

Assessing commonly recognized H₂/O₂ chemical reaction mechanisms at reheat gas turbine conditions

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Context and Objective

Among the technologies for fossil fuel power production with CO₂ capture “pre-combustion” removal of CO₂ and hydrogen combustion is one of the strong candidates. There is an increasing interest in developing non-diluted premixed or partially premixed hydrogen burners to avoid the higher cost and maintenance that comes with dilution. One possible near-term industrial application is the ALSTOM GT24/GT26 combustion system with the Sequential Environmental Vortex (SEV) burner [1]. To prevent ignition of the high-temperature fuel air mixture in the mixing region of the SEV, the residence time therein must not exceed the auto ignition delay time.

Accurate predictions of hydrogen combustion rely on high precision in the chemical mechanisms. The present study builds on previous work by Ströhle and Myhrvold [2] and investigates the performance of selected detailed chemical mechanisms at the high temperature and pressure conditions relevant to gas turbine and particularly reheat engine conditions. Generally, there is little data available at these conditions and a major part of the present work is limited solely to comparison between mechanisms.

Method, Results and Discussion

The ignition delay time is computed by solving the perfectly stirred closed reactor equations at constant enthalpy and pressure conditions using an in-house code where the CHEMKIN library is used for the property and source term calculations. Ignition delay is in this work defined by the time when a certain temperature increase is achieved.

The high-pressure shock tube data by Petersen et al. [3] are compared to ignition delay predictions in Fig. 1(a). All mechanisms follow the same trend where the ignition delay time increases with decreasing temperature, however, the GRI-Mech and the Leeds mechanism largely overpredict the ignition delay data. The Li, Ó Conaire and San Diego mechanisms give satisfactory agreement with the experiments in the lower temperature range and these three mechanisms also follow each other very well. At higher temperatures Konnov and Davis provide a slightly closer match with the experiments. Generally, all mechanisms overpredict the ignition delay time at higher temperatures with at least a factor 2.

The remaining work covers a temperature range from 1173 K to 1273 K, equivalence ratios from $\Phi=0.2$ to $\Phi=1.5$ and pressures up to 30 atm. Figure 1(b) shows the ignition delay plotted against pressure for an initial H₂-air mixture at a fuel-air ratio of $\Phi=0.75$ and temperature of 1273 K. The overprediction of the ignition delay time with the GRI-Mech and Leeds mechanisms, which mainly are developed for hydrocarbon chemistry, is at least partly attributed to the differences in the chain terminating reaction $H+O_2(+M)=HO_2(+M)$. Konnov, Ó Conaire and Davis predict the shortest ignition delay

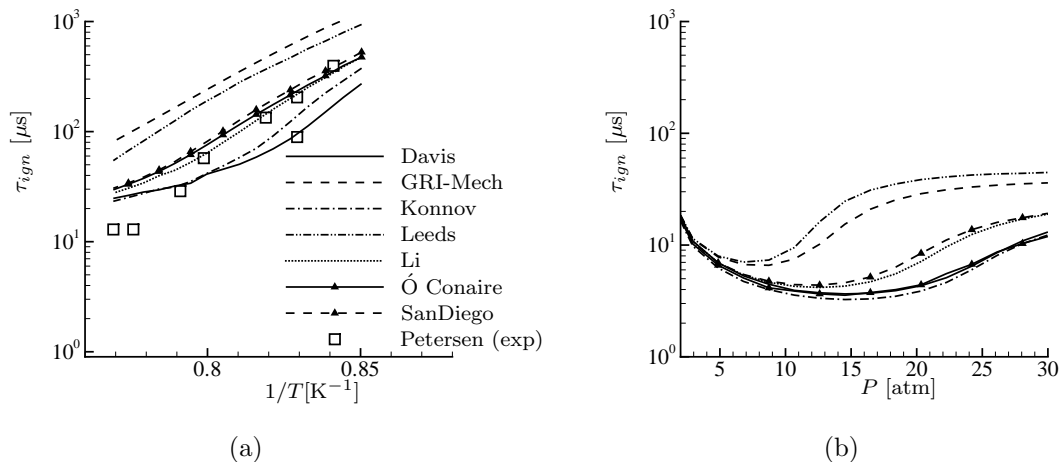


Figure 1: Ignition delay results with selected chemical mechanisms for (a) 2% H₂, 1% O₂, 97% Ar at 33 atm compared with shock tube data of Petersen et al. [3], and (b) H₂-air at $\Phi=0.75$ and $T=1273$ K.

times, while Li and San Diego follow each other closely somewhat above. It is interesting to note that, disregarding GRI-Mech and Leeds, the Davis mechanism predicts the longest ignition delay times at lean conditions (not shown here), while it predicts the fastest ignition at richer conditions. This may be attributed to differences in third-body efficiencies. Another interesting observation is that the Li and Ó Conaire mechanisms, which share the same inheritance in the Mueller mechanism, exhibit considerable differences. The Li and San Diego mechanisms are very close in behavior at all conditions considered, even though the chemical reaction coefficients of important reactions are notably different. A general observation is that the differences in ignition delay times between the dedicated hydrogen mechanisms Ó Conaire, Li and Konnov also are significant.

Conclusion

If the differences in ignition delay time and flame speed are related to the design of actual combustion equipment, as for instance the SEV burner by Alstom, the impact on cost will be significant. Hence, more experiments are needed to reduce the uncertainties in predictions with hydrogen mechanisms at the relevant high temperature and pressure conditions. The complete work has been published in [4].

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