

Experimental and Modeling Study of a Lean Premixed Isobutene/Hydrogen/Oxygen/Argon Flame

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Abstract

The experimental structure of a lean isobutene/hydrogen/oxygen/argon flame (2.7% iC_4H_8 , 4.5% H_2 , 83.0% O_2 , 9.8% Ar , $\phi=0.225$) has been determined by molecular beam mass spectrometry at low pressure (40 mbar). The detected species throughout the flame thickness were: H_2 , CH_3 , O , OH , H_2O , C_2H_2 , CO , C_2H_4 , CH_2O , O_2 , HO_2 , Ar , C_3H_4 , C_3H_6 , CO_2 , C_2H_4O , C_4H_6 , iC_4H_8 , C_3H_6O , C_4H_6O and C_4H_8O . The original model, validated against premixed rich CH_4 , C_2H_2 , C_2H_4 , C_2H_6 flames, has been extended by building a sub-mechanism taking into account the formation and the consumption of species involved in the isobutene combustion. It contains 520 reactions and 99 chemical species. There is a good agreement between calculated mole fraction profiles predicted by this mechanism, compared to experimental results.

Introduction

Isobutene is an important intermediate species produced from the pyrolysis and oxidation of isooctane, also MTBE and ETBE, which are used worldwide as octane enhancer. To be able to model correctly the combustion of these fuels in engines, it is necessary to understand more precisely the oxidation mechanism of isobutene.

In 1975, Bradley and West [1] studied the thermal decomposition of isobutene (mixtures of 0.1% and 0.5% in argon) in a single-pulse shock tube (1055 – 1325 K). The isobutene oxidation has been investigated by Brezinsky and Dryer [2] in a turbulent flow reactor, at atmospheric pressure. Curran et al. [3] studied the ignition of isobutene/oxygen/argon mixtures at equivalence ratios from 0.1 to 4 in a shock tube by measuring and modeling ignition delays behind reflected shock waves. In 1998, Dagaut and Cathonnet [4] investigated experimentally and numerically isobutene oxidation and ignition in a jet stirred reactor in the temperature and pressure ranges of 800 to 1230K and at 1 to 10 atm, respectively. Several isobutene studies in shock tube were performed in the last decade. Particularly, Bauge et al. [5] measured ignition delays of isobutene-oxygen-argon mixtures ($\phi = 1$ to 3) behind reflected shock waves at temperatures from 1230 to 1930 K and pressures from 9.5 to 10.5 atm. Santhanam et al. [6] observed dissociation and vibrational relaxation in shock waves in 2, 5, and 10% isobutene mixtures with krypton by using the laser-Schlieren technique. And very recently, Yasanuga et al. [7] studied pyrolysis and oxidation of isobutene behind shock waves in the temperature range of 1000 - 1800 K and at pressure between 1.0 and 2.7 atm. A reaction mechanism was elaborated and validated against experimental results.

To the best of our knowledge, isobutene flames have not yet been investigated in terms of their structure. The aim

of this work was to measure mole fraction profiles in a flat lean isobutene flame ($\phi = 0.225$) at low pressure, and to build a reaction sub-mechanism which will be incorporated to an already validated model for some rich hydrocarbons flames (methane, acetylene, ethylene and ethane) [8].

Experimental

A lean premixed isobutene/hydrogen/oxygen/argon flat flame (2.7% iC_4H_8 , 4.5% H_2 , 83.0% O_2 , 9.8% Ar), at equivalence ratio (ϕ) of 0.225, has been stabilized at 40 mbar on a Spalding-Botha type burner, 8 cm in diameter. The initial flow velocity was 53.4 cm/s. The experimental setup, which was described elsewhere [9], consists of a molecular beam mass spectrometer system (MBMS) developed to determine the structure of one-dimensional laminar premixed flames burning at low pressure. For every species, interferences from fragmentation during the electron impact or from overlapping of species with similar mass have been kept low or taken into account. The conversion of signal intensities to mole fractions has been performed by using a calibrated mixture for stable compounds and by estimating ionization cross-sections for carbon-containing radicals. About uncertainties, we estimate 5-10% at the maximum value for species with a mole fraction above 10 ppm and 20% for species with a mole fraction value below 10 ppm. However, because of some measurements have to be performed close to the ionization potential to avoid interferences, error bars could be larger. The detected species throughout the flame thickness were: H_2 , CH_3 , O , OH , H_2O , C_2H_2 (acetylene), CO , C_2H_4 (ethylene), CH_2O (formaldehyde), O_2 , HO_2 , Ar , C_3H_6 (propene), CO_2 , CH_3CHO (acetaldehyde), C_4H_6 (1,3-butadiene), iC_4H_8 (isobutene), C_3H_6O (acetone), C_4H_6O (1 propen-1-one, 2 methyl-) and C_4H_8O (prop-1-en-1-ol, 2 methyl- and propanal, 2 methyl-).

