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Development of a Reduced Multicomponent Jet Fuel Surrogate for Computational Fluid Dynamics Application

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Abstract : This study proposed four Jet fuel surrogate (S1, S2 S3, and 4) with careful selection of seven large hydrocarbon fuel components, ranging from C_9-C_{16} of higher molecular weight and higher boiling point, adapting the standard molecular distribution size of the actual jet fuel. The surrogate was composed of seven components, including n-propyl cyclohexane (C_9H_{18}), n- propylbenzene (C_9H_{12}), n-undecane ($C_{11}H_{24}$), n- dodecane ($C_{12}H_{26}$), n-tetradecane ($C_{14}H_{30}$), n-hexadecane ($C_{16}H_{34}$) and iso-cetane ($iC_{16}H_{34}$). The skeletal jet fuel surrogate reaction mechanism was developed by two approaches, firstly based on a decoupling methodology by describing the C_4 -C_{16} skeletal mechanism for the oxidation of heavy hydrocarbons and a detailed H_2 /CO/C_1 mechanism for prediction of oxidation of small hydrocarbons. The combined skeletal jet fuel surrogate mechanism was compressed into 128 species, and 355 reactions and thereby can be used in computational fluid dynamics (CFD) simulation. The extensive validation was performed for individual single-component including ignition delay time, species concentrations profile and laminar flame speed based on various fundamental experiments under wide operating conditions, and for their blended mixture, among all the surrogate, S1 has been extensively validated against the experimental data in a shock tube, rapid compression machine, jet-stirred reactor, counterflow flame, and premixed laminar flame over wide ranges of temperature (700-1700 K), pressure (8-50 atm), and equivalence ratio (0.5-2.0) to capture the properties target fuel Jet-A, while the rest of three surrogate S2, S3 and S4 has been validated for Shock Tube ignition delay time only to capture the ignition characteristic of target fuel S-8 & GTL, IPK and RP-3 respectively. Based on the newly proposed HyChem model, another four surrogate with similar components and composition, was developed and parallel validations data was used as followed for previously developed surrogate but at high-temperature condition only. After testing the mechanism prediction performance of surrogates developed by the decoupling methodology, the comparison was done with the results of surrogates developed by the HyChem model. It was observed that all of four proposed surrogates in this study showed good agreement with the experimental measurements and the study comes to this conclusion that like the decoupling methodology HyChem model also has a great potential for the development of oxidation mechanism for heavy alkanes because of applicability, simplicity, and compactness.

Keywords : computational fluid dynamics, decoupling methodology Hychem, jet fuel, surrogate, skeletal mechanism
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