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Kinetic Modeling of the Impact of *n*-Decane Aging on its Combustion Characteristics

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Abstract

In current aircrafts, jet fuels are used as coolants and their oxidation in the liquid phase (autoxidation) occurs before their combustion. Autoxidation changes the fuel composition and its physical properties. Despite its ubiquity, the effects of fuel autoxidation on its combustion characteristics remain unexplored in the literature. In this work, two validated detailed kinetic models for *n*-decane autoxidation and combustion are developed and used to explore these phenomena. Fuel autoxidation has a strong impact on ignition delays, fuel conversion and oxygenated combustion products because of hydroperoxides and alcohols formed during liquid phase oxidation.

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Introduction

In modern aviation, jet fuel is used as a source of energy for engines, but also as a coolant, hydraulic fluid and as a means of balancing and stabilizing the aircraft. It is used as a heat transfer fluid to cool hydraulic and lubrication systems, engines and even the airframe [1]. During its circulation in the different cooling systems of the aircraft, the jet fuel is subjected to temperatures up to 150°C with residence times of up to several seconds. Note that these cycles can be repeated during the recirculation of the jet fuel. Along all its chain of use, from its production to its injection in the combustion chamber, the jet fuel is in contact with air, which allows its saturation in dissolved oxygen [2]. Under these conditions, the oxidation of the fuel in the liquid phase is favored and its resistance to this phenomenon, called thermal oxidation stability, is a crucial criterion in jet fuels formulations. Jet fuels autoxidation leads to changes in its chemical composition, which, in turn, can modify its key physical properties, such as viscosity or freeze point. Deposit and gum formation are consequences of fuel autoxidation at higher extent of reaction and are one of the main adverse effect of liquid oxidation as it clogs the pumps, filters, pipes and heat exchangers [2]. The formation of solids originates from the polymerization of oxygenated molecules formed in the liquid phase oxidation process. The main primary oxygenated products of autoxidation are hydroperoxides which are also well known for weakening elastomer-components such as O-rings and hoses [1]. Standard tests are used to assess the thermal oxidation stability of jet fuels (ASTM D3241) and their peroxide number (ASTM D3703). Thermal oxidation stability standard tests are also in effect for gasoline (ASTM D525), diesel (ASTM D2274) fuels, and lubricants (ASTM D5763) [3]. The thermal oxidation stability constraints and the consequences of autoxidation on the physicochemical properties of jet fuels are therefore well established. However, its consequences on the combustion characteristics of fuels, in terms of reactivity and combustion products remain largely unexplored.

Streva et al. [4] experimentally studied the effects of gasoline-ethanol (E25) blends aging on the fuel properties. Fuels samples were stored in four automotive fuel tanks in a room with open window to the atmosphere and were analyzed in aging periods of 30 and 180 days. Research octane numbers was increased by 2 or 3 units after the first 30 days but by only 1 or 2 units after 180 days. These changes are difficult to explain but the authors note that it could influence the engine performance and exhaust emissions. Owczuck and Kolodziejczyk [5] reported experiments carried out at the Automotive Industry Institute in Poland to explore the effect of long-term storage on gasoline, diesel, and jet fuels. After 4 years of storage, the gasoline samples showed reduced RON and MON values. Zarghami et al. [6] measured the CO emission, unburned hydrocarbon (UHC), and particulate matter (PM) emissions from the

combustion of an aged liquid biofuel in a swirl burner. The liquid biofuel was naturally aged at 20°C for 24 months with analysis every 3 months. Biofuel aging was also accelerated at 80°C and, using viscosity analyses, an equivalent amount of aging was established with natural aging. For example, 31 hours of aging at 80°C is equivalent to 12 months of natural aging at 20°C. Combustion experiments showed that aging increased CO and UHC measurements. The longer aging periods (24 months) led to a considerably degraded fuel with poor combustion performances yielding high PMs levels. Hashimoto et al. [7] probed the effects of autoxidation of different alkanes on the cetane number. All the alkanes studied (*n*-decane, cetane, nonadecane, 2,2,4,4,6,8,8-heptamethylnonane, and 2,6,10,14-tetramethylpentadecane) were autoxidized at 150°C for up to 6 h. The authors quantified the extent of autoxidation of each alkane after aging with the measure of the total hydroperoxide concentration with an iodometric method. For *n*-decane, they showed that when the concentration of hydroperoxides reached 200 ppm in the autoxidation process, the cetane number was increased by 3 units. For 400 ppm, they measured an increase of 5.5 units.

