Progress Towards a Validated Cantera-based Turbulent Flame Speed Solver

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***Abstract*— The aim of this work is to develop a Cantera-based solver to predict turbulent flame speeds (S_T) in the wrinkled flamelet, corrugated flamelet and thin reaction zone regimes, in which Da> 1. With the modified solver S_T predictions for hydrogen/air and hydrogen/methane/air mixtures over the range of equivalence ratios $0.5 \leq \Phi \leq 1.0$, at initial temperature and pressure of T_i = 300 K and P_i = 1 atm were calculated. Comparison with experimentally-obtained values for hydrogen (H_2) and a 50/50 hydrogen/methane (H_2/CH_4) blend and a currently-used correlation for S_T shows satisfactory agreement.**

I. Introduction

Most industrially-applicable combustion occurs at turbulent conditions. The ability for researchers to validate their mechanisms at comparable conditions is highly desirable. Available one-dimensional flame speed solvers focus on laminar flames. These solvers are not capable of predicting turbulent flame speed (S_T) as they do not account for (1) enhanced transport, (2) reduction of available reaction volume, and (3) enhancement of effective reaction rate that are found in turbulent flow when compared to laminar. The aim of this work is to develop a Cantera-based S_T solver which will account for the properties listed above.

II. Metodology

The S_T solver is built on top of the existing unstretched freely-propagating, one-dimensional laminar flame speed (S_L) solver within Cantera 2.2a [1]. Enhancement of property transport due to turbulent mixing is modelled using a one-dimensional k-ε approach. Enhancement of effective reaction rate due to temporal temperature fluctuations is modelled using reaction rate correction factors that assume temperature distribution around a temporal mean. Reduction of available reaction volume due to the presence of fine turbulent structures is modelled using the eddy dissipation concept.

III. Experimental Setup

Experimental turbulent flame speed was measured using a spark-ignited cylindrical fan-stirred bomb at Texas A&M University [3]. Four centrally-located, equi-spaced fans produce homogeneous and isotropic turbulence with an average u' of 1.5 m/s and ℓ of 2.7 cm. Flame speeds were measured for H_2 and H_2/CH_4 over the range of equivalence ratios $0.5 \leq \Phi \leq 1.0$, at initial temperature and pressure of T_i = 300 K and P_i = 1 atm, respectively.

IV. Validation

The results from the modified solver were compared against the experimental data, as show in Figure 1. It can be seen that the solver captures both the magnitude and profile of the experimental flame speeds for both fuels. While more accurate at lean conditions the solver also predicts stoichiometric condition well for the H_2 flame. The opposite can be said for the H_2/CH_4 flame where results are more accurate at lean conditions. The broken line in Figure 1 is an algebraic correlation, by Muppala et al [4], between the laminar and turbulent flame speed, currently used by researchers. For both fuels the model's predictions are more accurate than the correlation.

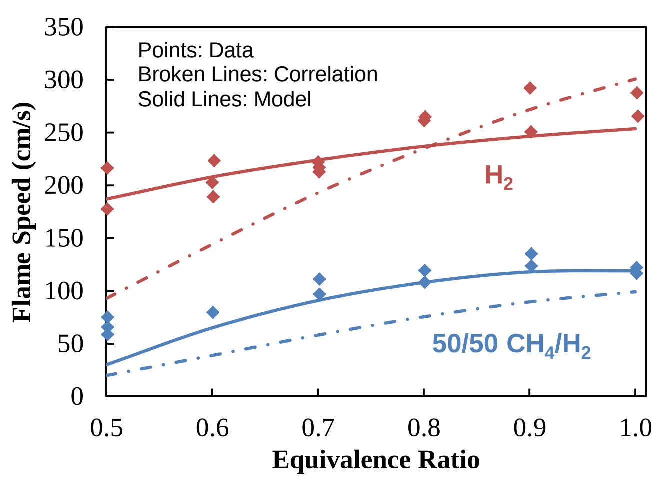

Figure 1 Comparison of experimental, algebraic correlations and computation flame speed data

