Reduction of a detailed chemical mechanism for a kerosene surrogate via RCCE-CSP

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A B S T R A C T

Detailed mechanisms for kerosene surrogate fuels contain hundreds of species and thousands of reactions, indicating a necessity for reduced mechanisms. In this work, we employ a framework that combines Rate-Controlled Constrained Equilibrium (RCCE) with Computational Singular Perturbation (CSP) for systematic reduction based on timescale analysis, to reduce a detailed mechanism for a jet fuel surrogate with n-dodecane, methylcyclohexane and m-xylene. Laminar non-premixed flamelets are utilised for the CSP analysis for different strain rates and therefore different scalar dissipation rate, covering the flammable region of strain rates for the surrogate fuel.

Two RCCE-reduced mechanisms are developed via an RCCE-CSP methodology, one with 17 and one with 42 species, and their accuracy is assessed in a range of cases that test the performance of the reduced mechanism under both non-premixed and premixed conditions and its dynamic response. These include non-premixed flamelets with varying strain rate, laminar premixed flames for a range of equivalence ratios and pressures, flamelets ignited by an artificial pilot or by hot air, and unsteady flamelets with time-dependent strain rate.

The profiles of both major and minor species, as well as important combustion characteristics such as the ignition strain rate and the laminar flame speed, are investigated. The structure of non-premixed flamelets is very well predicted, while the premixed flames are overall well predicted apart from a few deviations in certain species and an underprediction in the laminar flame speed. Apart from the large reduction in dimensionality, the reduction in computational time is also considerable (up to 19 times). As the detailed mechanism comprises 367 species and 1892 reactions, this paper presents the first application of RCCE to a mechanism of this size, as well as a comprehensive validation in a set of cases that include non-premixed and premixed laminar flames, atmospheric and elevated pressures and steady-state and dynamic response.

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1. Introduction

Design of jet engines for increased efficiency and reduced emissions is a time-consuming procedure, during which several different configurations and layouts are tested. An experimental approach to this design procedure is costly in terms of both time and resources. In contrast, turbulent combustion CFD with an accurate chemical mechanism provides all the required information for the design process. Benefits from turbulent combustion simulations can impact the efficiency for lower fuel consumption and longer engine life, as well as assist in the reduction of NO_x emissions and soot formation. The modelling of turbulent combustion in jet engines requires the accurate representation of a surrogate fuel, the development of a detailed chemical mechanism and lastly the development of a reduced chemical mechanism in order to incorporate comprehensive chemistry into turbulent combustion CFD. These aspects are discussed in the following paragraphs. :

1.1. Modelling of surrogate fuels

The most common aviation fuel for aircraft is kerosene, for both transport and military operations. The first challenge in modelling kerosene combustion, however, is the accurate representation of kerosene with a so-called surrogate fuel, as kerosene is a distillate product and therefore includes hundreds of components. These surrogate fuels resemble the most important characteristics of the real fuel, with most of them targeting either the physical properties, like density and viscosity, or the fuel's chemical properties, such as molecular weight and sooting tendency [1].

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The first attempts to model kerosene were the early works of Wood et al. [2] who used a 14-component surrogate fuel to model JP-4 (Jet Propellant 4) and Heneghan et al. [3] who represented JP-8 with a 12-component fuel; these studies focused on the thermal stability and distillation curve of the real fuels. The pioneering work of Gueret et al. [4] was the first to introduce a surrogate fuel with only three components related to the main hydrocarbon families, namely alkanes, cycloalkanes and aromatics, represented by 79% n-decane, 11% 1,2,4-trimethylbenzene and 10% n-propylbenzene, respectively. These components were selected after a chemical analysis of Jet-A1, and the surrogate fuel was later validated in a jet stirred reactor (JSR). No PAHs were included in their compact model with 56 species and 360 reactions, as the fuel was oxidised with global reactions straight to C_4 species or smaller.

Following these works, Dagaut et al. [5] used a single component surrogate fuel with n-decane to represent kerosene in a JSR at elevated pressures, while Doute et al. [6] used the same surrogate in premixed flames. The similarity observed in [5] was reasonably validated numerically with a detailed mechanism with 90 species and n-decane in [6]. The importance, however, of including an aromatic component in the surrogate fuel to model soot formation in a kerosene flame was also discussed in [7], where 10% toluene was added to 90% n-decane and resulted in reasonable agreement, similar to Maurice et al. [8] who used 78% n-decane and 22% ethylbenzene to predict the CO and NO_x emissions from a well-stirred reactor. The work of Lindstedt and Maurice [9] explored the potential of including the aromatic components benzene, toluene, ethylbenzene and ethylbenzene/naphthalene at 11%, accompanied by 89% n-decane as base component of the surrogate fuel, in a mechanism consisting of 193 species and 1085 chemical reactions. Benzene was found to have a disadvantage against the other components, and all the surrogates were compared in the experimental configuration of Doute et al. [6]. Most of these works are covered by the comprehensive review of Edwards and Maurice [1], which also highlights the necessity of multi-component surrogate fuels and the similarity of n-dodecane with kerosene in terms of physical properties. For a historical perspective, Edwards [10] describes the evolution of modelling of liquid fuels, the development of jet engines and the differences in batches of kerosene, along with the physical properties of liquid fuels and the specifications that should be checked.

