

Role of Volatility in the Development of JP-8 Surrogates for Diesel Engine Application

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ABSTRACT

Surrogates for JP-8 have been developed in the high temperature gas phase environment of gas turbines. In diesel engines, the fuel is introduced in the liquid phase where volatility plays a major role in the formation of the combustible mixture and autoignition reactions that occur at relatively lower temperatures. In this paper, the role of volatility on the combustion of JP-8 and five different surrogate fuels was investigated in the constant volume combustion chamber of the Ignition Quality Tester (IQT). IQT is used to determine the derived cetane number (DCN) of diesel engine fuels according to ASTM D6890. The surrogate fuels were formulated such that their DCNs matched that of JP-8, but with different volatilities. Tests were conducted to investigate the effect of volatility on the autoignition and combustion characteristics of the surrogates using a detailed analysis of the rate of heat release immediately after the start of injection. In addition, the effect of volatility on the spray dynamics was investigated by Schlieren imaging in an optically accessible rapid compression machine (RCM). The images supported the conclusions made in the IQT tests. Furthermore, apparent activation energies of JP-8 and surrogate fuels were determined based on the chemical delay periods, which could be considered as a new parameter for developing surrogate fuel.

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INTRODUCTION

According to the single fuel policy [1], all military diesel engines have to use JP-8, which is the commercial aviation fuel treated with additives to make it suitable for diesel engines operation. A better understanding of the autoignition and combustion characteristics of JP-8 and other alternate fuels in internal combustion (IC) engines is needed, to improve engine performance, emissions, and fuel economy [2, 3, 4]. Gaining this understanding via experimentation is very challenging because real fuels are composed of thousands of components for which the combustion mechanisms are not known. A reasonable approach is to develop a surrogate fuel with a defined composition that mimics the characteristics and properties of the real fuel. Generally, the surrogate fuel is supposed to have (i) a limited number of components, (ii) similarity in properties and combustion characteristics to the real fuel, (iii) high purity, and (iv) low cost. Due to the different interests of study, a surrogate fuel can be proposed to emulate certain properties of the real fuel [5]. Surrogate fuels can be typically classified as physical surrogates that match the physical properties of the real fuel, such as distillation curve,

density, and viscosity, and chemical surrogates that match the chemical properties of the real fuel, such as soot tendency, ignition delay, species, and etc [6, 7].

Many proposed surrogate fuels have been studied in different experimental devices [8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21]. A pressurized flow reactor (PFR) is widely used to investigate the Negative Temperature Coefficient (NTC) regime, reactivity and intermediate species during low temperature oxidation of fuels. Lenhart [6], Agosta [7], and Cemansky [9] found that strong NTC behavior was observed for all JP-8 samples. However, none of the surrogate fuels matched the start of the NTC regime with JP-8 samples although some surrogates provided the closest match to the reactivity. Moreover, the study suggested that increasing the overall aromatic content of a fuel would tend to decrease reactivity but cause no significant effects on the start of the NTC region. Dooley et al. reported that their first (n-decane/iso-octane/toluene) and second (n-dodecane/iso-octane/1, 3, 5-trimethylbenzene/n-propylbenzene) generation surrogate fuels produced a very similar concentration of low temperature species compared to the real fuel during low temperature

oxidation process although the first generation surrogate fuel was much more volatile than the second generation surrogate fuel [10, 11]. Based on previous studies, an important corollary is that two fuels should have very similar oxidation characteristics in fundamental experiments if the main combustion property targets are matched, such as derived cetane number (DCN), hydrogen-carbon ratio (H/C), molecular weight (MW), and threshold sooting index (TSI) [10, 11, 12, 13, 14, 15].

In order to examine global combustion kinetic behavior, shock tubes and rapid compression machines (RCM) are the most commonly used to obtain ignition delay (ID), pressure and rate of heat release (RHR) traces. Studies have shown that the IDs of surrogate fuels were very close to the actual fuel in a shock tube [10, 11, 12, 13, 16] although the two-stage ignition from the pressure and RHR traces exhibited a great difference from that of the actual fuel in a RCM [10, 11]. Other aspects of surrogate fuels have also been investigated in different types of experimental systems. Honnet [17] reported that the Aachen (n-decane/1, 2, 4-trimethylbenzene) surrogate fuel accurately reproduces the extinction strain rate and volume fraction of soot formation in laminar non-premixed flows. Humer [18] indicated that the extinction characteristics of Aachen and modified Aachen (n-dodecane/1, 2, 4-trimethylbenzene) surrogate fuels agree well with JP-8 in laminar non-uniform flows.