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The final flame temperature, measured by using Pt/PtRh10% coated thermocouples 0.1 mm in diameter and located close to the sampling cone tip, was 1720 K. The temperature profile has been corrected for radiation losses by the electrical compensation method [10]. Experimental uncertainties are estimated to ± 50 K.

Modeling

Previously, we have developed a reaction mechanism validated against premixed rich $C_2H_4/O_2/Ar$ flames ($\phi = 2.25$ and 2.50) which describes in detail the formation of soot precursors and more precisely the main pathways involving benzene [8]. In this work, we have extended the original model by building a sub-mechanism taking into account the formation and the consumption of species involved in the isobutene combustion. By using kinetic data from the literature, we were able to build a new mechanism containing 520 elementary reactions and involving 99 chemical species. (Note: The complete mechanism is available by contacting the authors at Veronique.dias@uclouvain.be or Jacques.vandoreen@uclouvain.be).

The numerical simulation of the mechanism of the investigated one-dimensional flames has been performed by using the Cosilab[®] software from SoftPredict [11]. Molecular and thermal diffusion are considered in this code. The modeling has been performed by using as input parameters the initial composition of the flame, the initial total mass flux and the experimental temperature profile measured in similar conditions as the mole fraction.

Results and Discussion

Figures 1-4, 6, 7 show experimental and simulated mole fraction profiles of chemical species detected in the lean isobutene flame (H_2 , CH_3 , O , OH , H_2O , C_2H_2 , CO , C_2H_4 , CH_2O , O_2 , HO_2 , Ar , C_3H_6 , CO_2 , CH_3CHO , C_4H_6 , iC_4H_8 , C_3H_6O , C_4H_6O and C_4H_8O).

Figure 1 presents experimental and calculated mole fraction profiles for main species: H_2 , iC_4H_8 , O_2 , H_2O , CO and CO_2 . We can observe an excellent agreement between experimental results and simulated ones.

From the model, the main consumption of isobutene is with the hydroxyl radical (OH): $iC_4H_8 + OH = iC_4H_7 + H_2O$ (R.438) by using the rate coefficient suggested by Yasunaga et al. [7], $k_{438} = 2.7 \times 10^{13} \exp(-1510/T)$ [$cm^3 mol^{-1} s^{-1}$]. The iC_4H_7 radical reacts with an hydrogen atom to produce methane and allene ($iC_4H_7 + H = CH_4 + aC_3H_4$ (R.520)), with $k_{520} = 6.31 \times 10^{13}$ [$cm^3 mol^{-1} s^{-1}$] from Santhanam et al. [6]. From allene, the radical propargyl is produced by the reaction R.171: $aC_3H_4 + OH = C_3H_3 + H_2O$, with $k_{171} = 2.0 \times 10^7 T^{2.0} \exp(-503/T)$ [$cm^3 mol^{-1} s^{-1}$] from Miller and Melius [12]. Then, C_3H_3 reacts with the hydroxyl radical to form the C_3H_2 radical (R.158: $C_3H_3 + OH = C_3H_2 + H_2O$ [12]). In this lean flame, C_3H_2 radical reacting with oxygen allows the formation of HCCO and CO, by the global reaction $C_3H_2 + O_2 \Rightarrow HCCO + H + CO$ (R.149), $k_{149} = 2.0 \times 10^{12}$ [$cm^3 mol^{-1} s^{-1}$] from Pauwels et al. [13]. Carbon monoxide is also produced from HCCO by the reaction

$HCCO + O_2 \Rightarrow CO + CO + OH$ (R.35), $k_{35} = 1.63 \times 10^{12} \exp(-432/T)$ [$cm^3 mol^{-1} s^{-1}$] from Peeters et al. [14]. Carbon monoxide is consumed by the classic pathway with the reaction $CO + OH = CO_2 + H$ (R.17), $k_{17} = 6.32 \times 10^6 T^{1.5} \exp(+250/T)$ [$cm^3 mol^{-1} s^{-1}$] from Baulch et al.'s evaluation [15].

