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Development of a surrogate and its comprehensive compact chemical kinetic mechanism for the combustion of Alcohol-To-Jet fuel

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Abstract
This study develops a compact high-fidelity chemical kinetic mechanism for a proposed surrogate of Alcohol-To-Jet fuel, capable of modelling ignition delay time, laminar flame speed, and species concentration. A combination of 85% iso-dodecane and 15% iso-cetane by wt% that is a close approximation to the real fuel composition was selected as the ATJ surrogate to investigate the simulation of the three given combustion properties. A relatively good agreement has been observed for ignition delay, laminar flame speed, and mole fraction of some species, between the simulation by the Chemkin-Pro software package and the available experimental data in the literature. The authors suggest that this proposed surrogate with its compact validated mechanism can be used by researchers to study the combustion behaviour of ATJ fuel including the investigation on the complex geometries of combustion system such as Equivalent Reactor Network Analysis which require a compact accurate chemical kinetic mechanism.

Keywords Jet fuels chemical kinetics · Skeletal mechanism · ATJ fuel · Ignition delay · Flame speed · Species concentration

Abbreviations

ATJ	Alcohol-To-Jet
atm	Atmosphere
CFD	Computational fluid dynamics
GHG	Green-house gases
IC12	Iso-dodecane
IC16	Iso-cetane
IDT	Ignition delay time
LES	Large eddy simulation

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LPST	Low pressure shock tube
MW	Molecular weight
NTC	Negative temperature coefficient
QOOH	Alkylhydroperoxy radicals
OOQOOH	Peroxy-alkylhydroperoxides
R	Fuel radicals
RCM	Rapid compression machine
RO2	Alkylperoxy radicals
SP	Smoke point

Introduction

Today, having a higher efficiency combustion with reduced emissions is a necessity, especially in the field of aviation which is facing a growing demand for the foreseeable future. There has been a huge growth of aviation kerosene (jet fuels) usage in air transportation during the recent decades that has caused serious environmental issues. As an example, the ten percent increment in the proportion of international aviation transport among the other sectors producing GHG emissions from 1990 to 2017 [1], shows the negative impacts of the usage growth in consumption of the aviation kerosene based fuels. This coincides with the increasing price of fossil fuel and the application of stricter rules for environmental protection worldwide, demonstrating the significance of developing technical solutions to address these issues. In this regard, researchers are focused on the improvement of the combustion efficiency of conventional jet fuels and investigating promising alternative candidates.

Using renewable alternative fuels is one of the promising approaches that not only help to improve the combustion efficiency, but also can satisfy the need to reduce or end the application of fossil fuels. By having a higher fuel quality, considerable emissions reduction can be achieved, but it requires to have a deep understanding of the chemical interactions in the combustion process of the alternative fuels. Moreover, for developing a satisfactory computational fluid dynamics (CFD) or large eddy simulation (LES) study of the fuels, as the important techniques of combustion investigation, a vital prerequisite is to have an accurate knowledge of chemical kinetics of combustion and develop a mechanism that successfully simulates the global combustion properties.

One of the promising aviation alternative fuels is Alcohol-To-Jet (ATJ) which can be extracted by hydrogenation, dehydration, and oligomerisation of alcohol. ATJ is produced commonly from iso-butanol feedstock and mostly composed of highly branched alkanes includes iso-dodecane (~ 85%) and iso-cetane (~ 15%). The properties of the fuel and its components are given in Table 1. This renewable drop-in jet fuel has been approved to be used in aviation sector, but can only be blended up to 30% with conventional fuels, mostly because of the lack of aromatic content and also having a relatively long ignition delay time that are not favourable for the engine operation.

In spite of its great importance, ATJ is not a well-analyzed fuel and not much attention has been given to the detailed understanding of the combustion process of

Table 1 The physicochemical characteristics of iso-dodecane, iso-cetane, and ATJ fuels [2, 3]

Fuel	DCN	MW (g/mol)	H/C ratio	Density (kg m^{-3})	Viscosity(cst)	Flash point (°C)	SP (mm)
Gevo ATJ	15.5	175.6	2.17	756	2.1	48	35
iso-dodecane	16.8	170.3	2.17	745	1.31	45	35.2
iso-cetane	15	226.4	2.13	784	4.7	69	31.2