The few studies of the literature show that aging of the liquid fuel has an impact on its combustion characteristics. All studies report an increased in reactivity through RON or cetane number measurements as a consequence of fuel aging. The impact of liquid fuel oxidation on the combustion pollutants remains mostly unexplored. In this work, we investigate the effects of fuel aging on its combustion, using detailed kinetic modeling and *n*-decane as surrogate fuel. Simulations of liquid *n*-decane oxidation are performed in a liquid phase batch reactor model with a recently validated detailed kinetic mechanism [8]. The composition of the liquid fuel at the end of the simulated aging period are then used as an input data for gas phase combustion simulations, using a new combustion kinetic model for *n*-decane and *n*-decanol. This work aims at better understanding the role of fuel aging on its combustion kinetics and, in particular, to investigate its potential impact on combustion pollutants.

Development of liquid- & gas-phase kinetic models

Fuel autoxidation and combustion are characterized by the same radical chain reactions. The kinetic mechanisms are therefore the same and the main differences are in the thermochemical and kinetic data. For combustion, kinetic models use ideal gas thermo-kinetic data, that are independent of the bath gas. In the liquid phase, these data become solvent dependent and a new data set must be used for each fuel. For this reason, the simulation of liquid phase oxidation has long remained an unachievable challenge. The pioneering work of Jalan et al. [9] showed that liquid phase oxidation kinetic models could be generated from gas-phase mechanism with a

correction of gas phase thermo-kinetic data based on the calculation of the Gibbs energy of solvation at infinite dilution ($\Delta_{solv}G$). Jalan et al. [9] first proposed to use a Linear Free Energy Relationships (LFER) of the literature to compute this quantity. The main drawback of this approach is that LFERs were only determined at 298 K and that most autoxidation applications occur at higher temperatures. Our group proposed to use Equations of State (EoS) to calculate $\Delta_{solv}G(T)$ [10] and applied this method to develop detailed autoxidation kinetic models for *n*-butane [11] and *n*-decane [8]. The latter mechanism is used in this work to simulate different extent of *n*-decane aging. The main features of this kinetic model and its performances are recalled here.

Modeling of liquid phase oxidation of *n*-decane

The autoxidation kinetic model of *n*-decane was developed using the following steps: (a) generation of a low-temperature gas phase combustion mechanism for *n*-decane with EXGAS [12]; (b) generated gas-phase thermochemical data were corrected by $\Delta_{solv}G(T)$ calculated with the UMR-PRU EoS [10]; (c) Kinetic data of H-abstractions from *n*-decane by RO• and ROO• radicals, initial O-O bond fissions of hydroperoxides and self-reactions of ROO• radicals were taken from new reaction rate rules, defined for *n*-butane autoxidation, established from literature review and *ab initio* calculations [11]. (d) The remaining kinetic data of the model are the original gas-phase rate constants. Diffusive corrections for bimolecular rate constants were found to be negligible. The kinetic model composed of 250 species and 1835 reactions was validated against several sets of experimental data measured in standardized autoclaves and in a semi-open reactor [8]. Simulations were performed in a liquid batch reactor with T, P and V fixed and the concentration of O₂ kept constant at 7.25×10^{-5} mol/cm³ [8, 9, 11]. Figure 1 presents new validations of this kinetic model against experiments reported by Hashimoto et al. [7] and Syroezchko et al. [13].