A secondary path of iC_4H_8 consumption is the reaction with the hydrogen atom: $iC_4H_8 + H = tC_4H_9$ (R.-502), $k_{502} = 8.30 \times 10^{13} \exp(-1922/T)$ [$cm^3 mol^{-1} s^{-1}$] from the Tsang's evaluation [16]. Tertiobutyl radical (tC_4H_9) isomerizes into iC_4H_9 (R.503), $k_{503} = 3.57 \times 10^{10} T^{0.88} \exp(-17413/T)$ [$cm^3 mol^{-1} s^{-1}$] from Matheu et al. [17]. By decomposition of this last radical, propene and methyl radical are produced: $iC_4H_9 = C_3H_6 + CH_3$ (R.504), $k_{504} = 7.0 \times 10^{12} \exp(-13190/T)$ [$cm^3 mol^{-1} s^{-1}$] from Warnatz's recommendation [18]. We should underline that the main C_3H_6 production comes directly from the isobutene through the reaction R.435, $iC_4H_8 + H = C_3H_6 + CH_3$ with the rate constant $k_{435} = 1.72 \times 10^{13} \exp(-1812/T)$ [$cm^3 mol^{-1} s^{-1}$] from Tsang and Walker [19]. The propene consumption (with oxygen atom) permits forming ketene (CH_2CO) and methyl radical: $C_3H_6 + O \Rightarrow CH_2CO + CH_3 + H$ (R.189), $k_{189} = 1.2 \times 10^8 T^{1.65} \exp(-165/T)$ [$cm^3 mol^{-1} s^{-1}$] from the Tsang's evaluation [20]. By the reverse reaction, ketene produces C_2H_3O ($CH_2CO + H = CH_3CO$ (R.-138), $k_{138} = 3.0 \times 10^{13} \exp(-4040/T)$ [$cm^3 mol^{-1} s^{-1}$] [27]) which forms methyl radical and carbon monoxide by decomposition: $CH_3CO = CH_3 + CO$ (R.139), with $k_{139} = 3.16 \times 10^{14} \exp(-6060/T)$ [s^{-1}] from Lifshitz and Ben-Hamou [27].

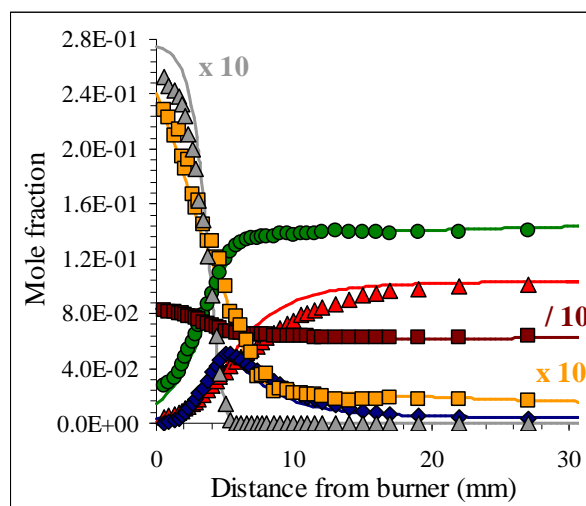


Figure 1: Experimental (symbols) and simulated (lines) mole fraction profiles of main species in the isobutene flame: iC_4H_8 (grey), H_2 (orange), O_2 (brown), H_2O (green), CO_2 (red) and CO (blue).

Figure 2 presents mole fraction profiles for O , OH and HO_2 radicals. The model predicts very well experimental data for the OH radical and underestimates slightly O and HO_2 radicals. We can underline the presence of O and OH in the post-combustion zone,

contrary to HO_2 radical which is produced and consumed in the flame front.

Methyl radical (CH_3), acetylene (C_2H_2) and ethylene (C_2H_4) mole fraction profiles are presented in Fig. 3. In the isobutene flame, these three species are intermediates with a formation and consumption in the flame front. We can see a very good agreement between simulated and experimental results. Indeed, the initial mechanism has been established and validated in rich premixed C_2H_4 flames [8] where ethylene was the reactant.

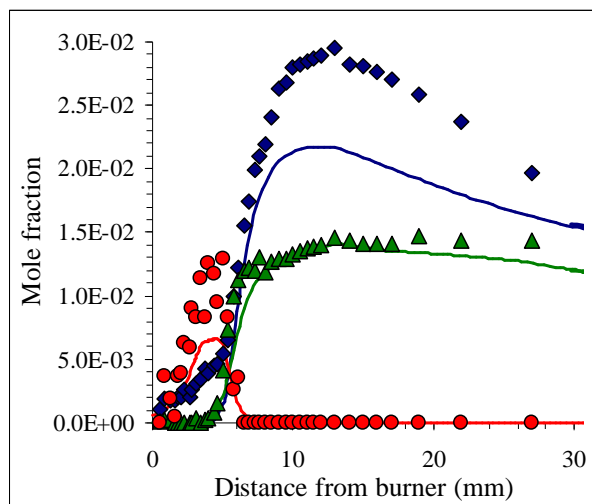


Figure 2: Experimental (symbols) and simulated (lines) mole fraction profiles of O (blue), OH (green) and HO_2 (red) radicals in the isobutene flame.

