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Methods and tools for the characterisation of a generic jet fuel

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Abstract

The demand for producing environmentally friendly jet fuels raises the question how to design a jet fuel that matches predefined properties. Targets to be matched are *e.g.* energy content or less harmful emission characteristics. A further major challenge for the production of new synthetic jet fuels is their availability for the required certification process in sufficient quantities within an appropriate time frame and at reasonable cost. This implies the need for tools for the formulation of synthetic jet fuels which have mostly a component pattern that differs from Jet A-1 made from crude-oil. In the present work, to address these challenges, a new approach will be presented in order to be able to design a synthetic jet fuel from scratch with preselected and well-defined physical and chemical properties: The development of a chemical kinetic reaction mechanism able to describe the oxidation of a generic fuel consisting of only a few representative components of the major molecule classes occurring in jet fuels. N-dodecane, cyclohexane, and isooctane were chosen as single fuel components, and their global combustion properties, *i.e.* laminar burning velocity and ignition delay time, were measured. These experimental data were used for the validation of the reaction mechanisms, first developed for each single fuel component, and then combined to the reaction mechanism for the generic fuel under consideration. The last step is the further optimization and reduction of the generic fuel reaction mechanism to ensure its suitability for the integration in numerical simulation to tackle the combustion of a synthetic fuel under practical conditions, *e.g.* in CFD simulations.

## 1. Introduction – Correlation between composition and properties of fuels

The use of crude oil based fuels is connected with different issues such as concerns about the security of supply and negative impacts on the climate as well as on the environment due to emissions of primarily carbon dioxide (CO_2), nitrogen oxides (NO_x) and soot. Several organizations of the aviation sector commit to reduce the emissions of CO_2 and NO_x up to 2050 drastically; for example, the International Air Transport Association (IATA) aims to reduce the CO_2-emissions by 50 % compared to 2005. The Advisory Council for Aeronautical Research in Europe (ACARE) aspire to a reduction of 75 % for CO_2-emssions and 90 % for NO_x-emissions, each referring to emissions in 2000 [1]. Besides technical and operational improvements, the use of alternative synthetic fuels is necessary to achieve these goals.

Over the last years, many ideas on new processes and technologies focusing on the production of synthetic jet fuels have been suggested. There are four main requirements for new jet fuels: (i) The demand for producing environmentally friendly jet fuels; (ii) New fuels have to be compatible with the currently used materials in the aircraft industry as well as with the existing jet engine technology; (iii) They should be fully interchangeable with the existing fuel infrastructure; and (iv) They must be available worldwide, at competitive prices. Points (ii) and (iii) are related to safety considerations and hence, all jet fuels must be certified, *e.g.* by ASTM [2]. One way to address these challenges is the design of a synthetic jet fuel that matches predefined properties, *e.g.* energy content or density so that the designed jet fuel passes the certification process without any additional revision, thus avoiding increasing costs and time delay to the market launch. Emission characteristics are not in the focus of the certification process yet, although they are an ever-growing concern due to environmental and health impacts.
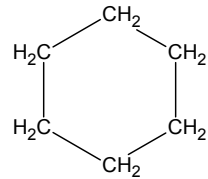
n-alkanes
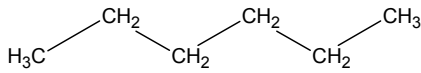
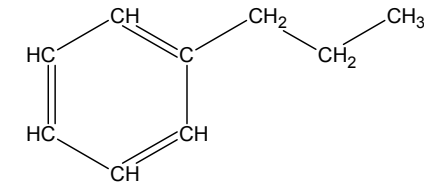## iso-alkanes
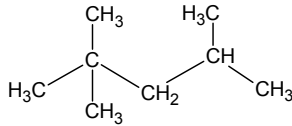
cycloalkanes

aromatics

Fig. 1 Structures of the four typical types of hydrocarbons present in conventional crude oil jet fuel (structures shown are only examples as molecules in jet fuels are usually larger in C-number)

For the design of a synthetic fuel having favoured properties, *e.g.* reduced emissions, a deeper knowledge about the correlation between the fuel composition and fuel properties as well as its combustion behaviour is essential. A further challenge arises as a jet fuel may consist of numerous components [2]; these can be classified in four basic types of hydrocarbons: n-alkanes, iso-alkanes, cycloalkanes, and aromatics – examples are shown in Fig. 1.

Every component is characterised by specific physical and chemical properties like density, boiling temperature, H/C ratio, and enthalpy of formation as well as sooting behaviour and further combustion properties. These properties differ depending on the specific molecule and including its carbon length and its degree of branching. Since a practical fuel like a jet fuel is a multicomponent mixture, the properties are defined by the characteristics of all fuel components [1, 2]. Because mixing and combustion are affected by the fuel properties, the system (aircraft - jet engine) and its emission pattern are influenced, too. Figure 2 illustrates this relationship between fuel components, fuel properties, and combustion process.

