KINETICS OF OXIDATION OF A REFORMULATED JET FUEL (1-HEXANOL/JET A-1) IN A JET-STIRRED REACTOR: EXPERIMENTAL AND MODELING STUDY.

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Abstract
The kinetics of oxidation of a reformulated jet fuel (commercial jet A-1/1-hexanol 90/10 % in mass) were performed using a fused-silica jet-stirred reactor over a range of experimental conditions (temperature: 560 to 1030K, pressure: 10 atm, mean residence time: 1 s, equivalence ratio: 0.5 to 2, initial fuel concentration: 1000 ppm). Concentration profiles of reactants, stable intermediates and final products were measured as a function of temperature. A chemical kinetic reaction mechanism consisting of 7011 reactions involving 2176 species was proposed to represent the data. It is based on previously proposed chemical schemes for the oxidation of 1-hexanol, n-decane, gasoline, and several jet fuels under similar conditions. The kinetic modeling showed reasonable agreement with the present data over the entire range of conditions considered in this study. Reaction paths analyses and sensitivity analyses were used to rationalize the results.

Introduction
Due to increasing global warming issues associated with increasing carbon dioxide emissions and limitation in petroleum availability, the interest for synthetic liquid fuels obtained via a variety of processes, including bio-processes, is of great interest. Beside fully synthetic jet fuel [1], blends of conventional kerosene with bio-derived chemicals have already been considered [2-4]. Among them, long carbon-chain alcohols are interesting since they could be produced in bio-processes [5-7] and mix well with petrol-derived fuels. Furthermore, they should be more stable than fatty acid methyl esters. However, so far no kinetic model was proposed for the combustion of such blends over a wide range of conditions, i.e. covering both cool-flame and high temperature oxidation regimes. Due to the complex composition of jet fuels, surrogate mixtures are frequently used for modeling their kinetics of oxidation[8]. Previously, a model fuel consisting of *n*-decane, *n*-propylcyclohexane, and *n*-propylbenzene was used [8-10]to represent Jet A-1. More recently, the oxidation of a synthetic paraffinic jet fuel (SPK) and a Jet A-1/SPK mixture was modeled with a more complex model fuel consisting of *n*-decane, *n*-propylcyclohexane, *iso*-octane, and *n*-propylbenzene[11].

In the present study, the kinetics of oxidation of a reformulated jet fuel mixture (1-hexanol mixture with a commercial Jet A-1) were measured. These experiments were performed in a jet-stirred reactor (JSR), in order to: (1) compare the chemical kinetics of oxidation of conventional and reformulated jet fuels, (2) provide new information on the kinetics of oxidation of a reformulated jet fuel over a broad range of conditions, and (3) propose and validate a detailed kinetic reaction mechanism for the oxidation of a reformulated jet fuel from low to high temperatures.

Experimental setup
The high-pressure jet-stirred reactor (JSR) used here is similar to that used earlier [12-14]. It consists of a fused silica (to minimize wall catalytic reactions) sphere of 33 cm^3 in volume,

equipped with four nozzles of 1 mm internal diameter for the injection of the gases achieving the stirring. It was located inside a regulated electrical resistance oven of ≈1.5kW wrapped with insulating ceramic wool and enclosed in a stainless steel pressure-resistant jacket allowing operation at high-pressure, i.e. up to 40 atm. A nitrogen flow of 100 L/h was used to dilute the fuel and avoid pyrolytic reactions before admission in the reactor. All gases were preheated before injection to minimize temperature gradients inside the JSR. The liquid fuel was atomized and vaporized before injection into the reactor using an in-house atomizer-vaporizer assembly maintained at ca. 550 K. The fuel and oxygen (99.995% pure, Air Liquide) were diluted by a flow of nitrogen (<50 ppm of O_2; <1000 ppm of Ar; <5 ppm of H_2, Air Liquide), and mixed at the entrance of the injectors. The experiments were performed at steady state, at a constant mean residence time of 1 s, the reactants flowing continuously in the reactor (Table 1).

