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Experimental Laminar Flame Speed Study of Nitrogen-diluted Diethoxymethane/Oxidizer Mixtures under Microgravity

R. Glaznev[1], F. Halter[2,3], J. Beeckmann[1], C. Chauveau[2]

[1] Institute for Combustion Technology, RWTH Aachen University, Germany
[2] CNRS ICARE, Orléans, France
[3] University of Orléans, France

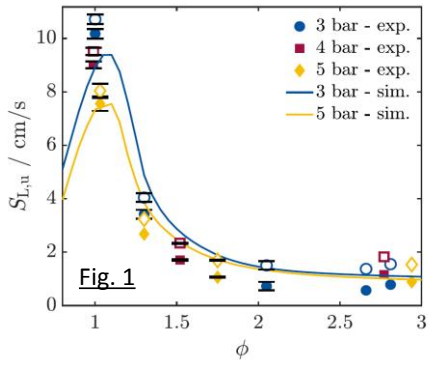
The global transition to minimum CO_2 emissions causes growing interest in alternative fuels. Various alternative energy carriers with low-temperature chemistry (LTC) are present in many applications. They differ from fuels without LTC by a wider flammability range and lower soot emissions complicating their fire detection[1]. Diethoxymethane (DEM, $C_5H_{12}O_2$) is a representative bio-hybrid fuel with complex low-temperature chemistry[1]. Diethoxymethane's laminar flame speed ($S_{L,u}$), a fundamental reactivity and exothermicity metric of a combustible mixture, is of key importance for kinetic model validation. Understanding the effect of low-temperature chemistry on DEM's laminar flame speed requires high-fidelity experiments in a wide range of conditions. Nitrogen dilution of the combustible mixture decreases the adiabatic flame temperature T_{ad} and thus favors low-temperature reaction pathways. For this, accurate experimental data on the fundamental combustion properties of DEM, such as the laminar flame speed, are required.

One of the most sophisticated experimental methods to measure $S_{L,u}$ is based on the acquisition of a centrally ignited outward propagating flame (OPF). This technique has gained widespread use, owing to the considerable pressure range it offers and the clearly defined stretch rate $K = {}^{2}/_{R_f} \frac{dR_f}{dt}$, where R_f denotes the flame radius. During the early stage of flame propagation, the flame front radius can be tracked using high-speed Schlieren/shadowgraphy optical techniques or Particle Image Velocimetry (PIV). Since the burned gas can be assumed motionless, the flame propagation speed with respect to the burned gas, $S_{L,b} = \frac{dR_f}{dt}$, is then calculated. Flame propagation speed S_L^b can be extrapolated to zero-stretch rate using linear or nonlinear methods. The laminar flame speed is then obtained using the mass continuity equation as $S_{L,u}^0 = \sigma S_{L,b}^0$, where $\sigma = \frac{\rho_b}{\rho_u}$ is the density ratio between burned and unburned gases. In this work, an experimental study of N_2-diluted spherically expanding DEM flames was conducted. Nitrogen dilution considerably decreases flame propagation speed, causing significantly increased experimental timescales[2]. The expansion of spherical flames is a complex process that can be influenced by radiation and buoyancy effects. These effects can cause the flame to deviate from its spherical shape, thereby challenging underlying post-processing analysis assumptions[2]. In order to distinguish the impact of radiation from the buoyancy-induced deformation, microgravity experiments were carried out during a parabolic flight campaign onboard the Airbus A310 Zero-G. The radiation-correction formula proposed by Yu et al.[3] was used to correct radiation heat losses in experimental laminar flame speed data. The experimental results were compared with planar, steady laminar flame speed simulations under adiabatic assumptions conducted using the 1D reactive computational fluid dynamics (CFD) solver FlameMaster and a reduced version of the kinetic mechanism by Jacobs et al.[1].

Results

The extracted laminar flame speeds are shown in Fig. 1 over the equivalence ratio (filled symbols). The lines in Fig. 1 represent laminar flame speeds obtained from the planar unstretched adiabatic premixed simulations using the kinetic mechanism by Jacobs et al.[1]. The total differences between radiation affected flame speeds and simulations are 10 % near stoichiometric conditions for $P_u = 3\ bar$ and become larger to approximately 50 % at fuel-rich conditions. These results were expected since the experimental data obtained are not yet radiation corrected. However, for $P_u = 5\ bar$ and $\varphi = 1$ uncorrected experimental S_L^u shows good agreement with the adiabatic simulation results, meaning that either radiation does not play a significant role for these particular conditions, or that the experimental data and kinetic mechanism require further analysis and potential improvement for the mixtures near stoichiometric conditions. Discrepancies between S_L^u-

calculations with the adiabatic assumption and experiments are observed for most conditions. The low flame speeds, below 10 cm/s, indicate that radiation must be corrected. The generalized empirical correlation by Yu et al.[3] is used to obtain radiation-free laminar flame speeds (open symbols). Recall that this model was developed by employing CFD and the statistical narrowband (SNB) model. It is also based on several types of fuels, from C1 to C8 hydrocarbon fuels, syngas H_2/CO at various ratios, and fuels containing oxygen functional groups such as dimethyl ether. A wide range of equivalence ratios and different initial pressures and temperatures were chosen to quantify the uncertainty associated with radiation. Moreover, the applicability of this formula for the N2-diluted flames was recently studied for ethanol[2]. Thus, the model is applied in the present study to DEM. It is given as:



$$\frac{S_{L,u}^{corr}}{S_{L,u}} = 1 + 0.82\left(\frac{S_{L,u}}{S_0}\right)^{-1.14}\left(\frac{T_u}{T_i}\right)\left(\frac{P_u}{P_i}\right)^{-0.3}, \quad \text{where} \quad S_0 = 1\ cm/s, \quad T_i = 298\ K \quad \text{and} \quad P_i = 1\ atm.$$

Radiation-corrected laminar flame speeds obtained are shown in Fig. 1 by open symbols. The corrected experimental results underpredict the simulation results by 25 % at ϕ = 1.3. The offset becomes negligible for 1.5 < ϕ < 2.1. A slightly larger discrepancy is observed for the richer mixtures ($\varphi > 2.5$), which can be explained by lower repeatability caused by the ignition challenges and more pronounced Lewis number effects. However, the obtained experimental data for $\varphi > 2.5$, which were extremely difficult to measure and post-processed very carefully, can be used as a reference data set to validate kinetic schemes of DEM.

Perspectives

Rayleigh scattering measurements can provide unique insights into radiation effect and temperature distribution inside ultra-slow spherically expanding flames. The first tests were conducted during the parabolic flight campaign in May 2023 (Table 1.). An example of temperature evolution of different stages of DEM flame propagation is presented in Fig. 2. More repetitions and further analysis are required for better understanding of the radiation effect.

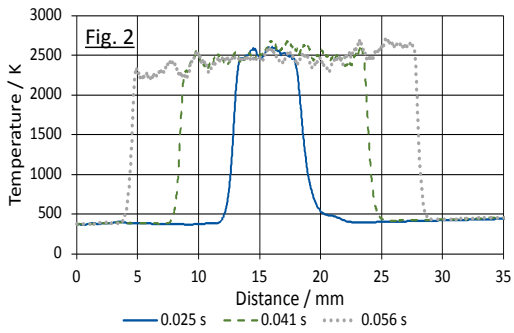


Table 1. Rayleigh scattering signal of ultra-slow flame at different time steps.

0.016 s	
0.034 s	
0.053 s	

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