In turn, if it is known how the combustion process, emissions etc. is affected by the properties of the single fuel components, it should be possible to design a synthetic jet fuel with predefined properties (as depicted by the dashed line in Fig. 2). Hence, this designer fuel is characterised by favoured and adjusted properties. This implies also the need for tools for the formulation of synthetic jet fuels with a component pattern that differs from crude-oil made Jet A-1.
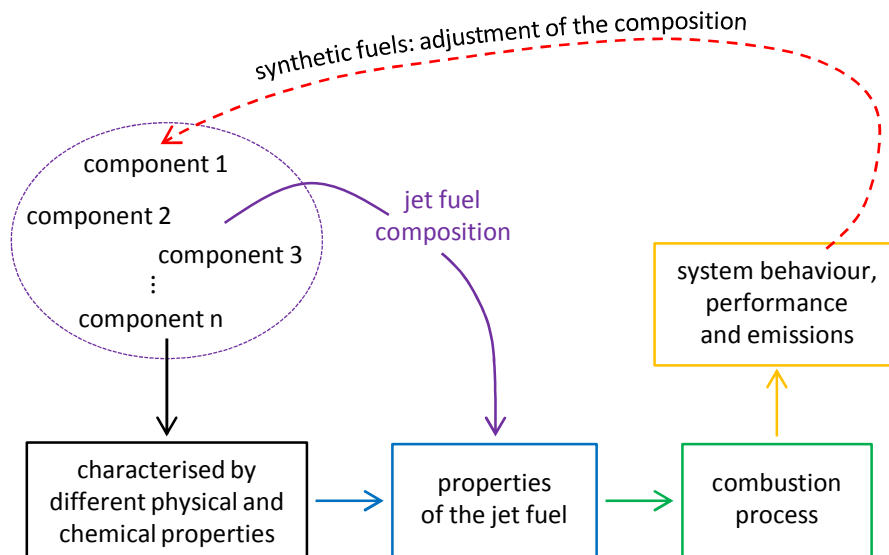

Fig. 2 Designed synthetic jet fuel: Understanding the influence of fuel properties on the combustion process as well as on the system behaviour and emissions

To investigate the influence of different fuel components, the project InnoTreib [3] was initiated by the German Aerospace Center (DLR) and Stuttgart University (StU), together with Technical University Hamburg-Harburg (TUHH). The project's overall goal was to develop a new approach enabling the design of a synthetic jet fuel with preselected and well-defined properties from scratch using a set of different tools. Experimental work as well as mechanism development and simulations belong to these tools.

As part of InnoTreib, the structure dependency of the global combustion properties, *i.e.* laminar burning velocity and ignition delay time, of three neat fuel components were investigated (see Section 2). Here, the molecule classes n-alkanes, iso-alkanes, and cycloalkanes were considered by using n-dodecane ($C_{12}H_{26}$), isooctane (2,2,4-trimethylpentane, C_8H_{18}), and cyclohexane (C_6H_{12}), respectively. Furthermore, a detailed reaction mechanism for a generic jet fuel (also known as surrogate) was developed (see Section 3) following by the aim to reduce the number of species in this mechanism to less than 60 species for the implementation in a CFD model. The consideration of aromatics was not included within InnoTreib since aromatics act as soot precursors. Consequently, it is important to understand the combustion properties of aromatic free fuels since the elimination of aromatics in fuels, thus called innovative fuels, offers a smart possibility to reduce the emission of particles and soot.

2. Experimental Tool – Investigation of global combustion properties

The investigation of the fundamental combustion properties, *i.e.* laminar burning velocity and ignition delay time, for n-dodecane, isooctane, and cyclohexane is strongly connected with the two aims: (i) To gain information about the effect of the molecular structure on fuel reactivity and (ii) to generate validation data for the development of the reaction mechanism of a generic fuel. Moreover, the laminar burning velocity and the ignition delay time provide key information about the combustion behaviour of the investigated fuels. Within the experimental work, fuel components beyond the InnoTreib-project, here n-propylcyclohexane, n-propylbenzene, and toluene, were measured, too, to examine the influence of the aromatic structures on the combustion properties.

2.1 Laminar burning velocity

The laminar burning velocity can be considered as a quantity for the flame propagation in a combustion process as well as for the reactivity of a fuel. More precisely, the laminar burning velocity is defined as the propagation velocity of the flame front into an unburned gas mixture (fuel-air-mixture). For a stable flame, equilibrium between the velocity of the inflow (unburned) gas mixture and the propagation velocity of the flame front is required. To generate a premixed flame, any liquid has to be vaporized first.

Using the cone angle method, according to the equation $S_u = v_u \cdot \sin \alpha$, the laminar burning velocity (S_u) is determined by the cone angle (α) measured from the premixed conical shaped flame and the velocity (v_u) of the unburnt fuel-air-mixture as illustrated in Fig. 3. This method was exploited previously for the measurements of several alternative jet fuels, *e.g.* Coal-to-Liquid, Gas-to-Liquid, Alcohol-to-Jet, and Farnesane, and is described in more details, including the experimental set-up, in earlier publications [4-11].
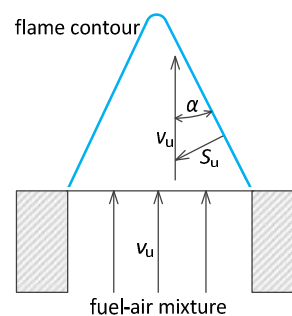

Fig. 3 Schematic how to determine the laminar burning velocity (S_u - laminar flame speed, v_u - gas velocity of the unburnt gas mixture, α - cone angle)

The experiments were carried out at constant pressure (1 bar) and preheat temperature (473 K); the fuel/air equivalence (φ)-range was varied between 0.6 and 2.0 as shown in Figs. 4 and 5. From Fig. 4 it is visible that n-dodecane (squares) and cyclohexane (triangles) have very similar burning velocities whereas for isooctane (rhombs) distinct smaller values were obtained. These differences are caused by the different structures of the molecules; a branched structure (isooctane) causes a minor reactivity reflected in a smaller burning velocity. For comparison, burning velocities of Jet A-1 were measured, too. These data (circles) lie between the neat components.