Table 1. Experimental conditions in the JSR

Initial mole fractions			φ	P/ atm
1-hexanol-Jet A1 mixture	O_2	N_2		
0.001	0.033	0.966	0.5	10
0.001	0.01542	0.98358	1	10
0.001	0.00771	0.99129	2	10

The temperature of the gases inside the JSR ranged from 560 to 1030 K. A high degree of dilution was used (1000 ppm of fuel corresponding to 10280 ppm of carbon), minimizing temperature gradients in the JSR and heat release. Thermocouple (0.1 mm Pt/Pt-Rh 10% wires located inside a thin-wall fused-silica tube) measurements showed a good thermal homogeneity along the vertical axis of the JSR (gradient < 3 K/cm).

The reacting mixtures were sampled via a low-pressure fused-silica sonic probe. The samples (≤50 Torr), were taken at steady temperature and residence time. They were analyzed on-line by Fourier Transformed Infra-Red spectrometry (FTIR) and gas chromatography-mass spectrometry (GC-MS), and off-line, after collection and storage at low-pressure (ca. 40 mBar) in 1 L Pyrex bulbs, by GC. The condensable compounds were analyzed on-line whereas permanent gases and volatile species were analyzed off-line. A heated glass piston chamber was used to pressurize the samples to 1 Bar in the GC injection loop. Gas chromatographs equipped with capillary columns (DB-5ms, DB-624, Plot Al_2O_3/KCl, Carboplot-P7), thermal conductivity detector (TCD), and flame ionization detector (FID), were used for species measurements. Compound identification was made via GC/MS analyses using an on-line ion trap detector (Saturn 2000, Varian) and an off-line quadrupole mass spectrometer (V1200, Varian), both operating in electron impact ionization mode (70 eV). On-line FTIR analyses (Nicolet Magna 550; 1 cm^{-1} resolution) were used to quantify H_2O, CO, CO_2, CH_2O, CH_4, and C_2H_4. For these measurements, the sampling probe was connected to a temperature controlled (140 °C) gas cell (2 m path length; 500 mBar) via a 6.35 mm O.D. deactivated stainless steal heated line (200 °C). A good repeatability of the measurements and a reasonably good carbon balance (100 ± 10%) were obtained in these series of experiments. No oxygen balance could be computed since numerous oxygenated intermediates could not be measured.

Computational methods

The PSR computer code of the Chemkin II library [15]was used for the kinetic modeling. It computes species concentrations from the balance between the net rate of production of each species by chemical reactions and the difference between the input and output species flow rates. The detailed chemical kinetic scheme used here derives from previous studies on the oxidation of liquid fuels (gasoline, diesel, SPK, and kerosene) and surrogates [8, 16-17]. Cross-reactions between the fuel components sub-schemes were included. For the kinetic modeling, a surrogate model fuel was used. In the computations, the fuel was represented by a mixture of *n*-decane (CAS 124-18-5), *iso*-octane (2,2,4-trimethyl pentane; CAS 540-84-1), *n*-propyl cyclohexane (CAS 1678-92-8), *n*-propyl benzene (CAS 103-65-1), and 1-hexanol (CAS 111-27-3). The model fuel composition was chosen on the basis of GC analyses and previous studies on SPK and SPK/Jet A-1 oxidation[11, 18]. The proposed kinetic reaction mechanism consisting of 7011 reactions involving 2176 species is available from the authors. The rate constants for the reverse reactions were computed from the forward rate constants and the equilibrium constants computed using the appropriate thermochemical data [8, 16-17]. The pressure dependencies of the unimolecular reactions and of pressure-dependent bimolecular reactions were taken into account when information was available (i.e., k(P,T)). Local 1st-order sensitivity analyses and reaction rate analyses, by computing the rates of consumption (R with a negative value) and production (R with a positive value) for every species, were performed.

Results and Discussion

In this study, the oxidation of reformulated kerosene was performed in a JSR. The fuel had a density of 0.807 g/cm^3 at room temperature and a global chemical formula of $C_{10.28}H_{20.85}O_{0.14}$. The composition of the Jet A-1 was determined to be ca. 24.1% *iso*-alkanes, 15% *n*-alkanes, 23.2% naphtenes (cycloalkanes), and 37.4% aromatics in mole. The composition of the surrogate model fuel used in the kinetic modeling is given in Table 2.

Table 2. Composition of the model fuel (initial fuel concentration = 1000 ppm).

