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14. ABSTRACT

Experimental and numerical studies are carried out to develop a surrogate that can reproduce selected aspects of combustion of JP-8. Surrogate fuels are defined as mixtures of few hydrocarbon compounds with combustion characteristics similar to those of commercial fuels. A mixture of n-decane and trimethylbenzene, called the Aachen surrogate, and a mixture of n-dodecane, methylcyclohexane, and o-xylene called Surrogate C are selected for consideration as possible surrogates of JP-8.

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Report Title

Combustion of JP8 in Laminar Premixed Flames

ABSTRACT

Experimental and numerical studies are carried out to develop a surrogate that can reproduce selected aspects of combustion of JP-8. Surrogate fuels are defined as mixtures of few hydrocarbon compounds with combustion characteristics similar to those of commercial fuels. A mixture of n-decane and trimethylbenzene, called the Aachen surrogate, and a mixture of n-dodecane, methylcyclohexane, and o-xylene called Surrogate C are selected for consideration as possible surrogates of JP-8.

Experiments under nonpremixed conditions are carried out employing the counterflow configuration. The fuels tested are JP-8 and the Aachen surrogate. Critical conditions of extinction, autoignition, and volume fraction of soot measured in laminar nonpremixed flows burning the Aachen surrogate are found to be similar to those in flames burning JP-8. Numerical calculations are performed using the chemical kinetic mechanism for the Aachen surrogate. The calculated values of the critical conditions of autoignition and soot volume fraction agree well with experimental data.

Experimental studies are carried out to characterize premixed combustion of jet fuels and its surrogates in laminar nonuniform flows. The counterflow configuration is employed. Studies are performed with a premixed reactant stream made up of prevaporized fuel, oxygen and nitrogen from one duct, and an inert stream of nitrogen from the other duct. Critical conditions of extinction are measured for JP-8, Aachen surrogate and Surrogate C. The measured critical conditions of extinction of these surrogates agree well with those for JP-8.

This study confirms that the Aachen Surrogate and Surrogate C are possible surrogates of JP-8.

List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Number of Papers published in peer-reviewed journals: 0.00

(b) Papers published in non-peer-reviewed journals or in conference proceedings (N/A for none)

Number of Papers published in non peer-reviewed journals: 0.00

(c) Presentations

Experimental Measurements of Extinction of Premixed Flames Burning High Molecular Weight Hydrocarbon Fuels, by Patrick Weydert, Ulrich Niemann, and Kalyanasundaram Seshadri, paper to be presented at the Spring Meeting of the Western States Section of the Combustion Institute, University of Southern California at Los Angeles, March 17-18, 2008.

Number of Presentations: 1.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts): 0

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts): 0

(d) Manuscripts

A Surrogate Fuel for Kerosene, by S. Honnet, K. Seshadri, and N. Peters, paper submitted for publication in the proceedings of the 32 Symposium International on Combustion, August 2008.

Number of Manuscripts: 1.00

Number of Inventions:

Graduate Students

NAME	PERCENT_SUPPORTED
None	
FTE Equivalent:	
Total Number:	**1**

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
None	
FTE Equivalent:	
Total Number:	**1**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
Kalyanasundaram Seshadri	0.18	No
FTE Equivalent:	**0.18**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
None	
FTE Equivalent:	
Total Number:	**1**

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period:	0.00
The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:......	0.00
The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:......	0.00
Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):......	0.00
Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:......	0.00
The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense	0.00
The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:......	0.00

Names of Personnel receiving masters degrees

NAME	
None	
Total Number:	**1**

Names of personnel receiving PHDs

NAME	
None	
Total Number:	**1**

Names of other research staff

NAME	PERCENT_SUPPORTED	
Stefan Helmuth Humer	0.21	No
FTE Equivalent:	**0.21**	
Total Number:	**1**	

Sub Contractors (DD882)

Inventions (DD882)

Combustion of JP-8 in Laminar Premixed Flames, Agreement Number: W911NF0610158

1 Statement of Problem Studied

The Department of Defense directive # 4140.25 dated April 12, 2004 mandates that "primary fuel support for land-based air and ground forces in all theaters (overseas and in the Continental United States) shall be accomplished using a single kerosene-based fuel, in order of precedence: JP-8, commercial jet fuel (with additive package), or commercial jet fuel (without additives)." A key challenge is to develop technologies for converting diesel-powered equipment employed by the US Army so that they can be powered by JP-8. This conversion is a complicated process. Many issues with fuel properties and performance have to be considered. They include autoignition, combustion, fuel injection, lubricity, and spray characteristics.