In Fig. 5, the results for the measured burning velocities of n propylcyclohexane (pentagons), n-propylbenzene (left triangles), and toluene (right triangles) are compared to the data obtained for Jet A-1. The aromatic fuel components toluene and n-propylbenzene have only slightly higher burning velocities than Jet A-1 has. In contrast to the aromatics, the difference for n-propylcyclohexane to Jet A-1 is similar to the results for cyclohexane and n-dodecane. The lower burning velocities of the aromatics considered can be explained by their typical structure as seen by the comparison of the measured burning velocities of n-propylbenzene with those of n-propylcyclohexane: the aromatic structure of n-propylbenzene leads to a lower reactivity that causes a lower burning velocity compared to n-propylcyclohexane.
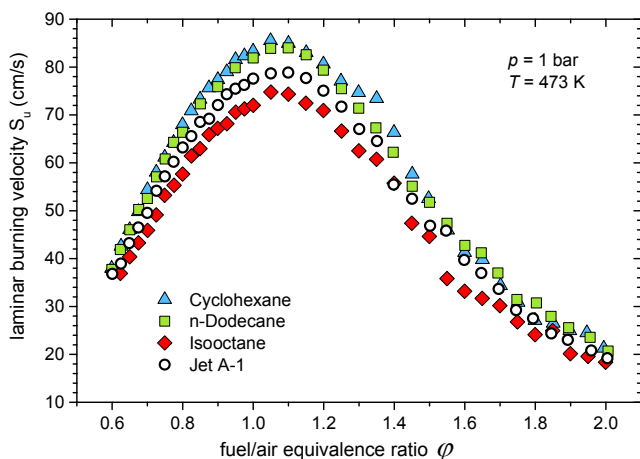
Fig. 4 Experimental results for the measurement of the laminar burning velocity of cyclohexane, n-dodecane, isooctane, and Jet A-1 (for reference); all fuels were premixed with air
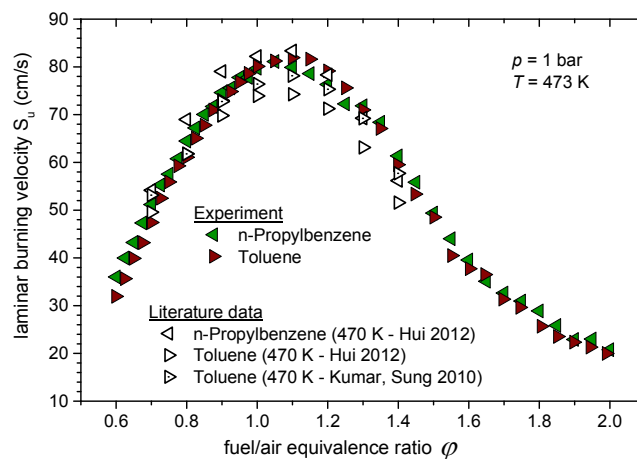

Fig. 5 Experimental results for the measurement of the laminar burning velocity of n-propylcyclohexane, n-propylbenzene, toluene, and Jet A-1; all fuels were premixed with air

Fig. 6 Comparison of the presented measurements of the laminar burning velocity of n-dodecane and isooctane with literature work (Kumar, Sung 2007 [12], Kumar et al. 2007 [13], Galmiche 2012 [14])

Fig. 7 Comparison of the presented measurements of the laminar burning velocity of n-propylbenzene and toluene with literature work (Hui 2012 [15], Kumar, Sung 2010 [16])
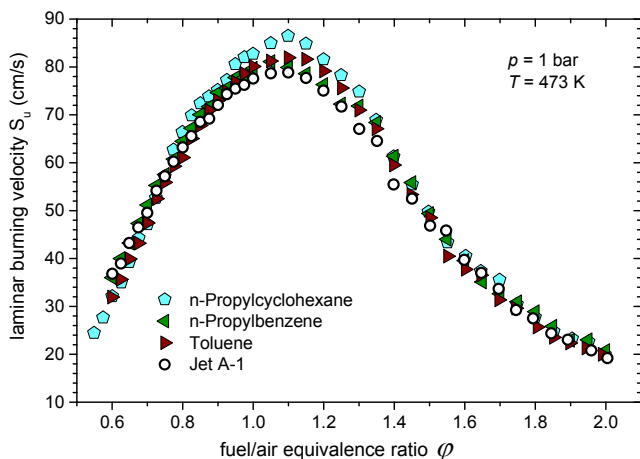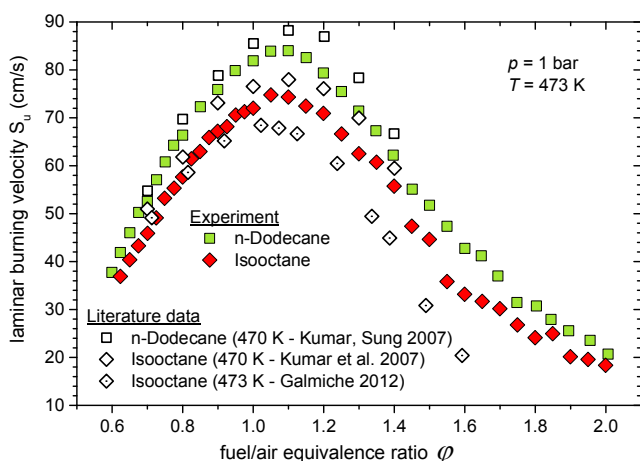
Since for a better clarity error bars are not given in Figs. 4-7 the reader is referred to section 4, Figs. 11a-d, where the single measurements for cyclohexane, n-dodecane, isooctane, and Jet A-1 are compared to the simulation. From these graphs is apparent that the uncertainties, derived from the maximum error, are similar for all fuels. In detail, the uncertainties of the measured laminar burning velocities amount to < 4 % in a wide φ-range from 0.6 to 1.5. Only for fuel rich mixtures, the uncertainties may increase to > 10 %. Thus, even though the differences of the laminar burning velocities between aromatics as well as cycloalkanes and n-dodecane, respectively, are small, there is a systematic trend to lower values for the burning velocity of aromatics especially within the range of the maxima. The uncertainties for the φ-values are in a range between ± 2 % and ± 4 %.