It should be noted that most of the surrogate work in PFR, shock tube, and RCM were conducted with fuels in the gas phase. However, few studies have shown differences in thermophysical properties of an actual fuel and its surrogate fuels, such as distillation curve, density, sound speed, viscosity, and thermal conductivity [19, 20, 21, 22, 23].

The literature review shows that surrogates for JP-8 have been developed, mostly, for gas turbine application [8, 9, 10, 11, 12, 13, 14, 15, 16]. However, these surrogates may not be suitable for diesel engines because fuel volatility has not been considered as a prime property of the surrogates. The surrogate fuels proposed by Violi [24] show a better fit of the distillation characteristics to mimic the volatility of JP-8. However, this study did not include experimental work to examine the effect of volatility on autoignition and combustion characteristics.

In diesel engines, fuel volatility has a strong impact on combustion, engine performance and emissions. Therefore, there is a need to investigate the role of volatility in surrogate development for diesel engine applications in terms of spray, autoignition, and combustion characteristics in multi-phase heterogeneous combustion conditions.

EXPERIMENTS

Optically Accessible Rapid Compression Machine

The RCM is mainly designed to emulate an engine compression stroke to make fundamental analysis of IC engine cycle combustion. Thus, it has the following advantages: (i) easy access of various optical diagnostic techniques, (ii) flexibility and accuracy in controlling the charge pressure and temperature, (iii) easy to clean windows. A detailed description and operating procedure have been provided in previous publications [25, 26, 27].

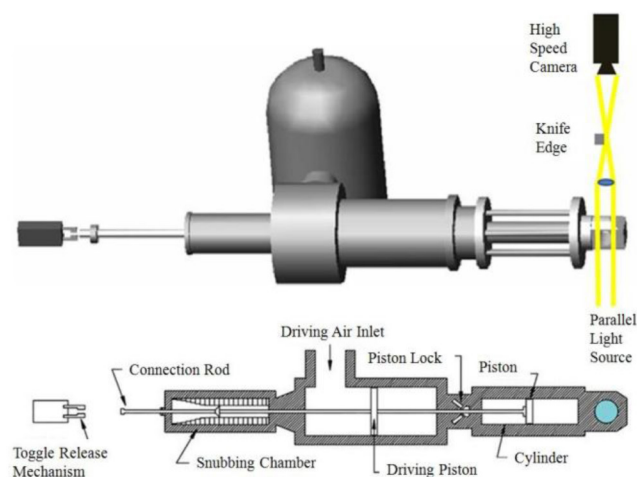


Figure 1. Schematic of rapid compression machine at Wayne State University

A schematic of the RCM is shown in Figure 1. Three pistons with different functions are mounted on a long connection rod and located inside three cylinders or chambers. The first piston on the left is in the snubbing chamber, which is filled with viscous hydraulic oil in the funnel shape chamber and provides the damping resistance of the compression stroke. The second chamber in the middle with pressurized shop air generates the force to perform a compression stroke. In this study, the driving air is set at 60 psi. The charge air contained in the third cylinder is compressed into a combustion chamber through a check valve and orifice when the compression stroke occurs. The charge air is pre-heated and kept at the pressure of 1 bar and temperature of 373 K. Once the charge air is compressed, the peak pressure can reach about 18 bar. In order to avoid turbulence interference during the Schlieren tests, the compressed air has settled down for about 10 seconds after the piston reached its top dead center (TDC). Thus, the corresponding pressure and mass average temperature at the injection signal are 15 bar and 600 K, respectively. A sample pressure history, with injection and camera signals, is shown in Figure 2.

