

Development of JP-8 Surrogates and their Validation using Ignition Quality Tester

Amit Shrestha, Ziliang Zheng, Tamer Badawy, and Naeim Henein
Wayne State University

Peter Schihl
US Army RDECOM-TARDEC

ABSTRACT

This paper presents a new approach for the development of six different JP-8 surrogates for application in diesel cycle simulation. The approach involves a step-wise formulation of 2-, 3-, and 4-component surrogates from a list of pure compounds which are selected based on several criteria. A MATLAB code is developed and is used in conjunction with the Ignition Quality Tester (IQT) and HYSYS software in order to formulate optimal surrogates.

The first part of the results shows a comparison between the calculated and the measured DCNs for six surrogates. The differences in the properties such as the density, volatility, lower heating value, H/C ratio, molecular weight, and threshold sooting index of the surrogates and the JP-8 are also highlighted. This is followed by the evaluation of the surrogates with respect to the target JP-8 fuel. The evaluation is made in terms of ignition delays and the rate of heat release at three different IQT test temperatures. Finally, the test results are examined to evaluate the validity of the development approach and the potential use of the IQT in the development and validation of the JP-8 surrogates for application in diesel engines.

CITATION: Shrestha, A., Zheng, Z., Badawy, T., Henein, N. et al., "Development of JP-8 Surrogates and their Validation using Ignition Quality Tester," *SAE Int. J. Fuels Lubr.* 7(1):2014, doi:10.4271/2014-01-9077.

INTRODUCTION

Due to the high thermal efficiency, high power density, and the capability of operating on conventional as well as alternate and renewable fuels, compression ignition (CI) engines are used in many applications, including heavy duty vehicles and passenger cars. However, variations in the composition of the fuels and the associated effects on combustion require the development of new control strategies and experimentation that are costly and time consuming. Diesel cycle simulations can be very effective in the efficient development of engines that can meet the production targets while operating on fuels of different physical and chemical properties. The most uncertain part in the simulation is the mechanism of combustion of distillate fuels. This shows the need for the development of surrogates of known combustion mechanisms for use in cycle simulation.

A surrogate fuel is a mixture of a handful number of pure compounds that can reasonably reproduce certain characteristics of the specific fuel of interest [1]. The presence of known compounds in the surrogate fuel enables one to study the compositional effects of the fuel on engine combustion process. Depending on the type of application, a surrogate may be developed to reproduce either the physical

or chemical characteristics of the target fuel [2, 3] or both. The target fuel for which a surrogate is the subject of the current study is JP-8, an aviation fuel which is also used in a variety of the U.S military diesel vehicles under their single fuel policy act. Unlike conventional diesel fuels, JP-8 has a wide specification, particularly its cetane number and volatility [2, 4].

Extensive research has been done in the development of aviation jet fuel surrogates for application in gas turbines, wherein the focus has been on the combustion in the gas phase. A detailed review of the previous studies on aviation jet fuel surrogates can be found in [5].

In order to formulate the surrogate, the first step is to match its properties with those of the target fuel. Some of these properties include volatility, hydrocarbon class compositions, density, hydrogen-to-carbon (H/C) ratio, cetane number (CN), molecular weight (MW), lower heating value (LHV), and sooting tendency. Matching hydrocarbon class compositions and distillation curve of the surrogate with that of the target fuel is an important part of the surrogate formulation [6, 7, 8, 9]. The distillation curve of a fuel can be used as a measure of its overall volatility [8]. The volatility is known to have significant effects on the evaporation of the fuel [6], which affects the

formation of the combustible fuel-air mixture. The density, surface tension, and viscosity are other important physical properties of the fuel that have important effects on spray atomization [10].

Several investigations have been done to emulate the thermo-physical properties of the target fuel [3, 11,12,13,14]. Huber et al. [3] considered density, speed of sound, viscosity, thermal conductivity, and cetane number as fundamental properties required to emulate the thermo-physical properties of the target fuels. In order to accomplish this task, they developed a surrogate mixture containing seven or more fuel components. On the other hand, Wood et al. [6] and Violi et al. [8] considered 14- and 7-component surrogate mixtures, respectively, to reproduce the physical as well as chemical properties of their target fuels. However, the number of fuel components in these surrogates is considered large from the stand point of kinetic modeling and three-dimensional computational analysis. Computational time increases by square of the number of the chemical species present in the kinetic model [15]. Therefore, one of the main targets of the current study is to develop JP-8 surrogate with the least possible number of fuel components.