V. MODELLING RESULTS

The solver was also used to compare NO_x and CO formation within a H_2/CH_4/air flame, as shown in Figure 2 and Figure 3. Enhanced transport causes a slower rise in temperature for the turbulent flames. As a result, laminar NO_x has a higher concentration due to the larger post flame zones in the laminar flames. For gas turbine conditions, turbulence increases the concentration of NO_x formed due to the presentence of temperature fluctuation (T') and it's influence on the rate constant. For this work T' has a small impact due to the low level of turbulence present, as shown in Figure 4. As a result, other turbulent phenomena have a larger effect on NO_x formation. Due to fast chemistry; CO has the same equilibrium concentration for both cases

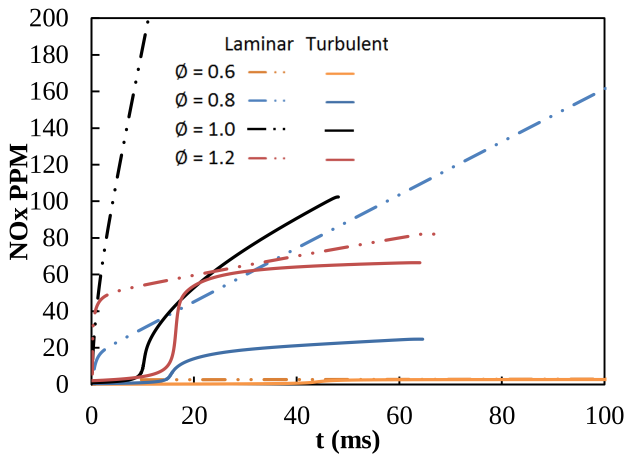

Figure 2 Comparison of laminar and turbulent NO_x production for a H_2/CH_4/air flame

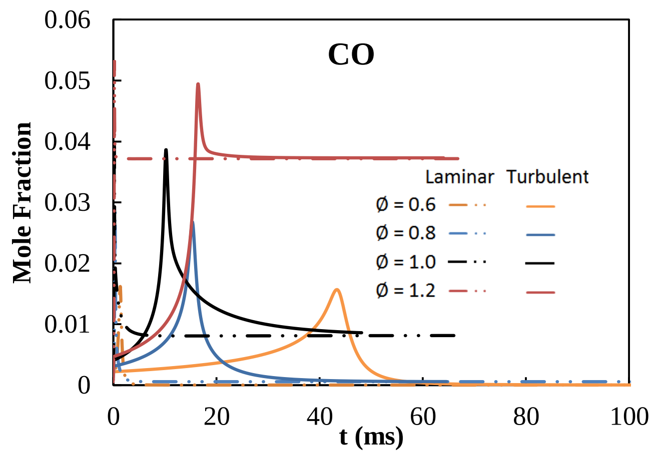

Figure 3 Comparison of laminar and turbulent CO production for a H_2/CH_4/air flame

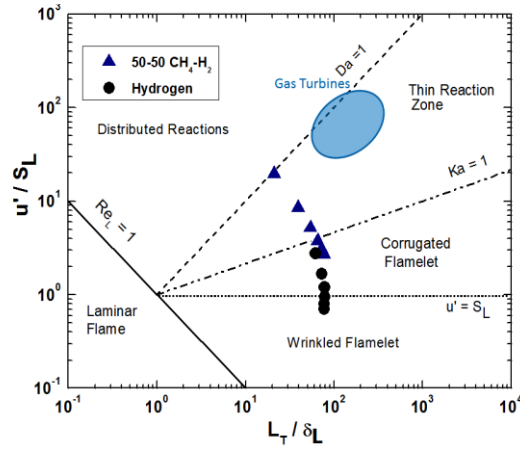

Figure 4 Borghi Diagram for the two flames and gas turbine conditions

VI. FUTURE WORK

Future work on the solver will aim to improve it's flexibility and robustness. With an improved solver, it will be further validated over a range of conditions, compositions and turbulent levels. An exploration of pollutant formation at a range of turbulent conditions will also be carried.

VII. CONCLUSIONS

Development of the new solver has shown it is possible to have a relatively computationally inexpensive 1D turbulent flame solver using Cantera. The solver was validated against turbulent flame speed and used to predict concentration of NO_x and CO.

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