this promising alternative drop-in fuel which is currently used in the aviation sector [4–7]. A limited number of investigations have been made to study the physical properties of ATJ and developing surrogate representations for these properties [2, 8]. Ignition delay of ATJ at relatively low temperatures were studied by Min et al. [9] where they experimentally investigated ignition delay of a range of jet fuels using a rapid compression machine (RCM) for just a limited number of low temperature points at 20 bar. Zhu et al. [10] investigated ignition delay times of conventional and alternative fuels behind reflected shock waves at 3 and 6 bar, for stoichiometric conditions, and provided data for ignition delay times of GEVO ATJ at just high temperatures. Later in 2016, Hass et al. [11] suggested a surrogate for ATJ fuel by using a 50/50 composition of iso-octane and iso-cetane, and developed a kinetic mechanism for simulation of the ignition delay against the experimental data provided by Zhu et al. [10]. The mechanism did not demonstrate a close emulation of the experimental ignition delay at high temperature. A shock tube study was conducted by Flora et al. [12] to provide data for the ignition delay of candidate drop-in replacement jet fuels including GEVO ATJ at 20 bar and a lean condition (0.5). Parise et al. [13] conducted a Shock tube/laser absorption measurement to study the decomposition of ATJ fuel in a shock tube, and obtained a multiple species time-history measurement for temperatures between 1070 and 1320 K and pressures between 1.3 atm and 1.5 atm. They used an iso-cetane mechanism as the representative of ATJ iso-parafins to simulate the experiments. Ritcher et al. [14] made experimental investigations on laminar burning velocity and ignition delay time of ATJ-SPK and Jet A-1. They reported similar ignition results for both fuel types at the initial pressure pinitial = 1.6 MPa, for two different equivalence ratios of 1.0 and 2.0, and the initial temperature between 800 and 1700 K. The result of laminar burning velocity at 473 K also showed a similarity between two fuels, at three pressures of 0.1, 0.3, and 0.6 MPa.

In recent years, a series of investigations were directly dedicated to ATJ fuel, and contributed to improving the combustion understanding of the fuel [15–21]. Guzman et al. [15] conducted Single pulse shock tube experiments to determine the pyrolytic and oxidative decomposition products of an alcohol-to-jet fuel at 4 bar nominal pressure, 2 ms nominal reaction time, and temperatures ranging from 900 to 1550 K. They developed a detailed iso-alkane kinetic model against the experimental results, and a good agreement was observed between the empirical and simulated data. They continued their research on the species concentration of ATJ fuel by blending it with n-heptane and F-24 fuel [16, 17]. They used various kinetic models in the literature to test the ability of the models to simulate the influence of the test conditions on the evolution of intermediate species. It was also reported that increment of the initial fuel load does not affect the results significantly, while, increasing the pressure reduces the mixture reactivity temperature. The blend of F24/ATJ was also studied by Kim et al. [18] who conducted rapid compression machine (RCM) experiments in order to analyse the effects of chemical composition and blend ratio on ignition delay at the pressures of 10, 20, and 30 bar, equivalence ratios of $\phi = 0.5$ and 1.0 in synthetic dry air, over a limited temperature range of 620 K to 720 K. The results demonstrated that autoignition is affected by different chemical structures and reactivity has a non-linear variation with respect to blending ratio, whereas there was no linear correlation between ignition characteristics and blending ratio. The effects of fuel blending on the first stage and overall ignition processes of the blend (F24/ATJ) was investigated by Mayhew et al. [19] at the pressures of 6 MPa and 9 MPa and the temperature of 825 K and 900 K. The results showed a longer ignition delay increasing non-linearly by increased volume fraction of ATJ, where 85% of the increment occurred in an extended first stage ignition duration and 15% of the increase in 2nd stage ignition delay. It is observed that blends consisting of 0–60% by volume of ATJ fuel produced nearly identical first stage ignition delays. Kim et al. [20] developed a data-driven chemical kinetic mechanism based on the HyChem approach to model ATJ ignition delay that they measured in a shock tube and RCM at just 2 MPa and stoichiometric condition. The model could emulate the empirical ignition delay at the certain points with a good agreement.

In spite of the recently published works dedicated to ATJ fuel, there is a lack of mechanism development that can provide a close simulation of all three important global combustion properties include ignition delay, flame speed, and species concentration, while having a compact size. Thus, this study tries to develop a compact mechanism covering the global combustion properties, with the aid of decoupling methodology, using the Chemkin-Pro software package, and the experimental results in the literature. In this regards, two iso-dodecane (IC12) and iso-cetane (IC16) mechanisms, developed by the authors of this study, have been applied as the surrogate for ATJ fuel, and with a composition of 85%wt IC12, and 15%wt IC16.

Mechanism development

Regarding current computational resources, the detailed mechanisms including thousands of species and reactions have a limited functionality and application due to their long computational time, even for usage in zero and one-dimensional modelling, or for the complex processes that cover mass, energy and momentum in modelling of an aero-engine with the aid of reaction chemical kinetics. To develop compact high-fidelity mechanism for ATJ fuel which can cover the key combustion properties, an approach should be applied that can cover both aims of having a minimal model and demonstrating a close simulation of the intended combustion parameters in comparison with experimental data. Since the decoupling methodology has been found to be an effective approach to provide a compact mechanism for heavy hydrocarbon fuels [21], it is applied in this study to provide a light weight mechanism for ATJ fuel. The method includes the coupling process of a C_0-C_n core mechanism, in a detailed format, to a C_n-C_m sub-mechanism in a simplified format. By using a simplified sub-mechanism of a heavy hydrocarbon that is well-developed, the number of species and reactions in the developed model is considerably reduced through the consideration of the required representative species for the prediction of the fuel combustion parameters.

