



Experimental and numerical investigation of atmospheric laminar premixed n-butane flames in sooting conditions



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ABSTRACT

Experimental and numerical investigation of atmospheric laminar premixed n-butane/O₂/N₂ flames operating at two equivalence ratios ($\phi = 2.16$ and 2.32) has been performed. Both flames produce soot particles. Mole fraction of reactants, stable intermediate and combustion products have been obtained using a quartz microprobe coupled to gas chromatography and infrared spectroscopy technique analysis. The temperature profiles were obtained by Laser induced fluorescence of nitric oxide. The experimental results showed that a weak variation of equivalence ratio in sooting conditions introduces an increase of benzene and some unsaturated aliphatic species peak mole fraction. Except for benzene, the peak species mole fraction increase does not exceed a factor of two. A new reaction kinetic model is proposed to predict gaseous species mole fraction. In addition to the good agreement observed with our experimental data base, the proposed mechanism predicts well the detailed data obtained in low pressure rich n-butane premixed flames and high temperature ignition delay times reported in the literature.

Reactions path analysis revealed that the first aromatic ring is controlled by C₄ + C₂ (nC₄H₅ + C₂H₂ = C₆H₆ + H) and C₃ + C₃ (self recombination of C₃H₃ radicals) reactions routes. C₄ + C₂ reaction path predominates in the reaction zone while C₃ + C₃ path tends to predominate in the post flame region. The impact of the equivalence ratio on both reactions and the main differences between our and three selected literature models are discussed.

1. Introduction

Many alternative paths to the burning of conventional fossil fuels are being investigated to produce energy in order to meet international commitments on CO₂ reduction. The use of biomass to propose modern fuels using significant quantities of bio fuels is a path that appears more and more credible. In recent years, studies of alcohols issued from biomass have been widely focused on ethanol because it can be produced in large quantities. However, more and more studies highlight the interest in using alcohols of larger carbon chain such as butanol [1–5]. According to Norton and Dryer [6] alcohols oxidation can exhibit some similarities with alkanes oxidation. The authors showed that oxidation of the alcohols involves H-transfer reactions leading to alkenes in similar ways to those of the corresponding alkane. Studies on the oxidation of large alcohols oxidation should then motivate new numerical and experimental studies and modeling on large alkanes oxidation.

Most investigations have been conducted on n-butane oxidation in premixed reactors especially in the case of jet stirred reactor [7–11].

The main studies on n-butane oxidation in JSR conditions have been reported by Dagaut's group and concerned the impact of n-butane or isobutane oxidation on NO depletion in a large equivalence ratio range and at atmospheric pressure. Various studies were also devoted to the global data (laminar flame speed and ignition times). Atmospheric laminar of premixed n-butane/air, ethylene/n-butane/air, n-butane/toluene/air counterflow flames were experimentally studied in a large of equivalence ratios ($0.5 \leq \phi \leq 1.9$) by Hirasawa et al. [12]. The laminar flame speeds were determined using digital particle image velocimetry (DPIV). The authors reported peak of n-butane velocity about 40 cm/s. Laminar flame velocities have been measured by using the heat flux method in the case of alkanes representative of natural gas oxidation by Bosschaert et al. [13] for different equivalence ratios ($0.6 \leq \phi \leq 1.6$). The reported values exhibited the following trend: isobutane (33.4 cm/s) < methane (35.7 cm/s) < n-butane (37.1 cm/s) < propane (39.5 cm/s) < ethane (40.7 cm/s). Recent measurements using heat flux method have been also reported by Dirrenberger et al. [14] for neat alkane flames (methane, ethane, propane, butane) and for their binary or ternary mixtures as representative of

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natural gas combustion. The peak value reported for n-butane is about 39 cm/s which confirmed the experimental values of Bosschaert et al. [13] whereas a disagreement could be observed with the older literature values probably due to the absence of correction for flame stretch.

Motivated by engine applications, various investigations have been performed in the case of ignition delay times at low temperature in Rapid Compression Machine conditions [15–18]. However only few investigations concerned ignition delay times at high temperature. Ogura et al. [19] measured ignition delay times in shock tube for n-butane and isobutane mixtures in 1200–1600 K temperature and 1.7–2.4 atm pressure ranges. Iso-butane ignition time was observed higher than that measured for n-butane (factor of 2). The authors attributed the difference of H atoms production efficiency by initiation reactions. Recently Zhang et al. [20] measured the ignition delay times in shock tube for C₁ up to C₄ alkanes/O₂ diluted by argon at stoichiometric composition. The ignition delay times of n-butane were observed close to those of propane and the difference of reactivity between the different alkanes was assigned to their aptitude to produce ethyl or methyl radicals.

The literature analysis reveals a crucial lack on the species mole fraction profiles in the sooting premixed n-butane flames. Only one investigation [21] has been conducted in sooting conditions as in the present work. In this investigation, mole fraction of various stable species were measured in a laminar premixed flat flame of n-C₄H₁₀/O₂/Ar in sooting conditions ($\Phi = 2.6$) at atmospheric pressure. The different isomeric forms considered as soot precursors such as unsaturated C₃ and C₄ could not be distinguished. A more recent investigation has been conducted by Oßwald et al. [22] in a low pressure rich and non-sooting premixed butane and iso-butane flames. The authors proposed a new detailed reaction mechanism to model their 35 experimental species mole fraction profiles obtained in iso and n-butane flames. Globally, a good agreement was found between the model and the experiments. One can note that the model tends to underestimate the stable intermediate species and to overestimate the reactive species. The position of the peak species mole fraction is correctly predicted in both flames when the temperature profile is shifted to take into account the probe perturbation.