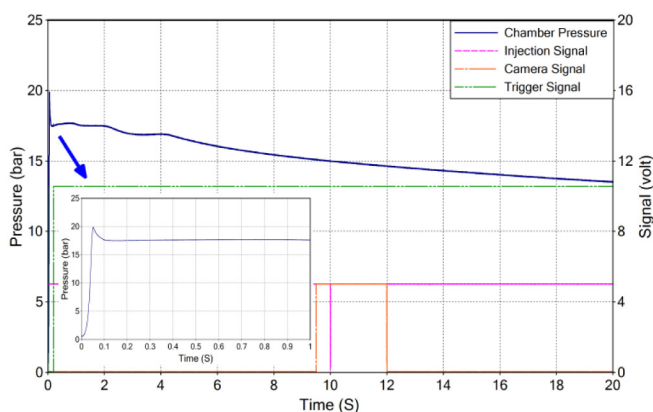


Figure 2. Sample signal traces of a rapid compression machine

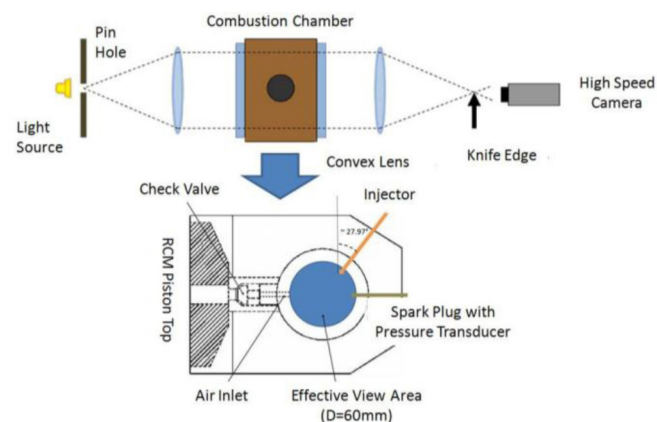


Figure 3. Schematic visualization setup for the combustion chamber of a rapid compression machine

The fuel sprays were studied in an optically accessible combustion chamber of the RCM under simulated, quiescent diesel engine conditions. A schematic of the Schlieren visualization setup along with the chamber is shown in Figure 3. The chamber is in a cylindrical shape with two quartz windows on both side ports, which allow line-of-sight imaging of the injected fuel spray. A common rail solenoid injector with a single-hole nozzle is mounted at an angle about 28° from the vertical axis, delivering the fuel into the center of the combustion chamber at the injection pressure of 100 bar. Due to the size of the chamber, the injection duration was well controlled to be the same for all the fuels and to avoid serious impingement on the walls and windows. This non-ignitable condition was selected intentionally to isolate the mixing and evaporation processes from the complex autoignition and combustion processes. In addition, a Kistler type 6117B spark plug with an integrated pressure transducer is installed on the horizontal axis.

A 70W projection lamp provided light source passing through a small pin hole, which was placed on the focal point of a convex lens. Thus, the point light source was converted to parallel light, which proceeded through the chamber where injection events take place, and reached another convex lens. A sharp knife edge was placed on the focal point of second lens to cut the refracted light beam, which was refocused to a high-speed

CMOS camera (Vision Research Phantom V310). Images were collected at approximate 10000 frame per second (FPS) and with 512 by 512 pixel resolutions. A detailed Schlieren setup has been provided in previous publications [28, 29, 30].

Ignition Quality Tester

The Ignition Quality Tester (IQT) [31] is widely used to measure the DCN of fuels for diesel engines. Also, DCN is considered as one of the critical properties in the investigation of surrogates for aviation fuels [10, 11, 14]. A detailed description of IQT at Wayne State University, as well as details of its operation, have been provided in previous investigations [32, 33].

As in the IQT study, a fuel was injected into the combustion chamber along the central axis of the body, which is pre-heated to the standard test temperature of about 828 K by nine cartridge-type resistance heaters. The charge air pressure and temperature are 2.137 ± 0.007 MPa and 818 ± 30 K, respectively [31]. The IQT is a high temperature combustion device that simulates compression temperatures in diesel engines but at a lower air pressure.

The IQT equipment was utilized in the present investigation as a platform to investigate the physical and chemical processes that lead to the autoignition of different fuels under well-controlled charge pressure and different temperatures. There are many definitions of the ignition delay period in the literature. All researchers agree on the start of injection (SOI) as the start of ID. However, several criteria have been used to define the end of ID or the start of combustion (SOC) [34, 35, 36, 37]. In the current investigation, the definition of ID specified in ASTM D6890 [31] was used as shown in Figure 4. It is the time elapsed from the SOI to the SOC. SOC in ASTM D6890 is defined as the time when the pressure in the chamber reaches 1.38 bar above the initial chamber pressure. This point is considered to be the "combustion recovery point" [38, 39].