The objective of the study described in this report is to understand those key aspects of combustion of JP-8 that are required to facilitate conversion of diesel-powered equipment to JP-8. JP-8 is a mixture of numerous aliphatic and aromatic compounds. The major components of this fuel are straight chain paraffins, branched chain paraffins, cycloparaffins, aromatics, and alkenes. The concentration of paraffins is on the average 60 % by volume, that of cycloparaffins 20 %, that of aromatics 18 %, and that of alkenes 2 %. It has been established that an useful approach is to first develop surrogates that reproduce selected aspects of combustion of JP-8. Surrogates are mixtures of hydrocarbon compounds. The hydrocarbon compounds used to construct the surrogate will depend on those aspects of combustion of JP-8 that the surrogate is expected to reproduce.

Experimental and numerical studies are carried out to develop a surrogate that can reproduce selected aspects of combustion of JP-8 in laminar nonpremixed and premixed flows. A mixture of *n*-decane and trimethylbenzene, called the Aachen surrogate, and a mixture of *n*-dodecane, methylcyclohexane, and *o*-xylene called surrogate C are found to reproduce many aspects of combustion of JP-8. The next section describes the important results obtained in this research.

2 Summary of the Most Important Results

The summaries of the important results are given in this section. Section 2.1 describes research carried out on nonpremixed flames. Section 2.2 describes studies carried out in premixed systems. The research described in section 2.1 has been submitted for publication in a peer-reviewed journal. A copy of the manuscript has been sent to the Army Research Office. A manuscript describing research described in section 2.2 is in preparation for submission to a peer-reviewed journal. A draft of this manuscript is attached to this report.

2.1 Experimental and Chemical-Kinetic Modeling Study of Combustion of Kerosene and its Surrogate in Laminar Nonpremixed Flows

This research is carried out in collaboration with Professor N. Peters at Institut für Technische Verbrennung, RWTH Aachen, D-52056 Aachen, Germany.

Experimental and numerical studies are carried out to develop a surrogate that can reproduce selected aspects of combustion of kerosene. Jet fuels, in particular Jet-A1, Jet-A, and JP-8 are kerosene type fuels. Surrogate fuels are defined as mixtures of few hydrocarbon compounds with combustion characteristics similar to those of commercial fuels. A mixture of *n*-decane 80 % and trimethylbenzene 20 % by weight, called the Aachen surrogate, is selected for consideration as a possible surrogate of kerosene. Experiments are carried out employing the counterflow configuration. The fuels tested are kerosene and the Aachen surrogate. Critical conditions of extinction, autoignition, and volume fraction of soot measured in laminar nonpremixed flows burning the Aachen surrogate are found to be similar to those in flames burning kerosene.

A chemical-kinetic mechanism is developed to describe the combustion of the Aachen surrogate. This mechanism is assembled using previously developed chemical-kinetic mechanisms for the components: *n*-decane and trimethylbenzene. Improvements are made to the previously developed chemical-kinetic mechanism for *n*-decane. The combined mechanisms are validated using experimental data obtained from shock tubes, rapid compression machines, jet stirred reactor, burner stabilized premixed flames, and a freely propagating premixed flame. Numerical calculations are performed using the chemical-kinetic mechanism for the Aachen surrogate . The calculated values of the critical conditions of autoignition and soot volume fraction agree well with experimental data. The present study shows that the chemical-kinetic mechanism for the Aachen surrogate can be employed to predict nonpremixed combustion of kerosene.