Therefore, a well-validated core detailed mechanism encompassing C0–C5 chemistry [22, 23] was coupled to the provided sub-mechanisms of iso-dodecane and iso-cetane. The sub-mechanisms are lumped version models with a limited number of species and reactions that can play an important role to produce a small-sized mechanism.

The validation of the sub-mechanisms have been discussed in our previous works [24, 25]. Indeed, the initial raw sub-mechanisms were extracted from a detailed mechanism in the literature [26] and revised by adding some missing reactions of iso-paraffin kinetic models, and by modifying some reaction rates. The details of the revisions can be found in the published works [24, 25].

Ignition delay

Simulation of the IDT of the developed mechanism for ATJ fuel was conducted at 20 bar and stoichiometric conditions, performed by the closed homogeneous batch reactor model in Chemkin-Pro, and compared to the available experimental data at three regimes of the low, intermediate and the high temperature (from 650 to 1250 K). Typical NTC behaviour was observed, in accordance with the experimental data. In general, the model demonstrates a relatively good agreement with the experimental data, though a discrepancy was observed at the intermediate temperature zone and extending into the cool flame region. Based on Fig. 1, considering the disagreement between two experimental results for ATJ fuel at high to moderate temperature zone, and also between the RCM empirical data for iso-dodecane and ATJ fuel (which includes around 90% IC12 in its structure), the discrepancy between the modelling and the experimental data for ATJ can be related to the experimental uncertainty of the measurement in RCM test of ATJ fuel. On the other hand, the lumped reactions and their associated rates in the sub-mechanisms which restrict the performance of a mechanism at some temperature points or pressure conditions, can have a contribution in the issue. The second scenario is more likely to be responsible for the discrepancy at 650 K, where there is not a significant difference between RCM data for iso-dodecane and ATJ fuel. More experimental data could help to reach a certain conclusion. Considering the discrepancy, the proposed kinetic model demonstrated an acceptable and reasonable behaviour in predicting the IDT.

Reaction pathway analysis is a tool that can provide a better understanding of reaction mechanisms by determining the contribution of each reaction to the production and consumption of every species with the aid of a rate-of-production analysis. Therefore, a reaction pathway analysis was performed based on the rate of production data produced within Chemkin-Pro, in stoichiometric conditions at 20 bar with a closed homogeneous batch reactor at 800 K as representative of low and

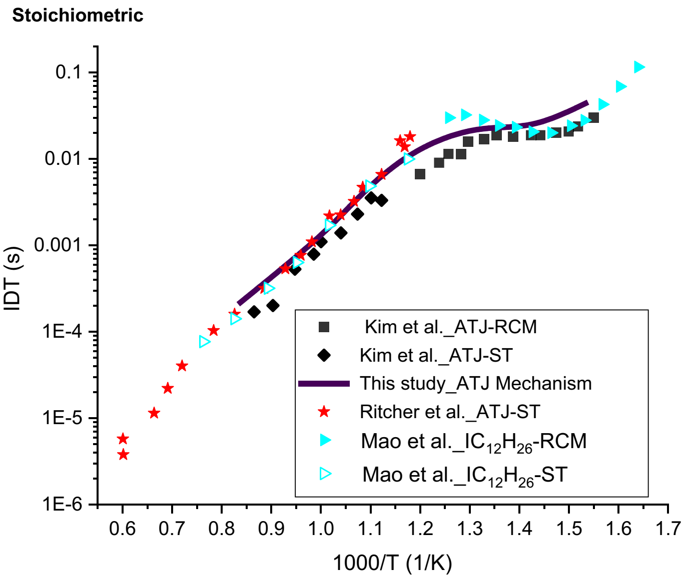

Fig. 1 Ignition delay time results of the developed mechanism of this study at P = 20 bar for stoichiometric conditions, against the shock tube and RCM experimental data of ATJ and iso-dodecane fuel species [14, 20, 27]

intermediate temperature regimes, and at 1200 K as representative of the high temperature regime.

The reaction pathway at low temperature for the model of this study discloses that, the chain branching reaction sequence starts after the generation of iso-paraffins alkylperoxy radicals (RO2) of ATJ fuel due to the first O2 addition to the fuel radicals (R) that are produced by the fuel H-atom abstraction, when most fuel is consumed particularly by the OH radical. The produced fuel radicals including iso-dodecane and iso-cetane radicals which have a heavily branched structure resulting a low reactivity, are depleted through the reaction channel of RO2 production. In comparison with normal paraffins, these iso-paraffins in the structure of ATJ fuel which undergoing impeded H-shifting due to the stable 5-membered transition state rings and have a very stable type of C-H primary bonds, need a larger amount of energy to break [20]. In the next stage, an intramolecular hydrogen abstraction converts the alkylperoxy radicals to the alkylhydroperoxy radical (QOOH) form of the fuel iso-paraffins which in turn generate peroxy-alkylhydroperoxides (OOQOOH) via a second O2 addition process. The production of cyclic ether and the concerted elimination reaction are the important side reaction channels which have a contribution to the consumption of QOOH and RO2 radicals. Similar to the iso-dodecane pathways at low temperature [24], the NTC behaviour of ATJ fuel arises due to a competition between the degenerate chain branching reactions and these side reactions. As can be seen from Fig. 1, ATJ fuel has a more pronounced high temperature regime resulting a narrower NTC region in comparison with conventional jet fuels, since a higher activation energy is needed for the reactions of H atom abstraction and alkyl radical oxidation [20]. Finally, the OOQOOH radical forms an OH radical and ketohydroperoxides of the fuel iso-paraffins which decompose to the β-scission products.