Initial concentrations (ppm)				
n-Decane	*iso*-Octane	n-Propylcyclohexane	n-Propylbenzene	1-Hexanol
316	82	378	245	144

Since *iso*-octane is much more branched than the *iso*-alkanes present in the fuel, as previously [11], a lower concentration of *iso*-octane was used in the model fuel.

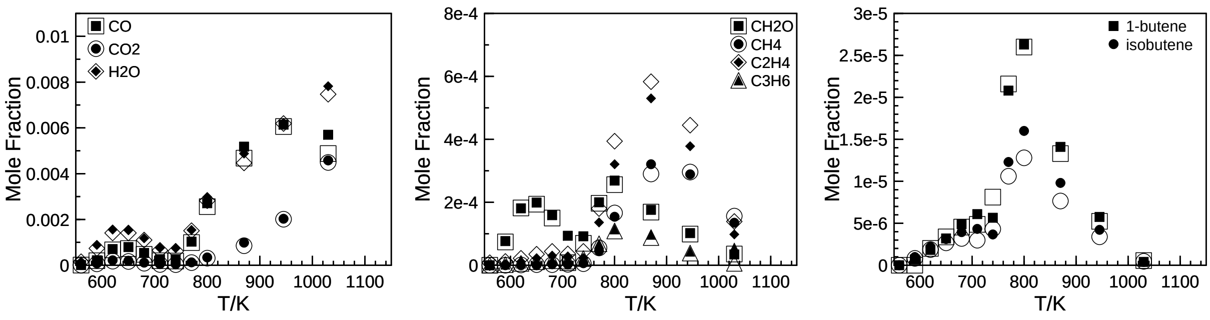

Figure 1. Comparison of experimental concentration profiles measured during the oxidation of Jet A-1 (closed symbols) and reformulated kerosene (open symbols) under the same conditions (φ=1, 1000 ppm of fuel, 10 atm, 1 s).

In the present experiments, the temperature was varied step-wise in the range 560–1030 K, keeping the residence time equal to 1s. This temperature range allowed the observation of the cool-flame oxidation regime (~560-760 K), the negative temperature coefficient (NTC,

~660-760 K) regime, and the high-temperature oxidation regime (>760 K). The experiments were performed for several equivalence ratios (φ=0.5, 1, and 2).

More than 17 species were identified and measured by CG/MS, FID, and TCD. Experimental concentration profiles were obtained for H_2, H_2O, O_2, CO, CO_2, CH_2O, CH_4, C_2H_6, C_2H_4, C_2H_2, C_3H_6, C_3H_4 (allene and propyne), 1-C_4H_8, i-C_4H_8, C_6H_6, toluene. Uncertainties for the measured concentrations based on analytical and systematic error were estimated to be ca. 10%. Other minor products detected (ppm level) were not quantified nor used in the kinetic modeling.

To evaluate the impact of fuel reformulation, we compared the concentration profiles measured from the oxidation of 100% Jet A-1 and the present reformulated kerosene (Figure 1.) As can be seen from that figure, the concentration profiles obtained for most of the measured species during the oxidation of the two fuels are very similar over the entire range of experimental conditions. Slightly lower concentrations of *iso*-butene and higher concentrations of ethylene were measured with the reformulated kerosene, due to dilution effect of 1-hexanol.

The concentration profiles obtained for the oxidation of the reformulated jet fuel were compared to the present model predictions. As introduced in the previous section, a detailed chemical kinetic reaction mechanism was used to represent the oxidation of the fuels. The mechanisms used previously for modeling the oxidation of a SPK jet-fuel[11] and 1-hexanol [7] were merged. The resulting scheme included both low- and high-temperature oxidation processes. The present model was also successfully tested for the oxidation of the pure surrogate fuel components under similar JSR conditions. Figures 2-4 show examples of the present results obtained at 10 atm for the oxidation of reformulated jet fuel.

