

Experimental Validation and Combustion Modeling of a JP-8 Surrogate in a Single Cylinder Diesel Engine

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ABSTRACT

This paper presents the results of an experimental investigation on a single cylinder engine to validate a two-component JP-8 surrogate. The two-component surrogate was chosen based on a previous investigation where the key properties, such as DCN, volatility, density, and lower heating value, of the surrogate were matched with those of the target JP-8.

The matching of the auto-ignition, combustion, and emission characteristics of the surrogate with JP-8 was investigated in an actual diesel engine environment. The engine tests for the validation of the surrogate were conducted at an engine speed of 1500 rpm, a load of 3 bar, and different injection timings. The results for the cylinder gas pressure, ignition delay period, rate of heat release, and the CO, HC, and NOx emissions showed a good match between the surrogate and the target JP-8. However, the engine-out particulate matter for the surrogate was lower than that for the JP-8 at all tested conditions. These findings are presented and discussed in the paper.

Additionally, a reduced surrogate fuel model was constructed and was implemented in three-dimensional CFD simulation for the predictions of the cylinder gas pressure, rate of heat release, and engine-out emissions of the tested surrogate. The CFD results were found to be in good agreement with the experimental data.

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INTRODUCTION

Due to the single fuel policy, military engines, originally developed to operate on conventional ULSD (Ultra Low Sulfur Diesel) fuel, are required to operate on JP-8 fuel (a petroleum based aviation kerosene fuel) [1]. For the diesel engine to operate properly on different fuels there is a need to optimize the combustion process and account for the physical and chemical properties of different fuels. Combustion optimization through experimentation is very expensive and time consuming. Therefore, CFD (Computational Fluid Dynamics) simulation could be effectively used for this purpose [2]. However, the use of the CFD codes for combustion optimization requires a kinetic model of the fuel, and the development of it is not feasible for actual fuels because they are composed of hundreds of hydrocarbons of different molecular structures. Therefore, research has been directed toward identifying fuel surrogates that would emulate the behavior of distillate fuels. Since the surrogate fuel consists of

a limited number of fuel species of known physical and chemical properties, its kinetic model can be developed to be used with the CFD codes.

Many kerosene surrogates have been proposed of which most of them have been developed to emulate the gas phase combustion characteristics, typical of jet turbine environment, of the target fuel. As a result, the surrogate validation is conducted using fundamental validation devices, such as shock tube [3, 4], pressurized flow reactor [3, 4, 5, 6, 7], and rapid compression machine [3, 4], where the fuel is pre-vaporized prior to its introduction in the combustion chamber. Therefore, these types of surrogates are developed with more emphasis on matching the chemical (rather than physical) properties of the target fuel. On the other hand, few surrogates have been developed considering both the physical as well as chemical properties of the target fuel, such as those developed by Violi et al. [8] and Wood et al. [9]. Therefore, surrogates are developed based on application [6-10].

In the present study, one of the goals was to validate a two-component JP-8 surrogate in a single-cylinder diesel engine. The surrogate, named as S2, is one of the six JP-8 surrogates developed for diesel engine application in a previous investigation [11]. The six surrogates were identified after they passed two tests. The first test was for matching the following properties - DCN (Derived Cetane Number), volatility, density, and lower heating value (LHV) - of the target JP-8. The second test was for matching the behavior of the surrogates and the target JP-8 in a constant volume combustion vessel under conditions close to those in an actual diesel engine. The constant volume combustion vessel is a part of the IQT (Ignition Quality Tester) used to determine the DCN of the fuel according to ASTM D6890 [12]. Therefore, the additional goal of the current investigation was to evaluate the potential use of IQT in the development and validation of surrogates. The evaluation is done based on the similarities of the autoignition, combustion, and emissions characteristics between the surrogate and the target fuel from the data obtained from the engine tests.

Further aim of this investigation was to construct a reduced surrogate fuel model for its use in 3D (three-dimensional) CFD simulation for the predictions of the engine test results of the surrogate. For this purpose, the detailed mechanism from CRECK Modeling [13] was considered. The mechanism consists of 466 species and 14631 reactions and was reduced using Chemical Workbench [14] software tool. The Chemical Workbench software tool offers several mechanism reduction modules [15], the most popular being directed relation graph (DRG), DRG with error propagation (DRGEP), path flux analysis (PFA), and computational singular perturbation (CSP). In the current study, the combination of PFA and CSP was utilized for efficient mechanism reduction. Briefly, PFA method is used for the reduction of the number of species and the associated reactions. In PFA, the contribution of any non-target species in the production and consumption flux of the target species is determined in terms of its importance index [15]. If the importance index of any species is smaller than the user-specified threshold value, then the species (and the associated reactions) are removed from the original mechanism. On the other hand, CSP is mainly to remove reactions and the associated species. In CSP, the importance index of any reaction that influence the target species is determined based on quasi-steady state concept for the group of coupled species. If the importance index of any reaction is smaller than the specified threshold value, then the reaction is removed from the original mechanism. Therefore, both methods require a user-specified initial set of target species and a threshold value between 0 and 1 for mechanism reduction. The target species are the set of important species that should be retained in the reduced mechanism. Readers are advised to refer [15] for the details of the PFA and CSP methods incorporated in the Chemical Workbench software. The mechanism reduction process was completed by a detailed validation of the reduced mechanism against its original mechanism.

