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### Full Length Article

# Laminar burning velocities of *n*-decane and binary kerosene surrogate mixture



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#### ABSTRACT

Laminar burning velocities of *n*-decane and binary kerosene surrogate mixture consisting of *n*-decane (80%) and benzene (20%) by liquid volume were determined at atmospheric pressure and initial gas temperatures of 338 and 358 K. The heat flux method was employed to measure the burning velocity in nonstretched flames and three kinetic mechanisms were used to simulate the results: JetSurF 2.0, and two models for kerosene developed at Politecnico di Milano: Skeletal Surrogate (121 species) and hightemperature detailed (ver. 1412). New measurements were compared with available literature results at 400 K by extrapolation, which was performed using calculated temperature dependence of the laminar burning velocity. The data determined with the heat flux method agree with some previous counterflow burner measurements and disagree with the data from spherical flames. The detailed mechanism from PoliMi was able to reproduce the present experiments the best. The increase of the burning velocity in the surrogate mixture compared to *n*-decane was found to be insignificant.

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#### 1. Introduction

Surrogate fuel blends are often used in laboratory experiments and in combustion modeling to reproduce important characteristics of real transportation fuels [1]. Fuel surrogates usually consist of a few class-representative hydrocarbons such as normal and branched alkanes, aromatics and cycloalkanes; the complexity of a particular blend depends on the number of combustion properties (targets) taken into account [1–3]. Most often binary and ternary blends were suggested as gasoline [4], diesel [5,6] and kerosene [7] surrogates, yet, in some cases a single species, *n*-decane, was used to make comparison with kerosene combustion characteristics, such as burning velocity [8].

First detailed and reduced kinetic schemes developed to model combustion of kerosene were based on *n*-decane mechanisms [9-12] and were compared with available data from shock tubes [11], jet-stirred reactors [12], as well as with flame structure [13] and limited flame speed measurements [14]. Several binary surrogates for kerosene based on *n*-decane were examined: *n*-decane + benzene [10,15,16], *n*-decane + toluene [10], *n*-decane + *n*-hexane [15], *n*-decane + ethylbenzene [10], *n*-decane +

*n*-propylbenzene [17], *n*-decane + propylcyclohexane [17], n-decane + trimethylbenzene [18]. Remarkably, none of these blends were tested to obtain laminar burning velocity, until very recent study of Comandini et al. [19], who investigated n-decane + butylbenzene and *n*-decane + propylcyclohexane flames. Note that the data obtained by Eberius et al. [20] for n-decane + *n*-propylbenzene using Bunsen burner cannot be considered reliable due to lack of curvature and stretch correction. Therefore, the primary goal of the present work was to provide accurate measurements of the burning velocity of *n*-decane and a binary surrogate mixture at the same conditions and to compare these with predictions of kinetic models. According to the data in Edwards and Maurice [21], the fraction of aromatic compounds in typical aviation fuels varies and can reach up to about 20% by volume. In the present study, a simple *n*-decane + benzene fuel blend was chosen following previous literature studies [10,15,16] and our recent work on benzene flames [22], with the goal to determine whether the aromatic content in the fuel has an influence on the laminar burning velocity of the surrogate. Therefore, the fractions of the aliphatic and aromatic components were selected to be 80% (n-decane) and 20% (benzene), respectively.

The laminar burning velocity, important characteristic of any fuel + air mixture, which depends only on stoichiometric ratio,  $\phi$ , temperature and pressure, was measured for *n*-decane in several recent works as summarized in Table 1. The studies ignoring



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Table 1
Stretch-corrected measurements of the burning velocity of <i>n</i> -decane + air mixtures.

Temperature, K	Pressure, atm	Eq. ratio	Method	Extrapolation	Source
500	1	0.6-1.4	Stagnation	Linear	Zhao et al. [24]
360, 400, 470	1	0.7-1.4	Counterflow	Linear	Kumar and Sung [25]
403	1	0.7-1.5	Counterflow	Computationally assisted non-linear	Ji et al. [26]
400	1	0.7-1.6	Spherical	Linear and non-linear	Singh et al. [29]
400	0.7-5	0.7-1.4	Spherical	Linear	Kim et al. [30]
400	1	0.6-1.5	Stagnation	Computationally assisted non-linear	Munzar et al. [31]
350-470	1-3	0.7-1.4	Counterflow	Non-linear	Hui and Sung [33]
403	1	0.6-1.5	Spherical	Non-linear	Comandini et al. [19]

stretch correction in Bunsen or spherical flames [14,20,23] are not included and not considered in the present work. First stretchcorrected measurements in stagnation flow configuration have been performed by Zhao et al. [24] at initial gas temperature of 500 K. Kumar and Sung [25] implemented counterflow flame configuration and selected three temperatures: 360, 400 and 470 K. They noticed that linear stretch correction yields around 2-3 cm/s higher values than the burning velocity derived using non-linear extrapolation, but still presented only linearly extrapolated values. Ji et al. [26] also implemented counterflow technique, yet applied computationally assisted non-linear extrapolation to zero stretch, which is currently considered to be an advanced approach for the counterflow data processing [27]. Ji et al. [26] compared their measurements at 403 K with the results of Kumar and Sung [25] and found significant discrepancy up to 10–15 cm/s in rich mixtures, which was partially attributed to the different methods of stretch correction.