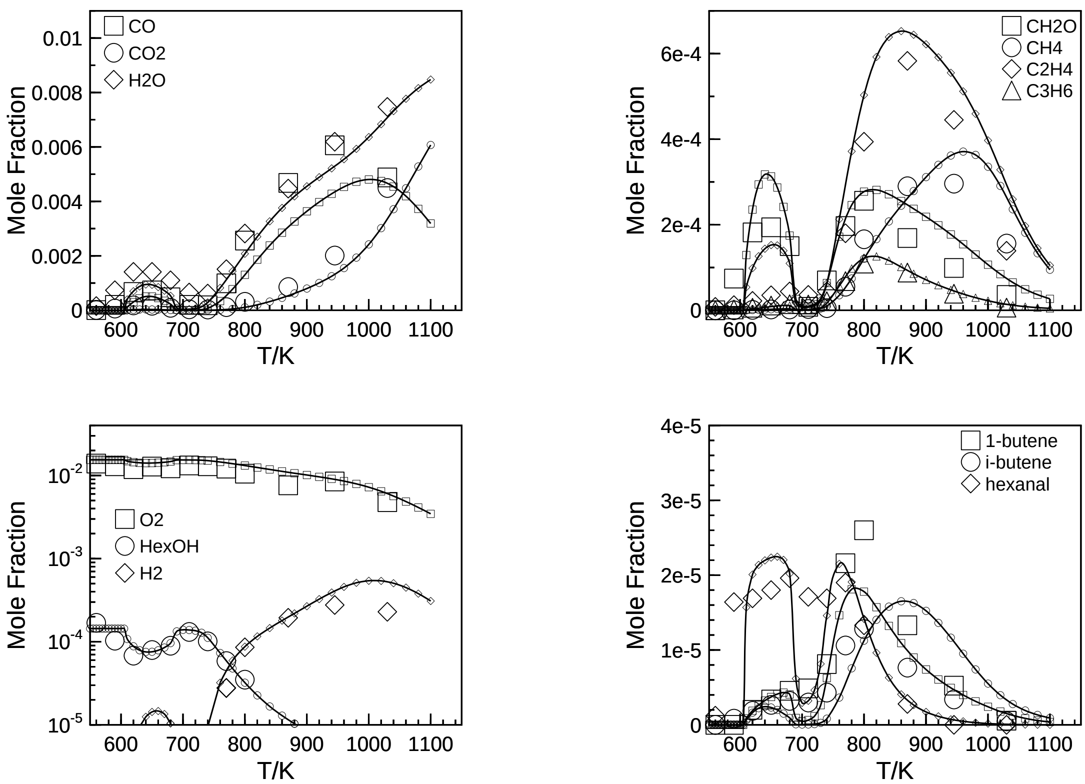

Figure 2. Comparison between experimental (large symbols) and computational (lines and small symbols) concentration profiles measured during the oxidation of reformulated kerosene (φ=1, 1000 ppm of fuel, 10 atm, 1 s).

As can be seen from these figures, the present model represents reasonably well the measured concentration profiles obtained for most of the species. However, it tends to over-estimate the formation of CH_2O, particularly under fuel-lean conditions. It also over-estimates the production of ethylene in fuel-lean conditions. It should be noted that the formation of hexanal (Figure 2), resulting from the oxidation of hexanol, is well-predicted by the present model.

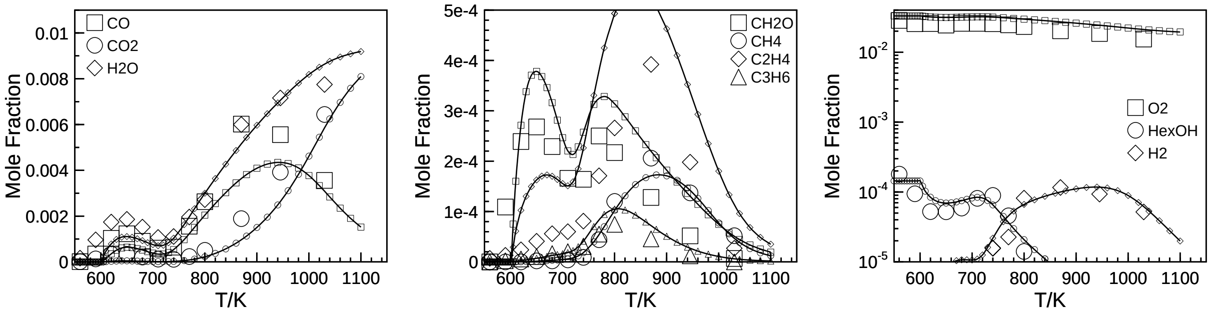

Figure 3. Comparison between experimental (large symbols) and computational (lines and small symbols) concentration profiles measured during the oxidation of reformulated kerosene (φ=0.5, 1000 ppm of fuel, 10 atm, 1 s).

