

# Development of an Experimental Database and Kinetic Models for Surrogate Jet Fuels

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**The engineering and scientific community has been searching for the identification of surrogate fuels that can reasonably represent the performance and emissions behavior of jet fuels (e.g., Jet A, JP-8) in engines. Many proposals exist in the literature, but there has been no consensus of opinion. It has been recognized that if the surrogate (or its) components were identified and agreed upon, then the research community could focus their resources on the development of chemical kinetic models for accurate representation of this surrogate. This manuscript reviews the findings and recommendations of a working group created by AFOSR, ARO and NIST to identify a surrogate fuel and/or its components. As a part of this study, the chemical kinetically limited processes within a gas turbine are identified. In addition, a palette of compounds is presented from which a surrogate fuel might be constructed. We initially suggested a simplified surrogate composed of n-decane, n-butylcyclohexane and n-butylbenzene and experiments were performed and**

**compared to reactivity data for jet fuels. Results indicate that this mixture is more reactive and difficult to extinguish than typical jet fuels. Some ideas for resolving these issues are discussed. Recommendations for future efforts are provided and a roadmap for the creation of surrogate fuel kinetics models is proposed.**

## I. Introduction

In 2003, Tsang and others<sup>1</sup> held a workshop with industry experts on the development of databases for real transportation fuels. As part of the discussions, the need for surrogate fuels was identified. Even prior to this date, there had been significant interest in the creation of surrogate fuels for testing, to provide a baseline for performance and emissions, and to provide a tool that could facilitate modeling. Federal agencies had indicated a willingness to fund research in this area; however, they were concerned about the proliferation of surrogate definitions and encouraged the community to reach a common understanding for the selection and identification of surrogates. Thus, in 2004, three working groups were created; one each for gasoline, diesel, and jet fuel. This paper presents a summary of the findings of the working group for surrogate jet fuels. The paper is directed towards simulation of chemical kinetic phenomena, although physical attributes of the fuel are discussed as well. Issues related to fuel spray effects and drop size distributions are outside the scope of this paper. Treatment of such effects, however, will be important for any practical application of results from this work. Results from the other (gasoline and diesel) working groups are reported separately<sup>2,3</sup>. Coincident with these efforts is the development of a collaborative effort<sup>4</sup> for predictive models of complex fuels in chemically reacting environments.

Several research groups have proposed surrogates of varying complexity that are valid for different applications. Single-component fuels may be adequate for simple applications like combustion efficiency, while more complex surrogates will undoubtedly be required for chemistry-dependent applications, such as soot formation and emissions, radiation loading, combustion staging, or lean-premixed-prevaporized applications. With a suitable number of components, it is also possible to simulate a fuel's physical properties (for example its distillation characteristics). Such issues will be relevant to preferential vaporization related phenomenon, including pool fire hazards<sup>5,6</sup>. A substantial number of surrogate fuel mixtures have been proposed already, evaluated in engines and in fundamental experiments, and studied numerically.

Computational combustion modeling is an essential, complementary tool to engine experiments. The combination of computational fluid dynamics (CFD) and detailed chemical kinetics provides the promise for optimizing engine performance. Consequently, chemistry models are needed to represent the combustion of jet fuel in practical devices such as gas turbine engines. In addition, there is a desire to apply such tools to other devices burning kerosene fuels (pulse detonation engines, JP-8-fueled diesels, RP-1-fueled liquid rocket combustors, and hydrocarbon-fueled scramjets) as well. Unfortunately, it is not possible currently to represent the complex chemistry of kerosene fuels in a chemical kinetic model that has been validated over the conditions of interest. Not only are the kinetics of all of the components not well determined, but possible chemical kinetic interactions among them are not understood. A large number of components in a surrogate fuel would lead to an unwieldy number of reactions, species, and thermochemical parameters. Even restricting the number of fuel species to less than ten results in a very large dimensional model. In fact the dimensional complexity of an engine combustion model and current computational resources limit the number of species that can be considered within engine combustion codes. One current target for scramjet combustion modeling is 20 species. As available computer power continues to escalate, this maximum number may well increase, as it still is not well established how many species are needed to simulate all aspects of combustor performance. There is also a trade-off between model fidelity, chemical kinetics, distillation matching, and computational complexity (even with reduction procedures) in applications. While the long-term goal to increase the number of species considered should remain, there are presently practical reasons to limit the number of pure components used to represent kerosene fuel chemical kinetics.

The present coordinated effort (the "Surrogate Fuels Working Group") represents an attempt to draw coherence to these efforts. The goal is to define a small number of kerosene-range hydrocarbon molecules that can be blended into useful experimental fuels and modeled computationally. The latter requires: a) laboratory combustion data (e.g., from flow reactors, shock tubes, combustion bombs, opposed flames, etc.) of sufficient quality to validate the kinetic models, b) identification of key species in these validation data sets, c) fundamental chemical kinetic, thermochemical, and physical property data, and d) identification of key kinetically-limited phenomena.