Dooley et al. [16, 17] emphasized the importance of matching the H/C ratio, CN, MW, and threshold sooting index (TSI). They reported that the H/C ratio is important with respect to the adiabatic flame temperature, local air-fuel stoichiometry, enthalpy of combustion, flame velocity, overall radical production, and premixed sooting. Other investigations that considered the H/C ratio as one of the important surrogate properties are [2, 9, 18, 19]. Dooley et al. [16, 17] also pointed out that the CN correlates with autoignition behavior, the average molecular weight strongly correlates with gas-phase fuel diffusive transport properties, and, finally, the TSI correlates with non-premixed sooting characteristics. Further, the importance of matching the sooting characteristics of the surrogate with that of the target fuel has been discussed in [8, 9]. However, Edwards and Maurice [7] reported that the soot formation also depends on trace species such as sulfur and metals, present in the target fuel, and these trace species cannot be exactly reproduced by a surrogate fuel.

Once the surrogate is formulated, it is important to validate its autoignition and combustion characteristics against those of the target fuel. For this purpose, different types of equipment have been used. A shock tube was used to study the autoignition behavior of the developed surrogate fuel [16, 19]. Similarly, the other commonly used equipment for validation is a pressurized flow reactor (PFR) or a variable pressure flow reactor (VPFR). These equipment allow the users to record the species concentration-time history of the fuel during its oxidation process. Several validation studies [2, 4, 16, 18,19,20] using these equipment have been done in order to assess the oxidation characteristics of the surrogate fuel with respect to its target fuel. The PFR has also been used to compare the reactivity of the surrogate and its target fuel [2, 8]. Also, a rapid compression machine (RCM) has been used for testing and validation purposes. Dooley et al. [16, 19] used the

device to study the two-stage ignition of their surrogate fuels. Likewise, other different types of systems have been used for the analysis of the strain rate at extinction in laminar non-premixed flows [21] and extinction limits analysis in a non-sooting counterflow diffusion flame [22] for surrogate validation. It is worth noting here that the validations in these devices - shock tube [23], rapid compression machines [23], and pressurized flow reactor [16] - were conducted using the fuel in gas phase. Therefore, the effects of spray atomization and vaporization relevant to CI engines autoignition and combustion are not considered. This statement can further be strengthened from the results obtained by Dooley et al. [16]. The comparison of the species concentration-time history of their first [19] and second [16] generation surrogates in VPFR showed close similarities in their oxidation characteristics although their first generation surrogate (composed of n-decane/isooctane/toluene) is more volatile than their second generation surrogate (composed of ndodecane/iso-octane/1,3,5-trimethylbenzene/n-propylbenzene). Therefore, because of the differences in the volatilities of these surrogates, it is likely that the combustion behavior of these two different surrogates would be different if the comparisons were made in CI engines where physical properties of the fuel have a strong impact on combustion. Hence, validation of the surrogate fuel in a practical heterogeneous combustion device where liquid fuel spray properties are contributing factors in initiating autoignition is of a major interest in this work. For this purpose, the Ignition Quality Tester (IQT) is used in the current investigation.

Hence, the current investigation attempts to develop multicomponent JP-8 surrogates, which can emulate the ignition delay (ID) and the rate of heat release (RHR) of the target JP-8 for diesel engine applications. A total of six surrogates are developed which are different either in the number of components or in the type of one of the components. The maximum number of components in a surrogate is limited to four such that a simplified surrogate kinetic model may be developed for 3D CFD simulation. All of these surrogates are formulated to match as closely as possible specific properties of the target JP-8 fuel. These properties are derived cetane number (DCN), volatility, density, lower heating value (LHV), hydrogen-carbon ratio (H/C), molecular weight (MW), and threshold sooting index (TSI). Out of these seven properties, the first four properties are prioritized over others. The order of priority for the rest of the properties from high to low follows H/C ratio, MW, and TSI. Prioritization of these properties is made mainly because of the two reasons. First, a highly simplified surrogate, such as the one with three or fewer number of fuel components, cannot match simultaneously all of these properties of the target JP-8. Second, the objective is to develop surrogates that can emulate the ignition delay and the RHR of the target JP-8 fuel in diesel engine-like combustion conditions for which the DCN, volatility, density, and LHV are considered to be of greater importance than other properties. This assumption, along with the methodology of the surrogate development, is

assessed by testing surrogates at different charge temperatures in the IQT, and comparing their performance against the target JP-8 fuel.

For the formulation of the surrogate mixtures, a MATLAB program, developed in-house, was used. As a note, although TSI has been considered as one of the important targeted properties, no emission analysis is performed in the current study. Therefore, this part of analysis is planned to be done in a follow-up work through engine testing.

