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Extending the predictions of chemical mechanisms for hydrogen combustion: Comparison of predicted and measured flame temperatures in burner-stabilized, 1-D flames

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ABSTRACT

A method is presented for extending the range of conditions for which the performance of chemical mechanisms used to predict hydrogen burning velocities can be evaluated. Specifically, by comparing the computed variation of flame temperature with mass flux in burner-stabilized flat flames with those obtained experimentally the predictive power of a chemical mechanism can be tested at constant equivalence ratio over a range of more than 700 K. Sensitivity analyses for the flame temperature shows changing importance of various reactions with mass flux. High-quality flame temperature data obtained by CARS is capable of discerning differences in rate coefficients smaller than their current uncertainty. The method is general, and can be used for other fuels as well.

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1. Introduction

One of the major goals of combustion science is the accurate prediction of combustion phenomena. Given the complexity of combustion processes, and the empirical manner in which most practical combustion systems are developed, the ability to predict flame stability and pollutant formation represents a substantial contribution towards the design and optimization of new combustion equipment. A major advance in the last few decades is the prediction of flame structure and propagation by direct numerical simulation using detailed chemistry and transport. In addition to uncertainties

regarding transport properties [1], uncertainty in the chemical mechanism used, individual reactions usually being known to no better than a factor of two [2], is a limiting factor in the accuracy of the simulation results. One of the methods for testing the predictive power of chemical mechanisms (as well as for optimizing them [3]) has been to compare numerical and experimental determinations of the free-flame burning velocity of one-dimensional flames. One well-known limitation to this use of burning velocity data is that the rates of only a relatively small number of reactions have significant influence on the calculated burning velocity [4]. When considering a mechanism for a specific fuel, another limitation is that, in

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general, the only parameters varied for mechanistic purposes are the equivalence ratio, pressure and mixture temperature. That the variation in flame temperature achieved is inextricably tied to the changes in these parameters results in a relatively limited sampling of parameters; thus, the contributions of the important reactions at stoichiometric conditions are only tested along the temperature profile ending at the (high) adiabatic stoichiometric temperature. A widened range of conditions with which the model predictions could be compared would clearly enhance the reliability of the simulations.

A particularly interesting challenge in this regard is predicting the behavior of hydrogen combustion. Hydrogen has the potential of becoming a major sustainable energy carrier [5,6], and improved combustion mechanisms will most certainly assist in the development of hydrogen burning equipment. In addition, the oxidation mechanism for hydrogen is relatively simple, and is an essential part of hydrocarbon oxidation mechanisms. Thus, a more accurate hydrogen mechanism will also improve the predictions of other fuels as well.

In this paper, we propose a method for extending the range of conditions for testing the performance of chemical mechanisms for hydrogen oxidation with respect to burning velocity. Specifically, we use a modified version of the method used by Kaskan [7] to derive overall activation energies: by varying the mass flux of fuel-air mixture to a flame stabilized on a porous-plug burner, we modulate the flame-burner heat flux, thereby varying the flame temperature over a wide range. Rather than deriving an “overall” flame parameter, we compare the variation in flame temperature with mass flux with that obtained from detailed flame calculations. Using coherent anti-Stokes’ Raman scattering (CARS) to measure temperature, an accuracy of better than 40 K can be achieved [8], offering the potential of highly reliable data.

2. Experimental method

Hydrogen-air flames were stabilized on a McKenna Products water-cooled sinter burner, similar to those used in previous investigations [8]. Here we used a bronze sinter (rather than stainless steel) because of the superior heat transfer through the sinter to the cooling water. The flow rate of the cooling water was 0.8 l/m. Since the heat flux in hydrogen flames is more than 6 times higher than that in methane flames, the stainless sinter was inclined to glow visibly, even at this flow of water. Gas flows were measured using calibrated mass flow meters, with an accuracy of 3%. The equivalence ratio was determined by measuring the oxygen concentration in the unburned mixture by means of paramagnetic detection. The CARS setup is described elsewhere [9]. The reproducibility of the measurements reported below was better than 30 K, and was determined mainly by the uncertainties in the mass flow meters. The accuracy was estimated by comparing measurements on near-adiabatic flames with the temperatures calculated at equilibrium, and was also better than 30 K. Vertical temperature profiles were measured by moving the burner relative to the laser beams in steps of 1 or 2 mm (depending on the steepness of the gradients) for 20 mm, starting at ~ 1 mm above the burner surface. The equivalence

ratios studied were 0.6, 0.8, 1.0 and 1.2. While the mass flux corresponding to the free-flame burning velocity was obtainable for $\phi = 0.6$, there was insufficient gas pressure to obtain significantly higher mass fluxes using the current burner. Thus, for richer flames the mass fluxes are below the free-flame value.

The experiments were modeled using the PREMIX code in the CHEMKIN II package [10], using various mechanisms (see below). In addition to the use of the “industry standard” GRI-Mech mechanisms [11,12], the calculations were performed with recently improved mechanisms for hydrogen combustion such as in refs. [13–15]. The temperature profiles obtained with these recent mechanisms lie, as a rule, between those calculated using GRI-Mech 2.11 and 3.0 mechanisms. To avoid clutter in the figures and to emphasize the major points, the discussion below is concentrated mainly on the results obtained using the GRI-Mech mechanisms. When using the GRI-Mech mechanisms, the carbon-containing part of the mechanism was removed to accelerate the calculations. Multicomponent diffusion and thermal diffusion were included in the calculations.

3. Results and discussion

Fig. 1 shows typical experimental temperature profiles for various equivalence ratios and mass fluxes, ρv . At the higher temperatures, the profiles continue to rise in the post-flame region due to slow radical recombination, while at temperatures below ~ 2000 K the profiles are flat over much of the measurement domain. The rapid decrease in temperature above 1.8 cm for $\phi = 0.6$, $\rho v = 0.0057$ g/cm²s is due to mixing with the nitrogen shroud at this very low mass flux. The uncertainty in the temperature measurement is shown in the figure; the predictions shown using GRI-Mech 3.0 [11] are excellent, and with few exceptions, being within the experimental error. Since most of the experimental profiles are flat, and the form of the calculated profiles at the higher temperatures mirror the experimental profiles very well, even though

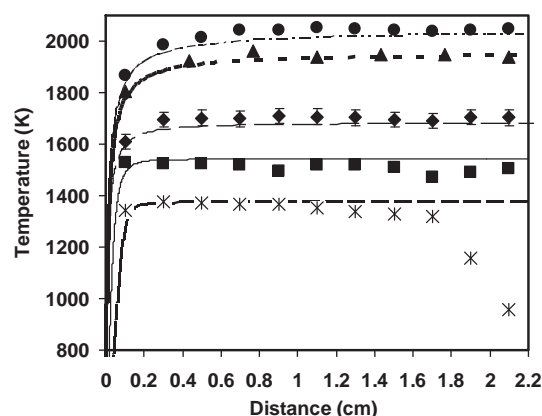


Fig. 1 – Vertical profiles of temperature in hydrogen-air flames. Points: measurements; lines calculations using GRI-Mech 3.0. ● - $\phi = 1.0$, $\rho v = 0.056$ g/cm²s; ▲ - $\phi = 1.0$, $\rho v = 0.042$ g/cm²s; ◆ - $\phi = 1.2$, $\rho v = 0.038$ g/cm²s; ■ - $\phi = 0.8$, $\rho v = 0.0105$ g/cm²s; * - $\phi = 0.6$, $\rho v = 0.0057$ g/cm²s.

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