



Full Length Article

Skeletal mechanism development for a 3-component jet fuel surrogate using semi-global sub-mechanism construction and mechanism reduction

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ABSTRACT

A skeletal mechanism with 110 species and 352 reactions is developed from a detailed mechanism that includes 369 species and 2691 reactions for a 3-component jet fuel surrogate which is composed of methylcyclohexane (MCH), n-dodecane and m-xylene. Firstly, the semi-global sub-mechanisms of MCH and n-dodecane are constructed to substitute the corresponding portions in detailed mechanism, the construction is guided by main reaction pathways and involves isomer lumping, parallel reaction lumping and reaction product substituting, the rate parameters of key reactions are tuned via genetic algorithm (GA) to fit ignition delays. Secondly, the aromatics and base sub-mechanisms are reduced by DRGEP and iterative sensitivity analysis (ISA). ISA calculates the sensitivity parameter for every objective and only removes the one with the lowest value in every iteration. This approach could remove redundant species and reactions effectively. The skeletal mechanism is validated against ignition delays in shock tube, laminar flame speeds and species concentration profiles in shock tube and plug flow reactor over a wide range of conditions. Furthermore, the skeletal mechanism is employed to simulate 3D jet fuel spray combustion and ignition delay times are validated against experimental data.

1. Introduction

Kerosene based jet fuels (Jet-A/Jet A-1/JP-8) are widely used in the aviation industry to power jet engines of aircraft. Jet-A and Jet A-1 are utilized in civilian aviation, JP-8 is a primary military jet fuel which includes a military-specific additive package to Jet A-1 [1]. Major chemical composition of these jet fuels are very similar [2], moreover, the ignition delays of JP-8 are found close to Jet-A over wide conditions [3] which indicates that the JP-8 additives have negligible influence on fuel chemical reactivity.

As typical petroleum-derived fuels, jet fuels consist of hundreds to thousands of components belonging to various types of hydrocarbons. In numerical investigations, realistic chemical kinetics is important for simulating fuel combustion characteristics, but the complexity of real fuels makes it infeasible to model every involved fuel component [4] therefore surrogate fuels with one or more representative components have been developed to mimic the combustion behavior of real jet fuels [5].

In Early studies, n-decane was commonly used as a single-component surrogate [6] based on its similarity with kerosene in oxidation rates under jet stirred reactor (JSR) [7,8] and premixed flame conditions [9]. The advantage of single-component surrogate is that compact

reaction mechanisms are usually available to integrate into 3D numerical simulations, for instance: Zeng et al. [10] developed a skeletal n-decane mechanism with 50 species and 210 reactions; Chang et al. [11] developed a highly reduced n-decane mechanism with only 40 species and 141 reactions using decoupling method. However, except for ignition quality, other chemical properties of jet fuels are poorly represented by single-component surrogate [12] such as average molecular weight, major chemical classes and smoke point.

To comprehensively emulate these characteristics, different groups proposed multi-component surrogates for kerosene with mated kinetic models. Honnet et al. [13] formulated a surrogate targeting the ignition and extinction behavior of jet fuel with 77.2% n-decane and 22.8% 1,2,4-trimethylbenzene by mole fraction. Dagaut et al. [14] found that a 3-component surrogate consisting of 74% n-decane, 15% n-propylbenzene and 11% n-propylcyclohexane by mole fraction showed best agreement with the JSR and flame data from Jet-A among the 4 candidate mixtures they tested. Humer et al. [15] developed a surrogate mechanism containing 3 components (43.3% dodecane, 31.0% toluene, 25.7% methylcyclohexane by mole fraction) to mimic the sooting behavior of JP-8. Dooley et al. [16] proposed a surrogate for Jet-A POSF 4658 with 0.4267n-decane, 0.3302 iso-octane and 0.2431 toluene by mole fraction, it was extensively tested in various combustion devices.

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Table 1
Sizes of some jet fuel surrogate kinetic models.

Reference	Species	Reactions
Honnet et al. [13]	122	900
Dagaut et al. [14]	209	1673
Humer et al. [15]	283	7878
Dooley et al. [16]	1599	6633
Malewicki et al. [17]	2080	8310
Kim et al. [18]	4263	18,000
Narayanaswamy et al. [19]	369	2691

Malewicki et al. [17] subsequently updated the POSF 4658 surrogate into the 2nd generation with 0.404n-dodecane, 0.295 iso-octane, 0.228n-propylbenzene and 0.073 1,3,5-trimethylbenzene by mole fraction. Kim et al. [18] developed a 4-component surrogate composed of 0.3862 n-dodecane, 0.1090 iso-cetane, 0.2924 decalin and 0.2124 toluene by mole fraction which could capture both the physical and chemical properties of Jet-A. Narayanaswamy et al. [19] proposed a surrogate consisting of 48.5% methylcyclohexane (MCH), 30.3% n-dodecane and 21.2% m-xylene by mole fraction. The sizes of kinetic models used in above studies are summarized in Table 1. As can be seen in Table 1, mechanisms for multi-component surrogates are often of a large size and could not be used in 3D numerical simulations due to prohibitively long computational time. For this reason, it is desirable to reduce the size of multi-component mechanisms without significant loss of accuracy on chemical properties.