PROPERTIES OF THE TARGET FUEL

The target fuel of interest for which surrogates are developed is a specific type of the jet propellant JP-8 used in military ground vehicles. From a surrogate development viewpoint, a major problem associated with the JP-8 fuel is its compositional variability [2, 4]. Detailed information on compositional variability of the JP-8 fuel can be found in [4].

Table 1 shows the hydrocarbon class composition and other properties of the target JP-8 fuel considered in this study.

Table 1. Hydrocarbon class composition and properties of the target JP-8

	Target JP-8
n-alkanes (vol%)	9.2
Iso-alkanes (vol%)	29.8
Cyclo-alkanes (vol%)	44.5
Aromatics (vol%)	12.6
Others (vol%)	3.9
Derived Cetane Number	50.1
H/C Ratio	1.93
Molecular Formula	C _{11.54} H _{22.26}
MW (g/mol)	160.96
Boiling Point Range (°C)	164.7-263.4
LHV (MJ/kg)	43.3
TSI	22.96
Density (g/cm ³)	0.797 (@ 25°C)
Viscosity @ 40°C, (cSt)	1.368

The distillation curve of the target JP-8 is shown in Figure 1. The start and end temperatures of the curve are 164.7°C and 263.4°C, respectively, as shown in Table 1.

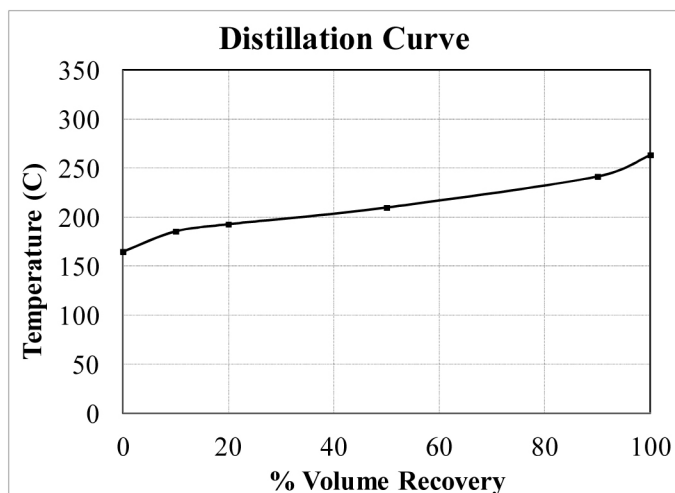


Figure 1. Distillation curve of the target JP-8

The standards used to identify the hydrocarbon class compositions and to determine other properties of the target JP-8 are shown in Table 2.

Table 2. Test standards used to identify/determine the properties of the target JP-8

Test Standards	Application
ASTM D1319	Identification of volume percent of aromatics and olefins
ASTM D2425	Identification of volume percent of normal-, iso-, and cyclo-paraffins
ASTM D 6890	Determination of DCN
ASTM D5291	Determination of carbon and hydrogen weight proportions
ASTM D86	Determination of distillation curve
ASTM D3338	Determination of lower heating value
ASTM D1298	Determination of density
ASTM D1322	Determination of smoke point
*CORE MW (method based on cryoscopy)	Determination of molecular weight

*CORE MW is the test method followed by Core laboratory, Texas, USA for the determination of molecular weight. The repeatability of the method was reported to be very accurate with percent standard deviation of 1.

TSI Calculation

ASTM D1322 is used to determine the smoke point of the target fuel. Smoke point is a measure of smoke producing tendency of the fuel. A fuel with high smoke point has lower tendency of producing smoke.

The equation, as defined by Calcote and Manos [24], was used to calculate the TSI of the fuel.

$$TSI = a \left(\frac{\text{Molecular Weight}}{\text{Smoke Point}} \right) + b$$

In the above equation, molecular weight is in gm/mol, smoke point is in mm, and 'a' and 'b' are apparatus specific constants. The unit of 'a' is mm*mol/gm and 'b' is dimensionless. The constants 'a' and 'b' are calculated from the measured smoke point data for different mixtures of toluene and 2,2,4-trimethylpentane.

METHODOLOGY OF SURROGATES DEVELOPMENT

Criteria for the Surrogate Development

1. Availability of the Kinetic Models of the Surrogate Components

The selected surrogate components must have their kinetic models available. In addition, the kinetic model for each

component must be available from a single source such that there exists consistency in the Arrhenius rate parameters for any given reaction, and transport and thermodynamic parameters for given species. These criteria are considered important because the ultimate goal of this study is to conduct 3D CFD analysis using surrogate mechanism.