For the measurements of n-dodecane, isooctane, n-propylbenzene, and toluene, a comparison to literature data is presented in Figs. 6 and 7 showing that the experimental data as obtained within this work are close to the data reported in literature, with small deviations. In detail, the data for n-dodecane and isooctane (Fig. 6) from Kumar and Sung [12] and Kumar et al. [13], respectively, each measured applying the counterflow technique, show higher laminar burning velocities. In contrast to this, the isooctane measurements from Galmiche et al. [14], who worked with a spherical expanding flame, yielded lower values for the laminar burning velocity. The comparison for the aromatics in Fig. 7 shows slightly higher values for the data from Hui et al. [15] for n-propylbenzene but lower values for toluene, which is also the case for the comparison to the data from Kumar and Sung [16]. In both works, the counterflow technique was used. From these comparisons it is concluded that there is no systematic deviation between data of laminar burning velocities resulting from measurements with the cone angle method and measurements performed with another methods.

2.2 Ignition delay time

The ignition delay time is defined as the time period between the initiation of the reactive system by a shock wave and the onset of ignition [8]; thus, it is determined during the initialization of the combustion process. The ignition process is characterised by the decomposition of (large) molecules resulting in the formation of radicals leading finally to a steep rise of the radical concentration, pressure, and temperature.

The measurements of the ignition delay times are performed in a shock tube behind reflected shock waves as described earlier [7, 8, 10, 11]. All ignition delay times given in the present work are derived as follows: The time difference between initiating the reactive system by the reflected shock wave and the peak of the excited CH*-radical concentration measured at a wavelength $\lambda = 431$ nm are determined as a function of the temperature for a given mixture composition. The φ-value and initial pressure p_{init}, which both also have an influence on the ignition delay time, were selected as $\varphi = 1.0$ and to approximately $p = 16$ bar, respectively. Furthermore, the fuel-air-mixtures were diluted 1:2 with nitrogen. The accuracy of the set-temperature is about ± 15 K [7].

The experimental results obtained within InnoTreib are presented in Fig. 8; besides the neat components, n-dodecane, isooctane, and cyclohexane, Jet A-1 was also measured. The experimental setup allows measurements of ignition delay times up to 30 ms depending on temperature. Within a previous study, the uncertainties for the ignition delay times were derived from the assumption that the pressure has an uncertainty of ± 10 % due to post shock compression effects. This results in accuracies between ± 6 % and ± 15 % [11], which are similar for all measurements of the ignition delay time performed in this shock tube.

All fuels show, at temperatures higher than 1000 K, a decrease of the ignition delay time τ with increasing temperature. Over the whole temperature range studied, n-dodecane (squares) and cyclohexane (triangles) show the shortest ignition delay times, isooctane the longest. These results correspond to the findings made for the laminar burning velocity: The branched structure of isooctane results in a lower reactivity leading to a longer ignition delay time. The values for Jet A-1 (circles) lie between those for n-dodecane and cyclohexane, respectively, and isooctane (rhombs) as well, especially at higher temperatures.

Interesting is the behaviour of the four fuels studied at temperatures lower than about 1000 K, a region called the NTC-area (NTC = Negative Temperature Coefficient). This distinctive feature of the oxidation of large hydrocarbons signifies a temperature zone in which the global reaction rate decreases with increasing temperature [17]. An NTC-area is characterised by a temperature region, where the ignition delay time values typically change only slightly with temperature.

As it is visible in Fig. 8, a strong NTC-behaviour was found for n-dodecane; thus, allowing measurements of individual ignition delay time data down to 650 K. Within

the available parameter range of the present work, no NTC-area was detected for isooctane and cyclohexane for temperatures as low as 800 K. In general, such a pronounced NTC-area as observed for n-dodecane is a characteristic feature of large n-alkanes. In addition, there are further literature studies available with no NTC-area for isooctane and cyclohexane reported, see *e.g.* for isooctane [18-21] and for cyclohexane [22-26], respectively. Depending on the specific experimental set-up and the specific molecule, it is possible to measure ignition delay time data in the low temperature area, down to temperatures as low as 600 K and 700 K, for isooctane *e.g.* [18, 19, 27-30] and cyclohexane *e.g.* [23, 31].
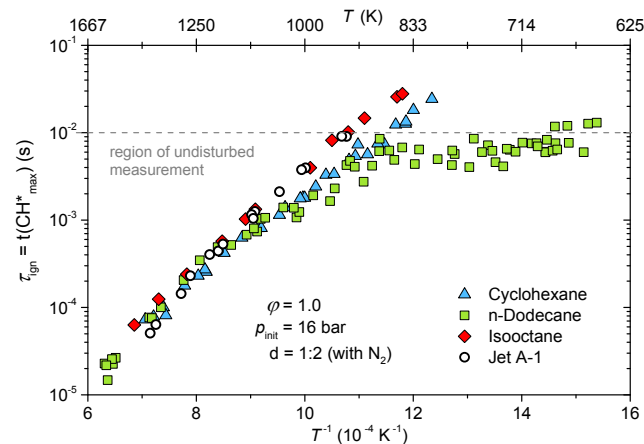
Fig. 8 Experimental results for the ignition delay time of cyclohexane, n-dodecane, isooctane, and Jet A-1 (for reference) in mixtures with air (the fuel-air-mixtures were diluted 1:2 with nitrogen)

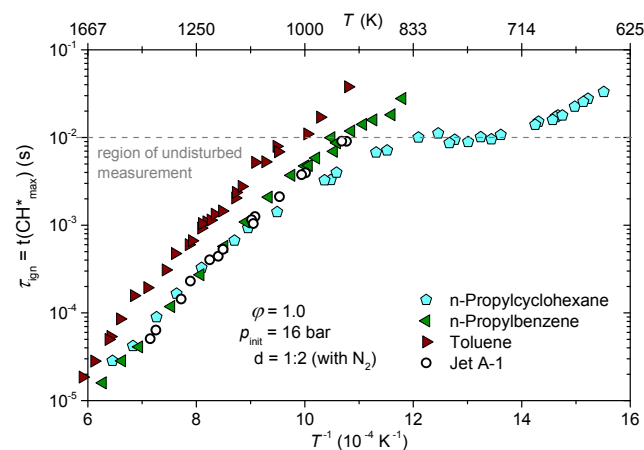**Fig. 9** Experimental results for the ignition delay time of n-propylcyclohexane, n-propylbenzene, toluene, and Jet A-1 in mixtures with air (the fuel-air-mixtures were diluted 1:2 with nitrogen)