2.2 Combustion of Jet Fuels and their Surrogates in Laminar Nonpremixed Flows

Experimental studies are carried out to characterize premixed combustion of jet fuels and its surrogates in laminar nonuniform flows. In the study described in section 2.1, and in a previous study supported by the U. S. Army Research Office, it was found that the Aachen surrogate made up of 80 % *n*-decane and 20 % trimethylbenzene by weight and Surrogate C made up of 60 % *n*-dodecane, 20 % methylcyclohaxane and 20 % toluene by volume at 298 K reproduce autoiginition and extinction characteristics of JP-8 in laminar nonpremixed flows. Here these surrogates are tested under premixed conditions. The counterflow configuration is employed. Studies are performed with a premixed reactant stream made up of prevaporized fuel, oxygen and nitrogen from one duct, and an inert stream of N_2 from the other duct. Critical conditions of extinction are measured for JP-8, Aachen surrogate and Surrogate C. The measured critical conditions of extinction of these surrogates agree well with those for JP-8. The experimental data confirms that these mixtures can be considered to be possible surrogates of JP-8.

Appendix: Combustion of JP-8 and its Surrogates in Laminar Premixed Flows

Abstract

Experimental studies are carried out to characterize premixed combustion of jet fuels and its surrogates in laminar nonuniform flows. In a previous study supported by the U. S. Army Research Office, it was found that the Aachen surrogate made up of 80 % *n*-decane and 20 % trimethylbenzene by weight and Surrogate C made up of 60 % *n*-dodecane, 20 % methylcyclohaxane and 20 % toluene by volume at 298 K reproduce autoiginition and extinction characteristics of JP-8 in laminar nonpremixed flows. Here these surrogates are tested under premixed conditions. The counterflow configuration is employed. Studies are performed with a premixed reactant stream made up of prevaporized fuel, oxygen and nitrogen from one duct, and an inert stream of N_2 from the other duct. Critical conditions of extinction are measured for JP-8, Aachen surrogate and Surrogate C. The measured critical conditions of extinction of these surrogates agree well with those for JP-8. The experimental data confirms that these mixtures can be considered to be possible surrogates of JP-8.

1 Introduction

The Department of Defense directive # 4140.25 dated April 12, 2004 mandates that "primary fuel support for land-based air and ground forces in all theaters (overseas and in the Continental United States) shall be accomplished using a single kerosene-based fuel, in order of precedence: JP-8, commercial jet fuel (with additive package), or commercial jet fuel (without additives)." A key challenge is to develop technologies for converting diesel-powered equipment employed by the US Army so that they can be powered by JP-8. This conversion is a complicated process. Many issues with fuel properties and performance have to be considered. They include autoignition, combustion, fuel injection, lubricity, and spray characteristics. Another application where conversion is required is unmanned aerial vehicles (UAV). Currently the UAVs in the field use gasoline or specialty fuels. The Army and other DOD services are in the process of developing technologies that would enable UAV's to operate on JP-8. It is very likely that UAV's will employ internal combustion engines that employ spark-ignition or compression-ignition.

JP-8 is a mixture of numerous aliphatic and aromatic compounds. The major components of this fuel are straight chain paraffins, branched chain paraffins, cycloparaffins, aromatics, and alkenes [1–8]. The concentration of paraffins is on the average 60 % by volume, that of cycloparaffins 20 %, that of aromatics 18 %, and that of alkenes 2 %. It has been established that an useful approach is to first develop surrogates that reproduce selected aspects of combustion of JP-8. Surrogates are mixtures of hydrocarbon compounds. The hydrocarbon compounds used to construct the surrogate will depend on those aspects of combustion of JP-8 that the surrogate is expected to reproduce. For example the hydrocarbon compounds in surrogates chosen to reproduce key aspects of combustion of JP-8 in aircraft gas turbine engines may not be the same as those required to reproduce combustion in diesel-powered equipment. The focus of this work is to develop surrogates that reproduce aspects of combustion of JP-8 that are required to facilitate conversion of diesel-powered equipment and equipment employing spark-ignition combustion to JP-8.