This manuscript first contains an overview of jet fuels and their characteristics, followed by a brief review of potential alternatives to jet fuels, prior work on surrogates and reference distillate fuels, methods for reduced

model development, and CFD implementations. Then, chemical kinetic targets for the surrogate fuel are discussed, a palette of possible components are presented, and needs of data sets from various experiments are identified. Finally, a roadmap for development of a surrogate JP-8/Jet A and associated chemical kinetic models are provided and related recommendations are presented.

## II. Overview on Jet Fuel Surrogates

There are a number of common jet fuels, summarized in Table 1. The airline and refining industries have been driving the effort to standardize all commercial jet fuels as “Jet A-1” (although the nomenclature varies internationally). This fuel is a complex mixture of hundreds (if not thousands) of hydrocarbons. Jet fuel specifications are “loose” enough that significant compositional variations exist between jet fuels that are nominally all “Jet A” or “JP-8”. The difference between Jet A-1 and JP-8 is simply an additive package to satisfy military requirements.

A starting point for surrogate development should be based upon a composition of a typical or average jet fuel. Unfortunately, variations in jet fuels are large. As an example, the variations in aromatics in JP-8 in 2004 are shown in Fig. 1 (Ref. 7). A recent “World Fuel Survey” was conducted under the auspices of the Coordinating Research Council, where 55 jet fuel samples (of Jet A, Jet A-1, JP-8, and JP-5) were obtained from locations world-wide<sup>8</sup>. The average composition is shown in Table 2, as obtained at WPAFB by the University of Dayton Research Institute using ASTM D2425 (Ref. 9). Typical GC-MS analyses of kerosene fuels identify perhaps 50% of the components, so ASTM D2425 was used to segregate the components into classes. The second column in Table 2 is for an “average” fuel made by mixing together equal volumes of Jet A from 5 different U.S. manufacturers. Typical compositions of Jet A, Jet A-1 and JP-8 fuels are sufficiently similar that the assumption of an “average” “jet fuel” based on Table 2 is reasonable. This argument is NOT equivalent to saying that all jet fuels will behave the same in a given situation or experiment. For example, the extreme 12% and 25% vol% aromatic fuels from fringes of the distribution in Fig. 1 will likely have different soot formation tendencies. Differences in other behavior (e.g., ignition or blowout) remain to be seen.

A good source for general information on jet fuels is the Chevron “Aviation Fuels” technical review; [http://www.chevrontexacoaviation.com/chevrontexacoaviation/tgam\\_prod/documents/Aviation\\_Tech\\_Review.pdf](http://www.chevrontexacoaviation.com/chevrontexacoaviation/tgam_prod/documents/Aviation_Tech_Review.pdf). This white paper discusses only surrogates for general purpose jet fuels and alternative (non-petroleum-derived) jet fuels. A general discussion of specialty kerosene fuels (such as JP-7 and RP-1) may be found elsewhere<sup>10</sup>.

While the majority of research engine tests utilize fuels that simulate the full distillation curve, it is often desirable to limit the chemical and/or physical complexity of the fuel to generate insight and understanding into the underlying fundamental processes. The simplest surrogate fuel consists of a single component, e.g., the use of n-decane as a jet fuel surrogate (e.g., see Ref. 11). However, in contrast to the usefulness of iso-octane and

**Table 1. Common characteristics of jet fuels**

Name	Specification	Description	Flash point, C	Freeze point, C
Jet A-1	ASTM D1655, UK DefStan 91-91	Standard commercial jet fuel	>38	<-47
Jet A	ASTM D1655	U.S domestic jet fuel	>38	<-40
JP-8	MIL-DTL-83133	U.S. military jet fuel (Jet A-1 + 3 additives)	>38	<-47
JP-5	MIL-DTL-5624	U.S. Navy high flash jet fuel	>60	<-46
TS-1	GOST 10227-86	Russian jet fuel	>28	<-50*

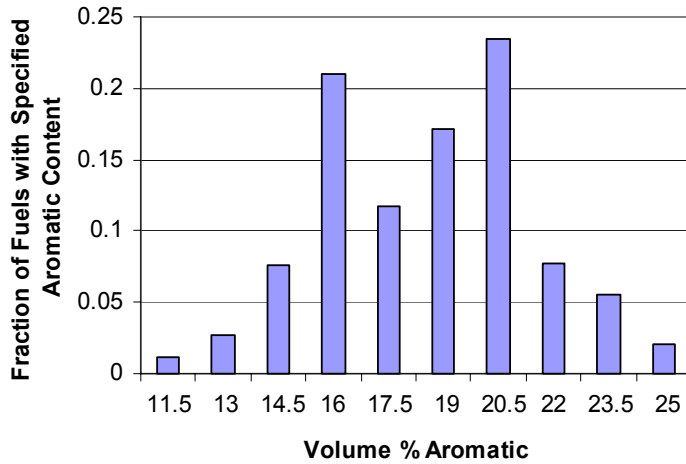
\* Russian test method for “chilling point”