Finally, the reduced multi-component surrogate fuel model was used with Reaction Design's FORTE simulation package [16] for conducting 3D CFD simulations. The simulated results, which include the ignition delay, combustion gas pressure, and engine-out emissions, were then compared with the surrogate test results obtained from the engine experiments.

PROPERTIES OF THE TARGET JP-8 AND SURROGATE FUELS

The surrogate S2 is composed of 60 percent n-dodecane and 40 percent 1,2,4-trimethylbenzene by volume [11]. The properties of the surrogate and its target JP-8 are shown in Table 1.

The distillation curves of the surrogate and the target JP-8 are shown in Figure 1. These distillation curves are obtained from the ASTM D86 measurements.

Table 1. Properties of the target JP-8 and surrogate fuels [11]

Fuels/Properties	JP-8	Surrogate S2
Derived Cetane Number	50.1	50.4
Density @ 25°C (g/cc)	0.797	0.802
Lower Heating Value (MJ/kg)	43.3	43.16
Hydrogen to Carbon Ratio	1.93	1.79
Molecular Weight (g/mole)	160.96	144.06
Threshold Sooting Index (TSI)	22.96	35.27

The distillation curves in Figure 1 together with the fuel properties data in Table 1 show that the key properties, such as the DCN, density, volatility, and heating values, of the surrogate are very similar to those of the target JP-8. As discussed in [11], these properties are deemed the most important for the surrogate that is developed for diesel engine applications, because these properties together have strong impact on the spray and evaporation characteristics, ignition delay, overall equivalence ratio, energy content per unit of fuel mass, and, to a great extent, engine-out emissions, which are the parameters of the major interest in diesel engine fuel test studies.

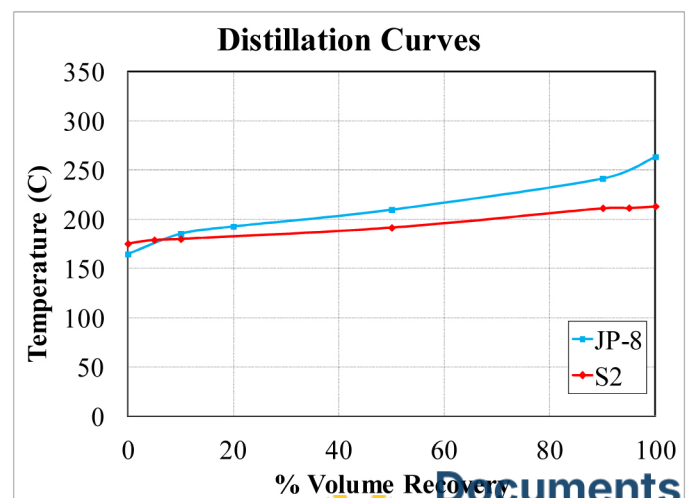


Figure 1. Distillation curves of the surrogate and target JP-8.

MECHANISM - REDUCTION AND VALIDATION

Reduction

The original mechanism was taken from CRECK Modeling [13]. The detailed mechanism (version 1212, December 2012) covers pyrolysis, partial oxidation, and combustion of hydrocarbon fuels up to C19 atoms. The mechanism consists of 466 species and 14631 reactions, which also includes NOx mechanisms. In the current investigation, this mechanism was reduced to 120 species and 1471 reactions, in steps as discussed below.

1. The original mechanism consists of the species having carbon atom numbers ranging from C1 to C19. Since the surrogate S2 consists of compounds having the highest carbon atom number 12 (C12), which is in n-dodecane, the species having carbon atom number higher than C12 were identified as redundant species in the original mechanism and were easily removed along with the related reactions using the DARS Basic [17] mechanism reduction module. This resulted in the reduced mechanism consisting of 408 species and 12587 reactions.
2. In the second step, Chemical Workbench software tool [14] with path flux analysis (PFA) [15] and computational singular perturbation (CSP) [15] reduction modules were utilized for further reduction.

