

**Effects of dilution on the Laminar Burning Characteristics of
Oxy-Dodecane mixtures with and without Hydrogen blending
and Oxy-Methane mixtures at elevated operating conditions**

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Abstract

N-Dodecane is an important representative in several surrogates of multicomponent fuels like gasoline and jet fuels. The choice of a surrogate fuel combination to estimate the combustion characteristics of a complex real fuel depends strongly on its individual component's physical, chemical, and combustion properties. Therefore, it is essential to have a precise reaction mechanism to predict the combustion characteristics, such as unstretched laminar burning velocity (LBV) and ignition delay times of the individual components of the surrogate fuel and the surrogate fuel itself. The combustion characteristics of (a) n-dodecane-air, (b) oxy-n-dodecane with diluents like N_2 , CO_2 , H_2O , and (c) n-dodecane- H_2 -air were less or not reported in the literature. The present work aims to fill the existing important gap. In this work, the unstretched LBV of n-dodecane at various operating conditions was measured using the freely expanding spherical flame (SPF) method. A new cuboidal combustion chamber (14.56 L) was constructed with 107 mm optical accesses on four sides. It had a dedicated heating system for elevated temperature experiments. Partial pressure method was used to prepare the combustible mixture inside the chamber. An electrical spark-ignition system was used to ignite the mixtures at the centre of the chamber. A high-speed shadowgraph system was used to image the spherical flame propagation. An in-house image-processing code was used to obtain the flame radius data from the flame images and subsequently the flame speed and flame stretch rate. Then, a non-linear stretch extrapolation scheme was used to find the unstretched flame speed, and finally, the unstretched LBV was estimated. The present rig was properly validated with the literature LBV data for CH_4 -air and n-decane-air mixtures at different operating conditions. A freely propagating planar flame model in CHEMKIN was used to simulate the unstretched LBV using various reaction mechanisms.

Initially, the unstretched LBV and burned gas Markstein length of premixed n-dodecane-air mixtures at pressure = 1-4 bar, temperature = 400-450 K, and $\phi = 0.8$ -1.4. The flame stability analysis of n-dodecane-air mixture at all the studied operating conditions quantified through burned gas Markstein length (L_b) emphasized that a transition of stable to unstable flame occurred at $\phi = 1.4$ due to thermo-diffusive effects. L_b was influenced significantly by an increase in pressure than temperature due to a substantial reduction in flame thickness. The comparison of measured unstretched LBV with available n-dodecane mechanisms indicated that JetSurF2.0, You et al., and PoliMi were the best candidates. Off-stoichiometric varieties of n-dodecane-air were more responsive to pressure and temperature

effects. Finally, the unstretched LBV of premixed n-dodecane-air mixtures increased/decreased with an initial temperature/ pressure hike. Raise in initial temperature increased the flame temperature and improved the flame propagation rate. An increase in initial pressure amended the reaction rate but decreased the flame propagation rate due to the dominance of three-body reactions and increased unburned gas density.

The second objective here was to measure the LBV and L_b of oxy-n-dodecane mixtures having high-flame temperatures safely by adding a third-party inert species. $(100-Z) \% (n\text{-C}_{12}\text{H}_{26} + (18.5 \text{ O}_2/\phi)) + Z\% (\text{N}_2/\text{CO}_2/\text{H}_2\text{O})$ mixtures were analysed at 400-450 K, 1-4 bar, $\phi=0.6-1.4$, and Z: (a) $\text{N}_2=55-75\%$, (b) $\text{CO}_2/\text{H}_2\text{O} = 65\%$. N_2 diluted mixtures were subjected to predominant thermal effects, whereas $\text{H}_2\text{O}/\text{CO}_2$ diluted mixtures were affected by all the real-time effects like thermal & chemical and thermo-diffusive effects. At 65% dilution, mixtures diluted with: (a) N_2 had the highest LBV due to the high-flame temperature, (b) CO_2 suppressed the LBV the most due to the thermal and chemical effects. Predicted LBV with You and JetsurF2.0 mechanisms showed excellent agreement with the present measurements. PoliMi's kinetic scheme always over-predicted the LBV in the rich mixtures. The diluted oxy-fuel mixtures generated stable flames with respect to thermo-diffusive effects at all the studied conditions. At a given thermodynamic condition, the flame's stability to the thermo-diffusive effects was the highest for mixtures diluted with steam, followed by N_2 and CO_2 due to their respective Lewis numbers. If the flame temperature attained was 2150 K or lower, the diluted oxy-n-dodecane mixtures at $\phi=1.4$ were affected by thermo-diffusive instability. The sensitivity of the chain termination reaction $\text{H}+\text{OH}+\text{M} \leftrightarrow \text{H}_2\text{O}+\text{M}$ showed a transition from negative to positive at 0% N_2 case.

The effects of hydrogen addition on the premixed laminar burning characteristics of n-dodecane reacting in air was the third objective of the present research. Approximately, the unstretched LBV increased three times at off-stoichiometric and two times for stoichiometric mixtures, as the mole fraction of hydrogen increased from 0-40% by volume in n-dodecane. Further, the simulation using JetsurF2.0 and You et al. predicted the LBV satisfactorily within uncertainty limits at all operating conditions, and PoliMi-1410 prediction accuracy varies with the equivalence ratio. The n-dodecane/air mixtures were unstable at rich equivalence ratios due to the lower mass diffusivity of n-dodecane and $\text{Le} < 1$, in contrast, H_2 blending transformed this unstable mixture to a stable mixture. H_2 addition resulted in an earlier onset of hydrodynamic instability due to a reduction in the flame thickness. In addition, sensitivity analysis was performed to identify the key reactions responsible for the enhanced reactivity

associated with H₂ addition. Reaction pathway and emission analysis shows the significant reduction of CO₂, and CO emissions.

The final objective of the current work was to investigate the dilution effect of steam, carbon dioxide, and nitrogen on the unstretched LBV and L_b of premixed (100-Z) % (CH₄ + (2O₂)/φ) + Z% (H₂O/N₂ /CO₂) mixtures at 300-453 K, 1-4 bar, equivalence ratio (φ)- 0.6-1.4, and Z was varied from 40-60% for steam and kept constant at 50% for CO₂/N₂. Present mixture formulation led to the comparison of the absolute dilution effect of each diluent at an identical mixture and thermodynamic conditions. The addition of 50% diluents significantly suppressed the flame propagation. It was the highest for CO₂ (87% as compared to no dilution) due to the simultaneous reduction in flame temperature and its kinetic effect, and it was followed by steam (69%) and N₂ (61%), and their suppression effect was primarily due to the reduction in the flame temperature. All the studied mixtures were stable to preferential diffusional instability as their: (a) Markstein length was positive and (b) the effective Lewis number of the mixtures were well higher than the critical Lewis number. Predicted LBV with GRIMech3.0 compared well with the experiments than FFCM-1. As the LBV increased beyond 150 cm/s, predicted LBV of both GRIMech3.0 and FFCM-1 showed significant deviation with the measurements.

Keywords: Laminar burning velocity, Flame stability, hydrodynamic instability, n-dodecane, dilution, effective Lewis number, hydrogen blending, oxy-fuel combustion