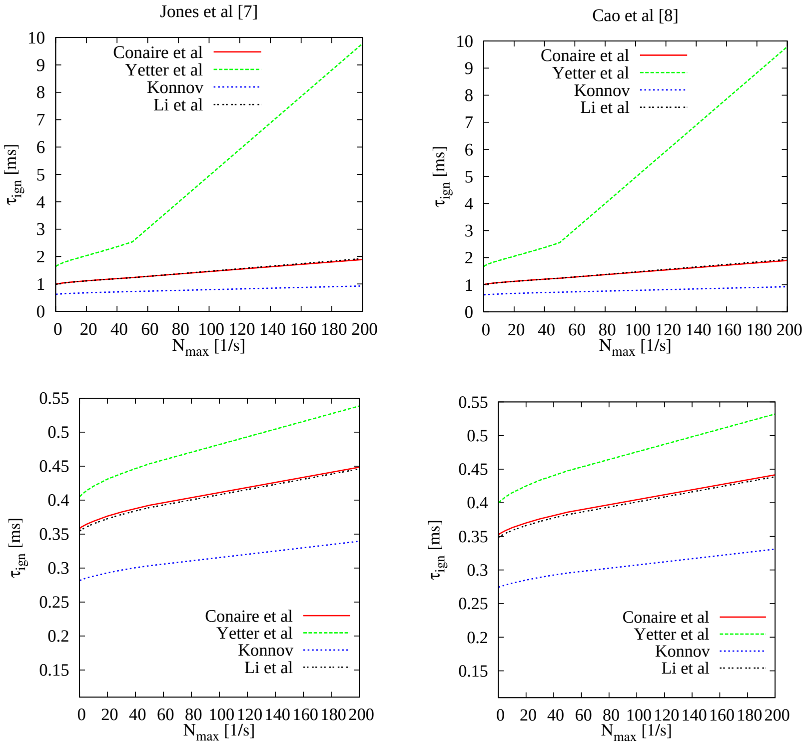

Figure 2: Influence of N_{max} on τ_{ign}, for two different auto-ignition criteria (top: $T_{cf} = 960K$, bottom: $T_{cf} = 1009K$)

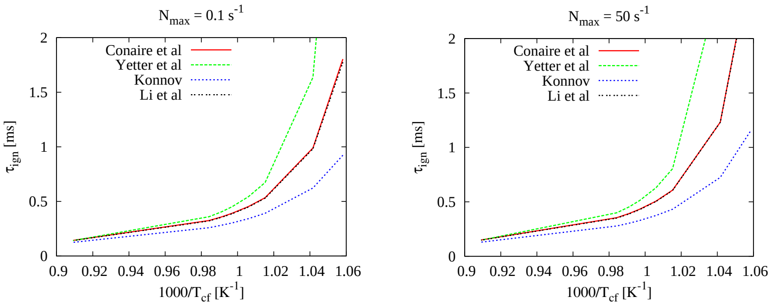

Figure 3: Influence of T_{cf} on the ignition delay time (ignition criterion taken from Jones et al [7])

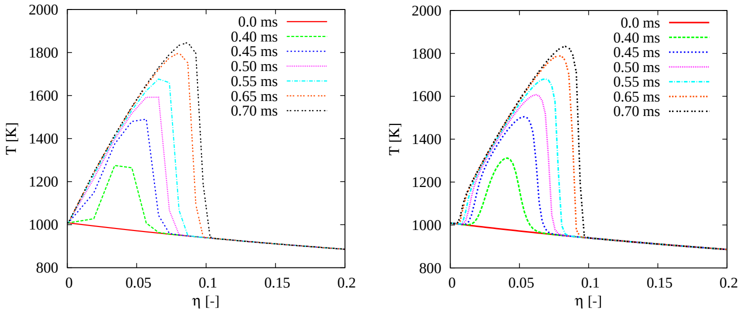

Figure 4: Conditional temperature evolution at $T_{cf} = 1009K$ and $N_{max} = 0.1s^{-1}$ at initial stages of ignition for the cases IGRID = 101 clustered around $Z_{ST} = 0.184$ (left), and for IGRID = 101 clustered around $Z = 0.03$ (right)

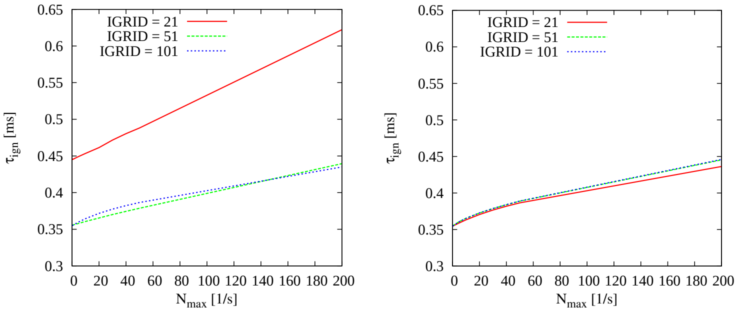

Figure 5: Ignition delay time for different resolutions in mixture fraction space calculated based on Jones et al [7], clustered around $Z_{ST} = 0.184$ (left), or $Z = 0.03$ (right)

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