In the high temperature regime, H atom abstraction has the greatest contribution to the combustion chemistry and the consumption of fuel. Unimolecular decomposition is the other important reaction channel having a significant weight in the high temperature reaction pathway. The produced fuel iso-paraffin radicals in the H abstraction stage generate alkylperoxy radicals through an O2 addition process. The iso-paraffin radicals of fuel also decompose to β-scission products, in which the C–C and C–H bonds of the iso-paraffins radicals are opened via β-scission leading to the production of olefins and alkyl radicals. Finally, through successive β-scission reactions, the olefins and alkyl radicals decompose to small molecules and radicals. The provided core mechanism has the role of depleting these small species, which demonstrates the significant impact of the core mechanism in the high temperature regime.

As it can be observed in Fig. 2, the key reactions relevant to the ignition of ATJ fuel at stoichiometric conditions for 800 K and 1200 K are identified and listed with the aid of sensitivity analysis.

At low temperature of 800 K, the generation of OOQOOH via the second O_2 addition, the isomerization of alkylperoxy, and the formation of ketohydroperoxides have the greatest promoting effect on the ignition delay. The decomposition of hydrogen peroxide which generates OH radicals is another key reaction with a promoting effect on the ignition delay time. Following the mentioned reactions, the H abstraction reactions are among the most important promoter reactions. The small species reactions producing two radicals also demonstrate a relatively srong promoting effect. On the other hand, the concerted elimination reaction of the alkylperoxy radicals decreasing the overall reactivity via the formation of more stable alkenes, and the formation of cyclic ethers demonstrate the strongest inhibiting impact. Due to the lower reactivity of the produced HO_2 radicals compared to the OH radicals which compensate a part of the decreased reactivity by the reaction of cyclic ethers, the concerted elimination that generates HO_2 radicals shows a more inhibiting effect than the cyclic ether reaction. Following the reaction of IC12-OOQOOH → O_2 + IC12-QOOH as the next strongest inhibitor reaction, the reactions of small species radicals that produce a more stable species are the other key reactions having an inhibitor role in the ignition of ATJ fuel.

As can be seen in Fig. 2, most of the strong promoter and inhibitor reactions at this temperature are the small species reaction of the core mechanism acknowledging the statement that the reactivity of the system in the high temperature regime is dominated by the reactions of the small species in the core mechanism. Those small species reactions producing more active radicals have the strongest promoting effect and the small species generating stable alkenes have the strongest inhibiting impact. The sensitivity analysis at 1200 K also demonstrates that the unimolecular decomposition and the formation of the alkylperoxy radicals have a very strong promoting effect, and the beta-scission of the fuel radicals demonstrates a strong inhibiting effect. While the reactions in the low temperature chain branching pathways that