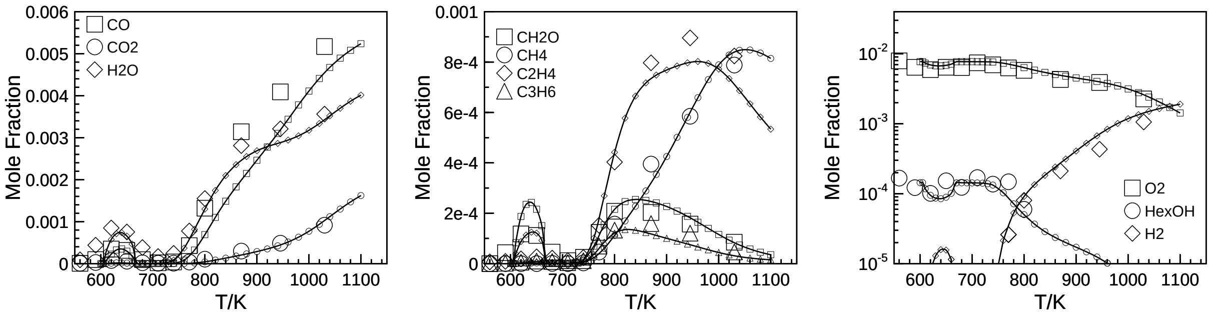

Figure 4. Comparison between experimental (large symbols) and computational (lines and small symbols) concentration profiles measured during the oxidation of reformulated kerosene (φ=2, 1000 ppm of fuel, 10 atm, 1 s).

Kinetic modeling was used to interpret the results. According to the present computations, at 800 K and stoichiometric conditions, 1-hexanol mainly reacts by metathesis with OH (91%) and to some extent with HO_2 (2.5%). Hexanal formation results from the oxidation of 1-hexanal:

3412. $CH_3CH_2CH_2CH_2CH(.)OH+O_2 \rightleftarrows C_5H_{11}HCO+HO_2$; R(hexanal)=0.75

Propylbenzene also reacts by metathesis with OH (76%) and to some extent with HO_2 (1.5%). Its reaction with H occurs through propyl elimination (1.5%):

2738. Pr-Benzene+H $\rightleftarrows$ $nC_3H_7+C_6H_6$

Propylcyclohexane also reacts via metathesis with OH (92%). *Iso*-octane mainly reacts by metathesis with OH (87%) and also with HO_2 (5.6%). The computations indicated that its oxidation is responsible for the formation of *iso*-butene. That formation occurs mainly via the following reactions:

2900. $tC_4H_9+O_2 \rightleftarrows iC_4H_8+HO_2$; $R(iC_4H_8)=0.483$

3093. 2,2,3-trimethyl-1-pentyl $\rightleftarrows$ $iC_4H_8+iC_4H_9$; $R(iC_4H_8)=0.039$

3097. 2,4,4-trimethyl-2-pentyl $\rightleftarrows$ $tC_4H_9+iC_4H_8$; $R(iC_4H_8)=0.232$

Among the main stable intermediates, ethylene formation occurs via decomposition of $C_2H_4O_2H$ and $C_2H_5O_2$:

231. $C_2H_4+HO_2 \rightleftarrows C_2H_4O_2H$; $R(C_2H_4)=0.294$

325. $C_2H_5O_2 \rightleftarrows C_2H_4+HO_2$; $R(C_2H_4)=0.08$

The decomposition of 1-C_5H_{11}, essentially produced from the oxidation of n-decane, also contributes to ethylene formation:

989. $1C_5H_{11} \rightleftarrows nC_3H_7+C_2H_4$; $R(C_2H_4)=0.05$

The decomposition 1-propyl-phenyl also yields ethylene:

2782. 1-propyl-phenyl $\rightleftarrows$ $C_6H_5CH_2+C_2H_4$; $R(C_2H_4)=0.132$

The oxidation of n-propylcyclohexane also contributes to ethylene formation, mainly through the decomposition:

6136. 2-$C_7H_{11} \rightarrow 2\ C_2H_4+C_5H_7$; $R(C_2H_4)=0.095$

Ethylene is mainly consumed via recombination with H and metathesis with OH under these conditions:

226. $C_2H_4+H(+M) \rightleftarrows C_2H_5(+M)$; $R(C_2H_4)=-0.537$

232. $C_2H_4+OH \rightleftarrows C_2H_3+H_2O$; $R(C_2H_4)=-0.275$

Methane is another important intermediate formed during the oxidation of reformulated jet fuel. It is mainly formed via reactions of methyl radicals with HO_2 and formaldehyde:

75. $CH_3+HO_2 \rightleftarrows CH_4+O_2$; $R(CH_4)=0.22$

199. $CH_2O+CH_3 \rightleftarrows HCO+CH_4$; $R(CH_4)=0.294$

Many other metathesis reactions of methyl radicals contribute to methane formation. Methane is essentially consumed by metathesis with OH:

77. $CH_4+OH \rightleftarrows CH_3+H_2O$; $R(CH_4)=-0.995$

Propene is formed by oxidation of propyl radicals. Among the most important reactions forming propene through oxidation of C_3H_7 radicals, one finds:

466. $nC_3H_7+O_2 \rightleftarrows C_3H_6+HO_2$; $R(C_3H_6)=0.159$
467. $iC_3H_7+O_2 \rightleftarrows C_3H_6+HO_2$; $R(C_3H_6)=0.067$
3821. $C_3H_6OOH1\text{-}2 \rightleftarrows C_3H_6+HO_2$; $R(C_3H_6)=0.199$

Propene is also produced by thermal decomposition of n-alkyl radicals derived from n-decane oxidation:

990. $2C_5H_{11} \rightleftarrows C_2H_5+C_3H_6$; $R(C_3H_6)=0.108$
2045. $2C_{10}H_{21} \rightleftarrows 1C_7H_{15}+C_3H_6$; $R(C_3H_6)=0.072$

The main oxidation route of propene is metathesis with OH (42%). 1-Butene is produced by oxidation of n-butyl radicals and decomposition of n-decyl and n-hexyl radicals, all released during n-decane oxidation:

706. $1C_4H_9+O_2 \rightleftarrows C_4H_8+HO_2$; $R(C_4H_8)=0.18$
1361. $3C_7H_{15} \rightleftarrows nC_3H_7+C_4H_8$; $R(C_4H_8)=0.087$
2046. $3C_{10}H_{21} \rightleftarrows 1C_6H_{13}+C_4H_8$; $R(C_4H_8)=0.307$

1-Butene oxidation mainly occurs via reaction with OH radicals (87%). Formaldehyde is produced by oxidation of vinyl and hydroxymethyl radicals and the decomposition of methoxy radicals:

2. $C_2H_3+O_2 \rightleftarrows CH_2O+HCO$; $R(CH_2O)=0.24$
161. $CH_2OH+O_2 \rightleftarrows CH_2O+HO_2$; $R(CH_2O)=0.087$
165. $CH_3O+M \rightleftarrows CH_2O+H+M$; $R(CH_2O)=0.267$

Its oxidation by OH and HO_2 yields HCO that, in turn, produces carbon monoxide:

198. $CH_2O+OH \rightleftarrows HCO+H_2O$; $R(CH_2O)=-0.685$
201. $CH_2O+HO_2 \rightleftarrows HCO+H_2O_2$; $R(CH_2O)=-0.138$
52. $HCO+O_2 \rightleftarrows CO+HO_2$; $R(HCO)=0.534$

CO mostly oxidizes by reaction with OH:

44. $CO+OH \rightleftarrows CO_2+H$; $R(CO)=-0.77$

Sensitivity analyses were also performed to identify the most influencing reactions. As can be seen from Figure 8, the most sensitive reactions involve small species pertaining to the C_0-C_2 sub-scheme. This result is actually in line with what was reported earlier in the literature for the oxidation of similar fuels in similar conditions. The recombination of HO_2 radicals tends to reduce the overall oxidation process (probed here by the formation of one of the final products, i.e. H_2O) at this temperature whereas the decomposition of H_2O_2 favors the overall oxidation by releasing the main oxidation agents, i.e. OH radicals:

$$2\ HO_2\ (+M) \rightleftarrows H_2O_2\ (+M)$$
$$H_2O_2\ (+M) \rightleftarrows 2\ OH\ (+M)$$

The kinetics of oxidation of propene and 1-hexene by OH are also influential.