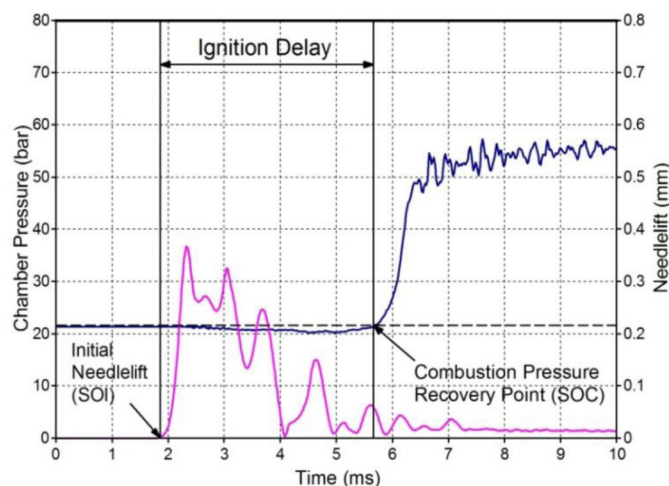


Figure 4. A sample of traces for the needlelift and chamber pressure depicting the definition of IQT ignition delay time

A schematic of IQT is shown in Figure 5. There are two thermocouples inside the combustion chamber along the axial direction. The first thermocouple measures the charge temperature close by the injector nozzle, and the second thermocouple is 7 cm downstream from the first one. The temperature gradient increases approximately 30 K from the first to the second thermocouple [39, 40]. The local area where combustion starts in the IQT is close to the pressure transducer [39]. In order to capture the change in temperature during the autoignition process, the thermocouple at position "a" was replaced with an Omega K-type fast response 0.002" diameter junction. The thermocouple is connected to a compensation circuit with an amplifier module (Analog Device 5B40).

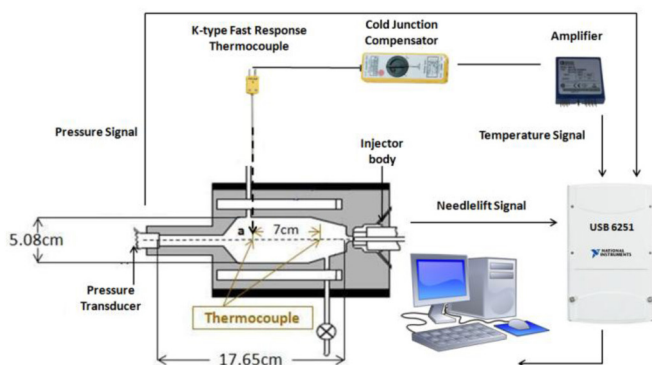


Figure 5. Schematic of IQT with a fast-response thermocouple and the additional DAQ system (based on reference [39])

An additional National Instrument (NI) high-speed multifunction data acquisition (DAQ) system was connected to the standard IQT system to expand the capability of obtaining data. The needlelift (N.L), pressure and temperature signals were simultaneously measured at a sampling rate of 1.25 MS/s. All the safety features were controlled by the standard IQT system.

Fuels

Volatility

Unlike conventional diesel fuel, JP-8 is not well classified and has a wide range of cetane numbers (CN) and volatility. The overall volatility of a fuel can be identified by its distillation curve [24]. In the current investigation, the distillation curve of a specific JP-8 fuel was measured at the Southwest Research Institute (SwRI) according to ASTM D86 [41], the other properties of JP-8 are shown in the Appendix. The distillation curves of the surrogate fuels were calculated using the Aspen HYSYS [42] software package, and the Peng-Robinson model was chosen to solve the state equations, based on ASTM D86.

Derived Cetane Number

In previous publications of surrogate development, the DCN of a surrogate fuel was calculated based on a linearity assumption between the volume fraction and the DCN of its components [21, 43]. However, calculated DCNs are not always consistent with measured DCNs [43]. Thus, the DCNs of all the surrogate fuels in the current study were measured in the IQT. The choice of the surrogate components was guided

by data published in the literature. In order to compare the effects of volatility on autoignition and combustion characteristics, some minor modifications were made to their volume percentages to keep the same DCNs of surrogate fuels. Meanwhile, other properties such as density, H/C, MW of the surrogate fuels were optimized to match the target JP-8 by using a MATLAB code. The detailed description was provided in a previous publication [43].