The results of the measurements of n-propylcyclohexane, n-propylbenzene, and toluene are presented in Fig. 9. The ignition delay times of

n-propylcyclohexane, n-propylbenzene, and Jet A-1 are nearly identical at temperatures higher than 1100 K. Similar to n-dodecane, NTC-behaviour was found for n-propylcyclohexane but with a slightly longer ignition delay time compared to n-dodecane. In contrast to all other fuels studied in the present work, toluene has a longer ignition delay over the whole temperature range. This finding is explained due to the shorter side chain (one C-atom) of toluene as the decisive difference to n-propylbenzene having a side chain of three C atoms.

3. Modelling tool – Development of a reaction mechanism

In principle, the combustion of any fuel can be described by a chemical kinetic reaction model consisting of many elementary reaction steps for describing the oxidation of the fuel components over intermediates to stable products, as a function of temperature, pressure, and fuel-air ratio. To model the combustion behaviour of a fuel mixture, all single components, in principle, have to be known – however, today, a direct modelling for a conventional jet fuel is not possible since it consists of a multitude of different species. Thus, the exact composition of a jet fuel is unknown and even if the concentrations of each component were known, it would be nearly impossible to include the oxidations reactions of all components in one mechanism.

With the assumption that all components belonging to the same molecule class (see Fig. 1) have similar combustion properties [2], the approach of a surrogate jet fuel can be used by choosing a representative component for each major molecule class existing in a jet fuel. Thus, any surrogate (model) fuel consists of only a few components

with well-known characteristics and oxidation behaviour for each component and moreover the characteristics of the surrogate are similar to a jet fuel [32]. Hence, a surrogate fuel is likewise a designer fuel in that sense that it should match specific properties of a jet fuel. The differences between designer and surrogate fuels lie in the way of use: A designer fuel is a synthetic fuel which is created for the technical use in aviation whereas a surrogate is used exclusively in research, with a well-known procedure for its development. In this study, the generic fuel is similar to a surrogate since its components were selected because of their specific molecular structure; their physical properties were of secondary importance.

The principle of development and validation of a reaction mechanism for a surrogate fuel is displayed in Fig. 10. The first issue is to select the components which are, in general, appropriate to reflect the combustion behaviour of a real fuel before starting the mechanism development. Then, it is important to define the target properties in which the surrogate fuel should match the real fuel, e.g. ignition delay time and/or C/H ratio. Then, further, a reaction mechanism for each single fuel component will have to be generated. With the knowledge about properties and mechanisms of the components, it is possible to create a detailed reaction mechanism for the surrogate consisting of the selected components. For the development as well as for the optimization of any mechanism, experimental determined combustion properties are required for the validation of the model. Once validated, the mechanism can be used for the implementation in a numerical simulation to predict the combustion process and the behaviour of a real fuel in a technical combustion chamber, e.g. a jet engine. To allow efficient CFD calculations, the use of a smart reaction model reduced with respect to number of species and reactions is essential.
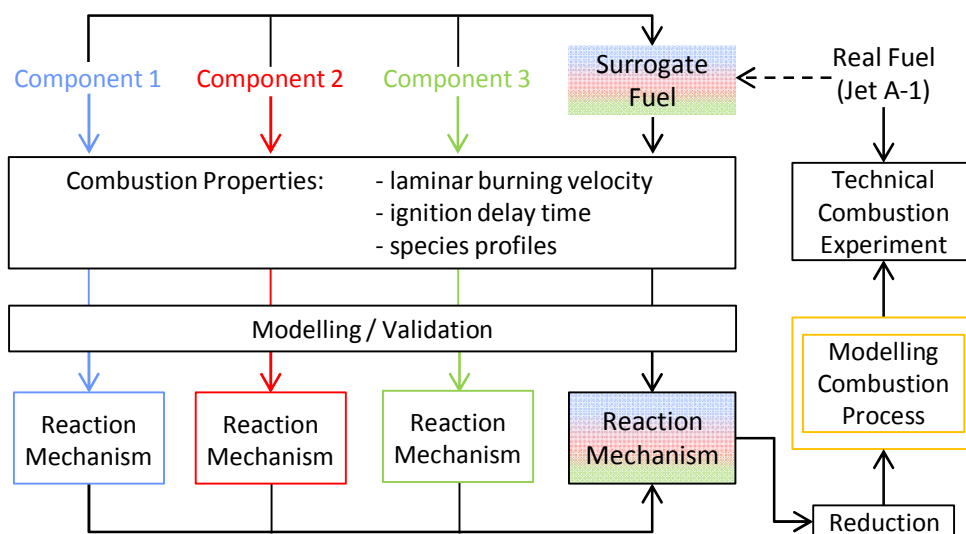

Fig. 10 Development of the reaction mechanism for a surrogate (generic) fuel which is used for numerical simulation of a real fuel, e.g. Jet A-1

Since a real fuel will be first vaporized and atomized before being burned in a jet engine, many individual fuel mixture compositions might exist, with the values for each single surrogate component ranging from 0% up to 100%, in principle. So the surrogate mechanism should be able to describe the combustion behaviour of numerous different fuel compositions.