2. Number of Surrogate Components

The maximum number of surrogate components should not exceed four. It is because a simplified surrogate mechanism, containing least possible number of chemical species, may be used for enabling time-efficient simulation analysis.

3. Boiling Points

The selection of fuel components should be made based on their boiling points. Since the surrogates developed in the current study are for diesel engine application, it is desirable to have the volatility, as defined by the distillation curve, of all surrogates as close as possible to that of the target JP-8.

4. Limit Only One Component from Each Hydrocarbon Class

The final criterion includes the selection of only one component from each hydrocarbon class, particularly for the 4-component surrogates.

Selection of Surrogate Fuel Components

The selection of surrogate components with available kinetic models is based on the mechanisms published by CRECK Modeling [25]. It should be noted that Lawrence Livermore National Laboratory (LLNL) also provides mechanisms for a variety of compounds, but we selected surrogate components based on the mechanisms published by CRECK Modeling because we found that the mechanisms for the components, which are more relevant to the formulation of Jet surrogates (particularly with respect to boiling point criterion), are not available from LLNL source. For example, in aromatics class, only toluene mechanism is available. The boiling point of toluene is about 110.5°C, which is much lower than the initial boiling point of the JP-8 fuel (164.7°C as shown in Table 1) considered in the current investigation.

Previous studies that demonstrate the use of the mechanism from CRECK Modeling can be found in [26].

The candidate components along with their boiling points are shown in Table 3.

In the n-alkanes category, n-decane, n-dodecane and n-hexadecane are listed. Although several previous studies considered both n-decane [2, 19, 21] and/or n-dodecane [4, 8, 16, 20, 21, 22] as suitable fuel components for their jet surrogates, in the current study, n-dodecane has been considered to be the first choice mainly because of the similarity of its physical properties to those of the jet fuels [5, 7, 27]. Some of these properties, as listed in [7], are density, viscosity, thermal conductivity, and heat capacity. The iso-alkanes in jet fuel are lightly branched [2, 28]. Alkanes with one-methyl branch, such as 2-methyldecane, could be a better choice if the kinetic model availability was not a constraint in

the current study. Based on the boiling point criterion, iso-cetane has been preferred over iso-octane. Similarly, the boiling point criterion also resulted in the choice of decalin over methylcyclohexane in cyclo-alkanes class.

Table 3. Chemical mechanisms source: CRECK Modeling, Ranzi et al. [25]

Molecular Class	Fuel Components Candidates	Boiling Points (°C)
Normal-Alkanes	n-decane	174
	n-dodecane	216
	n-hexadecane	287
Iso-Alkanes	Iso-octane	98.5
	Iso-cetane (2,2,4,4,6,8,8-heptamethylnonane)	240.2
Cyclo-Alkanes	Methylcyclohexane	101
	Decalin	187
Aromatics	Toluene	110.5
	Ethylbenzene	136
	Xylene	138.5
	n-propylbenzene	159
	1,2,4-trimethylbenzene	168

Most of the aromatics present in jet fuels are alkylbenzenes [2, 8]. Surrogate blends consisting of n-decane and alkylbenzenes are suitable to accurately predict major characteristics, including benzene profiles, of the kerosene flame [7]. Table 3 shows a list of the aromatic fuel species. The boiling point refinement shows that n-propylbenzene and 1,2,4-trimethylbenzene are suitable surrogate candidates than other species in the list. These two aromatic compounds have the same molecular weight and also close boiling points, 159°C for n-propylbenzene and 168°C for 1,2,4-trimethylbenzene. However, they have different molecular structure. In the current study, both of these aromatics are considered in the formulation of the JP-8 surrogates. The main reason for considering both aromatics is to find the differences in the autoignition and combustion characteristics of two surrogates that mainly differ in the aromatic type. Hence, the candidate components for surrogate formulation in this investigation are n-dodecane, iso-cetane, decalin, n-propylbenzene, and 1,2,4-trimethylbenzene. The molecular formula and structure of these components are shown in the table in Appendix A.

Surrogate Formulation Strategy

The surrogate formulation procedure is initiated in a step wise order starting from 2- to 3- to 4-component. This procedure is adopted for following reasons: (1) to demonstrate that as the number of components increase in the surrogate, they tend to match more closely the targeted properties of the JP-8. These properties are discussed in the following section of this paper. (2) to investigate the differences in the autoignition and combustion characteristics of the 2-, 3-, and 4-component surrogates that essentially have the same several targeted properties but differ in either the number or type of components. (3) to highlight the important properties that should be considered in the development of a surrogate for diesel engine applications.