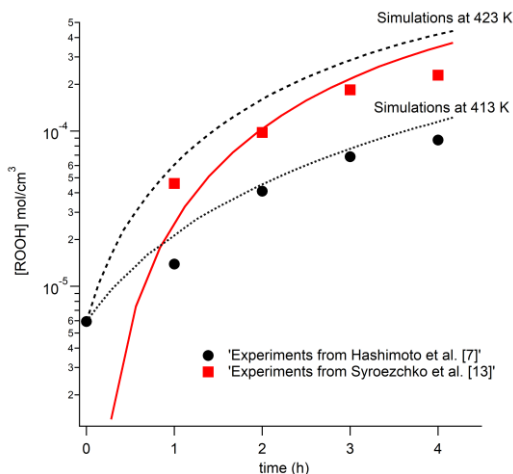


Fig. 1. Evolution of total hydroperoxides concentration during the autoxidation of *n*-decane. Symbols:

experiments from Hashimoto et al. [7] and Syroezchko et al. [13] at 423 K; solid line: simulations at 423 K with no ROOH at $t = 0$ s; dotted lines: simulations with [ROOH] = 5.9×10^{-6} mol/cm³ at $t = 0$ s ($T = 413$ and 423 K).

Both experimental data sets on *n*-decane autoxidation were measured at 423 K but are not in agreement. On average, the total quantity of ROOH measured by Syroezchko et al. [13] is 2.75 times larger than that of Hashimoto et al. [7], and our simulation are in better agreement with the former data (red line and symbols). Note that our model has already been validated against ROOH profiles from two other experimental studies [8]. Hashimoto et al. reported an initial concentration of hydroperoxides of 5.9×10^{-6} mol/cm³ before the autoxidation of *n*-decane. This initial concentration was included in our *in silico* initial composition. The simulations performed at 423 K overestimate their experimental data. If a shift of -10 K is applied in the simulations, we see that the experiments and simulation agree. One can wonder if such a shift is reasonable. Autoxidation experiments were performed on 1 L of *n*-decane sample, in a 1 liter three-necked flask equipped with a reflux condenser, heated with a mantle heater. Under those conditions, it seems reasonable to think that homogeneous isothermal conditions are not ensured. In addition, no information is given on the protocol used to measure hydroperoxides in oxidized fuels, in particular on the cooling of the samples. The temperature shift applied can therefore be deemed as reasonable. Figure 2 presents the evolution of the liquid composition as a function of the autoxidation time.

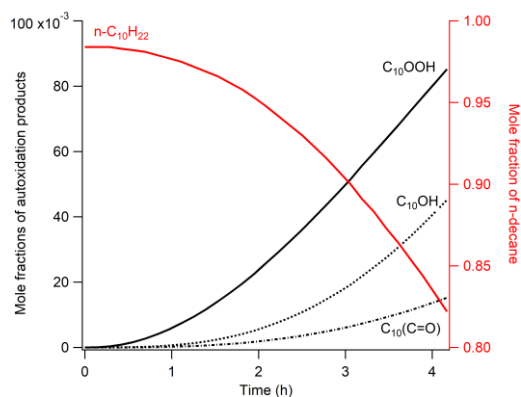


Fig. 2. Simulated *n*-decane conversion at 423 K and main autoxidation products profiles as a function of time. C₁₀OOH, C₁₀OH, and C₁₀(C=O) are lumped C₁₀ hydroperoxides, decanols and C₁₀ carbonyls (decanal and decanone).

The major autoxidation products of *n*-decane autoxidation are C₁₀ hydroperoxides, C₁₀ alcohols, C₁₀ with carbonyl groups. This is in agreement with the literature [8]. It can be noted that water is also a major product in the simulations, with a mole fraction very similar to that of C₁₀(C=O). At 1% *n*-decane conversion, the branching ratios of C₁₀OOH, C₁₀OH and C₁₀(C=O) are 0.86, 0.11, and 0.03, respectively.

Modeling of gas phase oxidation of *n*-decane

The low-temperature combustion kinetic model of *n*-decane was first generated with EXGAS [12]. The generated secondary mechanism was inspected to check if sufficiently comprehensive sub-mechanisms were generated to describe the combustion chemistry of C_{10} hydroperoxides, C_{10} alcohols, C_{10} with carbonyl groups. It was found that this generated model was lacking reactions for decanol. A subsequent kinetic model was generated with *n*-decane and decanol as reactants. This mechanism contains 1179 species and 6784 reactions and was then compared to experimental data of the literature. Figure 3 presents this comparison for experimental data measured in a Perfectly Stirred Reactor (PSR) [14].