Independent of the oxidation of any fuel to be described, a reaction mechanism features always the same structure: (i) It is composed of many elementary reactions; (ii) The combustion process is described starting from the reactants via the formation and decomposition of intermediate species up to the formation of the final combustion products (including pollutants); and (iii) Each reaction scheme is characterised by a systematic and hierarchic structure. Furthermore, to demonstrate the performance of the reaction model constructed, each reaction mechanism has to be validated with the help of reliable and relevant experimental data by the adjustment of kinetic and thermodynamic parameters as well as the examination of single species formation and decomposition pathways.

To reduce the computing time, the reduction of the reaction mechanism is important, especially if the mechanism should be implemented in a CFD-simulation: *e.g.* for the simulation of an aircraft combustor the computing time amounts to about 146 kCPUh using a mechanism with 119 species and 1022 reactions. If the mechanism is reduced to 79 species and 672 reactions the computing time is reduced by about a third, with 93 kCPUh.

For the reduction, unimportant species and reactions as well, are identified using the software package of *Chemical Workbench®* [33]. Another approach to reduce the size of a mechanism is the linear transformation model (linTM) [34] developed recently. Both applications allow the reduction of a mechanism, in particular the number of species, thus enabling its efficient use in CFD simulations. By eliminating species and reactions from the detailed reaction scheme, the calculation should yield similar results and agreement with the experimental data (targets are *e.g.* laminar flame speed, ignition delay time, and selected species profiles) compared to those obtained when using the original full mechanism.

4. Results of the modelling study

Within InnoTreib [3], it was decided to study a synthetic fuel without any aromatics to benefit from the improved environmental prospects aromatics-free fuels offer [1, 2]. Hence, in the present work, for the development of the reaction mechanism of a surrogate fuel to mimic a corresponding innovative fuel, n-dodecane, isooctane, and cyclohexane were chosen as representative components for the molecule classes of n-alkanes, iso-alkanes, and cycloalkanes, respectively. The exact molar composition of the surrogate fuel was chosen to reflect the typical composition of a jet fuel. Furthermore, to allow the integration of the reaction mechanisms developed within

InnoTreib [3] in a CFD program, reduced reaction models were constructed.

According to Fig. 10, the laminar burning velocity data at $p = 1$ bar and ignition delay time data of stoichiometric mixtures measured at $p \approx 16$ bar have been selected as targets; the results for the mechanism reduction are shown in Tab. 1. In the case of the surrogate fuel, it was not possible to reduce the mechanism to less than 60 species due to the need of containing an additional component. The use of an aromatic compound (toluene) to the surrogate was essential to predict the combustion behaviour of Jet A-1, which consist, besides n-alkanes, iso-alkanes, and cycloalkanes, of aromatics as described in section 1. As shown in Tab. 1, the reduction to less than 60 species was achieved for the reduction of the mechanisms of the single fuel components.

The comparisons between the detailed and reduced reaction mechanisms with the experimental data for each single component are presented in Figs. 11a-c for the laminar burning velocity and in Figs. 12a-c for the ignition delay time, respectively. Further, the developed reaction mechanism for the surrogate is compared to the measurements of Jet A-1, too (see Fig. 11d and Fig. 12d).

By using the reduced mechanisms for cyclohexane (Fig. 11a) and n-dodecane (Fig. 11b), respectively, the burning velocities are predicted with almost the same accuracy as by using the detailed model. For isooctane (Fig. 11c), the calculated values using the reduced mechanism show a shift to slightly higher φ-values.

Tab. 1 Number of species and reactions (in brackets) in the detailed and reduced reaction mechanisms for the single fuel components and the surrogate

Component	Number of species in mechanisms (number of reactions in brackets)	
	detailed	reduced
n-Dodecane	157 (1048)	55 (387)
Isooctane	114 (808)	50 (290)
Cyclohexane	129 (740)	50 (409)
Surrogate fuel *all 3 components*	170 (1024)	77 (438)

The developed reaction mechanism for the surrogate is compared to the measurements of Jet A-1, too. Since toluene as the selected aromatic model component was added to the mechanism, it is possible to perform calculations for an innovative generic jet fuel *and* for Jet A-1 as reference fuel using the *same* model. For these calculations, a surrogate composition of 40 % n-dodecane, 20 % cyclohexane, 25 % isooctane, and 15 % toluene was used.

Similar to isooctane, the calculation of the burning velocities of the surrogate with the reduced mechanism results in a shift to slightly higher φ-values compared to the experimental data as well as to the use of the detailed

mechanism (Fig. 11d). The differences between predicted ignition delay time data (see Figs. 12a-d) when using the detailed and the reduced reaction models are caused by the selected strong degree of reduction of the mechanism, in agreement to the findings on calculating burning velocities. The ignition delay time calculations of the pure fuel components using the detailed mechanism fit better to the experimental results (Figs. 12a-c). For all components, the reduced mechanisms are able to predict the ignition behaviour, too, especially at high temperatures (T > 1250 K). For cyclohexane (Fig. 12a), the temperature oxidation (T < 1000 K) is well described by the reduced mechanism, too. Although the mechanism for the surrogate is reduced to less than 50% of the original species number (see Tab. 1), the resulting deviation considering ignition delay time is smaller than for the pure fuel components (Fig. 12d).