Documents

Document Sharing Hub

Two series of surrogates are formulated. The first series contains n-dodecane, iso-cetane, decalin, and n-propylbenzene. The second series is different from the first in that instead of n-propylbenzene, 1,2,4-trimethylbenzene is used as an aromatic component.

Selection of Components for 2-Component Surrogates

A 2-component surrogate is the simplest surrogate that can be formulated. Previous studies, as reviewed in [5], demonstrated that the oxidation of the surrogate mixture containing n-decane and any aromatic compound higher than benzene (e.g. toluene, ethylbenzene) resulted in concentration profiles of the major species, intermediates, and benzene similar to those of kerosene fuels. Therefore, the choice of pure compounds is limited to one compound from n-alkane class and the other from aromatics. As a result, the first 2-component surrogate (denoted as S1) consists of n-dodecane and n-propylbenzene, and the second 2-component surrogate (denoted as S2) consists of n-dodecane and 1,2,4-trimethylbenzene.

Selection of Components for 3-Component Surrogates

The fuel components that are selected for the formulation of 3-component surrogates are n-dodecane, decalin, and n-propylbenzene (denoted as S3), and n-dodecane, decalin, and 1,2,4-trimethylbenzene (denoted as S4). Instead of iso-cetane, decalin is selected as third component mainly because of its lower boiling point. The idea is to formulate high to relatively low volatile surrogates as the number of fuel components increase from two to three. This also facilitates one to study the effect of volatility and molecular weight on the autoignition and combustion characteristics of surrogates in diesel engine like environment.

Selection of Components for 4-Component Surrogates

For the formulation of the 4-component surrogates, the final four components are n-dodecane, iso-cetane, decalin, and n-propylbenzene (denoted as S5) in the first series and n-dodecane, iso-cetane, decalin, and 1,2,4-trimethylbenzene (denoted as S6) in the second series.

Targeted Properties for Surrogates

The surrogates are desired to match the following properties: (i) ignition quality (DCN), (ii) volatility, (iii) density, (iv) lower heating value, (v) H/C ratio, (vi) MW, and (vii) TSI of the target JP-8 as close as possible. The importance of these properties is discussed below.

Ignition Quality

The DCN obtained from the IQT is used as a measure of ignition quality of surrogates and the target JP-8. The DCN is preferred over the cetane number obtained from the CFR

engine (ASTM D-613) because the IQT (i) is simpler to operate than the CFR engine, (ii) takes a fairly short time (approximately 20 min) to complete the test compared to a much longer time to make a test on the engine (iii) test is less expensive than the engine test, as it requires only about 100 mL of a fuel sample [30, 31], and (iv) tests have a higher repeatability and reproducibility [32, 33] than engine tests. The description of the IQT and the DCN calculations are given in details in a later section of the paper.

Volatility

JP-8 fuel is a complex mixture of hundreds of compounds with different boiling temperatures. The overall volatility of the fuel can be measured with respect to its distillation or boiling curve [8]. The distillation curve of the fuel is obtained by plotting its volume percent distilled at different temperature.

In the current investigation, the distillation curves of the surrogate fuels are obtained via HYSYS [34] simulation software. The simulation of distillation curves uses a Peng-Robinson fluid package to solve the equation of state. Once the compounds are defined, the distillation curves based on ASTM D86 is computed by the software. Also, the distillation curve of the target JP-8 was experimentally obtained using the same ASTM D86 standard. Hence, the volatility of the surrogate fuel is assessed by comparing its simulated distillation curve with the experimentally obtained distillation curve of the target JP-8.

Density

Liquid fuel density plays an important role in the liquid spray behavior and combustible mixture formation in diesel engines. In addition, during the injection process in the IQT, it is the volume of fuel that is kept the same for all the tested fuels. Given the same density, the mass of fuel injected should also be the same for all the surrogates and the target JP-8 fuel such that the overall equivalence ratio is maintained. Therefore, density has been prioritized over other properties, such as H/C ratio, MW, and TSI, in this investigation since the IQT is used for development and validation.

Lower Heating Value

It is the amount of energy released upon combustion of a specified amount of fuel. This property plays an important role in the validation of surrogate in CI engines. Therefore, for a given mass of fuel injected, the surrogate should be able to produce the same amount of energy as that of the target JP-8.

Hydrogen-to-Carbon Ratio, Molecular Weight, and Threshold Sooting Index

The importance of these properties in surrogate development is already discussed in the literature review. However, matching all of these properties between surrogate and target