**Table 2. Composition results for 55 “world survey” fuels<sup>9,\*</sup>**

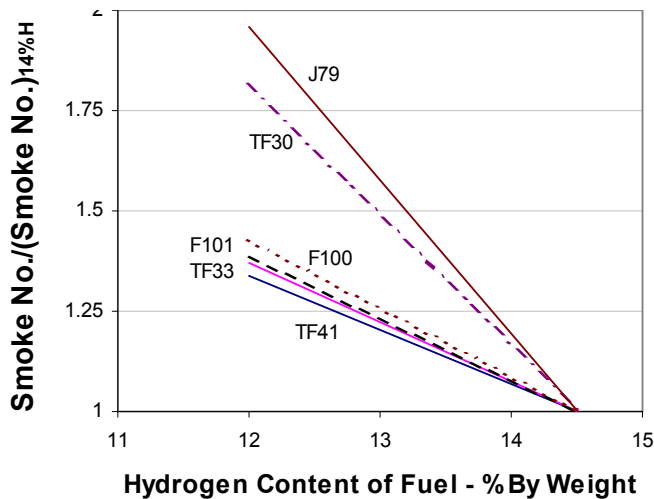
	World survey average, vol %	Composite Jet A blend
paraffins ( <i>n- + i-</i> )	58.78	55.2
Monocycloparaffins	10.89	17.2
Dicycloparaffins	9.25	7.8
Tricycloparaffins	1.08	0.6
alkyl benzenes	13.36	12.7
indans+tetralins	4.9	4.9
Naphthalene	0.13	<0.2
substituted naphthalenes	1.55	1.3

\*The ASTM procedure (D2425) also measures acenaphthenes, acenaphthylenes, tricyclic aromatics, and indenes, but these were below detection limits in all cases.

n-heptane as gasoline surrogates (through their widespread use as components of octane number reference fuels), there are no obvious corresponding surrogate fuel components or standard reference fuels for jet fuels. Jet fuels are “kerosene” fuels, with a typical boiling range of 160-260 C (Ref. 12). The jet fuel specifications (Jet A, Jet A-1, JP-8) control the 10% point of the distillation (<205 C) and the final boiling point (<300 C).



**Figure 1. Variation in aromatics (ASTM D1319) in JP-8 deliveries in 2004<sup>7</sup>.** The volume-averaged mean was 17.9 vol% aromatics. The X-axis is the vol % aromatics in the sample; the Y-axis is the fraction of the total deliveries that fall within the range. Thus, 23.4% of the fuel samples in 2004 had 20.5±0.75 vol% aromatics.



**Figure 2. Relationship between smoke number and weight % hydrogen in various engines<sup>15</sup>.**

fuel rich primary zones seem to be most sensitive to fuel composition effects on soot, while leaner-operating engines show less effect<sup>15</sup>. None of these studies, however, considered the impact on particle size, which has received increased attention recently.

### III. Additional Background Information

#### A. Alternative Fuels

One near-term need for surrogate kinetic models is to assess the impact of alternative (non-petroleum) fuels. Two such fuels include: a highly-isoparaffinic jet fuel derived from natural gas using the Fischer-Tropsch (F-T) process (F-T Jet A-1 or S-8)<sup>19</sup>, and a highly-naphthenic jet fuel derived from coal using a variant of a

In reality, traditional gas turbine engines are not particularly sensitive to fuel composition; hence there are no identified jet fuel characteristics that are required to maintain engine operability. Emerging engine technologies operating closer to stability limits are likely to exhibit stronger fuel sensitivity and use of (partial) premixing will inevitably lead to concerns relating to the auto-ignition characteristics of fuels. Jet fuel specifications have several composition limitations that have arisen as turbine engines have developed, such as a limit on aromatics (<25 vol% by ASTM D 1319) and naphthalenes (<3 vol% by ASTM D1840 when the smoke point is less than 25 mm). The JP-8 specification also calls for a hydrogen content greater than 13.4 mass %. Extensive NASA and AF-sponsored testing of fuels (including NASA’s ERBS, “Experimental Reference Broadened Specification”) in the late 70s and early 80s in various operational gas turbine engines found that physical (rather than chemical) properties of the fuel were the dominant factors in most aspects of gas turbine engine performance. Only for smoke (soot) emissions and combustor liner heating (through radiation from soot) were chemical properties important, and they seemed to be best correlated against overall fuel H/C ratio or hydrogen content<sup>13-15</sup> as shown in Fig. 2. These results were relatively independent of aromatic concentration or nature (e.g., single or fused rings). Others disagreed, typically citing naphthalene content as a secondary factor that could not be neglected<sup>16-18</sup>. Combustors with very

direct liquefaction process<sup>20</sup>. It is noted that any hydrocarbon source (coal, shale oil, biomass, etc.) can be used as the feedstock for the F-T process. An example F-T fuel is “S-8”, a synthetic jet fuel blended with JP-8 and flight tested in a B-52 in September and December, 2006. A surrogate for the F-T fuel would likely have an isoparaffin as a major component, while a surrogate for the naphthenic fuel would be rich in decalin and alkyl cyclohexanes. A broad chemical characterization of these fuels is provided in Table 3 (Ref. 9). A detailed analysis of the F-T Jet A-1 (or S-8) has been performed<sup>21</sup> using GC-MS that demonstrates that a large number of the paraffins are alkanes with one or two attached methyl groups.