In summary, all reaction mechanisms developed are able to reproduce the selected targets, *here* ignition delay time and laminar burning velocity. The differences in the calculations using the reduced and the detailed mechanisms as shown in Figs. 11 and 12 reflect the selected high and stepwise increasing degree of reduction in the number of species, here from 110 species (for n-dodecane even 157) to less than 60 (see Tab. 1). The deviations in the calculation of the laminar burning velocities are in the range of the experimental uncertainties; thus, less than 5 % over a wide φ-range, and up 20 % for fuel rich mixtures ($\varphi > 1.50$). Furthermore, the mechanisms are also capable to predict the ignition behaviour sufficiently well since the experimental and calculated values agree over a wide temperature range. However, the performance of the reduced mechanisms of n-dodecane and isooctane, respectively would benefit from an optimization at temperatures as low as 850 K and below.
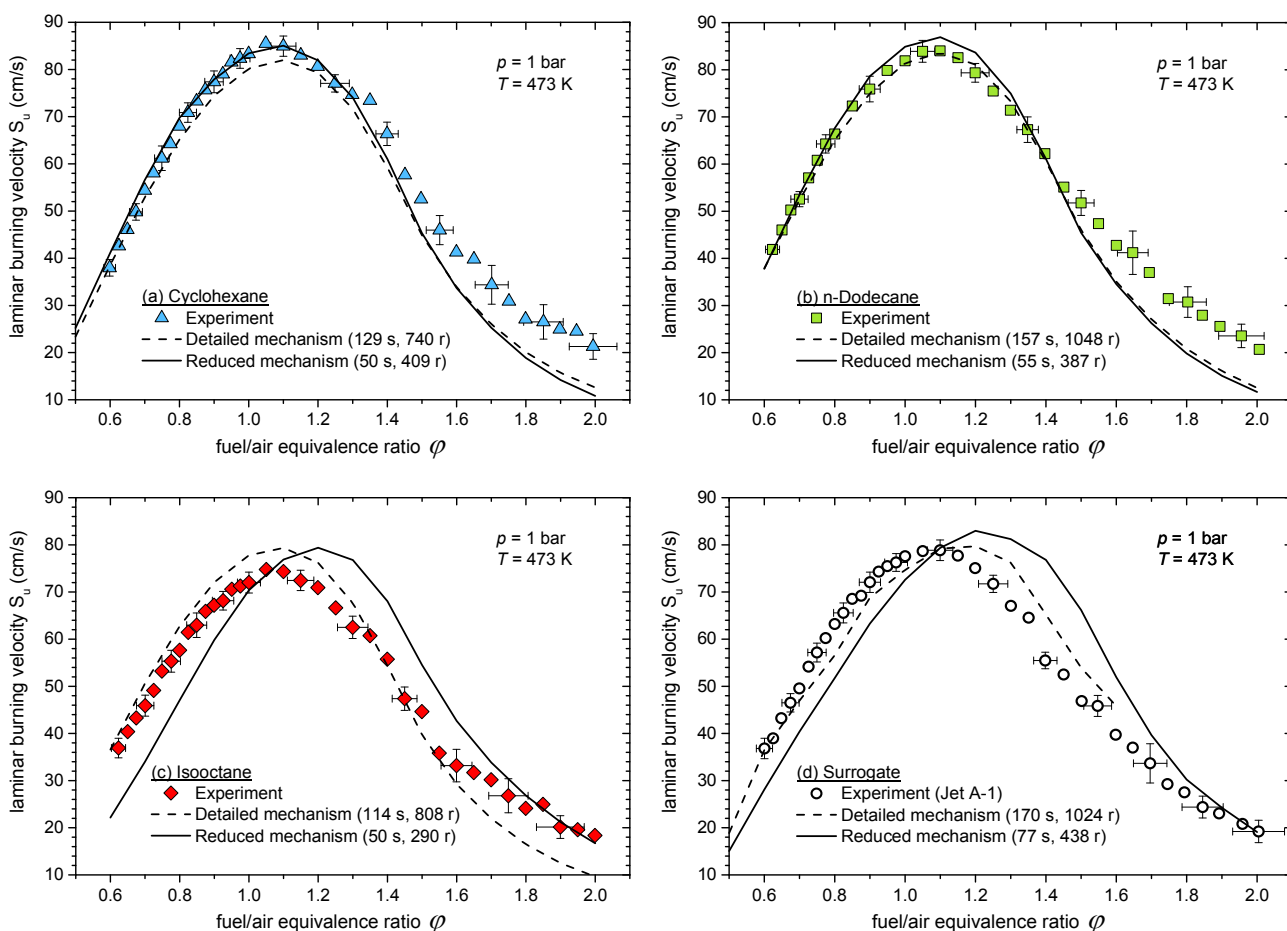

Fig. 11 Comparison between experiments (symbols) and calculations (lines) using the detailed (dashed) and reduced mechanism (full) for the determination of the laminar burning velocity of the single fuel components cyclohexane (a), n-dodecane (b), and isooctane (c) as well as for the surrogate fuel (composition: 40 % n-dodecane + 20 % cyclohexane + 25 % isooctane + 15 % toluene) using experimental data of Jet A-1 for comparison (d); in brackets: s = number of species, r = number of reactions