Edwards and Maurice [3] have defined two types of surrogates: physical surrogate and chemical surrogate. Physical surrogates are constructed to reproduce the physical properties of commercial fuels. Chemical surrogates generally have the same chemical-class composition of commercial fuels. They are constructed to reproduce selected aspects of combustion of commercial fuels. Two key aspects in developing chemical surrogates are (1) a clear definition of the aspects of combustion that the surrogate must reproduce, and (2) developing chemical-kinetic mechanism for the components in the surrogate. Starting from the pioneering work of Schulz [9], who proposed a 12-component surrogate mixture for JP-8, several investigators have proposed surrogates for jet fuels and kerosene [2–5, 10–21]. The components of surrogates of jet fuels often include a long chain aliphatic species and a cyclic compound. The aliphatic species is usually *n*-decane or *n*-dodecane [10, 13, 14, 16, 17]. The cyclic compound may be trimethylbenzene [10, 13, 16, 17] or propylbenzene [14]. The cyclic species methylcyclohexane, decaline, and 1-methylnaphthalene have also been selected as components of surrogates of jet fuels [2, 11]. Two component surrogates have been found to successfully reproduce many aspects of combustion of jet fuels [10, 13, 16, 17]. The temperatures of the air stream at autoignition as a function of the strain rate were measured in nonpremixed flows employing the counterflow configuration for kerosene and two-component surrogates made up of *n*-decane and trimethylbenzene [16, 17]. At a given value of the strain rate the air temperature at autoignition for a surrogate mixture of *n*-decane (60 %) and trimethylbenzene (40 %) by weight was higher than that of kerosene, while the air temperature at autoignition for a surrogate mixture of *n*-decane (80 %) and trimethylbenzene (20 %) by weight agreed with experimental data at low values of the strain rate [16, 17]. A surrogate of kerosene made up of *n*-decane (77 %) and mesitylene (23 %) by volume was used to study soot formation in laminar co-flow diffusion flames [13].

Recently several batches of JP-8 and Jet-A, and fifteen possible surrogates for JP-8 were tested in nonpremixed systems [10]. It was found that critical conditions of extinction and autoignition of JP-8 and Jet-A are similar. The surrogates of Jet-A and JP-8 were ranked employing the following criteria listed in the order of importance: (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. Among the surrogates tested, the surrogate H surrogate made up of *n*-decane (80 %) and trimethylbenzene (20 %) by liquid volume (*n*-decane 75 % and trimethylbenzene 25 % by weight), and a surrogate made up of *n*-dodecane (60 %), methylcyclohexane (20 %), and *o*-xylene (20 %) by liquid volume were found to best reproduce autoignition and extinction characteristics of JP-8 [10]. Surrogate H has a H/C ratio of 1.99. This compares well with the H/C ratio of 1.92 for JP-8. The autoignition characteristics of the surrogate H was found to agree best with JP-8 when compared to all the fifteen surrogates tested [10]. Its extinction characteristics agrees well with JP-8 [10].

2 Experimental Apparatus and Procedures

The liquid fuels tested here are vaporized by injecting them 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 is placed close to the nozzle, and the other at the exit of the vaporizer chamber. Flow rates of gases are adjusted by computer-regulated mass flow controllers. Flow lines going from the vaporizer to the counterflow burner are heated to prevent condensation inside the lines. A detailed description of the burner is given elsewhere [22, 23].

Figure 1 shows a schematic illustration of the counterflow configuration. Studies are carried out by injecting a premixed reactant stream made up of prevaporized fuel, oxygen and nitrogen from one duct, and an inert-gas stream of N_2 from the other duct. The prevaporized fuel include, JP-8, components of surrogates of JP-8, and possible surrogates of JP-8. The mass fraction of fuel, the mass fraction of oxygen, the temperature, and the flow velocity in the premixed reactant stream at the exit of the duct are $Y_{\mathrm{F},1}$, $Y_{\mathrm{O}_2,1}$, T_1, and V_1, respectively. The temperature and the flow velocity in the inert-gas stream at the exit of the duct are T_2 and V_2, respectively. The strain rate, a, is defined as the normal gradient of the normal

