Combustion of Jet Fuels and its Surrogates in Laminar Nonuniform Flows

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Abstract

Experimental studies are carried out to characterize nonpremixed combustion of jet fuels and a number of its surrogates in laminar nonuniform flows. The counterflow configuration is employed. Critical conditions of extinction and autoignition are measured for JP-8, Jet-A, and Fisher Tropsch (FT) JP-8. Thirteen surrogates of JP-8 and one surrogate of FT JP-8 are tested. It is found that critical conditions of extinction and autoignition of JP-8 and Jet-A are similar, while FT JP-8 is more reactive than JP-8 and Jet-A. Among the surrogates tested, the Aachen surrogate made up of *n*-decane (80 %) and trimethylbenzene (20 %) by liquid volume, and the UCSD surrogate made up of *n*-dodecane (60 %), methylcyclohexane (20 %), and *o*-xylene (20 %) by liquid volume best reproduce extinction and autoignition characteristics of JP-8. Surrogate G made up of *n*-decane (60 %) and iso-octane (40 %) by liquid volume best reproduces the combustion characteristics of FT JP-8.

Keywords: jet fuel, surrogate, autoignition, laminar flow

1. Introduction

Developing chemical-kinetic models that describe combustion of commercial fuels is of practical importance [1, 2]. Practical fuels, for example, gasoline, diesel, and jet fuels comprise hundreds of aliphatic and aromatic hydrocarbon compounds. The focus of the present work is on jet fuels. The major components of jet fuels are straight chain paraffins, branched chain paraffins, cycloparaffins, aromatics, and alkenes [3, 4]. The average composition is 29 Vol.% aromatics, 30 Vol.% cycloparafins, and 41 Vol.% parafins [5] depending on the crude oil and distilation process. JP-8 is a ”kerosene” fuel used by the U.S. Air Force. Detailed chemical-kinetic mechanisms describing combustion for many of the components in JP-8 are not available. A useful approach in developing chemical-kinetic mechanisms for jet fuels is to first develop surrogates for these fuels. Surrogate fuels are defined as mixtures of few hydrocarbon compounds whose relative concentrations can be adjusted so that the physical and chemical properties pertinent to combustion approximate those of commercial fuels [2]. Previous studies [6–9], suggested 5 or more components for a jet fuel surrogate. In this study the focus is on even more simplified mixtures of 2 to 3 components.

2. Specific Objectives

Here, an experimental investigation is carried out with the aim of developing an appropriate surrogate for JP-8 and Fisher Tropsch (FT) JP-8. The counterflow configuration is employed. Critical conditions of extinction and autoignition are measured for various jet fuels in nonpremixed systems. Similar measurements are made for potential surrogates of these fuels.

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Proceedings of the European Combustion Meeting 2009

2.1. Experimental Apparatus and Procedures

Figure 1 shows a schematic illustration of the experimental setup. The liquid fuels are vaporized using a vaporizer, where fuel gets injected by a spray nozzle into a heated chamber by an air blast nozzle. The temperature is kept about 20 K above the boiling range to assure that all its components are vaporized. Two thermocouples are used to monitor the temperature inside the vaporizer. One located next to the spray nozzle, the other one at the exit of the vaporizer chamber. The flow rates of gases are adjusted by computer-regulated mass flow controllers. The flow lines going from the vaporizer to the counterflow burner were heated to prevent condensation inside the lines. A detailed description of the burner is given elsewhere [10, 11].

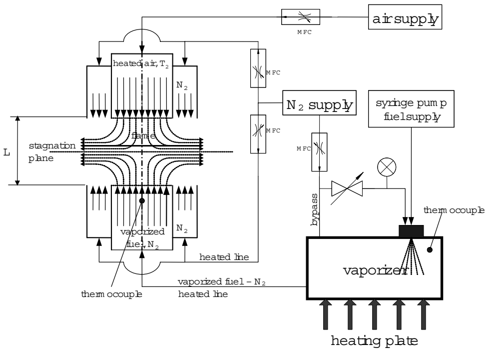

Fig. 1: Schematic illustration of the experimental setup. The figure shows the counterflow flow field and the air, nitrogen, and fuel feed systems and the vaporizer.