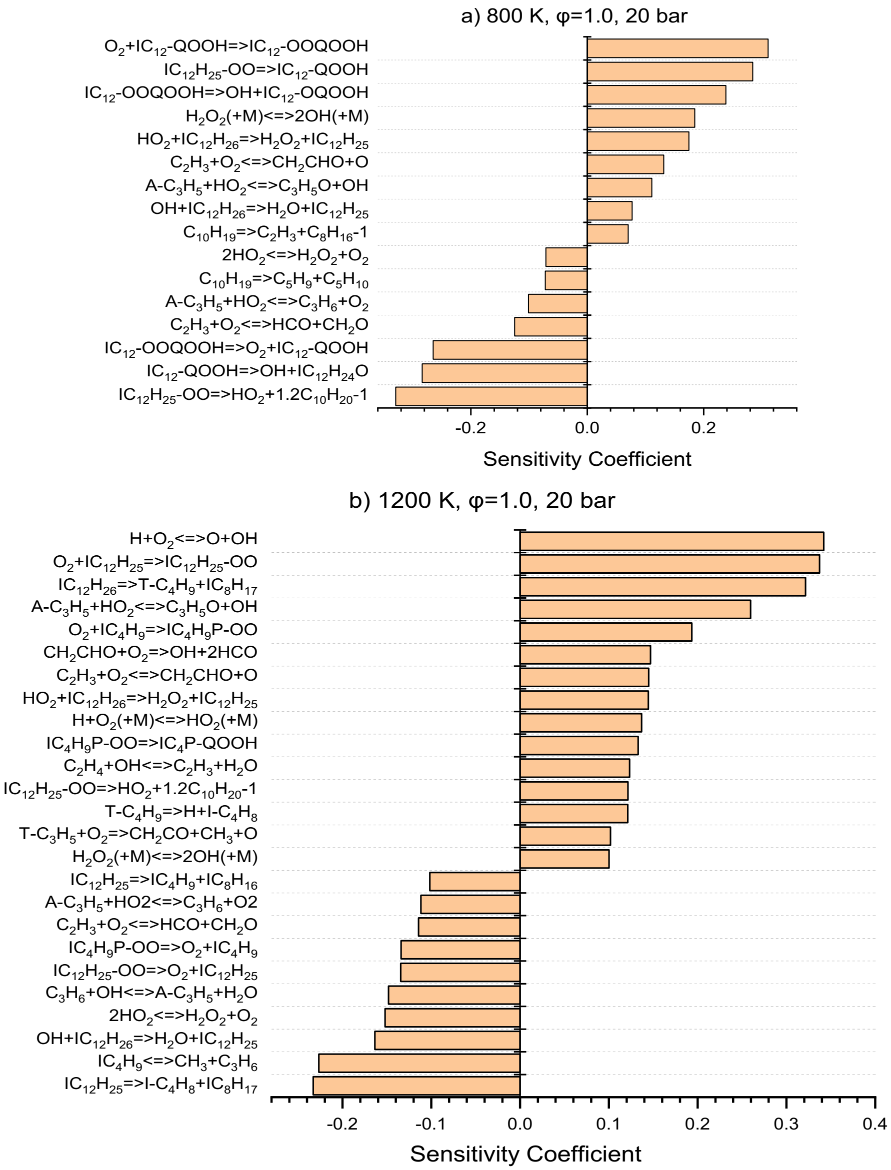

Fig. 2 Sensitivity analysis at 20 bar for stoichiometric condition at **a** low and **b** high temperatures

have a significant promoting or inhibiting effect at 800 K are not in the list of the top sensitive reactions at high temperature, H abstraction reactions by HO_2 and OH are still demonstrating a promoting and inhibiting effect at 1200 K.

Species mole fractions

Modelling of the mole fractions of the main products of ATJ fuel oxidation was conducted in the closed homogenous batch reactor in Chemkin-Pro using the developed mechanism for this study, and compared against the available experimental results [15] at the nominal pressure of 4 bar, reaction time of 2.2 ms, and over a temperature range of 900 to 1550 K. The experiment was conducted for a mixture of ATJ and O_2 diluted in argon, in a low pressure shock tube (LPST), while the initial fuel concentration was 52 ppm at a stoichiometry of 0.27.

As it is illustrated in Fig. 3, similar to the experimental profile of iso-dodecane [24], its consumption begins around 950 K, and continues to decay until around 1200 K where it is completely consumed, although there may be some subtle differences to the experiment in that experimentally it starts to decay at slightly lower temperature and not be completely consumed until slightly higher temperature. Subsequently, the consumption of IC12 which is mainly responsible for the consumption of ATJ fuel leads to the production of the hydrocarbon intermediates over that temperature range, which in turn react to produce CO and then CO_2. The simulations for most species in Figs. 3, 4, 5, 6 and 7 demonstrate in general a reasonable and in some cases very good agreement with the experimental measurements, and could capture the three parameters of the production, the decay, and the magnitude compared to the experiment. This is to be expected as they are dictated by the behavior of the fuel itself which is well captured by the model. Discrepancies arise from two principal causes, firstly as a result of the processes are applied for lumping

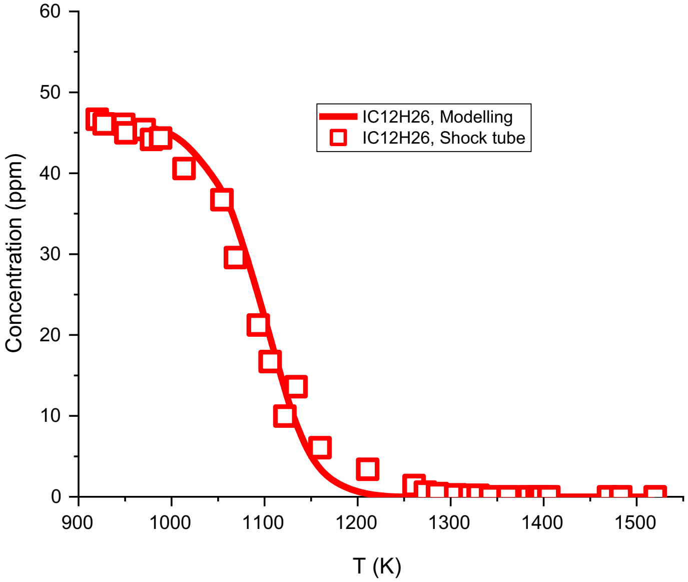

Fig. 3 Simulation results of IC12H26 concentrations for the developed mechanism of this study, against the low pressure shock tube experimental data for reaction time of 2.2 ms, at 4 bar over the temperature range of 900 to 1550 K [15]