**Table 3. Alternative fuel composition<sup>9</sup>.**

	F-T Jet A-1 (S-8)	Coal-based jet fuel
Paraffins	99.7	0.6
Monocycloparaffins	<0.2	46.4
Dicycloparaffins	0.3	47.0
Tricycloparaffins	<0.2	4.6
alkyl benzenes	<0.2	0.3
indans+tetralins	<0.2	1.1
Naphthalene	<0.2	<0.2
substituted naphthalenes	<0.2	<0.2

### B. Reference Distillate Fuels

Unlike gasoline research, which has often employed a set of reference fuels, jet fuel research does not have a similar set of reference fuel of varying composition. In the early 1970s, the Air Force had a number of fuels set aside for research, but this “Air Force Fuel Bank” has long-since been exhausted or discarded. The difficulty of creating jet reference fuels with varying composition but well-controlled physical properties was illustrated in a NASA-sponsored<sup>22</sup> effort in the early 1980s. It was found to be difficult to vary composition without changing physical properties (viscosity, surface tension). Given the tendency of distillate fuels to degrade during long-term storage, it is also difficult to ensure consistency over time.

### C. Previous Work on Surrogates for Jet Fuels

Experimental and modeling results for a wide variety of jet fuel/kerosene surrogates have been described in the literature (earlier reviews are available<sup>23,24</sup>). One reason for the large variation in surrogate composition is the wide variety of jet fuel applications, and the wide variation in composition sensitivity of these applications. In contrast to gasoline engines, where heptane/iso-octane surrogates have been employed since the 1920s for knocking/octane number estimation, surrogates have only recently been employed for gas turbines. Wood et al.<sup>24</sup> published work in the late 1980s describing the performance of a number of JP-4 and JP-5 surrogates. These surrogates were burned in a swirl-stabilized laboratory combustor, where the intent was to match fuel boiling range and composition. This required surrogates with more than 10 components (12 for the JP-5 surrogate), many of which were quite expensive. The surrogates matched the burning behavior of the full-boiling-range fuels, aside from soot formation. A similarly complex 12-component surrogate was developed by Schulz during the same period for liquid phase oxidation studies<sup>25</sup>. Schulz’ conclusion was that surrogates were not useful for these liquid-phase studies, where rate of oxidation and deposition are controlled by trace species rather than bulk fuel composition. For liquid phase properties across a wide temperature range, it has been found that using dodecane in a physical code such as Supertrapp to calculate fuel properties produces results comparable to the sparse experimental data<sup>26</sup>. Modeling of multi-phase behavior such as vaporization would require a more complex surrogate.

Focusing only on combustion applications, surrogate modeling and experimental results have been published for premixed flames<sup>5,27</sup>, flow/stirred reactors<sup>11,28,29</sup>, pool fires<sup>6</sup>, counterflow diffusion flames<sup>30,31</sup>, and shock tubes<sup>32</sup>. This by no means is a complete list. In fact, early work in the ‘70s and ‘80s focused on development of simplified (e.g., two-step) kinetics models for propane and for heptane to assist in simulations. Even a very coarse chemical kinetic model for Jet-A<sup>46</sup> was constructed that understandably provides a very poor representation of fuel-rich chemistry.

Dagaut et al.<sup>11</sup> modeled kerosene combustion in low-temperature jet-stirred reactors using *n*-decane as a reference hydrocarbon while neglecting the aromatic components and captured major species profiles adequately. Guerèt et al.<sup>28</sup> modeled kerosene oxidation via quasi-global models for *n*-decane, and an aromatic component (*n*-propylcyclohexane, trimethylbenzene, xylene, toluene, or benzene). Concentration profiles of molecular species in the flow reactor were similar for the surrogate and kerosene; however, the need for further refinement of the aromatic models was recognized. A number of studies compared various aromatic compounds in surrogates, generally concluding that alkyl-substituted aromatics were the best aromatic components<sup>47-52</sup>.

**Table 4. Example of surrogate make-up from various groups**

	UCI	Violi 1	Violi 2	Drexel	CSE	REI
<u>Composition</u>	vol%	vol%	vol%		mol?	mole%
<u>n-paraffins</u>						
n-decane	2.5		25		74%	32.6
n-undecane	0					
n-dodecane	25	30	25	varies		34.7
n-tridecane	10					
n-tetradecane	5	20	20			
n-pentadecane	5					
<u>iso-paraffins</u>						
iso-octane		10	5			
iso-cetane				varies		
<u>cyclo-paraffins</u>						
methyl cyclohexane		20	5	varies		16.7
n-propyl cyclohexane					11	
n-heptyl cyclohexane	11					
n-pentyl cyclohexane	11					
decalin	11.5			varies		
<u>aromatics</u>						
toluene			20			
m-xylene		15				
1,3 diisopropyl benzene	3				15	
n-propyl benzene						16
n-butyl benzene						
1-phenyl hexane	5			varies		
tetralin	9.5	5				
1-methyl naphthalene	1.5			varies		

A number of recent investigations<sup>5,30</sup> of surrogates have been based on the six-component “Violi” surrogates. As shown in Table 4, these surrogates are intermediate in complexity between the 12-component Wood et al surrogate (labeled “UCI” in Table 4) and the simpler two-component aliphatic/aromatic surrogates of (for example) Guerèt et al.<sup>28</sup>. Similar in complexity are the extensive investigations at Drexel involving a large number of variations of a 6-component surrogate<sup>53</sup>. The Drexel surrogates are notable for including a component from all of the major compound classes – n-paraffins, iso-paraffins, one- and two-ring cycloparaffins, and one- and two-ring aromatics. Several other recent surrogate investigations, such as the ones labeled CSE<sup>54</sup> and REI<sup>32</sup> in Table 4, have taken the “smaller is better” approach to surrogates.

