# BURNING VELOCITIES AND A HIGH TEMPERATURE SKELETAL KINETIC MODEL FOR N-DECANE OXIDATION

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Laminar flame speeds of n-decane/air mixtures were determined experimentally over an extensive range of equivalence ratios at 500 K and at atmospheric pressure. The effect of $N_2$ dilution on the laminar flame speed was also studied at these same conditions. The experiments employed the stagnation jet-wall flame configuration with the flow velocity field determined by Particle Image Velocimetry (PIV). Reference laminar flame speeds were obtained using linear extrapolation from low to zero stretch rate. Predictions of the experimental data using existing published kinetic models were found to be in poor agreement, including the partially reduced skeletal mechanism for n-decane pyrolysis and oxidation of Zeppieri et al. (S.P. Zeppieri, S.D. Klotz, F.L. Dryer, *Proc. Combust. Inst.,* 28 (2000) 1587-1595). The analyses of these results further support that laminar flame speed data for large carbon number alkanes primarily constrains the kinetic sub-mechanisms for hydrogen/carbon monoxide oxidation and small carbon containing species with carbon number generally less than 3. Revision of the Zeppieri et al. model by updating the hydrogen/oxygen and small carbon number $C_1$-$C_3$ sub mechanisms, thermochemistry and elementary rates results in acceptable prediction of the experimental results. Predictions using the revised model were found to reproduce data used in validating the original model including high temperature, atmospheric pressure flow reactor pyrolysis and oxidation, high pressure shock tube ignition delay, and stirred reactor measurements. The revised model predictions also agree well with atmospheric pressure, burner stabilized flame data and recently published shock tube ignition delay measurements at both low and high pressure.

As noted above, the present mechanism is developed for high temperature applications where the reactions of radicals with oxygen that are of significance to two-stage ignition phenomena are not of importance. Recent work on in our laboratory on kinetic modeling of two-stage large alkane oxidation suggests that without first developing robust high temperature mechanistic features, the resulting coupling precludes construction of predictive models for low and intermediate temperature kinetics. Addition of low and intermediate temperature submechanisms to the present high temperature mechanism is the subject of current work in our laboratory and will result in a wide range mechanism for n-decane oxidation for applications involving two-stage ignition as well as high temperature oxidation phenomena.
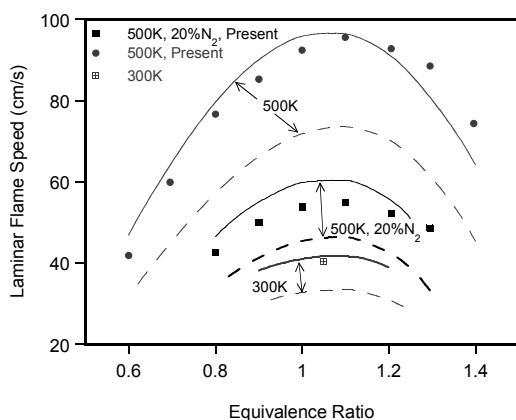


Fig. 1    Atmospheric pressure laminar flame speeds for *n*-decane/air mixtures. Symbols: 500 K and 500 K with 20% $N_2$ dilution - present experimental data; 300 K - P. Wagner, G.L. Dugger, *J. Am. Chem. Soc.* 77 (1955) 227 (extrapolated based on two higher temperature measurements); lines: model predictions (dashed line-Zeppieri et al., solid line - present *n*-decane model).
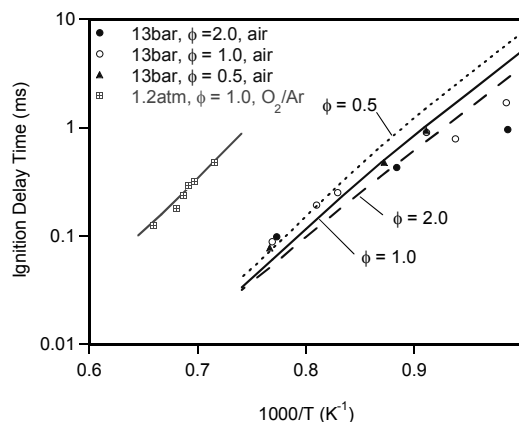
Fig. 2    Comparison of experimental (symbols) and computed (lines) ignition delay times for *n*-decane. Mixture compositions used in the experiments: 0.2% *n*-decane-$O_2$-Ar (D.C. Horning, D.F. Davidson, R.K. Hanson, *J. Propulsion Power*, 18 (2002) 363-371; D.C. Horning, *A Study of the High-Temperature Autoignition and Thermal Decomposition of Hydrocarbons*, Report No. TSD-135, 2001, Stanford University. and *n*-decane/air (U. Pfahl, K. Fieweger, G. Adomeit, *Proc. Combust. Inst.*, 26 (1996) 781-789).