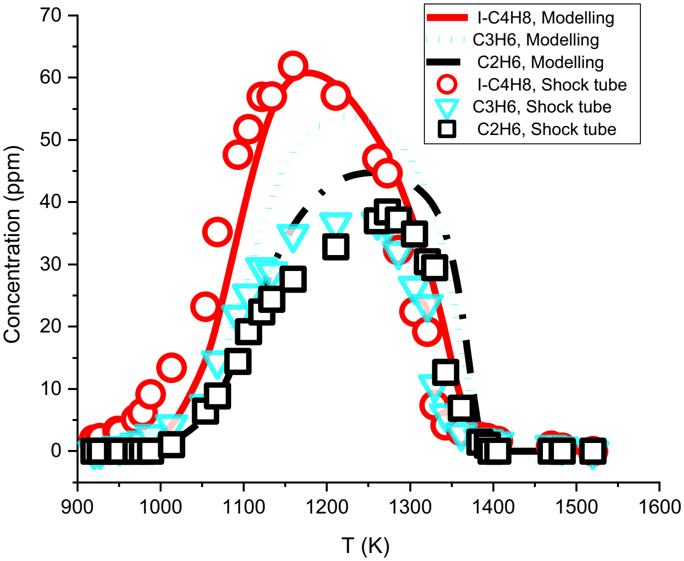

Fig. 4 Simulation results of I-C4H8, C3H6, and C2H6 concentrations for the developed mechanism of this study, against the low pressure shock tube experimental data for reaction time of 2.2 ms, at 4 bar over the temperature range of 900 to 1550 K [15]

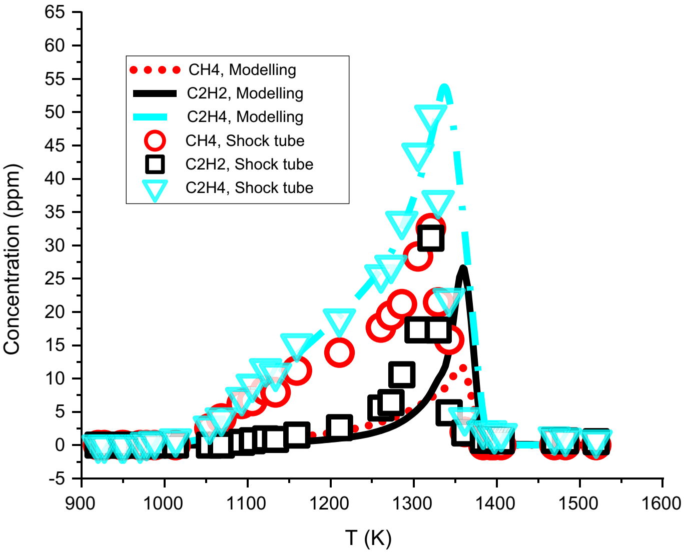

Fig. 5 Simulation results of CH4, C2H2, and C2H4 concentrations for the developed mechanism of this study, against the low pressure shock tube experimental data for reaction time of 2.2 ms, at 4 bar over the temperature range of 900 to 1550 K [15]

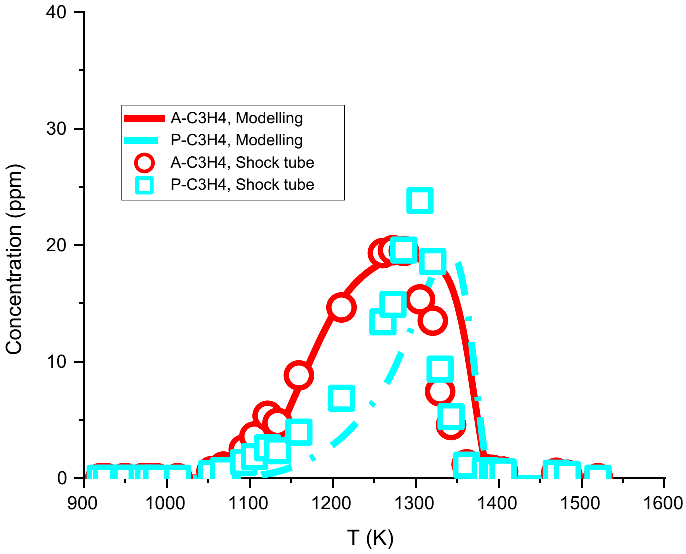

Fig. 6 Simulation results of A-C3H4 and P-C3H4 concentrations for the developed mechanism of this study, against the low pressure shock tube experimental data for reaction time of 2.2 ms, at 4 bar over the temperature range of 900 to 1550 K [15]