This brief review illustrates

the wide variety of current surrogates being employed to model jet fuels. This wide variation in surrogate partially led to the formation of the surrogate fuels working group, with a goal of better focusing limited resources into a smaller number of surrogates.

#### D. Reduced Models for Surrogates

For simulations of reacting flow in practical and complex geometries, detailed chemical kinetic mechanisms consisting of hundreds of species and thousands of reactions are much too large for current solution techniques and computers. The need for reduced chemical kinetic mechanisms is common to all practical fuels – a detailed discussion of such methods can be found in the corresponding papers<sup>2,3</sup> on gasoline and diesel surrogates, respectively.

#### IV. Kinetic Limitations for Selection of Surrogate Fuel and Validation Data

Fundamental chemical kinetic models applicable to jet fuel surrogates have few validation data sets available and very few studies that compare real fuels and surrogate mixtures for fundamental target conditions. These limitations must be addressed to assist developing surrogate fuel models that, in turn, can provide the information required for developing smaller dimensional models.

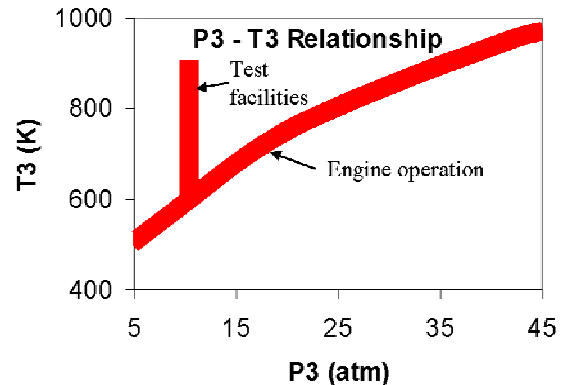
**Table 5. Kinetic limitations for jet fuels in gas turbine engines**

Kinetically-limited concern	Application	Generic Experiment/ characteristic	phi		Tinlet (K)		P3 (atm)		other	Priority (H,M,L)
			lean lmt	rich lmt						
Heat release rates	all	Flow reactors, stirred reactors	lean lmt	rich lmt	350	900	0.3	35		H
Combustion dynamics	all	ht rise rates, turbulent	lean lmt	rich lmt	350	1100	0.3	35		H
Fuel type effect	all	sensitivity to all above	lean lmt	rich lmt						H
NOx (RL)	Aeroengine	C/H ratio of fuel			450	900	4	35		H-
Flame stability	Augmentor	Extinction SR for premixed and non-premixed laminar	lean lmt	rich lmt	350	1100	0.3	6		H-
Soot/Particulate Matter (formation)	Aeroengine	PAH, C2H2 formation, H-atoms	1.5	3	600	900	10	35		H-
Flame propagation, structure	all	laminar flame speed	lean lmt	rich lmt	350	1100	0.3	35		H-
Turbulent/kinetic interactions	all	turbulent flame propagation, DNS simulations??	lean lmt	rich lmt	350	1100	0.3	35	?<u'/u'<?	H-
Soot/Particulate Matter (oxidation)	Aeroengine	OH, O2	0.75	1.5	600	900	10	35		M+
NOx (LP)	IGT	Superequilibrium O-atom for premixed flames	lean lmt	0.6	450	900	4	35	LPP for liquid fuel, Tflame	M
Lean Blow Off	Aeroengine	Extinction SR for premixed and non-premixed laminar flames	lean lmt	0.6	450	600	4	10		M
CO	IGT, Aeroengine	CO profiles near extinction conditions	lean lmt	0.6	450	700	4	15		M
Oxidation of fuel-rich gases	Aeroengine	fuel-rich air vs air in premixed opp jet	1.1	rich lmt	450	900	4	35		M
Altitude relight	Augmentor/ Aeroengine	ignition delay (1000-1500K)	lean lmt	rich lmt	250	400	0.2	2	estimated ranges	M
Altitude relight	Augmentor/ Aeroengine	minimum ignition energy	lean lmt	rich lmt	250	400	0.2	2		L+

In order to determine the best composition for a surrogate fuel, one needs to specify the use of the surrogate fuel. Specifically, parameters that need to be predicted accurately need to be identified. Ideally, accuracy levels for each of these parameters should also be established. These parameters are often termed “targets”. Example targets for surrogate fuels include fuel properties (chemical composition, C/H ratio, density, evaporation characteristics), engine characteristics (ignition, blow out, heat release, performance prediction, design guidance, emissions), and laboratory data (from premixed flames/shock tubes/stirred reactor/flow reactors) on species evolution, ignition characteristics, and flame properties (pre-mixed laminar flame speeds/extinction, diffusion flame properties, sooting characteristics under flame conditions, etc.). The availability/provision and breadth of fundamental targets will strongly influence the choice of compounds that can be utilized in constructing surrogate fuel models. Moreover, it is important to confirm that “typical” jet fuels behave similarly for the target conditions.