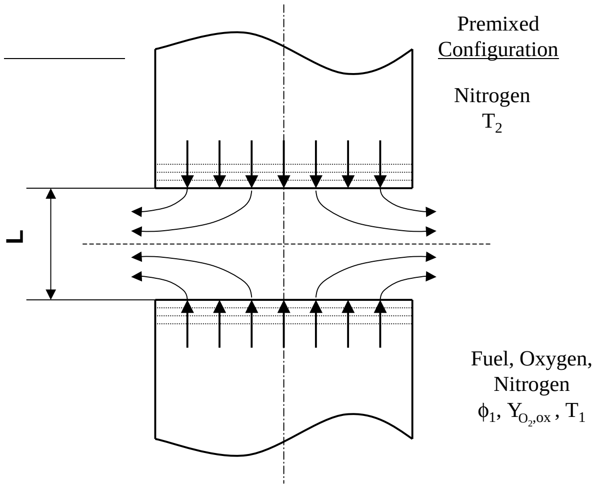

Figure 1: Schematic illustration of the counterflow configuration.

component of the flow velocity. The value of a changes along the axis of symmetry. The value of a is discontinuous across the stagnation plane. On the premixed reactant stream side of the stagnation plane the strain rate is represented by a_1, and on the inert-gas stream side of the stagnation plane, the strain rate is represented by a_2. The conditions under which these experiments are conducted are such that the flame is stabilized on the premixed reactant stream side of the stagnation plane. The strain rate on the premixed reactant stream side of the stagnation plane be given by [24]

$$a_1 = \frac{2|V_1|}{L}\left(1 + \frac{|V_2|\sqrt{\rho_2}}{|V_1|\sqrt{\rho_1}}\right). \tag{1}$$

Here ρ_1 and ρ_2 represent the density of the premixed reactant stream and inert-gas stream, respectively. In the experiments, the momentum of the counterflowing streams are approximately maintained at the same value to ensure that the stagnation plane is at mid-plane between the two 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 [24].

The experiments are conducted at a pressure of 1.013 bar. The premixed reactant mixture, made up of fuel, air, and nitrogen, is characterized by the equivalence ratio, $\phi = \nu_{O_2} Y_{F,1} W_{O_2}/(Y_{O_2,1} W_F)$, where W_F and W_{O_2} represent the molecular weights of fuel and oxygen, respectively, and $\nu_{\mathrm{O_2}}$ is the stoichiometric oxygen/fuel mole ratio. The quantity $Y_{\mathrm{O_2,x}} = Y_{\mathrm{O_2,1}}/(Y_{\mathrm{O_2,1}} + Y_{\mathrm{N_2,1}})$ is a measure of the dilution of air with nitrogen. In a reactive mixture of fuel and air the value of $Y_{\mathrm{O_2,x}}$ is 0.233. The experiments are carried out for $Y_{\mathrm{O_2,x}} = 0.18$, T_1 between 483 K and 488 K, and $T_2 = 298\,\mathrm{K}$. A premixed flame is stabilized in the mixing layer between the counterflowing streams for values of the strain rate less than $a_{1,\mathrm{E}}$, where $a_{1,\mathrm{E}}$ is the value of the strain rate, a_1, at extinction. In addition the velocity of the premixed reactant stream at the exit of the duct, V_1, must be greater than the laminar burning velocity, to prevent flashback. The flow velocity of the inert-gas stream is increased until extinction takes place. data is obtained showing $a_{1,\mathrm{E}}$ as a function of ϕ. The accuracy of the strain rate is ± 10 % of recorded value and that of the fuel mass fraction and oxygen mass fraction ± 3 % of recorded value. The experimental repeatability on reported strain rate is ± 5 % of recorded value.

The fuels tested are:

- Reference fuels: *n*-heptane, *n*-decane, *n*-dodecane, methylcyclohexane, trimethylbenzene, *o*-xylene
- JP-8 POSF 4177 (obtained from Wright Patterson Air Force Base (WPAFB)),
- Fuel mixtures: Possible surrogates of JP-8:
    1. Surrogate C: 60 % *n*-dodecane, 20 % methylcyclohexane, 20 % *o*-xylene by volume at 298 K: $H/C = 1.92$.
    2. Aachen surrogate: *n*-decane 80 %, trimethylbenzene 20 % by weight, $H/C = 2.00$.