It can be seen that the kinetic model developed in this study is able to accurately simulate the experimental data reported by Biet et al. [14]. The addition of a comprehensive decanol sub-mechanism has an impact on the simulated species profiles in Figure 3, compared to the generated model without decanol.

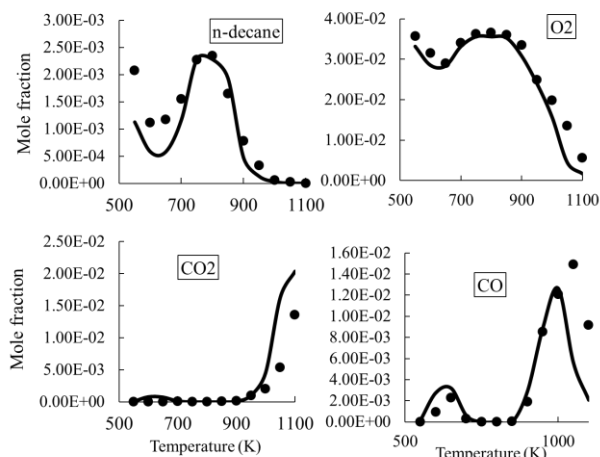


Fig. 3. Experimental (symbols) and simulated (line) species profiles of *n*-decane oxidation in a PSR (residence time of 1.5 s, 1 atm, stoichiometric mixture of 0.23 mol.% C_{10} in He).

In particular, it slightly improved the simulated mole fractions of *n*-decane in the 800 - 1000 K temperature range. Figure 4 presents validations of the model for the autoignition delays of *n*-decane.

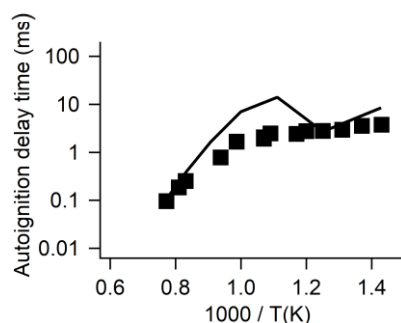


Fig. 4. Experimental [15] (symbols) and simulated (line) autoignition delay times of *n*-decane/air stoichiometric mixtures at $P = 13$ bar.

The new *n*-decane/decanol detailed combustion kinetic model is able to predict the ignition delay times of *n*-decane for temperatures ranging between 700 and 1300 K. The validation of the mechanism under these conditions allows us to establish that the simulation results of the impact of aging on the fuel reactivity and pollutants will be qualitatively reliable.

Impact of fuel aging on its auto-ignition delays

We first quantify the chemical impact of the fuel aging on its ignition delays. Using the liquid phase oxidation model, *n*-decane was aged to different extents, from 0.1 to 10% conversion of the fuel. The composition of the fuel mixture at the end of the aging process was then used as an input in the ignition delay simulations. Figure 5 presents the simulated mole fractions of the main autooxidation products as a function of *n*-decane conversion.

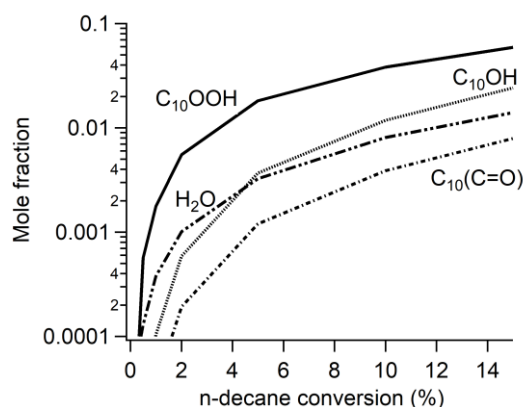


Fig. 5. Product branching ratios as a function of *n*-decane conversion. Pure *n*-decane autooxidation at 413K.

From the simulations, it appears that the C_{10} products branching ratios remain similar with *n*-decane conversion. When higher aging of *n*-decane are reached, the decomposition of hydroperoxides become non-negligible and increases the branching ratio of decanols. For high conversion, the branching fraction of water is also shown to decrease.