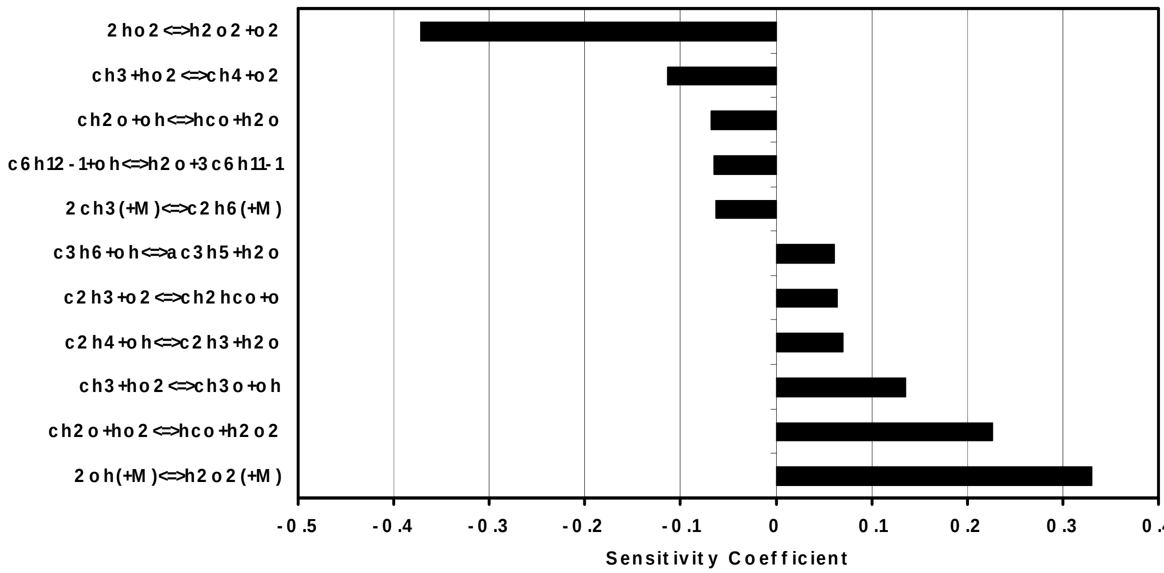

Figure 8. Sensitivity spectrum for H_2O during the oxidation of a synthetic jet fuel in a JSR at 10 atm, τ= 1s, φ= 1, and 800K.

Conclusion

The main objectives of this study were achieved. We compared the chemical kinetics of oxidation of conventional and reformulated jet fuels, showing very little differences. The kinetics of oxidation of reformulated jet fuel (commercial jet A-1/1-hexanol 90/10 % in mass) carried out in a fused-silica jet-stirred reactor over the temperature range 560 to 1030K, at a pressure of 10 atm, for equivalence ratios ranging from 0.5 to 2, an initial fuel concentration of 1000 ppm, and a fixed residence time of 1 s yielded a large set of data. Concentration profiles of reactants, stable intermediates, and final products were measured as a function of temperature. A chemical kinetic reaction mechanism consisting of 7011 reactions involving 2176 species was proposed to represent the data. It is based on previously proposed chemical schemes for the oxidation of 1-hexanol and several kerosene fuels under similar conditions. The kinetic modeling showed reasonable agreement with the data over the present range of conditions. The results were analyzed performing sensitivity analyses and reaction paths analyses.

Further kinetic modeling of reformulated jet fuel ignition and flame speeds are still needed to fully assess the validity of the proposed model. The use of an *iso*-alkane less branched than *iso*-octane should be considered in future the kinetic modeling. That should be possible thanks to recent studies on the oxidation of 2-*iso*-alkanes [19].

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