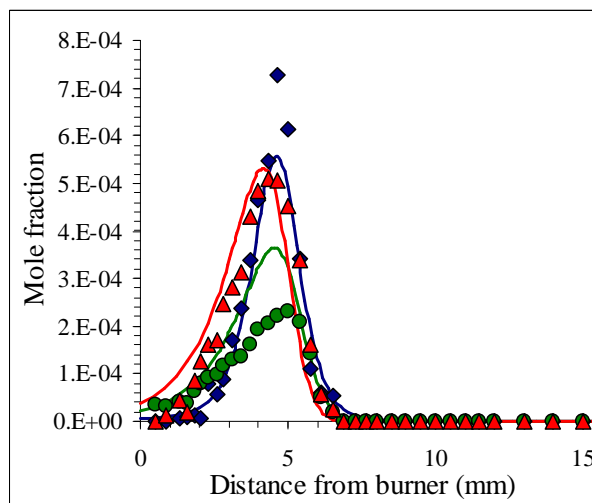


Figure 3: Experimental (symbols) and simulated (lines) mole fraction profiles of CH_3 (blue), C_2H_2 (green) and C_2H_4 (red) radicals in the isobutene flame.

Figure 4 shows experimental and simulated mole fraction profiles of propene (C_3H_6) and 1,3-butadiene (C_4H_6). The simulated profile of propene agrees very well with the experimental one. For C_4H_6 , the model underpredicts significantly the maximum value. We can justify this observation by the number of isomers for

C_4H_6 species at the $m/e = 54$. Indeed, only 1,3-butadiene is present in the mechanism but it is likely that others C_4H_6 species like 1,2-butadiene, 1-butyne or 2-butyne, etc, must be included. As it is written above, the main formation of propene comes from the reaction of isobutene with hydrogen atom ($i\text{C}_4\text{H}_8 + \text{H} = \text{C}_3\text{H}_6 + \text{CH}_3$, R.435 [19]). Propene is the main intermediate during the combustion of isobutene. Along the mechanism, 1,3-butadiene is produced from the decomposition reaction of the $n\text{-C}_4\text{H}_7$ radical: $n\text{-C}_4\text{H}_7 = \text{C}_4\text{H}_6 + \text{H}$ (R.302), $k_{302} = 2.28 \times 10^{52} \text{T}^{-12} \exp(-25770/\text{T})$ [$\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$] from Wang and Frenklach [21]. C_4H_6 reacts with the oxygen atom to produce the C_3H_5 radical: $\text{C}_4\text{H}_6 + \text{O} = \text{C}_3\text{H}_5 + \text{HCO}$ (R.286), $k_{286} = 6.0 \times 10^8 \text{T}^{1.45} \exp(+433/\text{T})$ [$\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$] from Adusei and Fontijn [22].

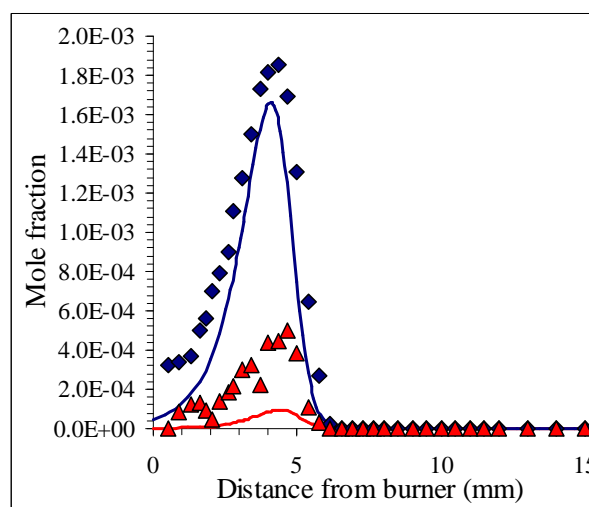


Figure 4: Experimental (symbols) and simulated (lines) mole fraction profiles of C_3H_6 (blue) and C_4H_6 (red) radicals in the isobutene flame.

In Fig. 5, the reaction pathways of major reactants and intermediates are schematized. We can see two main pathways: from $i\text{C}_4\text{H}_7$ radical and from $t\text{C}_4\text{H}_9$ radical. In this kinetic scheme, only isobutene, propene, carbon monoxide and carbon dioxide have been measured and allow to test the reliability of the model by comparison with experimental profiles.