Identification of the application of the modeling is also an important issue. A number of applications/customers (and a relative time frame for need) have been identified by the working group and include:

- Alternative (non-petroleum-derived) fuels [near-term]
- Gas turbine main combustor/augmentor stability [near term]
- Gas turbine engine emissions prediction and control [near term]



**Figure 3. Temperature and pressure regimes of interest for engine operation and testing.**

- Scramjet ignition/extinction [near-term]
- Jet fuels in HCCI engines [mid-term]
- PDE performance [mid-term]
- Soot mitigation [long-term]

The working group has focused primarily on applications to traditional gas turbine engine systems, although others are encouraged to compile needs for alternative applications. A list of kinetically-controlled phenomena is provided in Table 5. These priorities were reviewed and qualitatively ranked by experienced staff from several engine manufacturers. The priorities (ranked as high, medium, low) were selected for importance of simulating the characteristics of a real fuel. In addition, types of laboratory experiments that could be used to quantify fuel and surrogate fuel characteristics are suggested and experimental ranges of interest are listed.

The temperature and pressure ranges cited in Table 5 encompass a huge domain. The reality is that data is really required only in a limited space throughout the stated domain. For example, consider the curves in Fig. 3, which shows the area of interest for typical engines and for example test facilities. A model for a surrogate also should be validated under conditions of the test facilities, as test results need to be extrapolated to engine operating conditions.

In addition to testing of individual components for mechanism development, the performance of proposed surrogate fuels should be tested in zero or one-dimensional configurations. A failure to reproduce data in those configurations would be an indication that the surrogate is not performing well. Zero-dimensional experiments obtained in flow reactors and shock tubes will be essential for assessing the performance of the surrogate in the absence of fluid mechanics. One-dimensional experiments, which are ideally obtained in stagnation flow flames, would provide additional validation. Laminar flame speeds have been traditionally used to test the high-temperature flame response. However, there is now experimental and computational evidence<sup>33</sup> that processes that control flame speeds and flame extinction are different. Hence, while a surrogate and the real fuel may have very similar laminar flame speeds (usually the case), their extinction response can differ significantly. Thus, it is likely that the validation of surrogate fuels should consider both the phenomena of flame propagation and extinction. While atmospheric data is a good starting point for both zero- and one-dimensional experiments, clearly engine-like conditions (see Table 5 and Fig. 3) are a necessity. Validation data on individual surrogate components is needed to differentiate between errors due to inadequate surrogate compositions and errors due to mechanistic limitations.

## V. Surrogate and Component Study

### A. Combined Surrogate “Palette”

A product of the working groups is a recommended list of surrogate fuel components from which to develop mechanisms. Table 6 is the current list (palette) of components, including an assessment of relevance and mechanistic understanding. The various species are characterized in two ways: 1) relevance to jet fuel powered practical systems, and 2) current understanding of the mechanism and availability of thermo-physical and transport properties. These assessments and characterizations are based on a preliminary, limited survey and evaluation of the readily available literature and work known to the authors. A partial listing of resource material beyond the cited references is included in the appendix. Please note that a comprehensive literature review was not attempted as part of this effort, so this is by no means a complete list.

It seems logical to focus effort on the most relevant and least understood species. For jet fuels, the specification boiling range limitations indicate that most of the species in the fuel have carbon numbers from 10-14. Odd numbered alkanes are not listed, principally since there is limited experimental data on such molecules. Note, however, that an odd alkane may well create a greater number of odd carbon fragments, which may affect soot formation pathways. Separate analyses have indicated that jet fuels typically average about 20 vol% n-paraffins, hence the palette contains n-decane, n-dodecane, and n-tetradecane.

A typical fuel has about 35-40% iso-paraffins. The iso-paraffins have carbon numbers of 10-14. Iso-octane and iso-cetane, although having carbon numbers outside this range, were included in Table 6 because they are available at reasonable cost and are commonly used as reference fuels. Isododecane (2,2,4,6,6 pentamethyl heptane) is also commercially available and is apparently used in cosmetics. Thus, some experimental data and kinetic models exist for the highly-branched iso-paraffins (especially for iso-octane). However, recent analyses indicate that jet fuel iso-paraffins are better approximated by less-highly-branched molecules. Due to the complexities of distillate fuels, it is difficult to identify every hydrocarbon in the fuel. Recent GC-MS data from WPAFB indicates most of the identified iso-paraffins have one or (at most) two branches. NIST has found<sup>21</sup> similar results for the F-T Jet A-1 (S-8) synthetic jet fuel. The distribution of the iso-paraffins in JP-8 is



similar. We conclude that molecules such as methyl decane are much more representative as jet fuel components than iso-octane, and thus would warrant addition to the surrogate palette. However, these jet-fuel-range iso-paraffins are prohibitively expensive and difficult to obtain – some initial finds were ~\$1/mg. Exxon sells isoparaffinic solvent blends that could be used as a cost effective alternate, assuming that the chemical make-up can be identified and remains stable over time. The table includes 2-methylundecane as a representative of the isoparaffins.