Singh et al. [28,29] studied spherical flames at 400 K and employed linear and non-linear stretch correction methods. In agreement with previous observations, linear stretch correction overestimated burning velocities, yet the difference was in the range of 0.3–2 cm/s decreasing towards rich mixtures. Kim et al. [30] extended the pressure range of the measurements in spherical flames up to 5 atm keeping the same initial temperature of 400 K and using linear stretch extrapolation.

Munzar et al. [31] combined stagnation flow configuration experiments with computationally assisted non-linear extrapolation to zero stretch using JetSurF 2.0 kinetic scheme [32]. Their measurements were found in good agreement with the data of Singh et al. [29] in lean flames, while notably above the data of Ji et al. [26] in very rich mixtures. Hui and Sung [33] implemented counterflow technique with non-linear stretch correction and covered extended temperature and pressure ranges. The burning velocities of *n*-decane were somewhat midway between the results of Kumar and Sung [25] and Ji et al. [26] in rich flames. Finally, Comandini et al. [19] investigated spherical flames using nonlinear stretch correction at 403 K. They provided thorough comparison of all available data at initial temperature of 400 (403) K, and concluded that all results from spherical flames [19,29,30] were in agreement with each other, while some of the burning velocities determined in the counterflow configuration [25,33] had higher values. The reason for that was unclear.

Various factors reviewed by Egolfopoulos et al. [27] may affect reliability of the experimental data and contribute to uncertainties of the burning velocity measurements depending on the experimental method and data processing procedure. Eliminating the need for stretch correction may potentially help in elucidating the reasons of the data inconsistency. Therefore in the present work the heat flux method was implemented and the burning velocities of *n*-decane and binary kerosene surrogate mixture consisting of *n*-decane (80%) and benzene (20%) by liquid volume were determined at atmospheric pressure.

#### 2. Experimental details

The measurements of the burning velocity of *n*-decane + air and *n*-decane + benzene + air mixtures were performed on the same experimental setup as in our recent paper on benzene + air flames [22]. Due to low vapor pressure of *n*-decane, no measurements at standard conditions were possible, therefore, the unburned gas temperature ( $T_g$ ) was set to values of 338 and 358 K. For the same reason, the range of equivalence ratios was limited to  $\phi = 0.7-1.3$ . The fuels (*n*-decane and benzene) were provided by Sigma-Aldrich Sweden AB, with stated purity higher than 99%.

The heat flux method allows stabilization of flat adiabatic flames on a perforated burner due to possibility of balancing heat transfer between the flame and the burner plate. The edge of the burner plate is kept preheated to 368 K by a water circuit in the burner head, controlled by a water bath. The temperature difference between the burner plate and the unburned mixture forces positive heat flux from the plate to the gas, which is balanced by the negative heat flux from the flame back to the plate. Van Maaren et al. [34] developed an analytical expression which relates the radial temperature distribution in the burner plate and the net external heat flux *q* to/from the burner plate. The radial temperature profile is measured by a set of T-type thermocouples, and by varying the unburned gas speed  $V_{g}$ , the flame can be stabilized under sub-adiabatic conditions (q < 0,  $V_g < S_L$ ), super-adiabatic conditions (q > 0,  $V_g > S_L$ ) or near-adiabatic conditions ( $q \approx 0$ ,  $V_g \approx S_L$ ). Then the burning velocity is obtained by interpolation near  $V_g = S_L$ .

Details of the experimental and data processing procedures can be found in [22] and other papers referred therein. High boiling point of *n*-decane (about 174 °C) required to keep all gas lines with fuel + air mixture at elevated temperatures to avoid condensation. In addition to the heated hose used to transport the mixture to the burner, heat insulation and additional hot water circuit were installed around the joints.

The description of the uncertainty evaluation procedures can be found in [35]. As for benzene + air mixtures [22], adiabatic flames of *n*-decane are prone to cellular instabilities, therefore, the burning velocity was determined by extrapolation from stable subadiabatic flames with the method described in [36]. An example of the procedure for the case of *n*-decane + air at  $\phi = 1.1$  is presented in the Supplementary material. The extrapolation range, i.e. the difference between the last recorded unburned gas velocity  $V_g$  and  $S_L$ , increased with  $\phi$  from about 4 cm/s at  $\phi = 1-7$  cm/s at  $\phi$ = 1.3. The extrapolation procedure of [36] results in asymmetric overall uncertainties in  $S_L$ , i.e. they consist of positive and negative components,  $\Delta S_L^+$  and  $\Delta S_L^-$ . In the following they are tabulated separately and shown in figures as asymmetric error bars.

#### 3. Modeling

Following our recent work on benzene flames [22] three general-purpose kinetic mechanisms were tested: JetSurF 2.0 [32], and two models for kerosene developed at Politecnico di

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