In the burner a fuel stream made up of prevaporized fuel and nitrogen is injected from the fuel-duct, and an oxidizer stream of air is injected from the oxidizer-duct. These jets flow into the mixing layer between the two ducts. The exit of the fuel-duct is called the fuel boundary, and the exit of the oxidizer-duct the oxidizer boundary. The mass fraction of fuel, the temperature, and the component of the flow velocity normal to the stagnation plane at the fuel boundary are represented by $Y_{\mathrm{F},1}$, T_1, and V_1, respectively. The mass fraction of oxygen, the temperature, and the component of the flow velocity normal to the stagnation plane at the oxidizer boundary are represented by $Y_{\mathrm{O}_2,2}$, T_2, and V_2, respectively. The tangential components of the flow velocities at the boundaries are presumed to be equal to zero. The distance between the fuel boundary and the oxidizer boundary is represented by L. The velocities of the reactants at the boundaries of the counterflow burner are presumed to be equal to the ratio of their volumetric flowrates to the cross-section area of the ducts. The temperature of the fuel stream and the temperature of the oxidizer stream at the boundaries are measured using thermocouples.

The value of the strain rate, defined as the normal gradient of the normal component of the flow velocity, changes from the fuel boundary to the oxidizer boundary [12]. The characteristic strain rate on the oxidizer side of the stagnation plane a_2 is presumed to be given by [12]

$$a_2 = \frac{2|V_2|}{L}\left(1 + \frac{|V_1|\sqrt{\rho_1}}{|V_2|\sqrt{\rho_2}}\right). \qquad (1)$$

Here ρ_1 and ρ_2 represent the density of the mixture at the fuel boundary and at the oxidizer boundary, respectively. Both flows are mass balanced to ensure that the stagnation plane is in the center between the two ducts, so that there is no heat transfer from the flame to the ducts. Equation 1 is obtained from an asymptotic theory where the Reynolds numbers of the laminar flow at the boundaries are presumed to be large [12]. Critical conditions of extinction are presumed to be given by the strain rate, $a_{2,\mathrm{e}}$, and the mass fraction of fuel at the fuel boundary. Critical conditions of autoignition are presumed to be given by the strain rate, $a_{2,\mathrm{I}}$, the temperature of the oxidizer stream, $T_{2,\mathrm{I}}$, and the mass fraction of fuel at the fuel boundary.

The fuels tested were:

- Multicomponent fuels:
    1. JP-8 (obtained from China Lake), JP-8 POSF 4177 (obtained from Wright Patterson Air Force Base (WPAFB)), JP-8 POSF 3773 (obtained from WPAFB).
    2. Jet-A (obtained from San Diego Airport), Jet-A POSF 3602 (obtained from WPAFB) , Jet-A POSF 3638 (obtained from WPAFB), Blend POSF 4658 (obtained from WPAFB).
    3. Fisher Tropsch JP-8 (obtained from WPAFB).
- Fuel mixtures (liquid volume): Possible surrogates of JP-8:
    1. Surrogate A: 60 % *n*-decane, 20 % methylcyclohexane, 20 % toluene. $H/C = 1.93$.
    2. Surrogate B: 60 % *n*-decane, 20 % methylcyclohexane, 20 % *o*-xylene. $H/C = 1.93$.
    3. Surrogate C (UCSD surrogate): 60 % *n*-dodecane, 20 % methylcyclohexane, 20 % *o*-xylene. $H/C = 1.92$.
    4. Surrogate D: *n*-decane 50 %, butylcyclohexane 25 %, butylbenzene 25 %. $H/C = 1.92$.
    5. Surrogate E: *n*-decane 34 %, butylcyclohexane 33 %, butylbenzene 33 %. $H/C = 1.84$.

6. Surrogate F: *n*-decane 60 %, butyl-cyclohexane 20 %, butylbenzene 20 %. $H/C = 1.97$.
7. Aachen Surrogate: *n*-decane 80 %, trimethylbenzene 20 %. $H/C = 1.99$.
8. Modified Aachen Surrogate: *n*-dodecane 80 %, trimethylbenzene 20 %. $H/C = 1.97$.
9. Surrogate N1: *n*-decane 80 %, propylbenzene 20 %.
10. Surrogate N2: *n*-decane 70 %, propylbenzene 30 %.
11. Drexel Surrogate 1: *n*-dodecane 26 %, iso-cetane 36 %, methylcyclohexane 14 %, decaline 6 %, and 1-methylnaphthalene 18 %. $H/C = 1.82$.
12. Drexel Surrogate 2: *n*-dodecane 43 %, iso-cetane 27 %, methylcyclohexane 15 %, and 1-methylnaphthalene 15 %. $H/C = 1.87$.
13. Utah Surrogate: *n*-dodecane 30 %, *n*-tetradecane 20 %, iso-octane 10 %, methylcyclohexane 20 %, o-xylene 15 %, and tetraline 5 %. $H/C = 1.93$.