Experimental and simulated mole fraction profiles of light oxygenated species like CH_2O and CH_3CHO are presented in Fig. 6. The simulation of acetaldehyde (CH_3CHO) is excellent compared to experimental profile. For the formaldehyde (CH_2O), the model overestimates by a factor of 30% the experimental maximum mole fraction value. However, the shape and the position of the calculated profile agree well with that measured.

Acetaldehyde is produced from the C_2H_5 radical via the reaction with oxygen atom R.144: $\text{C}_2\text{H}_5 + \text{O} = \text{CH}_3\text{CHO} + \text{H}$, $k_{144} = 6.62 \times 10^{13}$ [$\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$] from Baulch et al. [15]. Indeed, isobutene forms directly C_2H_5 by $i\text{C}_4\text{H}_8 + \text{O} = \text{C}_2\text{H}_5 + \text{CH}_3\text{CO}$ (R.486), $k_{486} = 4.50 \times 10^{12}$ [$\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$] from Yasunaga et al. [7]. Acetaldehyde reacts

mainly with the hydroxyl radical to produce finally a methyl radical, carbon monoxide and water ($\text{CH}_3\text{CHO} + \text{OH} = \text{CH}_3 + \text{CO} + \text{H}_2\text{O}$, R.57 [18]). Formaldehyde is formed by the well know important reaction R.81: $\text{CH}_3 + \text{O} = \text{CH}_2\text{O} + \text{H}$ [15].

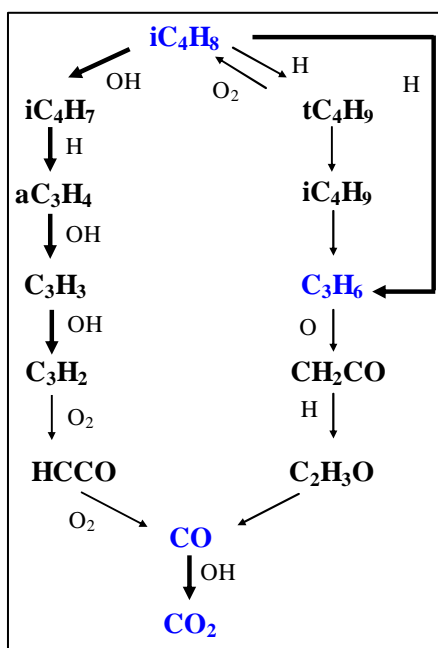


Figure 5: Reaction pathways of formation for important intermediate species in the lean isobutene flame. (Detected species are presented in blue).

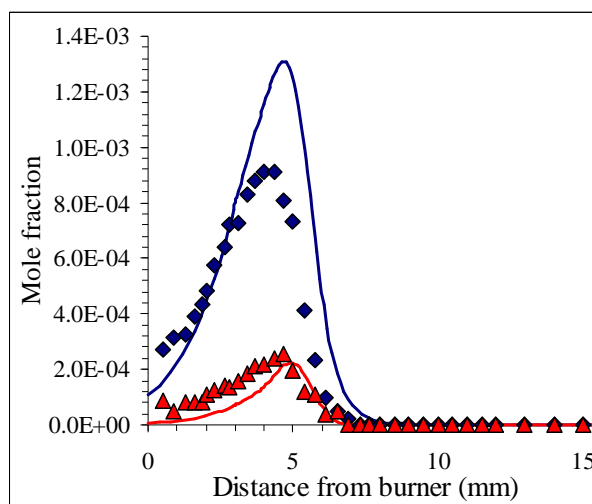


Figure 6: Experimental (symbols) and simulated (lines) mole fraction profiles of CH_2O (blue), and CH_3CHO (red) in the isobutene flame.

Figure 7 presents mole fraction profiles for the heaviest oxygenated species detected, that is to say, $\text{C}_3\text{H}_6\text{O}$ for acetone, $\text{C}_4\text{H}_6\text{O}$ for 1 propen-1-one, 2 methyl- ; and $\text{C}_4\text{H}_8\text{O}$ for prop-1-en-1-ol, 2 methyl- ($\text{pC}_4\text{H}_8\text{O}$) or propanal, 2 methyl- ($\text{mC}_4\text{H}_8\text{O}$). By mass spectrometry, we obtain experimental profiles for each m/e ratio and the identification of species is performed by comparison with previous isobutene studies presented in the

literature [3, 4, 7]. Considering the location of the mole fraction maxima and the shape of profiles, we can suggest that these three species are oxygenated species. According to the m/e , we can identify acetone ($m/e = 58$), 1 propen-1-one, 2 methyl- ($m/e = 70$), $(\text{CH}_3)_2\text{CCHOH}$ and $(\text{CH}_3)_2\text{CHCHO}$ ($m/e = 72$). For the last species, we cannot determine precisely, what is the chemical structure dominative, so both compounds are considered in the mechanism. Both $\text{C}_4\text{H}_8\text{O}$ simulated mole fraction profiles are summed up to be compared to the experimental one. We should underline the predominance by a factor of 14 of the $(\text{CH}_3)_2\text{CCHOH}$ ($\text{pC}_4\text{H}_8\text{O}$) mole fraction compared to the $(\text{CH}_3)_2\text{CHCHO}$ ($\text{mC}_4\text{H}_8\text{O}$) one.