In the present work, a reduction strategy combining semi-global sub-mechanism construction and mechanism reduction is proposed to reduce the 3-component surrogate mechanism developed by Narayanaswamy et al. [19] (referred to below as the original mechanism). This mechanism contains 369 species and 2691 reactions and has been extensively validated for both low and high temperature conditions, which is a good candidate to start with. Sub-mechanisms of large fuel molecules are replaced by several semi-global reactions to reduce mechanism size, then DRGEP and iterative sensitivity analysis (ISA) are used to remove redundant species and reactions. The final skeletal mechanism consists of 110 species and 352 reactions and is validated against the original mechanism and various experimental data.

2. Skeletal mechanism development

The original mechanism is modular assembled which consists of C₀-C₄ base chemistry [20], substituted aromatics sub-mechanism [21], low T and high T sub-mechanisms for both MCH [22] and n-dodecane [23]. In detailed mechanism of large hydrocarbons, cracking process of the fuel molecule is rather complex because large numbers of intermediate isomers are produced and their successive oxidation pathways should all be included [24,25]. It has been found that semi-global schemes describing the oxidation of heavy hydrocarbons with only a few representative species and reaction pathways can well reproduce ignition delay and species concentrations if the reaction pathways are chosen and tuned properly [26–28]. To minimize the mechanism size in this work, semi-global sub-mechanisms of MCH and n-dodecane are constructed and substitute the corresponding portions in the original mechanism.

2.1. Construction of MCH semi-global sub-mechanism

MCH semi-global sub-mechanism includes reactions of MCH and its naphthenic derivatives. In the original mechanism, H-abstraction from MCH by any radical produces 5 isomers via parallel reactions, these isomers are lumped into a representative methylcyclohexyl radical named MCHR in this work, the rate coefficient of the lumped reaction is the sum of corresponding coefficients in the original mechanism.

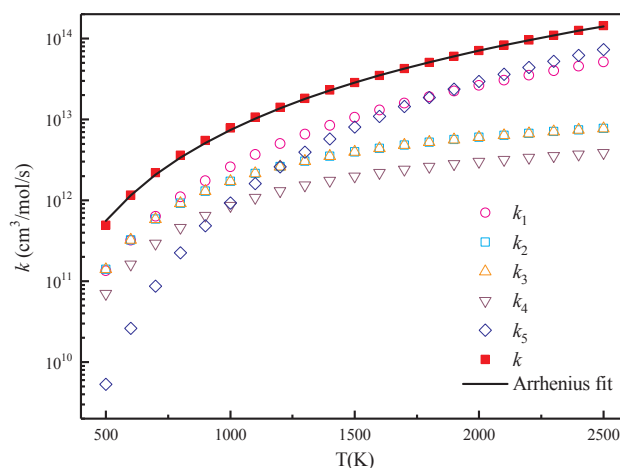
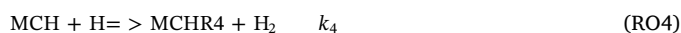
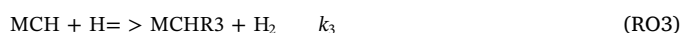
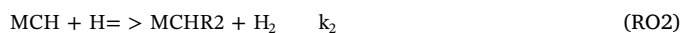
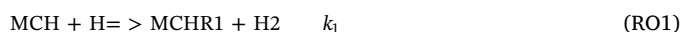
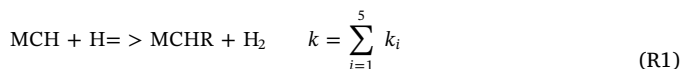


Fig. 1. Generation of lumped reaction rate parameters. $k_1(T) - k_5(T)$ (Hollow symbols) are calculated from corresponding rate parameters in original mechanism, $k(T)$ (solid symbols) are first obtained by summing $k_1(T) - k_5(T)$ and then used to fit Arrhenius equation to generate rate parameters of R1.



For instance, RO1–RO5 are H-abstraction reactions by H atom from MCH in the original mechanism, $k_1 - k_5$ are their rate coefficients, then the lumped reaction R1 is expressed as below.



Rate parameters of R1 are derived from curve fitting. As shown in Fig. 1, k_1 – k_5 are first calculated at $T = 500$ K and summed to form a k (500), then increase the temperature progressively to calculate a series of $k(T)$ values until $T = 2500$ K, Arrhenius equation is finally fitted using nonlinear least-square regression for these $k(T)$ values and the optimal pre-exponential factor, temperature exponent and activation energy of reaction R1 are obtained. Parallel H-abstraction reactions from MCH are all lumped by using this method.

Consumption reactions of MCHR are based on the main reaction pathways in the original mechanism. At high temperature, the ring opening of methylcyclohexyl radicals produces 5 different C₇ alkenyl radicals, these pathways are all inherited here as R2–R6 listed below:



Initial rate parameters of these reactions are derived from related reactions in the original mechanism. Adjustments are subsequently performed with the assumption that relative distribution of these alkenyl isomers are constant, i.e. each initial pre-exponential factor of R2–R6 is multiplied by a coefficient α_i with the constraint $\alpha_i \in (0,1)$, $\sum_{i=2}^6 \alpha_i = 1$. α_i values are evaluated by using the genetic algorithm (GA), which is a commonly used method in optimizing rate coefficients [29,30], to minimize the total relative error of ignition delays for jet fuel surrogate/air mixture between the current and the original mechanism at target conditions. Considering that low

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