Here H/C is the molar ratio of hydrogen to carbon.

3 Results

The strain rate at extinction, $a_{1,\mathrm{E}}$, as a function of the equivalence ratio ϕ are shown in Figs. 2, 3, 4, and 5. In these figures the lines represent experimental data.

Figure 2 shows the extinction characteristics of *n*-heptane, *n*-decane, *n*-dodecane, and methylcyclohexane are nearly the same. Figure 3 shows that at a given value of ϕ, the value of $a_{1,\mathrm{E}}$ for *o*-xylene is larger than that for trimethylbenzene. Thus *o*-xylene is more difficult to extinguish in comparison to trimethylbenzene. Figure 4 compares the extinction

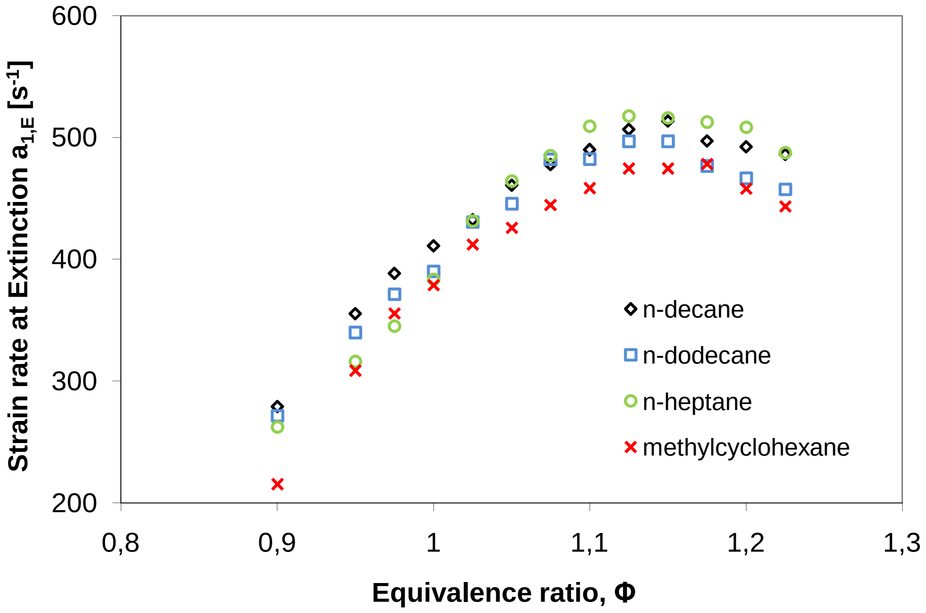

Figure 2: The strain rate at extinction as a function of the equivalence ratio. The figure shows data for the alkanes, *n*-heptane, *n*-decane, *n*-dodecane, and methylcyclohexane. The data is obtained for $Y_{\mathrm{O_2,x}} = 0.18$, T_1 between 483 K and 488 K, and $T_2 = 298$ K.