- Fuel Mixtures (liquid volume). Possible surrogate of F-T JP-8.
  1. Surrogate G: *n*-decane 60 %, iso-octane 40 %. $H/C = 2.22$.

3. Results and Discussion

3.1. Extinction of Flames

In the extinction experiments the temperature of the fuel stream is 473 $(\pm\, 10)$ K, and the temperature of the oxidizer stream, is 298 K. The distance between the fuel duct and the oxidizer duct is 10 mm. At some selected value of of the mass fraction of fuel, $Y_{\mathrm{F},1}$, the flame is stabilized at a strain rate $a_2 < a_{2,\mathrm{e}}$, where $a_{2,\mathrm{e}}$ is the strain rate at extinction. The strain rate is slowly increased until extinction is observed. The accuracy of the strain rate is $\pm\,5$ % of recorded value and that of the fuel mass fraction $\pm\,3$ % of recorded value. The experimental repeatability on reported strain rate is $\pm\,5$ % of recorded value.

Figure 2 shows experimental data for jet fuels. Extinction characteristics of different batches of JP-8 and different batches of Jet-A are similar. F-T JP-8 is harder to extinguish. Figure 3 compares experimental extinction data for potential surrogates of JP-8 with that for JP-8. The extinction characteristics of the surrogates are placed in three groups: Group 1 best, Group 2 good, Group 3 significant differences. The surrogates placed in these groups are:

- Group 1: Drexel Surrogate 2, Utah Surrogate, Aachen Surrogate, and Modified Aachen Surrogate.

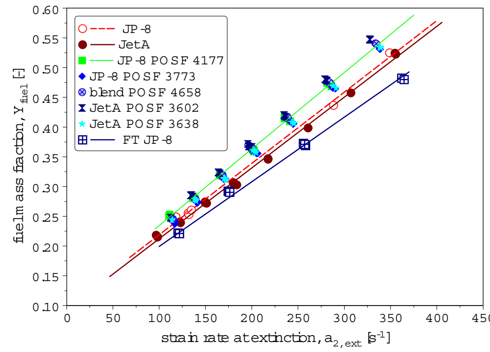

Fig. 2: The mass fraction of fuel as a function of the strain rate at extinction. The symbols represent experimental data, and the lines are best fits to experimental data. The figure compares extinction characteristics of various batches of JP-8, Jet-A, and FT JP-8.

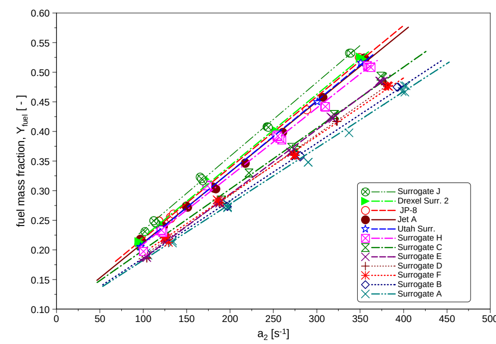

Fig. 3: The mass fraction of fuel as a function of the strain rate at extinction. The symbols represent experimental data, and the lines are best fits to experimental data. The figure compares extinction characteristics of various surrogates of JP-8.

- Group 2: Surrogate C, and Surrogate E.
- Group 3: Surrogate D, Surrogate F, Surrogate B, and Surrogate A.

Figure 4 shows that the extinction characteristics of surrogate G agrees well with those for F-T JP-8.