The work on surrogate fuels, which use n-decane as a main component, was continued by other researchers as well. Dagaut [11] used a surrogate fuel with 74% n-decane, 15% n-propylbenzene and 11% propylcyclohexane, which is different to Gueret et al. [4], and developed a detailed mechanism with 207 species to model a JSR under atmospheric pressures and lean and rich conditions. Another modification to Gueret et al. [4] was introduced by Honnet et al. [12] to develop the Aachen surrogate fuel with 80% n-decane and 20% trimethylbenzene to predict ignition times, flame speeds and non-premixed flames. Honnet et al. also updated the mechanism from Bikas and Peters [13], which was initially developed for n-decane combustion, and derived a new one with 122 species. This mechanism was also implemented in a multiphase LES study with Jet-A [14] using non-premixed and premixed flamelets.

Humer et al. [15] developed a detailed mechanism with 283 species and a lumped version with 173 species for testing different surrogate fuels based on different alkanes (n-decane, n-dodecane), different aromatics (o-xylene, toluene) and methylcyclohexane, and concluded that the n-dodecane/o-xylene/methylcyclohexane fuel provided higher accuracy than the n-decane/toluene/methylcyclohexane surrogate, while the aromatic component was found not to have significant difference, something that was also noticed by Lindstedt and Maurice [9] for toluene, ehtylbenzene and naphthalene. In the same work [15], few more surrogate fuels were also compared in the same configuration including the Drexel surrogate [16], the Utah surrogate [17] and the surrogate fuel developed in [2], which included five, six and twelve components, respectively.

The works of Colket et al. [18] and Dagaut and Cathonnet [19] were milestones in the development of jet fuel surrogates. Colket et al. [18] reviewed existing surrogate fuels and compared experimentally the most well-known ones for ignition and extinction along with a new surrogate consisting of 50% n-decane, 25% propyl-benzene and 25% propylcyclohexane, which was also tested at high pressure and lean conditions. Dagaut and Cathonnet [19] reviewed kinetic mechanisms and experimental data for kerosene, highlighting the importance of soot for environmental, military and design reasons and the significant influence of an aromatic component in the surrogate fuel. Regarding the experimental work on surrogate fuels and fuel components, the work of Ranzi et al. [20] reviewed the laminar flame speeds of several hydrocarbon fuels, including large alkanes (n-decane, n-dodecane), cycloalkanes and aromatics, and provided a database for the components of jet fuel surrogates.

It was only recently [21] that the first systematic method for the development of a surrogate fuel was suggested given specific targets, in this case towards chemical kinetics characteristics including soot tendency; an abstract approach was also attempted in [2]. Dooley et al. [21] suggested a four-component surrogate fuel, developing their previous surrogate fuel [22] to match the combustion properties of kerosene over a wide range of conditions including variable pressure flow reactor, diffusion flames, ignition delay times at high pressure, laminar flame speed and soot volume fractions. Kim et al. [23] developed two surrogate fuels using a systematic method similar to Dooley et al. [21], but targeting the physical properties of kerosene; they studied the influence of different cycloalkanes comparing methylcyclohexane and decalin and the surrogate fuels were found to reproduce most of physical and chemical properties under examination. Narayanaswamy and co-workers also identified the necessity of a systematic way for the developement of a surrogate fuel and introduced a methodology to select the composition of the surrogate components through an optimisation of specific targets, in this case for the chemical representation of the real fuel [24]. Most of the above mentioned surrogate fuels are shown in the following Table 1.

As briefly described in the previous paragraphs and also in [18], research still needs to be undertaken in the field of surrogate fuels in order to conclude to targets to be used for improved design of jet engines and reduced emissions. Systematic methods are indeed the only solution to the problem of identifying the composition of the surrogate fuel, but no suggestions exist for selecting the number of components in the surrogate fuel to represent the different hydrocarbon families and which components should be selected.

1.2. Detailed mechanisms

Some of the pioneering works regarding the development of surrogate fuels and detailed chemical mechanisms were discussed in the previous paragraph, while here some works that suggested only kinetics for known surrogates are reviewed. Patterson et al. [26] used a chemical mechanism including parts of GRI mechanism and others, with 85 species and 440 chemical reactions. This mechanism was validated in a JSR configuration and in premixed flames (compared with the results from Doute et al. [6]) and non-premixed flames at high strain rates, using the surrogate fuel from Lindstedt and Maurice [9]. The surrogate fuel from Violi et al. [17] was used in [27].

A detailed mechanism for the oxidation of n-dodecane was suggested in [28] and tested for burning velocities, ignition times and pyrolysis. The mechanism was based on USC Mech-II with an addition of 60 species, containing 171 species and 1306 reactions,