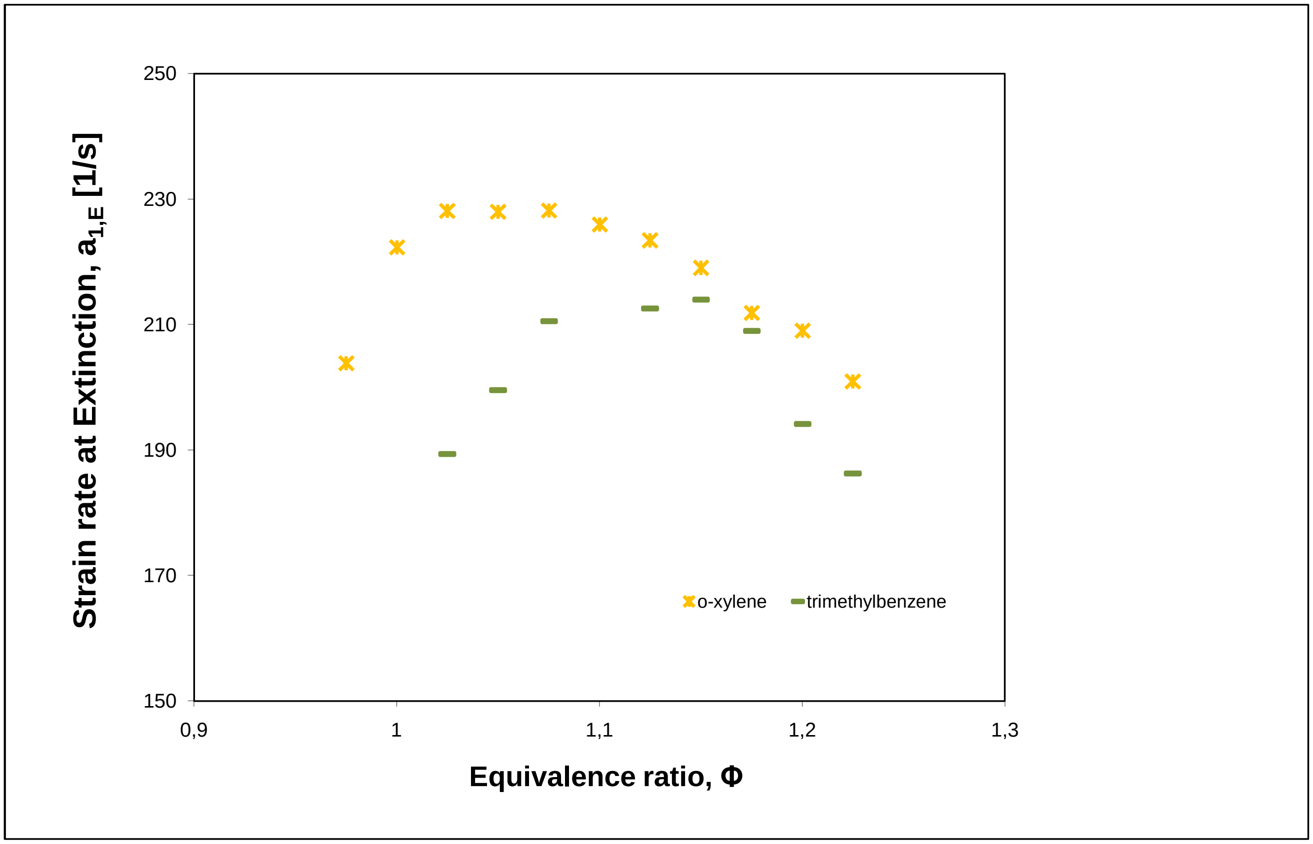

Figure 3: The strain rate at extinction as a function of the equivalence ratio. The figure shows data for the aromatics, *o*-xylene, and trimethylbenzene. The data is obtained for $Y_{\mathrm{O_2,x}} = 0.18$, T_1 between 483 K and 488 K, and $T_2 = 298$ K. The symbols represent experimental data.