**Table 6. Fuel surrogate components**

	Relevance to Practical Systems	Understanding of Mechanism		Understanding of Properties	
	Jet	Low & Intermediate Temperatures	High Temperatures	Thermo-physical	Transport
<b>Straight-chain Alkanes</b>					
n-decane	A	B	A-	A	A
n-dodecane	A	B	A-	A	A
n-tetradecane	A	B	B	B+	B
n-cetane (n-hexadecane)	B	B	B	B+	B
<b>Branched-chain Alkanes</b>					
iso-octane (2,2,4-trimethylpentane)	B	A-	A	B+	B
isododecane (2-methylundecane)	A	D	D	D	D
iso-cetane (2,2,4,4,6,8,8-heptamethylnonane)	B	B	B	B-	C+
<b>Cycloalkanes</b>					
methylcyclohexane	B	C	B+	B+	B
decalin	B	D	D	B	B-
<b>Single-ring Aromatics</b>					
toluene	C	C	C	A	B+
propyl benzene	A	C	C	B	B
o-xylene	C+	C	B	B	B
p-xylene	C+	C	B	B	B
m-xylene	C+	C	B	B	B
trimethylbenzene	B	D	D	D	D
<b>Multi-ring Aromatics</b>					
tetralin	C+	D	C	B+	B-
1-methylnaphthalene	B	C	C	B	C
<b>Legend</b>					
	A	B	C	D	F
Relevance to Practical Systems	Very important	Important	Possible surrogate, but not crucial		No relevance
Understanding of Mechanism	Detailed mechanism that has been verified	Mechanism, but not fully verified	Mechanism, but with major discrepancies	No mechanism	
Thermo-physical Properties	Data available (density to 0.3 %).	Sufficient data for model (density to 3 %)	Limited data only	Extremely limited/no experimental data, predictive model feasible.	No data or predictive model available
Transport Properties	Correlations available for viscosity, diffusivity, thermal conductivity (5%)	Data available for models (5-10%)	Limited viscosity and/or thermal conductivity data	Extremely limited/no experimental data; predictive model possible.	No data or predictive model available

There is ample evidence that ignition of pure fuels is highly dependent upon the amount of branching (with increased branching suppressing ignition) – as evidenced by the octane numbers for n-heptane (0), 2,4 dimethyl pentane (62), and 2,2,3 trimethyl butane (140) (Ref. 34). There is evidence that soot formation has the opposite trend with the number of branches, with the normal paraffins having the lowest tendency to produce soot<sup>35</sup> even

at the same H/C ratio. The effect of iso-paraffins on the combustion behavior of complex mixtures like jet fuels is not evident at this point, but it seems to be a key point for the surrogate fuel community to investigate.

Jet fuels contain measurable quantities of monocycloparaffins (e.g., butyl cyclohexane) and dicycloparaffins (hence, decalin is in the palette). The role of cycloparaffins in jet fuel combustion mechanisms is not clear. Wood et al<sup>24</sup> performed combustion measurements on surrogates with and without cycloparaffins (which were removed due to cost) and found little impact of the cycloparaffins on the combustion of the surrogates, aside from some small changes in soot levels, which were explained by the increase in surrogate H/C ratio when the cycloparaffins were replaced with n-paraffins. The Aldrich catalog lists butyl cyclohexane at \$310/500 mL.

The largest aromatic fraction in jet fuels are the alkyl benzenes, hence the inclusion of the various benzene isomers in Table 6. Trimethylbenzene has been included also, as it may be a useful molecule to tune extinction and ignition limits, based on recent experimental results discussed later. The small quantity of two-ring aromatics in jet fuel is represented by 1-methyl naphthalene in Table 6. It remains to be demonstrated which of these components is needed for a given model situation.

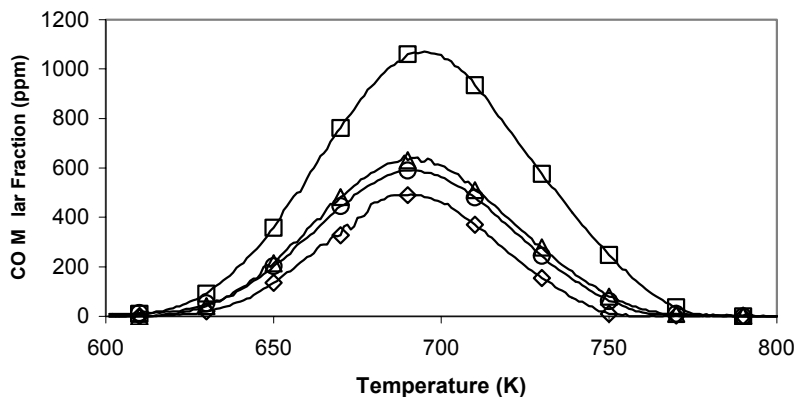
Since most of the validation data will be obtained in devices with prevaporized fuel, it is presumed that the initial surrogate efforts should focus on the chemistry, rather than matching the fuel boiling range. This approach allows the use of simpler surrogate mixtures of fewer components for which both mechanisms and validation targets are reasonably established and/or can readily be generated. Unfortunately, this approach will not likely produce a surrogate that is able to simulate the performance of a real fuel under practical conditions due to a miss-match of fuel physical properties. Since it is theoretically possible to simulate the boiling point curves within the computational codes, relaxation of the boiling point constraint may prove to be an important simplifying assumption that allows nearer term progress on the development of reaction kinetics.