In Fig. 7, we observe a good agreement between simulated and experimental mole fraction profiles. For $\text{C}_4\text{H}_6\text{O}$ and $\text{C}_4\text{H}_8\text{O}$, maximum calculated profiles are shifted of 1.2 mm and 0.8 mm, respectively, toward burnt gases compared to measured profiles.

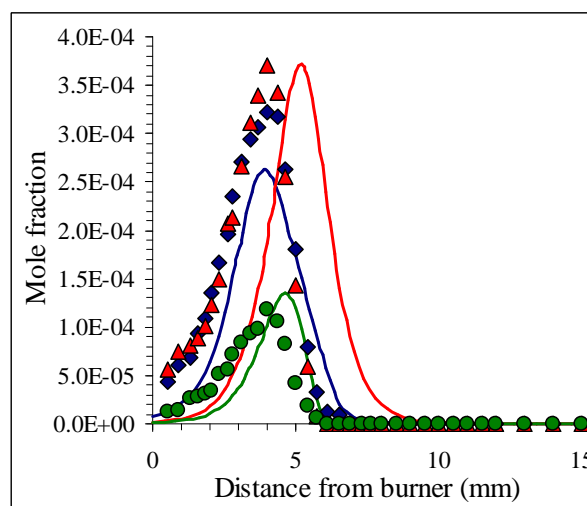


Figure 7: Experimental (symbols) and simulated (lines) mole fraction profiles of $\text{C}_3\text{H}_6\text{O}$ (blue), $\text{C}_4\text{H}_6\text{O}$ (red) and $\text{C}_4\text{H}_8\text{O}$ (green) in the isobutene flame.

The formation and consumption for these three species can be described in detail. From isobutene, $\text{pC}_4\text{H}_8\text{O}$ is produced by the reaction R.499: $\text{iC}_4\text{H}_8 + \text{O} = \text{pC}_4\text{H}_8\text{O}$ from Dagaut et Cathonnet [4], with a rate constant divided by two ($k_{499} = 5.0 \times 10^7 T^{1.28} \exp(+543/T)$ [$\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$]). By isomerisation, $(\text{CH}_3)_2\text{CCHOH}$ ($\text{pC}_4\text{H}_8\text{O}$) forms $(\text{CH}_3)_2\text{CHCHO}$ ($\text{mC}_4\text{H}_8\text{O}$): $\text{pC}_4\text{H}_8\text{O} = \text{mC}_4\text{H}_8\text{O}$ (R.497), $k_{497} = 4.0 \times 10^{13} \exp(-28790/T)$ [$\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$] [4]. By decomposition, both $\text{C}_4\text{H}_8\text{O}$ species produce iC_3H_7 radical: $\text{pC}_4\text{H}_8\text{O} = \text{iC}_3\text{H}_7 + \text{HCO}$ (R.498), $k_{498} = 6.0 \times 10^{13} \exp(-28790/T)$ [$\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$] [4]; and $\text{mC}_4\text{H}_8\text{O} = \text{iC}_3\text{H}_7 + \text{HCO}$ (R.500), $k_{500} = 2.44 \times 10^{16} \exp(-42325/T)$ [$\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$] [4].

As we described previously, the iC_4H_7 radical comes directly from the reaction of OH with isobutene, R.438: $\text{iC}_4\text{H}_8 + \text{OH} = \text{iC}_4\text{H}_7 + \text{H}_2\text{O}$ [7]. And the iC_4H_7 radical reacts with oxygen atom to form $\text{C}_4\text{H}_6\text{O}$ ($(\text{CH}_3)_2\text{CCO}$): $\text{iC}_4\text{H}_7 + \text{O} = \text{C}_4\text{H}_6\text{O} + \text{H}$ (R.488). The rate coefficient is estimated by analogy with the reaction $\text{CH}_3\text{CHCH}_2 + \text{O}$

$\Rightarrow \text{CH}_3\text{CHCO} + \text{H} + \text{H}$, $k_{488} = 1.74 \times 10^{11} \text{T}^{0.7} \exp(-1495/\text{T}) [\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}]$ from the Tsang's evaluation [20]. The main consumption of $\text{C}_4\text{H}_6\text{O}$ produces $\text{C}_3\text{H}_6\text{O}$ via the reaction: $\text{C}_4\text{H}_6\text{O} + \text{O} = \text{C}_3\text{H}_6\text{O} + \text{CO}$ (R.517). To estimate the rate constant, we have considered the reaction $\text{C}_3\text{H}_6\text{O} + \text{O} = \text{C}_3\text{H}_5\text{O} + \text{OH}$ from Herron [23], with $k_{517} = 1.0 \times 10^{13} \exp(-3020/\text{T}) [\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}]$.