Figure 6 presents the variations in ignition delay times as a function of the extent of aging.

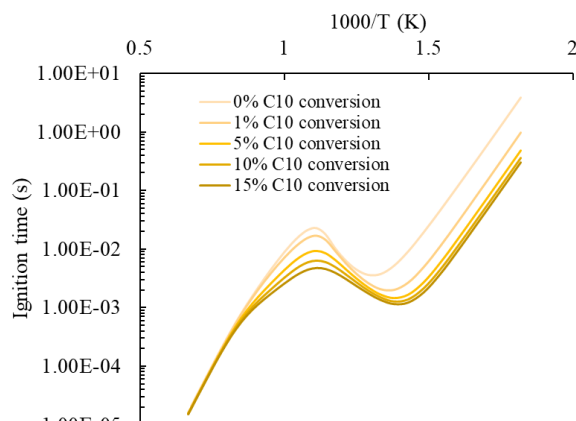


Fig. 6. Autoignition delay times, at 10 atm, of a stoichiometric mixture of *n*-decane / O₂ in air, for different extents of liquid *n*-decane aging.

The effect of fuel aging is clearly highlighted in Figure 6. The more *n*-decane is converted in its autoxidation, the shorter are the ignition delay times, for temperatures up to 1100 K. Above this temperature, ignition delay times are found to be independent of the extent of fuel aging. The most important effect on reactivity are observed between 550 and 700 K, where only 1% of liquid *n*-decane conversion leads to an ignition delay shorter by a factor of 4. Aging is also shown to slightly affect the Negative Temperature Coefficient (NTC) region, with a less pronounced NTC as the extent of aging is advanced. The increased reactivity of the fuel as its aging occurs probably originate in the presence of hydroperoxides in the aged liquid. Figure 7 presents ignition delay times as a function of temperature for three initial compositions: #1 is pure unaged *n*-decane, #2 is aged *n*-decane with the predicted modeling composition after aging (1% *n*-decane conversion) and #3 is the same as #2, but with no hydroperoxides in the input.

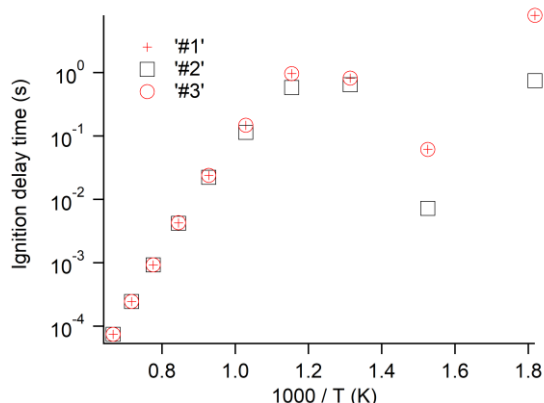


Fig. 7. Simulated ignition delay times of stoichiometric *n*-decane / air mixtures at 1 atm. #1 is unaged *n*-decane, #2 is aged *n*-decane at 1% fuel conversion, and #3 is aged *n*-decane without C₁₀OOH.

Figure 7 clearly shows that the liquid fuel impact of aging on its ignition delays is mainly due to the presence of hydroperoxides. The composition of aged *n*-decane used in simulation #2 includes *n*-decane, C₁₀OOH, C₁₀OH, C₁₀(C=O) and H₂O, while simulation #3 is the same without C₁₀OOH. This brute force sensitivity analysis shows that when hydroperoxides are removed from the initial composition used for the gas phase combustion, aged and unaged *n*-decane ignition delay times are the same from 550 to 1100 K.

Impact of fuel aging on its combustion products

The impact of fuel aging on its combustion products was investigated using the same method as above, but with the combustion process simulated in a

PSR. The conditions selected for the combustion in this reactor are the same as those presented in Figure 3 for pure *n*-decane: residence time of 1.5 s, 1 atm pressure, and a stoichiometric mixture of 0.23 mol.% C₁₀ in He. Figure 8 presents the effect of different extents of aging on the conversion of *n*-decane during its combustion in the gas phase.