3.2. Autoignition of Flames

The parameters that influence autoignition are:

1. Composition of the fuel stream, $Y_{\mathrm{F},1}$
2. Temperature of the fuel stream, T_1
3. Composition of the oxidizer stream, $Y_{\mathrm{O}_2,2}$
4. Temperature of the oxidizer stream, T_2
5. Strain rate a_2
6. Pressure, p

The experiments are conducted at $T_1 = 473$ K, $Y_{\mathrm{O}_2,2} = 0.23$ (air), $p = 1.013$ bar. Two sets of measurements were obtained. In one set the value

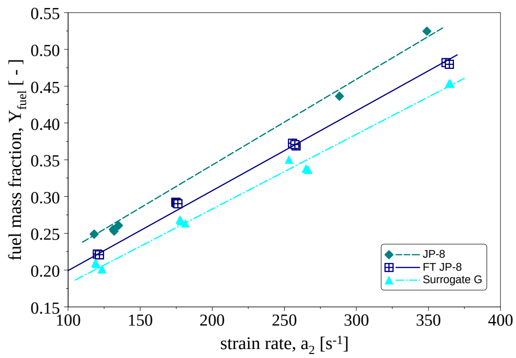

Fig. 4: The mass fraction of fuel as a function of the strain rate at extinction. The symbols represent experimental data, and the lines are best fits to experimental data. The figure compares extinction characteristics of a surrogate and FT JP-8.

of $Y_{\mathrm{F},1}$ was maintained at a constant value of 0.4. the values of T_2 were measured for various values of a_2. In the other set a_2 was maintained at a constant value of $550\,\mathrm{s}^{-1}$. Here the value of T_2 was measured for various values of $Y_{\mathrm{F},1}$. The experimental accuracy of the measured value of T_2 is $\pm 30\,\mathrm{K}$ and that of a_2 is $\pm 7\,\%$ of recorded value, and $Y_{\mathrm{F},1}$ is $\pm 3\,\%$ of recorded value. The experimental uncertainty (repeatability) for T_2 is $\pm 4\,\mathrm{K}$ of recorded value for a given mass fraction of fuel. The transient autoignition process, at any critical condition, was observed using a high speed camera. Only data where autoignition takes place around the axis of symmetry were recorded. Figure 5 shows photographs of

Fig. 5: High speed photograph of onset of autoignition. The fuel is JP-8 with $a_2 = 427\,\mathrm{s}^{-1}$, $Y_{\mathrm{F},1} = 0.4$, $T_1 = 483\,\mathrm{K}$, $Y_{\mathrm{O}_2,2} = 0.23$, and $T_2 = 1225\,\mathrm{K}$.

the transient autoignition process recorded by a high-speed camera at 500 frames per second. The fuel is JP-8 with $a_2 = 427\,\mathrm{s}^{-1}$, $Y_{\mathrm{F},1} = 0.4$, $T_1 = 483\,\mathrm{K}$, $Y_{\mathrm{O}_2,2} = 0.23$, and $T_2 = 1225\,\mathrm{K}$. The image on the left shows a faint illumination around the axis of symmetry. This is onset of autoignition. The image on the right shows a steady flame.

Figures 6 compares the critical conditions of autoignition of JP-8, Jet-A and F-T JP-8. It shows that the autoignition characteristics of JP-8 and Jet-A are similar, while F-T JP-8 is easier to ignite.

Figure 7 shows that the autoignition characteristics of different batches of JP-8 are the same. Similar results for Jet-A are shown in Figure 8.

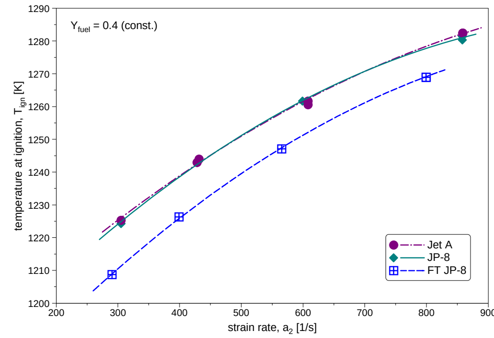

Fig. 6: The temperature of the oxidizer stream at autoignition as a function of the strain rate at fixed values of $Y_{\mathrm{F},1} = 0.4$. The symbols are experimental data. The lines are best fit. The figure compares of autoignition characteristics of JP-8, Jet-A, and F-T JP-8

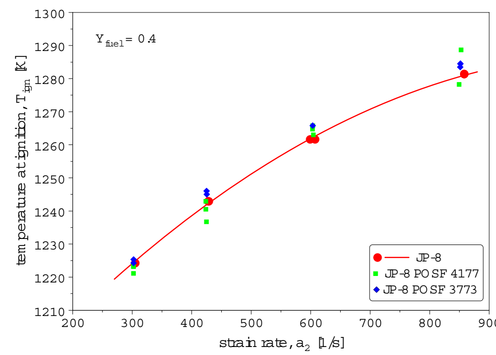

Fig. 7: The temperature of the oxidizer stream at autoignition as a function of the strain rate at fixed values of $Y_{\mathrm{F},1} = 0.4$. The symbols are experimental data. The lines are best fit. The figure compares of autoignition characteristics of various batches of JP-8.