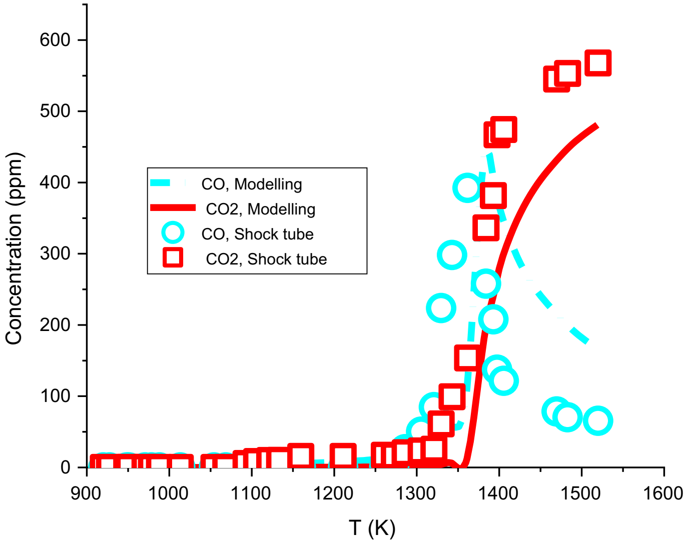

Fig. 7 Simulation results of CO and CO2 concentrations for the developed mechanism of this study, against the low pressure shock tube experimental data for reaction time of 2.2 ms, at 4 bar over the temperature range of 900 to 1550 K [15]

procedure in the mechanism development such as the elimination of the fuel radicals reactions and the lack of enough precision in the approximation used for the lumped reaction rates, and secondly the uncertainty in the reaction rates of the chemical reactions that the less-understood highly branched iso-alkanes undergo. These manifest themselves as subtle differences in species magnitude, such as C_3H_6 and C_2H_6 in Fig. 4, and/or variation in behavior with temperature such as for C_2H_2 and CH_4 in Fig. 5, and for CO and CO_2 in Fig. 7.

Laminar flame speed

The simulations of the laminar flame speed illustrated in Fig. 8 were conducted at 1 and 3 bar for the unburned combustion temperature of 473 K and a range of equivalence ratios (0.7 to 1.4). The results were compared to the results of the available experimental data for ATJ fuel [14]. It is observed that the mechanism emulates the laminar flame speed of the empirical data very closely at both pressures. In spite of the good general agreement between the modelling and empirical data, there are a little under-estimation and over-estimation at some points, and the discrepancies are considerable for equivalence ratios of 0.7 and 1.4, at 3 bar. Apart from the experimental uncertainty for the data, the issue demonstrates that the small reactions of the core mechanism which are mostly responsible for the simulation of flame speed can just show an acceptable simulation in a limited range of equivalence ratio, higher than 0.7 and lower than 1.4, for 3 bar or higher pressures.

In order to identify the most important reactions affecting the laminar flame velocity, sensitivity analysis was conducted using Chemkin-Pro for laminar flame speed at equivalence ratio of 1 and the pressures of 1 and 3 bar. As can be observed from Fig. 9, the dominant chain branching reaction of $H + O_2 \rightleftharpoons O + OH$ generating

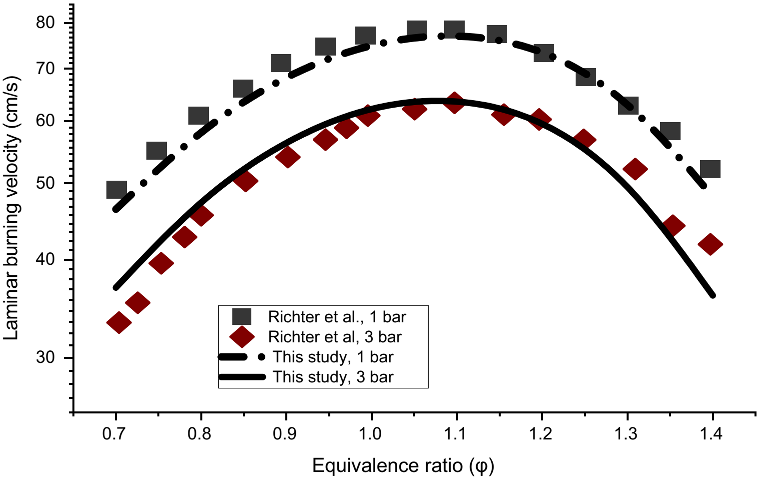

Fig. 8 Laminar flame speed simulation results of the developed mechanism of this study at the unburned temperature of 473 K, against the experimental data of ATJ fuel at a pressure of 1 and 3 bar [14]