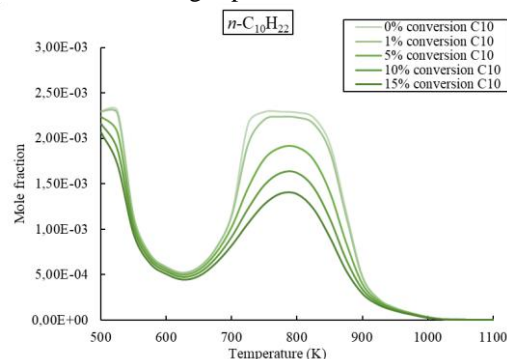


Fig. 8. Simulated gas phase *n*-decane profile in a PSR (residence time of 1.5 s, 1 atm, stoichiometric mixture of 0.23 mol.% C₁₀ in He) as a function of its liquid phase aging, expressed in % conversion of *n*-decane).

Fuel aging before its combustion is found to dramatically affect its reactivity. From 500 to 550 K, an increased extent of aging slightly increases the fuel conversion. Between 700 and 900 K, the most pronounced effects are observed. Pre-aging of the fuel changes the NTC region with an increase of reactivity observed compared to fresh *n*-decane. Figure 9 displays the evolution of the mole fractions simulated for C₁₀ hydroperoxide and C₁₀ alcohol and shows that different behaviors are observed in the different temperature zones.

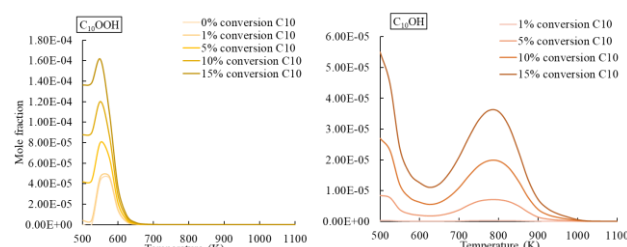


Fig. 9. Simulated C₁₀OOH (decane hydroperoxides) and C₁₀OH (decanol) profiles from *n*-decane oxidation in a PSR (residence time of 1.5 s, 1 atm, stoichiometric mixture of 0.23 mol.% C₁₀ in He) as a function of its liquid phase aging, expressed in % conversion of *n*-decane).

The simulations show that the more advanced is the extent of fuel aging, the more important is the hydroperoxides mole fraction peak at 575 K. The initial values of C₁₀OOH mole fractions at 500 K reflect the variation in the hydroperoxides quantity at the end of each extent of aging that are used in the gas phase composition input. The mole fraction of decanol is negligible up to an extent of aging of 1% liquid *n*-decane conversion. Above this level of conversion, a marked peak of decanol appears at 800 K.

Figure 10 presents the evolution of the main combustion products as a function of the fuel pre-aging.

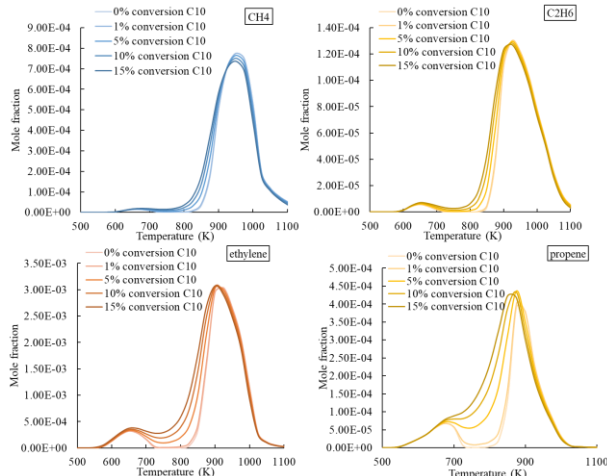


Fig. 10. Simulated products profiles from *n*-decane oxidation in a PSR (residence time of 1.5 s, 1 atm, stoichiometric mixture of 0.23 mol.% C₁₀ in He) as a function of its liquid phase aging, expressed in % conversion of *n*-decane).

