An experimental and reduced modeling study of the laminar flame speed of jet fuel surrogate components

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HIGHLIGHTS

- Premixed flames of three jet fuel surrogates are stabilized in a stagnation flow.
- Experimental centerline velocity profiles obtained using particle image velocimetry.
- Laminar flame speeds are determined using a direct comparison method.
- A reduced chemical kinetic model is developed and validated against detailed model.
- Predictive capabilities of kinetic models for laminar flame speed are assessed.

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ABSTRACT

The laminar flame speed is an essential combustion parameter used in the validation of chemical kinetic mechanisms. In recent years, mechanisms tailored for jet fuel surrogate components have been partially validated using the laminar flame speeds of pure components, which were derived using both linear and non-linear extrapolation techniques. However, there remain significant deviations between the results from different studies that motivate further investigation. In this study, laminar, atmospheric pressure, premixed stagnation flames are investigated for the surrogate fuels n-decane, methylcyclohexane and toluene, which are representative of the alkane, cycloalkane and aromatic components of conventional aviation fuel, respectively. Numerical simulations are directly compared to velocity profile measurements to assess the predictive capabilities of the recently proposed JetSurF 2.0 chemical kinetic mechanism. Simulations of each experiment are carried out using the CHEMKIN-PRO software package together with the detailed mechanism, with accurate specification of the necessary boundary conditions from experimental measurements. Furthermore, a skeletal version of the detailed mechanism is deduced for improved computational speed using a species sensitivity reduction method, here referred to as Alternate Species Elimination (ASE). Toluene experimental data are further compared to a detailed toluene mechanism, termed the Stanford mechanism. The experimental and numerical reference flame speeds are used to infer the true laminar flame speed of the compounds following a recently proposed direct comparison technique that is similar to a non-linear extrapolation to zero flame stretch. JetSurF 2.0 and the skeletal ASE mechanisms demonstrate excellent overall agreement with experiment for n-decane and methylcyclohexane flames, for which the original model was optimized, but poor agreement for toluene, which was not an optimization target. Improved agreement for toluene is observed between the Stanford mechanism and experiment. Results confirm that the direct comparison method yields consistent laminar flame speed data irrespective of the reactivity accuracy of the chemical kinetic model employed. The laminar flame speed results from this study are essential for the further development of chemical kinetic mechanisms and contribute to the surrogate modeling of jet fuel combustion.

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1. Introduction

The combustion of kerosene-type aviation fuels cannot be easily modeled because of their complex and variable composition where, similar to gasoline and diesel fuels, there are hundreds to thousands of different hydrocarbon components present within the real fuel. Such a complex mixture effectively prohibits numerical simulations and necessitates the development of surrogate fuels, which is an ongoing process in the combustion research community [1–4]. The fuels considered for this study are n-decane, methylcyclohexane, and toluene, which are all candidate jet fuel

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surrogate components [5–8]. *n*-Decane has a similar, but just slightly higher, hydrogen to carbon ratio to that observed in jet fuel, which allows for blends consisting of decane and much lower H/C ratio aromatics to match the target fuel [1,4]. In addition, it has been selected as a surrogate component due to its prominent chemical functional group in fossil-derived fuels. Methylcyclohexane has been used as a representative constituent for the cycloalkanes found in jet fuel, however its impact on the combustion properties of mixtures is largely unknown [4,8,9]. Toluene, the simplest alkyl-benzene, is an often-used surrogate for diesel, and has emerged as a jet fuel surrogate component to represent the aromatic content of commercial aviation fuel [10]. Aromatics have typically been added to jet fuels to improve the physical qualities of the fuel, such as preventing seal degradation, however toluene addition has also been shown to affect combustion properties. Specifically, the radical pool produced from toluene and its effect on the production of OH radicals has been shown to influence the flame speed and extinction strain rate in proposed surrogate mixtures [11–13].

The laminar flame speed is a global indicator of the reactivity of a specific fuel-air mixture and is used as a defining parameter for turbulent flame propagation, making it a high priority for the aviation fuel research community [4]. The laminar flame speeds of the fuels listed above have been experimentally and numerically studied by several groups [5–7,14]. However, deviations in experimental results between groups, as well as the sparse availability of data, motivates further investigation of these critically important surrogate fuel components.