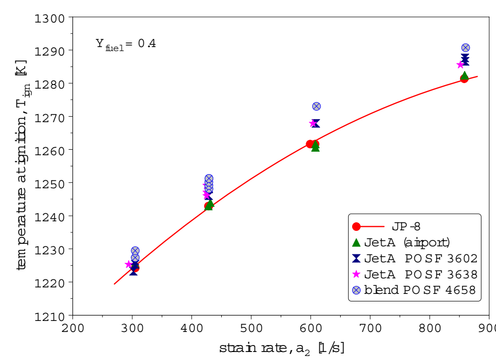

Fig. 8: The temperature of the oxidizer stream at autoignition as a function of the strain rate at fixed values of $Y_{\mathrm{F},1} = 0.4$. The symbols are experimental data. The lines are best fit. The figure compares of autoignition characteristics of various batches of Jet-A.

Figures 9 and 10 compare experimental autoigni-

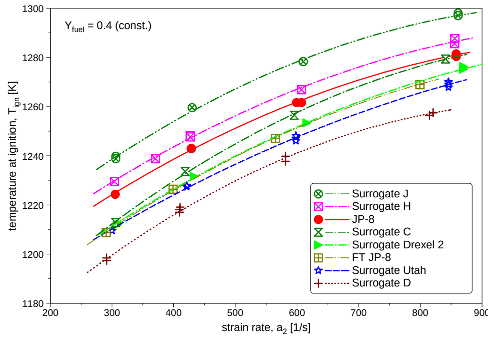

Fig. 9: The temperature of the oxidizer stream at autoignition as a function of the strain rate at fixed values of $Y_{\mathrm{F},1} = 0.4$. The symbols are measurements. The lines are best fit. The figures compares autoignition characteristics of various surrogates of JP-8.

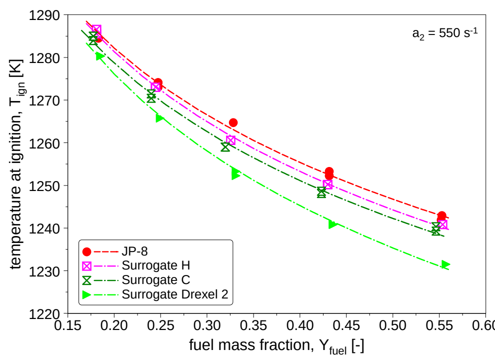

Fig. 10: The temperature of the oxidizer stream at autoignition as a function of the mass fraction of fuel in the fuel stream, $Y_{\mathrm{F},1}$ at a fixed value of the strain rate $a_2 = 550\,\mathrm{s}^1$. The symbols are measurements. The lines are best fit. The figures compares autoignition characteristics of various surrogates of JP-8.

tion data for potential surrogates of JP-8 with that for JP-8. The autoignition characteristics of the surrogates are placed in three groups: Group 1 best, Group 2 good, Group 3 significant differences. The surrogates placed in these groups are

- Group 1: Aachen Surrogate.
- Group 2: Surrogate C, Drexel Surrogate 2, and Modified Aachen Surrogate, Utah Surrogate,
- Group 3: Surrogate D, Surrogate N1, Surrogate N2.

Figures 11 and 12 show that the autoignition characteristics of surrogate G agrees well with those for F-T JP-8.

