



Systematic analysis and reduction of combustion mechanisms for ignition of multi-component kerosene surrogate

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Abstract

Currently, most detailed chemical kinetic mechanisms for combustion are still not comprehensive enough and update of key reaction rate is still required to improve the combustion mechanisms. The development of systematic mechanism reduction methods have made significant progress, and have greatly facilitated analysis of the reaction mechanisms and identification of important species and key reactions. In the present work, time-integrated element flux analysis is employed to analyze a skeletal combustion mechanism of a tri-component kerosene surrogate mixture, consisting of *n*-decane, *n*-propylcyclohexane, and *n*-propylbenzene. The results of element flux analysis indicate that major reaction pathways for each component in the surrogate model are captured by the skeletal mechanism compared with the detailed mechanism. After that, sensitivity analysis (SA) and chemical explosive mode analysis (CEMA) are conducted to identify the dominant ignition chemistry. The SA and CEMA results demonstrate that the ignition of *n*-decane and *n*-propylcyclohexane is sensitive only to the oxidation chemistry of H₂/CO and C1–C4 small hydrocarbons, while the ignition of *n*-propylbenzene is very sensitive to the initial reactions of *n*-propylbenzene and related aromatic intermediates. This demonstrates that the hierarchic structure should be maintained in the reduction of detailed mechanism of substituted aromatic fuels. The skeletal mechanism is further reduced by combining the computational singular perturbation (CSP) method and quasi steady state approximation (QSSA). A 34-species global reduced mechanism is obtained and validated over a wide range of parameters for ignition.

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1. Introduction

Kerosene is a mixture of a large number of hydrocarbon compounds with different classes of

chemical structures, such as alkanes, aromatics, and cycloalkanes, and a wide range of molecular weights. Because of the limitation in available computational resources to deal with combustion processes of a large number of components in real kerosene, a surrogate mixture containing two to five pure compounds is usually adopted to mimic kerosene combustion behaviors [1–8]. In order to develop reliable chemical kinetic mechanisms for

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real fuels, comprehensive kinetic mechanisms have been developed for certain single-component compounds [9–24]. For linear and branched alkanes, it is generally recognized that detailed kinetic mechanisms are well-established [9–12]. However, for cycloalkanes and aromatic compounds, the ring structure in these fuels introduces additional kinetics pathways, and the development of comprehensive kinetic mechanisms for these hydrocarbon fuels is still in progress [13–24]. When detailed mechanisms for each component in the surrogate are established, they can be combined together to mimic combustion behaviors for real fuels. However, these detailed mechanisms of kerosene are highly complicated and numerical investigations are severely restricted to some zero- and one-dimensional applications. In order to couple the combustion chemistry of kerosene with large-scale computational fluid dynamics (CFD) simulations, mechanism reduction is critical in combustion community [25]. Mechanism reduction has been extensively studied and various methodologies have been developed as reviewed in Ref. [25]. The first step in mechanism reduction is skeletal reduction [26], which removes unimportant species and reactions from the detailed mechanism. It should be noted that no matter what methods are adopted for skeletal mechanism generation, the realistic chemical kinetics and the major reaction pathways should be maintained in order to achieve reliable skeletal mechanism. When skeletal mechanism has been generated, model reduction methods, such as the quasi-steady state approximation (QSSA) [25–27] can be performed more effectively.

Based on the above considerations, the first goal of the present work is to scrutinize how well the skeletal mechanism can reproduce the reaction pathways compared with the detailed mechanism. The detailed mechanism for the three-component kerosene surrogate mixture used in the present work is developed by Dagaut et al. [1,2], and includes 209 species and 1673 reversible reactions. The skeletal mechanism with 106 species and 382 reactions generated in our previous work [28] by using the DRG method combined with the iterative screening and structure analysis (ISSA) method is adopted. The three-component surrogate consists of *n*-decane (denoted as NC₁₀H₂₂, 74% molar fraction), *n*-propylbenzene (PHC₃H₇, 15%), and *n*-propylcyclohexane (CYC₉H₁₈, 11%), which are typical representative compounds of linear alkane, aromatics, and cycloalkanes in kerosene. The second objective is to clarify dominant ignition chemistry of the three different hydrocarbon fuels. This is achieved by using sensitivity analysis (SA) [29] and the chemical explosive mode analysis (CEMA) [30,31]. Furthermore, the skeletal mechanism is further reduced to facilitate CFD simulations. The paper is organized as following: Section 2 presents the methodologies

used in this work; analysis and comparison of results based on the detailed and skeletal mechanism are performed in Section 3; validation and discussion of the global mechanism are presented in Section 4, and main conclusions are summarized in Section 5.

2. Methodologies

2.1. Time-integrated element flux analysis

The concept of element flux analysis, proposed by Revel et al. [32], provides a general methodology to identify reaction pathways under certain simulation condition with minimal computational effort. The method is briefly outlined as following.

The instantaneous element flux for each element (such as C, H, O) from species *k1* to *k2* through reaction *i*, denoted as $\dot{A}_{i,k1 \rightarrow k2}(t)$, can be calculated using the following equation [32]:

$$\dot{A}_{i,k1 \rightarrow k2}(t) = q_i(t) \frac{N_{A,k1} N_{A,k2}}{N_{A,i}} \quad (1)$$

where $q_i(t)$ is the instantaneous reaction rate of reaction *i* at time *t*, $N_{A,k1}$, $N_{A,k2}$, and $N_{A,i}$ are the number of atom *A* in species *k1*, species *k2*, and reaction *i*, respectively.

The total transformation for element *A* from species *k1* to *k2* in a mechanism consisting of *I* elementary reactions and *K* species at instantaneous time *t* can be calculated through the summation of contributions from all reactions:

$$\dot{A}_{k1 \rightarrow k2}(t) = \sum_{i=1}^I \dot{A}_{i,k1 \rightarrow k2}(t) \quad (2)$$

To derive global information, a time-integrated flux indicator is proposed [33,34]:

$$\bar{A}_{k1 \rightarrow k2} = \int_0^\tau \dot{A}_{k1 \rightarrow k2}(t) dt \quad (3)$$

Consequently, the time-integrated contribution of reaction *i* to the flux of element *A* from *k1* to *k2*, and the normalized weight of element flux from *k1* to *k2* to the total out flux of species *k1* can be easily identified with Eqs. (4) and (5), respectively:

$$\hat{A}_{i,k1 \rightarrow k2} = \frac{\bar{A}_{i,k1 \rightarrow k2}}{\bar{A}_{k1 \rightarrow k2}} = \frac{\int_0^\tau \dot{A}_{i,k1 \rightarrow k2}(t) dt}{\int_0^\tau \dot{A}_{k1 \rightarrow k2}(t) dt} \quad (4)$$

$$\hat{A}_{k1 \rightarrow k2} = \frac{\bar{A}_{k1 \rightarrow k2}}{\sum_k^K \bar{A}_{k1 \rightarrow k}} = \frac{\int_0^\tau \dot{A}_{k1 \rightarrow k2}(t) dt}{\sum_k^K \int_0^\tau \dot{A}_{k1 \rightarrow k}(t) dt} \quad (5)$$

2.2. Brute force SA and CEMA

Brute force SA is a useful method to identify important reactions which have the largest affects

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