

Response to reviewer comments

We highly appreciated the suggestions and comments from the reviewer to improve the overall quality of the work. We have attached the point-to-point responses to the reviewer's questions as follows. Detailed corrections on the manuscript can be found in the Supplementary Material of this submission with the name as 'Revised manuscript with changes marked'.

Reviewer #1

This paper developed a new four-component jet fuel surrogate (n-dodecane/iso-octane/iso-547 cetane/decalin/toluene) by formulating with a property optimizer. A reduced and robust kinetic chemical mechanism (containing 124 species and 590 reactions) that could be directly employed in practical engine combustion simulations is also developed for the presented surrogate. The mechanism is validated by comprehensive experimental data including ignition delay time (IDT) determined in shock tube and rapid compression machine (RCM), species mole fractions measured in premixed flames and jet stirred reactor (JSR), and laminar flame speeds. The comparison results between the predictions and measurements indicated that the current kinetic mechanism is capable of reflecting the oxidation process of real jet fuel and could be applied in practical engine computational fluid dynamic (CFD) simulation. All my concerns are list below:

(1) The innovation of this paper is not well displayed, it's better to list the contributions one by one. In addition, the research results are limited to the validation of each component and the surrogate fuel mixture, and do not involve the quantitatively analysis of the agreement between calculated values by surrogate and measured data of target jet fuel.

Response 1

Thanks for your good suggestions. We will provide a Highlights to the editor. The innovations of the current work are listed as follows:

1. A new four-component jet fuel surrogate was proposed based on a property optimizer.
2. Both physical and chemical properties of target fuel were emulated by the surrogate.
3. A reduced kinetic mechanism for the fuel surrogate was developed.
4. The mechanism was validated by comprehensive experimental data.

Besides, in the section 4.5, the comparison of ignition delay times, species mole fractions and laminar flame speeds were conducted for the newly developed JFS surrogate and the target jet fuel POSF-4658. We add some quantitatively analysis of

the agreement between calculated values by surrogate and measured data of target jet fuel in the section 4 of the revised manuscript.

(2) This paper is not well organized, which can make readers confused. Only a brief description of the related results of different researchers is given in the introduction and none of them analyze nor clarify the related problems in the study of the development of jet fuel surrogates and their corresponding kinetic mechanisms.

Response 2

Thanks for your comments. Actually, the shortcomings of the previous studies and the research gap were concluded in the third paragraph of the Introduction section. Nevertheless, we have added more analysis about the referred studies in the Introduction section to improve the paper.

(3) It is recommended that quantitatively analysis of the agreement between calculated values by surrogate and measured data of target jet fuel should be presented in detail. Meanwhile, the physical surrogate model is necessary to validate the performance of the surrogate jet fuel under practical conditions.

Response 3

Thanks for your good suggestions. The quantitatively analysis of the agreement between the calculated values and measurements has been presented in our revised manuscript. Besides, we have validated the surrogate model with the previously published experimental data of jet fuel, which is sufficient in terms of the completeness and relevance of the current validation work. As for the implementation of the current model with CFD simulation in practical conditions, the corresponding work will be conducted in the near future.

(4) Other details: the choices of the LHV of JP-8 fuel and surface tension of Jet-A used as the references are lack of theoretical basis; the format of Table 4 is not standardized.

Response 4

Thanks for your comments. As stated in our paper (Page 4, lines 130 to 133), the measurement of LHV and surface tension of POSF-4658 cannot be found in other references, hence we choose the LHV of JP-8 fuel and surface tension of Jet-A as the references which is completely inspired by the previous published researches^[1-3]. In the previous researches^[1-3], the authors adopted the same approach to deal with this problem. Besides, Table 4 has been combined and adjusted to be standardized.

Reference:

- [1] Kim D, Martz J, Violi A. A surrogate for emulating the physical and chemical properties of conventional jet fuel. *Combust Flame* 2014;161:1489–98;
- [2] WB Yu, WM Yang, KL Tay, FY Zhao. An optimization method for formulating model-based jet fuel surrogate by emulating physical, gas phase chemical properties and threshold sooting index (TSI) of real jet fuel under engine relevant conditions. *Combustion and Flame*, 2018, 193, 192-217.

[3] W Yu, F Zhao, W Yang, K Tay, H Xu. Development of an optimization methodology for formulating both jet fuel and diesel fuel surrogates and their associated skeletal oxidation mechanisms. *Fuel*, 2018, 231, 361-372.