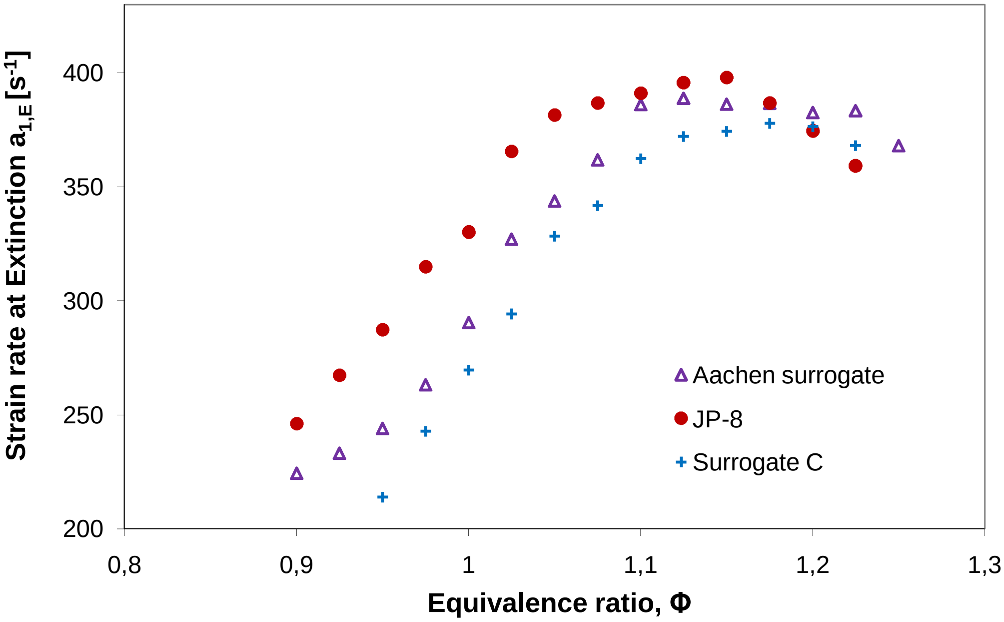

Figure 4: The strain rate at extinction as a function of the equivalence ratio. The figure shows data for the JP-8 (POSF 4177), Aachen surrogate, and surrogate C. The data is obtained for $Y_{O_2,x} = 0.18$, T_1 between 483 K and 488 K, and $T_2 = 298$ K. The symbols represent experimental data

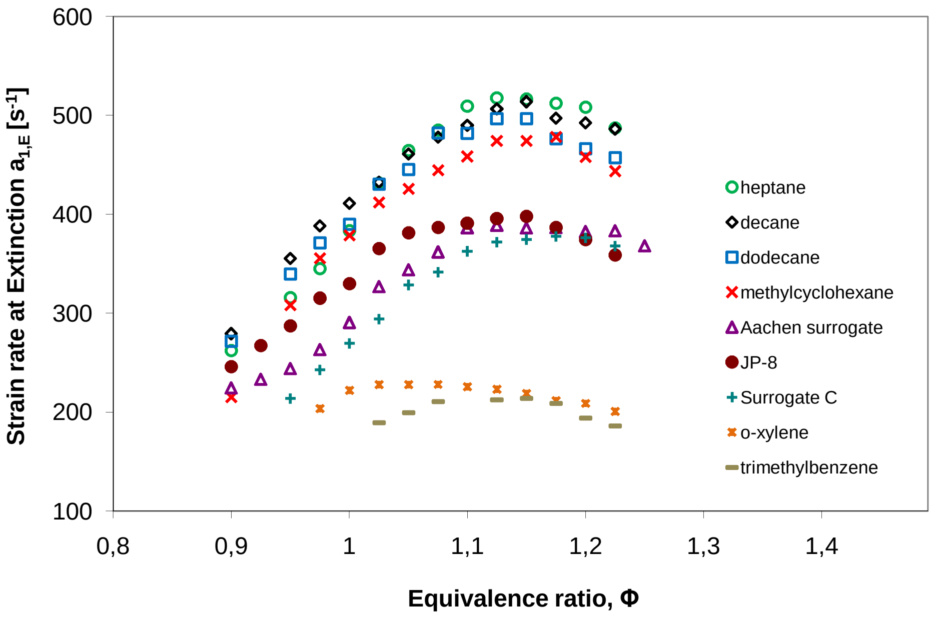

Figure 5: The strain rate at extinction as a function of the equivalence ratio. The figure shows data for the JP-8 (POSF 4177), its surrogates, and reference components. The data in this figure is reproduced from Figures 2, 3, and 4 obtained for $Y_{O_2,x} = 0.18$, T_1 between 483 K and 488 K, and $T_2 = 298$ K. The symbols represent experimental data

characteristics of surrogate C and the Aachen surrogate with those of JP-8. The critical conditions of extinction for the surrogates agree reasonably well with those of JP-8. The critical conditions of extinction in Figs. 2, 3, and 4 are plotted in Figure 5. It shows that in general alkanes are more difficult to extinguish in comparison to aromatics. JP-8 and its surrogates are more difficult to extinguish in comparison to the aromatics, while they are easier to extinguish when compared with the alkanes.

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