The main criterion in the reduction was to keep the maximum difference (error tolerance) between the ignition delays of the original and the reduced mechanisms under $\pm 10\%$. Mechanism reduction was initiated using PFA method. The initial set of target species selected were the fuel species (n-dodecane and 1,2,4-trimethylbenzene), air (O_2 and N_2), HO_2 , O, H, OH, H_2O , CO_2 , CO, NO, NO_2 , and inert species (He and Ar). The conditions for the reduction included equivalence ratio of 0.5 (for 50-50 mole fractions of n-dodecane and 1,2,4-trimethylbenzene) and different temperatures (500-800 K).

To begin with, the initial threshold value was kept small and the reduction was performed for 408 species and 12587 reactions. The reduction was done in a step-wise manner by increasing the initial threshold value gradually, thus removing less important species and reactions, until the error tolerance in the ID exceeds $\pm 10\%$. This was a straight forward process which resulted in the reduced mechanism consisting of 188 species and 4216 reactions for the threshold value of 0.005. Any further increment in the threshold value resulted in the reduced mechanism with more than $\pm 10\%$ error in the ID. Therefore, the additional reduction using PFA was done in an iterative manner, wherein the threshold value was increased by a small number such that the reduction would result in the elimination of only one species at a time from the 188 species mechanism. The eliminated species was recorded and the comparison of the ID of the newly reduced mechanism was made with that of the parent mechanism

(188 species in this case). If the difference in the ID of these mechanisms at any validation point was in excess of $\pm 10\%$ then the recorded species was added to the list of initial target species and was retained in the reduced mechanism. In the next step, the threshold value was increased again by a small number and the newly eliminated species was recorded. If the comparison of the IDs of the newly reduced mechanism and the parent mechanism showed ID difference within $\pm 10\%$ error, then the species was considered unimportant and was disregarded along with the associated reactions. Hence, in other words, a sensitivity analysis was performed to quantify the effect of each species on ID. The process was continued until no further reduction could be made within $\pm 10\%$ ID error tolerance. Although this was a very exhaustive manual process, it, however, turned out to be a very useful approach for mechanism reduction as it resulted in the significant reduction of the species as well as reactions. The reduced mechanism finally obtained using this approach consisted of 126 species and 1765 reactions.

Eventually, the CSP reduction was applied to 126 species and 1765 reactions mechanism using the same set of target species and reduction conditions as were used in PFA reduction earlier. The CSP threshold value of 0.018 resulted in 120 species and 1471 reactions with ID error tolerance within $\pm 10\%$.

Hence, with respect to 408 species mechanism, a reduction of 71% was achieved.

Validation

For the validation of the reduced mechanism against the original mechanism, a constant volume homogeneous reactor with different temperature, pressure, and equivalence ratio conditions was simulated from zero to 10 milliseconds using DARS Basic for the mixture (50-50 mole fractions) of n-dodecane and 1,2,4-trimethylbenzene. These conditions are typical of diesel engine operations and are shown in Table 2.

For mechanism validation, the ignition delay (ID) was defined as the time corresponding to the maximum temperature change [18]. The comparisons of the IDs of the original and the reduced mechanisms at all the validation points, as listed in Table 2, are shown in figures in Appendix A. It is of note that the unit of ID shown on Y-axis of each figure is the absolute value of ID in milliseconds, and not in the logarithmic scale. The results show close agreement in the IDs of the original 466 species and both the reduced mechanisms: 408 species obtained in step 1 and 120 species obtained in step 2. Also, it is observed in these figures that the IDs of the reduced 120 species mechanism is in better agreement with the IDs of the original mechanism at higher temperatures than at lower temperatures. At lower temperatures, the reduced mechanism has slightly shorter ID, however, within $\pm 10\%$ allowed error. Overall, both the reduced mechanisms very closely reproduce the ID values of the original mechanism at all validation points.

Table 2. Conditions used for the validation of the reduced mechanism

Test Variables	Variables Range
Temperature (K)	700 - 1300 ($\Delta T = 50$)
Pressure (bar)	40, 60, 80
Equivalence ratio (Φ)	0.5, 1.0, 2.0

Further validation includes the comparisons of the oxides of Nitrogen (NO and NO_2) of the original and the reduced mechanisms, and they are shown in figures in [Appendix B](#). It is observed in these figures that the reduced mechanisms closely reproduce the mole fractions of the NO and NO_2 of the original mechanism.