Density

In a multi-phase heterogeneous combustion system, density is a very important factor for autoignition process because a fuel is injected by volume in diesel engines. Also, the same density of a fuel implies the same mass of fuel injected into the combustion chamber, which is related to the global equivalence ratio and heating value. Thus, the density of surrogate fuels was optimized to match the target JP-8.

Lower Heating Value

Lower heating value (LHV) is the amount of energy released during combustion of the specified amount of a fuel, and it is very important to diesel engine applications. Thus, the LHVs of surrogate fuels were optimized to match the target JP-8.

Hydrogen-Carbon Ratio

H/C ratio is closely related to the adiabatic flame temperature, local air-fuel stoichiometry, enthalpy of autoignition reactions, flame speed, etc [44]. Thus, the H/C ratios of surrogate fuels were optimized to match the target JP-8.

Other Properties of Surrogates

The average MW is correlated with fuel diffusion processes in the gas phase [45]. Threshold Sooting Index (TSI) is an overall measure of the tendency for soot formation. Thus, these properties of surrogate fuels were optimized to be close to the target JP-8 although the correlation between TSI and particulate matter formation in diesel engines is not known at the present time.

The following six fuels were tested in the current study: (i) JP-8, a military aviation fuel; (ii) surrogate fuel #1 [10], denoted as "SF1"; (iii) surrogate fuel #2 [17, 18, 46], denoted as "SF2"; (iv) surrogate fuel #3 [18, 43], denoted as "SF3"; (v) surrogate fuel #4 [47], denoted as "SF4"; and (vi) surrogate fuel #5 [6, 24], denoted as "SF5". It should be noted that the selection of pure components was guided by the previous publications and the minor modification was made to match the properties of current JP-8 batch at Wayne State University (WSU). The properties and composition (volume basis) of tested fuels are listed in Table 1. The pure components used in this study are as follows: (a) n-hexadecane, as "n-C16", (b) n-dodecane, as "n-C12", (c) n-decane, as "n-C10", (d) 2, 2, 4, 4, 6, 8, 8-heptamethylnonane (iso-cetane), as "I-C16", (e) 2, 2, 4-trimethylpentane (iso-octane), as "i-C8", (f) decahydronaphthalene, as "decalin", (g) methylcyclohexane, as "MCH", (h) 1, 2, 4-trimethylbenzene, as "TMB", (i) m-xylene, as "xylene", and (j) toluene. The detailed pure component information is shown in the Appendix.

Table 1. Properties of JP-8 and surrogate fuels with their composition

Fuel Composition						
	JP-8	SF1	SF2	SF3	SF4	SF5
n-C16	-	-	-	-	-	1
n-C12	-	-	-	60	36	49
n-C10	-	54	66	-	14	-
i-C16	-	-	-	-	24	16
i-C8	-	30	-	-	-	-
decalin	-	-	-	-	-	19
MCH	-	-	-	-	8	-
TMB	-	-	34	40	-	11
xylene	-	-	-	-	-	4
toluene	-	16	-	-	18	-
Fuel Properties						
DCN	49.24*	49.51*	49.1*	49.28*	49.4*	49.36*
Density (g/ml)	0.802*	0.74	0.78	0.802	0.774	0.805
LHV (MJ/kg)	43.2*	44.1	43.4	43.2	44.1	43.7
H/C	1.93*	2	1.86	1.79	1.98	1.93
MW (g/mol)	161*	122	133	144	142	157
TSI	22.96*	14.6	28.94	35.27	16.32	22.19

*measured

RESULTS AND DISCUSSION

Distillation Curves of the Surrogates and JP-8

Prior to simulating the distillation curves for the surrogate fuels developed in this investigation, the accuracy of Aspen HYSYS software predictions were compared with distillation curves developed experimentally at SwRI. Figure 6 shows a fairly good agreement between the predicted and measured data for SF1, SF2, and SF3. Thus, Aspen HYSYS is recommended to be used in the surrogate development for diesel engine applications.