In this paper the chemical structure of two flat sooting premixed n-butane flames have been studied. Both flames were stabilized at atmospheric pressure and two equivalence ratios (2.16 and 2.32). Visually, it was observed that a slight increase in the equivalence ratio increased very strongly the yellow brightness of the flame characteristic of the presence of soot. In the present work, the impact of this weak increase of the equivalence ratio on the first aromatic ring and its precursors is examined. The impact on larger aromatics and soot volume fraction will be discussed in a forthcoming paper.

2. Experimental setup

2.1. Chemical flame structure

Two laminar atmospheric premixed fuel-rich n-butane/O₂/N₂ flames have been studied. The initial conditions of the studied flames are given in Table 1. The purity of n-butane and oxygen is higher than 99.5% while it is 95% for nitrogen. Yellow luminous radiation

Table 1
Conditions of the studied flames. Flow rates are given in STM conditions.

Φ	Total flow total (L/h)	N ₂ shield flow (L/min)	N ₂		O ₂		n-C ₄ H ₁₀	
			Flow (L/h)	%	Flow (L/h)	%	Flow (L/h)	%
2.16	757.1	50.0	424.0	56.0	250.0	33.0	83.1	11
2.32	734.4	50.0	400.2	54.5	246.3	33.5	87.9	12

characteristics of soot emission is found to start from 2 mm above the burner surface for both flames ($\Phi = 2.16$ and $\Phi = 2.32$).

Both flames were stabilized on a 6 cm diameter water-cooled McKenna burner. The burner was constituted by an internal bronze porous plug where the reactants mixture is fed, surrounded by a coaxial bronze porous ring flushed with nitrogen to shield the flame from surrounding ambient oxygen. A stainless steel disk placed at 16 mm from the burner surface, with shape and diameter similar to the burner porous plate was used to stabilize the fuel-rich flame in its upper part. A sampling probe was vertically translated at different heights (one dimensional flame) above the burner surface to collect combustion products and stable intermediate species.

The chemical structure of both sooting flames has been determined by means of a quartz micro-probe sampling system (tip diameter equal to 126 μ m) coupled with Fourier Transform InfraRed spectroscopy (FTIR), for the quantification of water, and on-line gas chromatographic techniques, which allowed to preliminarily determinate the in-flame mole fraction of O₂, CO, H₂ and C₁-C₇ light hydrocarbons (from methane to toluene). Hydrocarbon species were analysed with a HP-Plot Al₂O₃ capillary column (Φ 0.32 mm) and a flame ionisation detector (FID). Hydrogen, oxygen, nitrogen and carbon monoxide are separated in a molecular sieve 5A column (Φ 0.53 mm) and detected with a thermal conductivity detector (TCD). Helium was used as a carrier gas, except for hydrogen measurement which used nitrogen as carrier gas to improve the sensibility. The species were directly calibrated before each measure with cold known concentration standards. Analyses of H₂O and CO were performed by (FTIR) with a spectrometer NEXUS THERMO-OPTTEK as described in [23]. Calibration of water was carried out by preparing various H₂O-N₂ mixtures by using the saturated vapor water pressure at room temperature and atmospheric pressure. In the case of CO₂, we failed to obtain a linear response of FTIR and then its mole fraction profile is not reported and carbon balance could not be controlled.

All the sampling line was heated ($T = 120$ °C) and kept at sub-ambient pressure to reduce water and high molecular weight compounds wall condensation and adsorption. To improve the thermal stability of the system, a Pyrex cylinder (14 cm height, 1 cm thickness and 24 cm diameter) and an additional metallic grid were placed directly on the stabilizing disk, to avoid peripheral flames ignition. A scheme of the experimental setup used can be found in our previous paper [24].

Uncertainties are around 10% for major species (O₂, CO, H₂, and CH₄) and 20 % for minor and H₂O.

2.2. Gas temperature measurements by multiline NO-LIF thermometry

Laser induced fluorescence (LIF) is a laser diagnostic allowing in situ measurements of flame temperature with a high spatial resolution. The technique relies on the excitation of several rovibronic transitions of a fluorescent molecule using a tunable laser source and to the subsequent collection of the fluorescence signal. Among the species used for thermometry, NO is a good candidate because this molecule can be seeded as a tracer in the reactive mixture, allowing the measurement of the complete temperature profile from the burner surface to the burnt gases [25]. The temperature can be determined from the best fit between the experimental excitation LIF spectrum and a library of simulated spectra calculated on a large range of temperatures [26]. Calculation takes into account experimental parameters such as baseline, experimental line shape, bandwidth, pressure, collisional broadening and temperature.

NO LIF thermometry was shown to be well suited for stationary flames from low pressure to high pressure as previously detailed in [25,27–29]. Furthermore, capability of multi-line NO-LIF thermometry has also been demonstrated to measure the temperature of sooting flames by exciting transitions from the A-X(0,0) of NO around 225 nm [28–30]. Special care must be undertaken to prevent spectral

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