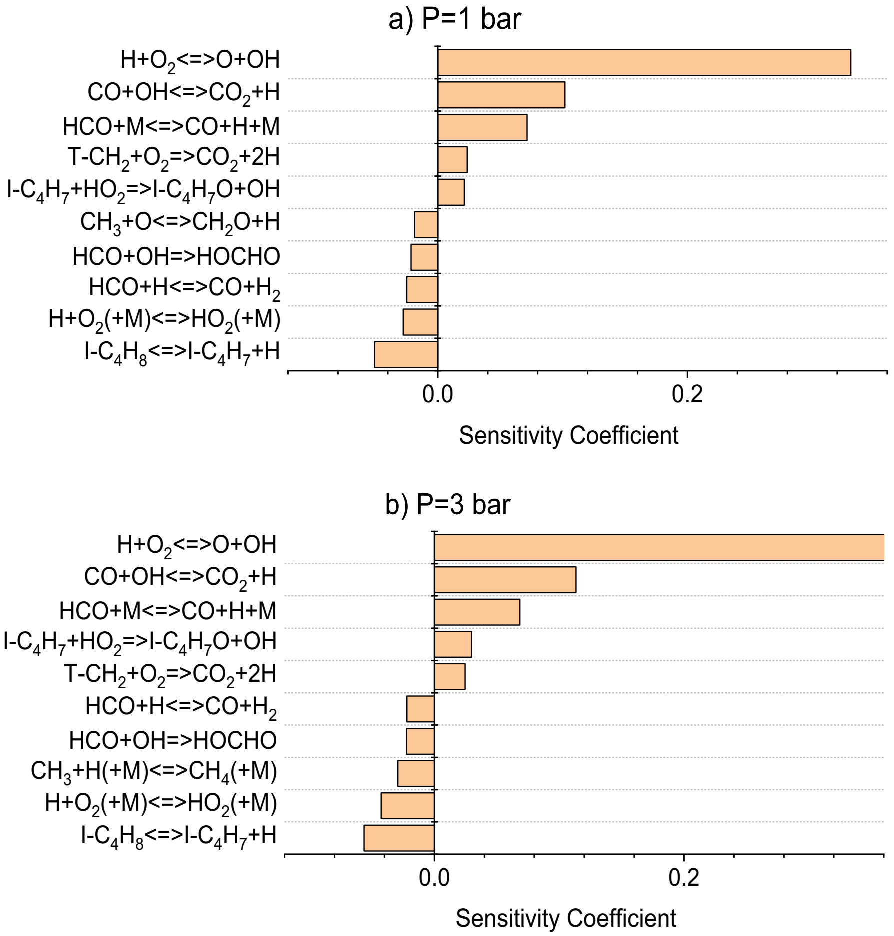

Fig. 9 Sensitivity analysis of laminar flame velocity of ATJ/air mixture at 443 K and equivalence ratios of 1, for 1 bar (**a**) and 3 bar (**b**)

OH and O radicals and having a great contribution to the flame with self-propagation characteristics [28], the main oxidation of CO and the production of CO as the chain propagation and the chain initiation reactions that lead to the production of H radicals, are the most important elementary reactions for the laminar flame velocity of an ATJ/air mixture. As the above mentioned reactions generate many active radicals of H, O, and OH, they have a promoting role on the laminar flame speed and increase it.

Among the inhibiting reactions for 1 and 3 bar, the decomposition of iso-butene, and the terminating reactions of the core mechanism such as $H + O_2\ (+M) \rightleftharpoons HO_2\ (+M)$ and $HCO + H \rightleftharpoons CO + H_2$ which have a suppressing impact on the flame speed due to the termination of the radical chain process, and demonstrate a strong negative sensitivity coefficients.

Conclusion

Using the decoupling methodology and developed lumped sub-mechanisms, a compact reaction kinetic mechanism covering both the low and high temperature regimes was developed for predicting the combustion characteristics of ATJ fuel as an important alternative jet fuel. The produced iso-paraffin sub-mechanisms of iso-dodecane and iso-cetane as the main components in the structure of ATJ fuel were coupled to a well validated core mechanism to simulate ignition delay, laminar flame speed, and species mole fractions. The mechanism could follow closely the experimental data of ignition delay over the low-to-high temperature and it is in reasonable agreement for stoichiometric conditions at 20 bar, in spite of the discrepancy observed for intermediate and cool flame temperature regions which can be related to the experimental uncertainty, since there is discrepancy between the experimental data of different sources and the uncertainty related to the RCM experiment. The simulations of the laminar flame speed at 1 and 3 bar demonstrated a general good agreement with the experimental data. The analysis of the reaction pathways and the sensitivity analyses were provided to gain a deeper understanding of the ATJ fuel developed mechanism. In addition to ignition delay and laminar flame speed, modelling was conducted for species concentration of ATJ fuel oxidation, as the other important combustion property. Simulation for the main species concentration of a mixture of ATJ/O_2 diluted in argon was conducted against the experimental results at the nominal pressure of 4 bar, reaction time of 2.2 ms, a temperature range of 900 to 1550 K, $\varphi = 0.27$, and the initial fuel mole fraction of 52 ppm, in a low pressure shock tube. The results showed a good agreement between the modelling and the experimental data for the mole fraction of most main oxidation products of ATJ fuel. In regard with the predictive capability of the developed model in the simulation of the three important combustion parameters, and its compact size, the authors suggest the mechanism is suitable for use in functional kinetic investigations and also for more complex applications including the investigation on the complex geometries of combustion system with the aid of the Equivalent Reactor Network Analysis.

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Declarations

Competing interests The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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