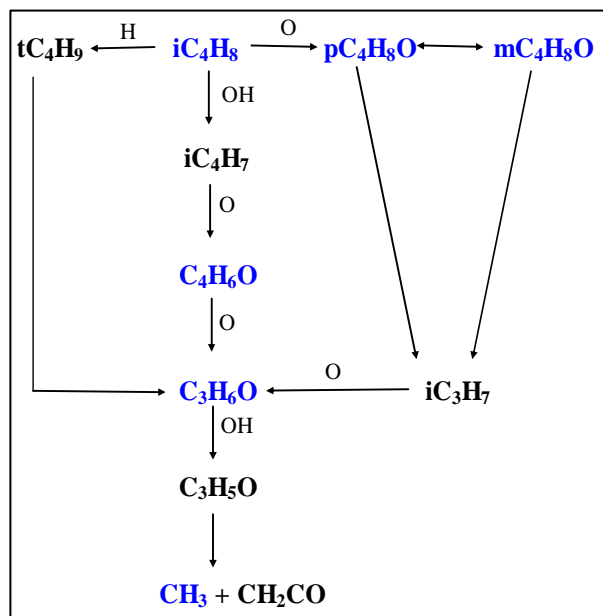


Figure 8: Reaction pathways of formation for oxygenated species: $\text{C}_3\text{H}_6\text{O}$, $\text{C}_4\text{H}_6\text{O}$ and $\text{C}_4\text{H}_8\text{O}$, in the lean isobutene flame. (Detected species are presented in blue).

Acetone is also produced through the reaction of the iC_3H_7 radical with the oxygen atom: $\text{iC}_3\text{H}_7 + \text{O} = \text{C}_3\text{H}_6\text{O} + \text{H}$ (R.512), $k_{512} = 4.82 \times 10^{13} [\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}]$ from the Tsang's evaluation [24]; and from the reaction $\text{tC}_4\text{H}_9 + \text{HO}_2 \Rightarrow \text{C}_3\text{H}_6\text{O} + \text{CH}_3 + \text{OH}$ (R.507), $k_{507} = 1.80 \times 10^{13} [\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}]$ from Dagaut and Cathonnet [4], but with a minor contribution. The acetone consumption allows the formation of $\text{C}_3\text{H}_5\text{O}$ radical by the reaction: $\text{C}_3\text{H}_6\text{O} + \text{OH} = \text{C}_3\text{H}_5\text{O} + \text{H}_2\text{O}$ (R.514), $k_{514} = 2.0 \times 10^{13} \exp(-1510/\text{T}) [\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}]$ from Sato and Hidaka [25]. The decomposition of $\text{C}_3\text{H}_5\text{O}$ radical produces a methyl radical and ketene (CH_2CO): $\text{C}_3\text{H}_5\text{O} = \text{CH}_3 + \text{CH}_2\text{CO}$ (R.487), $k_{487} = 2.0 \times 10^{13} \exp(-16160/\text{T}) [\text{s}^{-1}]$ from Lesoil [26].

The reaction pathway for these three oxygenated species ($\text{C}_3\text{H}_6\text{O}$, $\text{C}_4\text{H}_6\text{O}$ and $\text{C}_4\text{H}_8\text{O}$) is presented in Fig.8.

Conclusions

The lean premixed $\text{iC}_4\text{H}_8/\text{H}_2/\text{O}_2/\text{Ar}$ flame has been studied by molecular beam mass spectrometry at the equivalence ratio of 0.225 at low pressure (40 mbar). We have measured experimental mole fraction profiles of these detected species: H_2 , CH_3 , O , H_2O , C_2H_2 (acetylene), CO , C_2H_4 (ethylene), CH_2O (formaldehyde), O_2 , HO_2 , OH , Ar , C_3H_6 (propene), CO_2 , CH_3CHO (acetaldehyde), C_4H_6 (1,3-butadiene),

iC_4H_8 (isobutene), $\text{C}_3\text{H}_6\text{O}$ (acetone), $\text{C}_4\text{H}_6\text{O}$ (1 propen-1-one, 2 methyl-) and $\text{C}_4\text{H}_8\text{O}$ (prop-1-en-1-ol, 2 methyl- and propanal, 2 methyl-).