4. Conclusions

The surrogates of JP-8 are ranked employing the following criteria listed in the order of importance:

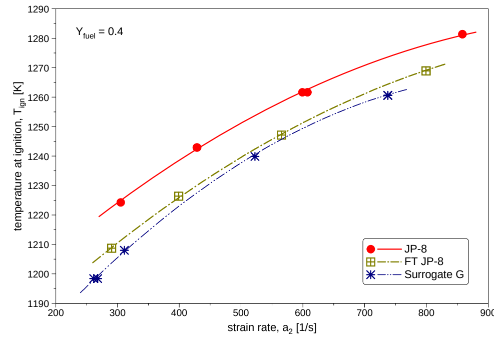

Fig. 11: The temperature of the oxidizer stream at autoignition as a function of the strain rate at fixed values of $Y_{\mathrm{F},1} = 0.4$. The symbols are measurements. The lines are best fit. The figures compares autoignition characteristics of a surrogate of F-T JP-8

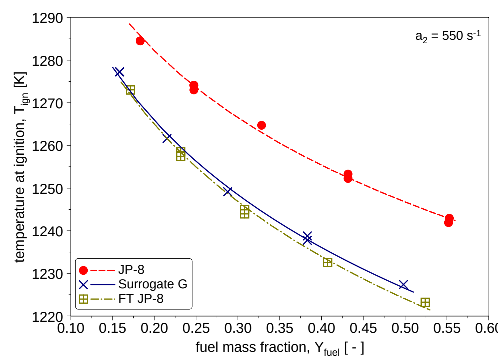

Fig. 12: The temperature of the oxidizer stream at autoignition as a function of the mass fraction of fuel in the fuel stream, $Y_{\mathrm{F},1}$ at a fixed value of the strain rate $a_2 = 550\,\mathrm{s}^1$. The symbols are measurements. The lines are best fit. The figures compares autoignition characteristics of a surrogate of F-T JP-8

(1) how well they reproduce critical conditions of autoignition, (2) how close is the hydrogen to carbon ratio to that of JP-8, (3) simplicity (availability of chemical kinetic mechanisms), and (4) how well they reproduce critical conditions of extinction. Using this criteria the surrogates are listed in the following order:

1. Aachen Surrogate,
2. Surrogate C,
3. Drexel Surrogate 2, and Modified Aachen Surrogate.

The Aachen Surrogate has a H/C ratio of 1.99. Its autoignition characteristics agrees best with JP-8 when compared to all surrogates tested here. Its extinction characteristics agrees well with JP-8. Professor Peters at RWTH Aachen, Germany has measured the volume of soot formed and it is similar to those for JP-8. The Aachen surrogate has only two components. The chemical kinetic mechanism for *n*-decane is well known (Bikas and Peters C&F 126, 1456, 2001). There is a need to compare the low and intermediate temperature chemistry of this surrogate with those for JP-8.

Surrogate C (also called the UCSD surrogate) has H/C ratio of 1.92. This is very close to that of JP-8. The components in the surrogate match the classes of fuel in JP-8. Its autoignition characteristics agrees very well with JP-8. Its extinction characteristics agrees with JP-8, although some differences are observed. It has only three components. Many investigators are developing chemical kinetic mechanisms for the components. There is a need to compare the low and intermediate temperature chemistry of this surrogate with those for JP-8. Surrogates C1 and Surrogate B1 include 1-methylnaphthalene therefore rates of soot production during combustion of these surrogates may be closer to those for JP-8.

The Drexel Surrogate 2 has a H/C ratio is 1.87. Its autoignition characteristics agrees well with JP-8. Its extinction characteristics agrees best with JP-8 in comparison to all surrogates tested. The chemical kinetic mechanisms for the components still are early stages of development. The low and intermediate temperature chemistry of this surrogate agrees well with those for JP-8 (shown by investigators at Drexel).

The Modified Aachen Surrogate has a H/C ratio is 1.97. Very close to that of JP-8. Its autoignition and extinction characteristics agrees well with JP-8. It has only two components. Many investigators are developing chemical kinetic mechanisms for the components. There is a need to compare the low and intermediate temperature chemistry of this surrogate with those for JP-8.

Overall the Aachen surrogate and Surrogate C (UCSD surrogate) appear to best reproduce the combustion characteristics of JP-8. Surrogate G reproduces the combustion characteristics of F-T JP-8.

Assuming that an approximate chemical formula of $C_{12}H_{23.3}$ can be used for JP-8, surrogates that have a close hydrogen to carbon ration to 1.94 and similar density as the commercial fuel reproduce the extinction and autoignition behavior of JP-8 very closely.

Acknowledgments

The research at the University of California at San Diego was supported by the U. S. Army Research Office, grant # W911NF-04-1-0139. Program manager Dr. Ralph A. Anthenien Jr, PhD, PE.

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