Fig. 12 Comparison between experiments (symbols) and calculations (lines) using the detailed (dashed) and reduced mechanisms (full) for the determination of the ignition delay time of the single fuel components cyclohexane (a), n-dodecane (b) and isooctane (c) as well as for the surrogate fuel (composition: 40 % n-dodecane + 20 % cyclohexane + 25 % isooctane + 15 % toluene) using experimental data of Jet A-1 for comparison (d); in brackets: s = number of species, r = number of reactions
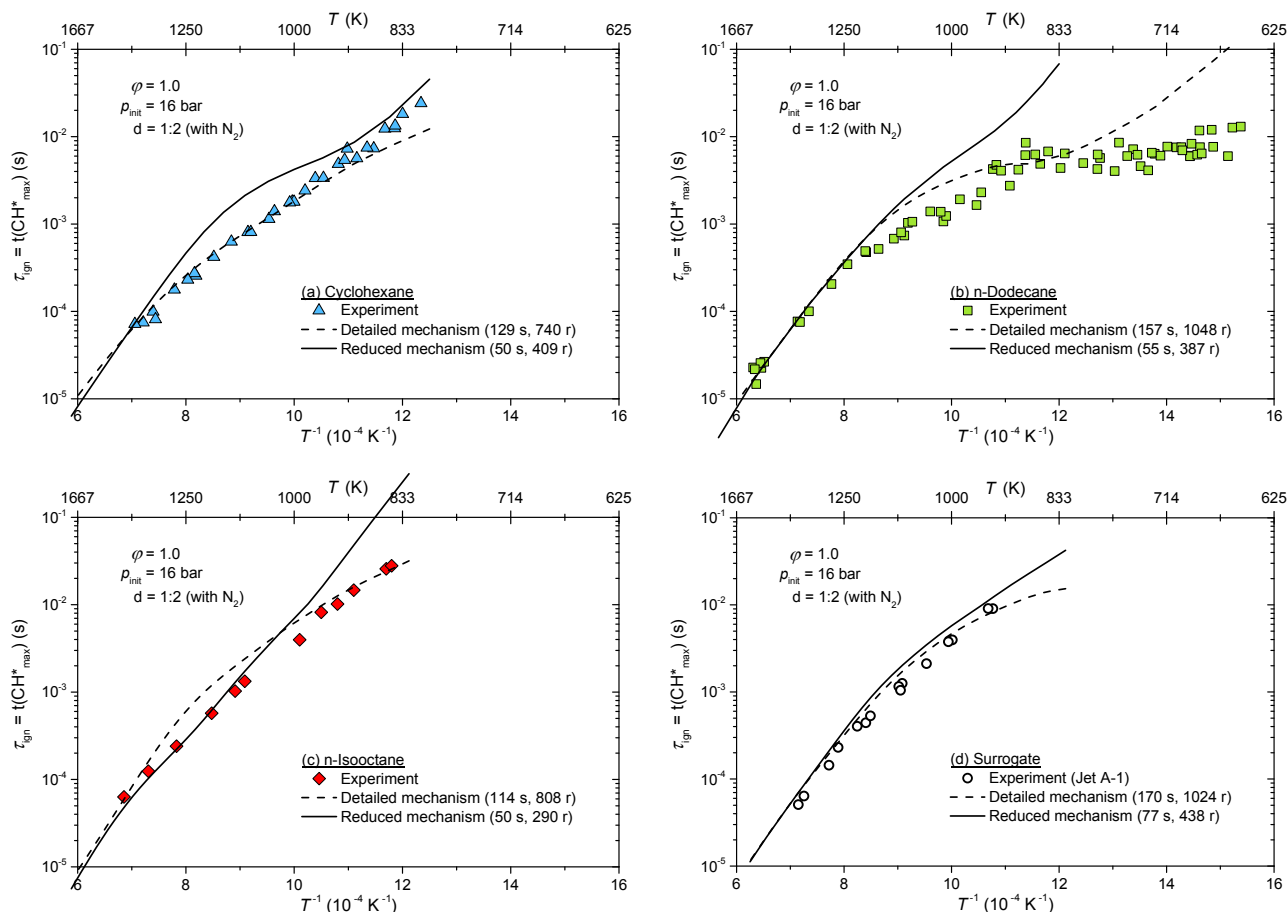
5. Conclusion

As part of the InnoTreib project, an innovative generic jet fuel (surrogate) was developed, defined by preselected properties leading to a more environmentally friendly combustion with reduced emissions of soot and further pollutants. The components selected for the generic fuel were n-dodecane, cyclohexane, and isooctane, representing each a major molecule class (n-alkanes, cycloalkanes, and iso-alkanes) present in a jet fuel (see Fig. 1). Aromatics were not considered since they are major soot precursors – the combustion of an innovative fuel must result in emissions as low as possible.

For the development, validation, and optimization of reaction mechanisms, the fundamental combustion properties laminar burning velocity and ignition delay time were measured for each pure component. With the help of these experimental data it was possible to develop (i) a detailed reaction mechanism for each surrogate component as well as (ii) a reduced reaction mechanism by decreasing the number of species and reactions of the detailed model. The reduced models predict the selected

combustion properties reliably. Based on the detailed reaction mechanisms of the components, the mechanism for the surrogate was generated and reduced following the same method as applied for each single component reaction mechanism.

The measurements were performed not only for the single fuel components but also for conventional Jet A-1 and, in addition, for further pure components, namely n-propylcyclohexane, n-propylbenzene, and toluene. The results indicate that isooctane and the aromatics have a lower reactivity than n-dodecane, cyclohexane, and n-propylcyclohexane which is caused by the different structures of the molecules. Based on these findings it is in principle conceivable that aromatics do not represent an indispensable ingredient of a synthetic fuel with regard to the combustion behaviour; for example, isooctane (or other branched saturated hydrocarbons) can lower the surrogate's burning velocity and increase the surrogate's ignition delay time at the same time.

The comparison between the experimental data and the calculations using the full and the reduced mechanisms shows good, comparable results since they are in

the same range with respect to the deviations of the target data. Both mechanisms are able to describe the laminar burning velocity data as well as those of the ignition delay time. The deviations occurring by using the reduced mechanisms are caused by the selected high degree of reduction the number of species (to less than 60) which was required for a further implementation in numerical simulations. Nevertheless, the reduced mechanisms are able to predict the combustion properties, especially for a generic fuel; however, at low temperatures, the calculation of the ignition delay time of n-dodecane is not satisfying.

In summary, it was shown that the development of alternative fuels is possible without aromatics, at least with respect to laminar burning velocities and ignition delay times of the studied surrogate and its single fuel components, since these combustion properties are very similar to those of a Jet A-1 fuel. Moreover, single fuel components well-known in the sense of their combustion behavior are necessary for the development of a surrogate reaction mechanism allowing not only the calculation of combustion properties but also the implementation in a CFD-simulation. The developed reduced reaction mechanism conduced to the specific investigation of alternative synthetic fuels; integrated in a CFD-simulation this mechanism enables the prediction of the combustion in a jet turbine under practical conditions.

6. Acknowledgment

7. Literature

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