The simulation shows that the main products of combustion can be affected by the aging of the fuel. Methane and ethane mole fractions are affected in the 750 – 950 K temperature region. Aging of the liquid fuel leads to higher mole fractions and shifts by about 50 K the production of methane and ethane towards the lower temperatures. Fuel autoxidation effects on ethylene and propene are even more pronounced. For temperatures ranging between 680 and 900 K, pre-aging of the liquid fuel at 1% conversion leads to higher productions of propene and ethylene, by a factor of 5 at 800 K. For higher conversions of liquid *n*-decane, the differences are orders of magnitude. As presented in Figure 11, the effects of aging are less pronounced for CO and CO₂.

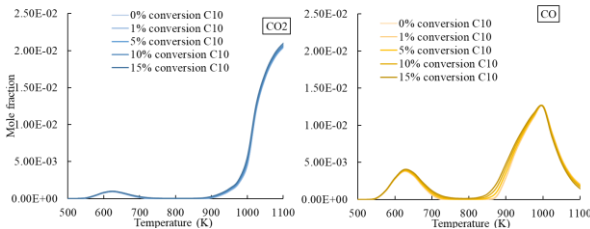


Fig. 11. Simulated products profiles from *n*-decane oxidation in a PSR (residence time of 1.5 s, 1 atm, stoichiometric mixture of 0.23 mol.% C₁₀ in He) as a function of its liquid phase aging, expressed in % conversion of *n*-decane).

CO₂ profiles remain the same for all the extent of aging explored. For CO, differences are observed between 825 and 975 K, and for 5% conversion of *n*-decane, an increase of a factor of 2.5 in the mole fraction is observed at 875 K.

The production of several combustion products is enhanced by the aging of the liquid fuel. Table 1

presents the increase factors between the simulated products for unaged and aged (1% conversion) *n*-decane, for the most affected combustion products.

Table 1. Comparison of predicted mole fractions of combustion products for fresh *n*-decane combustion and “1% conversion” aged *n*-decane, at 800 K. PSR simulations under the conditions of Fig. 8.

	Fresh C ₁₀	Aged C ₁₀ (1% conversion)	Ratio
H ₂ O	10.7 ppm	53.6 ppm	5
H ₂ O ₂	3.7 ppm	14.6 ppm	4
CH ₂ O	0.5 ppm	4.3 ppm	8
CH ₃ CHO	0.2 ppm	1.4 ppm	7

The simulations show that the quantity of minor products such as formaldehyde or acetaldehyde can increase by almost one order of magnitude for 1% conversion of liquid *n*-decane. Despite being produced in small quantities, these compounds can possess a high toxicity and the level of increase due to fuel aging can have dramatic effects on the environment and the human health. The cause of such increases in the quantity of combustion products is due to the accelerated conversion of the fuel induced by the presence of hydroperoxides.

Conclusion

In this work the first rigorous and comprehensive simulations of the impact of liquid phase oxidation of a hydrocarbon fuel on its combustion characteristics have been performed. *n*-Decane was chosen as the surrogate fuel. A validated detailed kinetic model for its autoxidation was used and further validated against another set of experimental data ([ROOH] as a function of time). It was found that this model is able to predict the formation of hydroperoxide with a good level of confidence. The *n*-decane autoxidation model was then used to age the fuel to different extents. The liquid phase composition after each aging was used as an input for combustion simulations. A new *n*-decane combustion kinetic model was developed for this purpose. It includes the combustion sub-mechanisms of lumped decanol, decane hydroperoxides and lumped decane with a carbonyl group. Comparisons with experimental data on *n*-decane combustion showed that the model is able to satisfactorily predict ignition delay times and species profiles in PSR. The combination of the liquid- and gas-phases kinetic model in the simulations showed that aging can dramatically impact the reactivity and the combustion pollutants of the fuel. The more the autoxidation reaction progresses, the more the fuel reactivity increases at low temperature, in terms of shorter ignition delay times and increased conversion. Combustion products were also shown to be affected by the fuel aging. In particular, combustion pollutants that are present in sub-ppm amounts when burning fresh fuel can be increased by an order of magnitude after aging the fuel to a low extent. This point remains

totally unexplored in the literature and deserve more attention as such low quantity pollutant can be highly toxic at low concentration.

Acknowledgments

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