CFD Tool, Models, and Assumptions

The Reaction Design's FORTE simulation package [16] was used for the simulation of the engine test conditions. The software code features advanced chemistry solver modules, such as dynamic cell clustering (DCC), for faster computations even with a relatively large sized mechanism consisting of more than 100 species [19, 20]. In DCC, a set of cells with high similarities in their thermo-chemical states are grouped together to form a cluster. The extent of similarities between cells is defined by the user-specified temperature and equivalence ratio dispersion thresholds. For instance, if the user sets the temperature and equivalence ratio (Φ) dispersion thresholds of 10 K and 0.05, respectively, then all the cells within these dispersion thresholds are treated similar and are grouped into a cluster, and the calculation is done for a cluster rather than for all the cells within the cluster. Hence, this reduces the computational time. Moreover, as compared to a case with dispersion thresholds of 5 K and $\Phi = 0.05$, the case with dispersion thresholds of 10 K and $\Phi = 0.05$ will have smaller number of clusters and therefore it will result in faster CFD calculations, however, with lower accuracy. For the case with dispersion thresholds of 0 K and $\Phi = 0.0$, no cluster is formed (meaning DCC is deactivated), and the solver computes the properties of each cell rather than cluster at every calculation time step. In the current study, the temperature and equivalence ratio dispersion thresholds used were 5 K and 0.05, respectively. These thresholds are smaller as compared to those used in [19, 20].

The FORTE simulation package also offers advanced spray models. In the current investigation, nozzle-flow model [21] was used for spray initialization. Based on the several inputs, including mass flow rate of the fuel, this model determines the spray cone angle, instantaneous discharge coefficient, effective injection velocity, and effective exit area of the flow. The effective exit area of the flow is then used to calculate the initial liquid droplet size [21]. For spray atomization and droplet breakup, Kelvin-Helmholtz/Rayleigh-Taylor (KH-RT) hybrid breakup model was used [22]. The KH-RT model considers the breakup in two steps: primary and secondary breakup. The

Kelvin-Helmholtz model considers the primary breakup of the intact liquid core of the fuel jet, whereas the Rayleigh-Taylor model in conjunction with the Kelvin-Helmholtz model predicts the secondary breakup of the individual liquid drops [22]. After the secondary breakup, the size distribution of child drops is estimated using Rosin-Rammler distribution [22]. In order to enhance spray predictions of the KH-RT model, an unsteady gas jet model [21] was selected in the simulation. The unsteady gas jet model eliminates the grid-size dependency of the KH-RT model, which is mainly caused due to the error in predicting the liquid-gas relative velocity. In other words, the use of gas jet model allows one to use a relatively coarser mesh without significantly affecting the accuracy of spray calculations. For the collision of droplets, radius of influence (ROI) model [21] was used. Unlike O'Rourke collision model where spray particles collide only if they reside in the same computational cell, the ROI model allows a droplet A to collide with another droplet B if the droplet A is within the radius of influence of the droplet B [21]. Hence, this approach removes the dependency of the droplet collision process on mesh-size as well as time-step. In addition, FORTE's wall impingement model [21] was used in order to account for droplet-wall interaction (stick, rebound, spread, and splash of a droplet with respect to wall). The wall film model of O'Rourke and Amsden [21] was used in order to account for wall film dynamics influenced by spray impingement, wall conditions, and near-wall gas flows.

Further, a Reynolds Averaged Navier-Stokes (RANS) based modified Re-Normalized Group Theory (RNG) k - ϵ turbulent model [21, 23] was used to account for in-cylinder turbulent flows. The original RNG k - ϵ model [24] is an extended version of the standard high Reynold's number k - ϵ model, wherein the k equation is the same as that of the standard k - ϵ model, but the ϵ equation has one extra term that accounts for non-isotropic turbulence [21]. Also, the original RNG k - ϵ model was developed for an incompressible flow [23], whereas the flow in compression ignition engine is compressible [25]. Therefore, Han and Reitz [23] modified the RNG ϵ -equation to take into account the effect of flow compressibility. Thus, this modified RNG k - ϵ model was used in the simulation.

For simulating turbulence effects on combustion kinetics, FORTE's generalized turbulence-chemistry interaction model was activated during the CFD calculations.

The computational domain consists of one-sixth sector mesh as shown in [Figure 2](#). One-sixth sector mesh was created because the injector has six nozzle holes, and it is centrally and axi-symmetrically located in the combustion chamber. Hence, sector-geometry, as compared to the full-geometry, simulation is computationally time-efficient. The sector mesh consists of 17809 cells at bottom dead center (BDC) with grid size of about 1.2 mm in the radial direction. Since the crevice region was not included in the sector mesh, therefore, FORTE's crevice model was used to accurately predict the motored gas pressure obtained from the engine experiments.

All the simulations were carried out from the intake valve