The distillation curves calculated using Aspen HYSYS software for the five surrogate fuels of Table 1 are shown in Figure 7, along with the curve measured for JP-8. SF1 is the most volatile surrogate fuel followed by SF4. The high volatility of SF1 is related to high volatility of its components, such as 2, 2, 4-trimethylpentane and toluene, which affects the volatility particularly at low temperatures. It is worth noting that low temperature evaporation is very critical to diesel engine performance [48]. The SF2 shows almost a straight line due to the close boiling points of 1, 2, 4-trimethylbenzene (169 °C) and n-decane (174 °C) [49]. SF3 shows a very close trend to JP-8 with a difference of about 10 °C. With an increasing number of surrogate components, a better fit of the distillation curve was achieved such as with SF5 which matches the JP-8 curve from the initial to final boiling points.

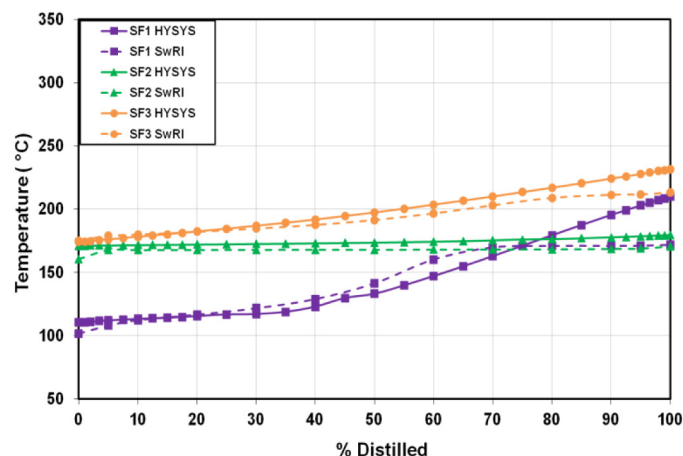


Figure 6. Comparison of distillation curves developed using HYSYS simulation and SwRI experimental results for three surrogate fuels.

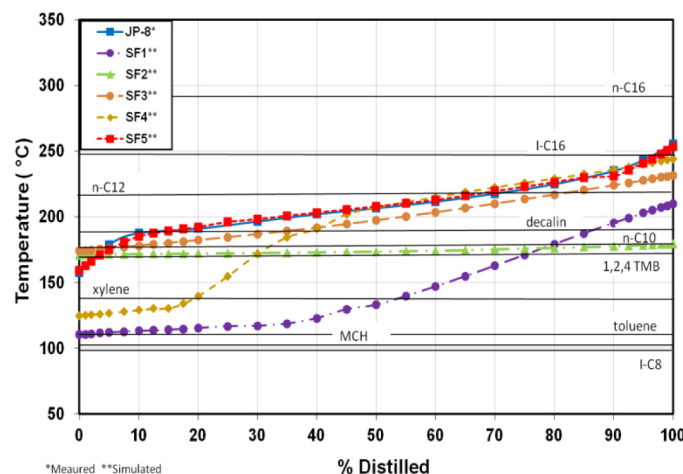


Figure 7. Comparison of distillation curves between JP-8 and surrogate fuels

Optically Accessible Rapid Compression Machine

The effects of volatility on the spray characteristics of each surrogate fuel and JP-8 were examined in the RCM at a charge pressure of 15 bar and a temperature of 600 K. The SOI was determined in the images by one frame prior to the first appearance of the initial jet. The high-speed Schlieren images were processed to obtain the spray penetration and projected vapor area. The raw Schlieren images showed a dark vaporized jet over a bright background, which is difficult to analyze because the background is not uniformly bright between each test. Further, it is quite challenging to define the vapor boundary just based on raw images. Thus, in the current study, a MATLAB based image processing code has been developed for this analysis [30]. A raw image was subtracted from a background image to reduce the effect of inhomogeneity of the light source, which also eliminated black spots caused by dust on the windows and the lens. In addition, a threshold (7% of maximum intensity) was applied for boundary calculation. In this study, spray penetration was defined as the length from the nozzle tip to the tip of the spray plumes, which indicates how far the spray travels with respect to time. Further, the averaged penetrations of each fuel are compared in the results section.