A sub-mechanism for isobutene taking into account the formation and the consumption of species involving in the iC_4H_8 combustion is elaborated according to several models from literature. Added to the original model [8], the complete mechanism contains 520 elementary reactions and 99 chemical species. The comparison between simulated and experimental mole fraction profiles allows the validation of this new model for a lean isobutene flame.

The future work consists to test the reliability of this mechanism in a rich isobutene flame to extend its validity range.

Acknowledgements

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References

- [1] Bradley, J.N., West, K.O., *J. Chem. Soc. Faraday Trans.*, 72:558-567 (1975).
- [2] Brezinsky, K., Dryer, F.L., *Combust. Sci. Technol.*, 45:225-232 (1986).
- [3] Curran, H.J., Dunphy, M.P. Simmie, J.M., Westbrook, C.K., Pitz, W.J., *Proc. Combust. Inst.*, 24:769-776 (1992).
- [4] Dagaut, P., Cathonnet, M., *Combust. Sci. Technol.*, 137:237-275 (1998).
- [5] Bauge, J.C., Battin-Leclerc, F., Baronnet, F., *Int. J. Chem. Kinet.*, 30:629-640 (2000).
- [6] Santhanam, S., Kiefer, J.H, Tranter, R.S., Srinivasan, N.K., *Int. J. Chem. Kinet.*, 35:381-390 (2003).
- [7] Yasunaga, K., Kuraguchi, Y., Ikeuchi, R., Masaoka, H., Takahashi, O., Koike, H., Hidaka, Y., *Proc. Comb. Inst.*, 32:453-460 (2009).
- [8] Dias, V., Renard, C., Van Tiggelen, P.J., Vandooren, J., *European Combustion Meeting*, Orléans - France, p.221 (2003).
- [9] Vandooren, J., Branch, M.C., Van Tiggelen, P.J., *Combust. Flame*, 90: 247-258 (1992).
- [10] Wagner, H.Gg., Bonne, V., Grever, T., *Z. Phys. Chem.*, 26: 93 (1960).
- [11] COSILAB®, The Combustion Simulation Laboratory, Version 2.1, www.SoftPredict.com, Rotexo GmbH & Co. KG, Haan (Germany), 2007.
- [12] Miller, J. A., et Melius, C. F., *Combust. Flame*, 91: 21-39 (1992).
- [13] Pauwels, J.-F., Volponi, J. V., Miller, J.A., *Combust. Sci. Technol.*, 110-111:249-276 (1995).
- [14] Peeters, J., Van Look, H., et Ceursters, B., *J. Phys. Chem.*, 100: 15124-15129 (1996).
- [15] Baulch, D. L., Cobos, C. J., Cox, R. A., Esser, C., Frank, P., Just, Th., Kerr, J. A., Pilling, M. J., Troe, J., Walker, R. W., et Warnatz, J., *J. Phys. Chem. Ref. Data*, 21 (1992),

- [16] Tsang, W., *J. Phys. Chem. Ref. Data*, 19:1-68 (1990).
- [17] Matheu, D.M., Green Jr., W.H., Grenda, J.M., *Int. J. Chem. Kinet.* 35:95-119 (2003).
- [18] Warnatz, J., *Combustion Chemistry*, ed. W.C. Gardiner, Jr., pub. Springer-Verlag, NY, (1984).
- [19] Tsang, W.; Walker, J.A., *Proc. Comb. Inst.*, 22:1015-1022 (1988).
- [20] Tsang, W., *J. Phys. Chem. Ref. Data*, 20:221–273 (1991).
- [21] Wang, H., and Frenklach, M., *Combust. Flame*, 110: 173–221 (1997).
- [22] Adusei, G. Y., and Fontijn, A., *J. Phys. Chem.*, 97:1406–1408 (1993).
- [23] Herron, J.T., *J. Phys. Chem. Ref. Data*, 17:967 (1988).
- [24] Tsang, W., *J. Phys. Chem. Ref. Data*, 17 (1988).
- [25] Sato, K., Hidaka, Y., *Combust. Flame*, 112:291-311 (2000).
- [26] Lesoil, H., “Comparaison de la structure de flammes d’acétone et de propionaldéhyde en milieu riche”, Dissertation, Université catholique de Louvain, 1995.
- [27] Lifshitz, A., Ben-Hamou, H., *J. Phys. Chem.*, 87:1782-1781 (1983).