Several different experimental configurations for the measurement of laminar flame speed exist, including the twin flame burner, the spherical bomb method, and the classical bunsen burner. In geometries where a stagnation flow is employed, the flow streamlines diverge as the flow stagnates, leading to a flame stabilized in a strained flow field [15]. For such geometries, it is common to make measurements of a large set of stretched experimental flames and extrapolate the results to zero flame stretch to correct for stretch related effects, yielding the laminar flame speed, S_L [5,6,16]. In a stagnation flame apparatus, the local velocity minimum that exists just upstream of the flame is commonly referred to as the reference flame speed, $S_{u,ref}$, and is used as the characteristic rate of flame propagation for an experimental flame, e.g. [5,16–18]. The flame stretch rate, K, is based on the imposed flow conditions of the system, and has been shown to be equal to the maximum axial velocity gradient in the cold flow upstream of the flame, $\partial u_z/\partial z$, or twice the radial velocity gradient, $\partial u_r/\partial r$, at this location [19]. The reference flame speed and stretch rate are then used to extrapolate to a condition of zero stretch.

The traditional approach to obtain laminar flame speed is to linearly extrapolate the measured reference flame speeds plotted against the measured flow strain rates to the speed at zero strain rate. This approach has been found to yield satisfactory results when the Karlovitz number is small, $Ka < 0.1$, and tends to overpredict the laminar flame speed otherwise [20].

More recently, non-linear extrapolations have been shown to correct for errors due to thermal expansion, typically leading to lower laminar flame speeds, especially for rich flames [5,16]. One such technique makes use of the slightly non-linear trend of data over a wide range of strain rates [11]. To accomplish this, a large set of experimental data is used, with an appreciable scatter of $S_{u,ref}$ vs K bounding the polynomial curve fit. Another technique, developed by Egolfopoulos and colleagues, is to use numerical simulations to investigate the generic effect of strain rate on reference flame speed, generating a continuous curve of $S_{u,generic,sim}$ vs K over a wide range of strain rates [5]. A best fit of this trend with the experimental $S_{u,ref}$ vs K data, together with the simulated laminar flame speed, is used to extrapolate the experimental data to zero strain.

A limitation of these extrapolation techniques is the large sample set of $S_{u,ref}$ values at variable K required for each experimental condition, leading to physical constraints when generating data for the validation of chemical kinetic mechanisms. Furthermore, in the case of twin flames, boundary conditions are observed only at the nozzle exits, and the resulting laminar flame speed values do not include the associated uncertainty present in the experimental measurements, such as variations in equivalence ratio or nozzle exit temperatures from flame to flame.

Recently, an alternative approach for the determination of laminar flame speed has been demonstrated by Bergthorson et al. [18]. Instead of attempting to correct experimental velocity profiles or $S_{u,ref}$ values for stretch-related effects, a one-dimensional axisymmetric streamfunction hydrodynamic model coupled with a comprehensive chemical kinetic mechanism is used to directly simulate the experimental conditions to obtain a predicted $S_{u,ref}$ value with the exact same hydrodynamic stretch conditions of the experimental data. Previous work has shown excellent agreement between model and experiment for stretched flames using several chemical kinetic models for (C1–C3)–hydrocarbon–air flames, so long as the boundary conditions are specified using experimental measurements [18,21,22].

Furthermore, it has been demonstrated that the relationship between $S_{u,ref}$ and K is accurately predicted by the hydrodynamic model, and the ability to capture this trend is independent of the reactivity predicted by the mechanism employed [18,23]. Consequently, any difference in the reference flame speed predicted by the model is solely due to differences in reactivity between the model and experiment. This difference in reactivity can be applied to the simulated laminar flame speed found using the chemical kinetics model, allowing for the true laminar flame speed of the mixture to be inferred [18]. The resulting estimate of the true laminar flame speed is effectively equivalent to that which would be obtained using a non-linear extrapolation, but should provide higher accuracy through the specification of all model boundary conditions from experimental measurements. Uncertainty and variations in the inlet boundary conditions can also be directly simulated and accounted for, which is not possible when linear or non-linear extrapolations of stretched flame speed data are used to generate the laminar flame speed. This direct comparison of numerical simulations against experimental data is an example of the approach promoted by Connelly et al. [24], whereby simulations are used to account for systematic effects inherent in any experiment, rather than attempting to correct the data to compare to an idealized model.

This work makes use of the direct comparison method to determine the laminar flame speed of *n*-decane, methylcyclohexane, and toluene–air mixtures at a preheated temperature of 400 K and atmospheric pressure over a wide range of equivalence ratios. The independence of the inferred laminar flame speeds on the chemical kinetic model employed is investigated by using a detailed and reduced version of the JetSurF 2.0 chemical kinetic mechanism for *n*-decane and methylcyclohexane [25], as well as a third independent detailed mechanism for toluene oxidation, termed the StanD mechanism [26]. Furthermore, the results are compared to laminar flame speed data available in the literature.

2. Experimental method

A jet-wall apparatus, shown in Fig. 1, was constructed to perform the flame velocity measurements in this study. The jet-wall geometry was selected due to the stability of the resulting flames, and the precise knowledge of the stagnation-point location and its associated boundary conditions, and is similar to the geometry applied previously by the authors with (C1–C3)–hydrocarbon–air