## B. Preliminary Selection of a Surrogate

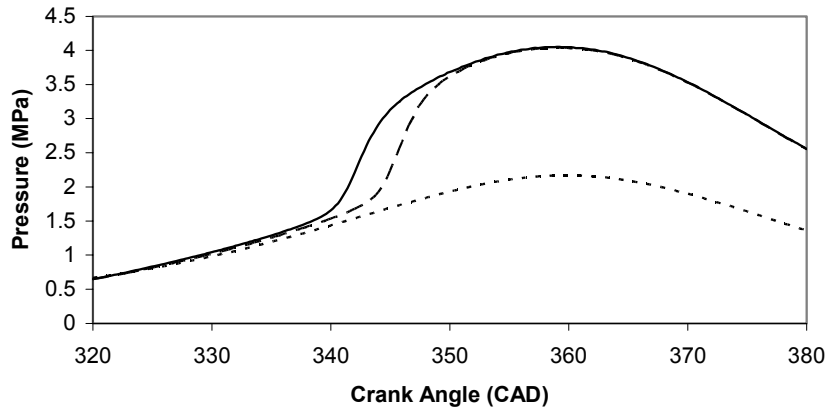
A preliminary surrogate was selected for testing. Initially, suggestions by Violi, et al<sup>5</sup>, Eddings, et al<sup>6</sup>, and others for components selections of eight or more were considered. Alternatively, we argued for the value of a simpler surrogate definition, with the understanding that such a mixture would not reproduce physical properties including vaporization characteristics.

Our reasons, included potential overlap of components with an early diesel fuel surrogate selection, a similar approach under consideration by the European community, and the surrogate selection could expand as necessary. Our constraints were also simple and straightforward; match the H/C ratio of fuels, and set the aromatic content at the limit of jet fuel regulations (25%, by liquid volume). The latter constraint was employed to approach the smoke characteristics of real fuels. The target H/C molar ratio was identified to be 1.92, which is close to the mean value (1.91) reported for JP8 (<http://www.desc.dla.mil/DCM/Files/2005PQISreport.pdf>) for 2005. Ranges vary year to year but the variation is estimated to be 0.05.

Based on these criteria and the components originally selected by the diesel group, we identified a preliminary surrogate as 50% n-decane, 25% n-butyl benzene, and 25% n-butylcyclohexane (volume liquid percentage). Experiments using this blend were performed at three laboratories and the results were compared to results from JP-8 samples provided by Wright-Patterson Air Force Base as well as other surrogate examples. Note that the set of experiments performed here are indicative of experiments that should be performed, although they have not yet been optimized to specifically match or span the ranges of interest as listed in Table 5. Hence, the set of experiments as presented here should be considered a starting point for a full evaluation.



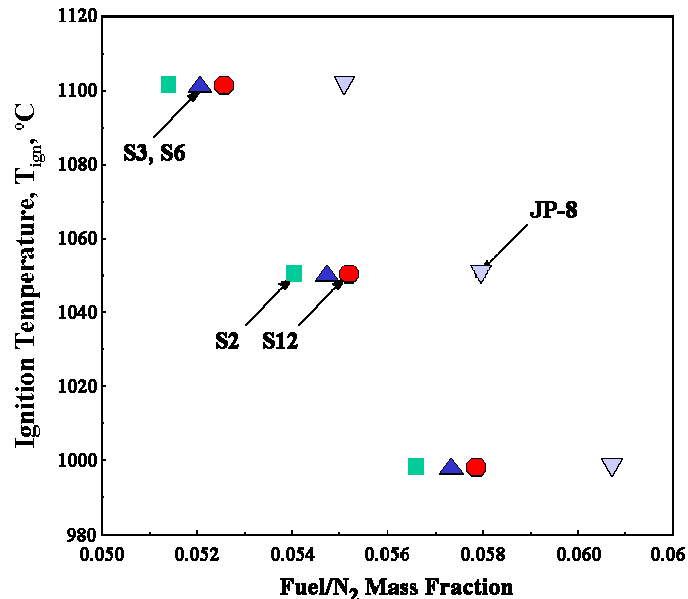
**Figure 4. Carbon monoxide (CO) molar fraction in a pressurized flow reactor.** (square) 50% n-decane / 25% n-butylbenzene / 25% n-butylcyclohexane; (triangle) “average” JP-8 POSF #3773; (circle) JP-8 POSF #3684; (diamond) JP-8 POSF #4177.



**Figure 5. Autoignition in a single cylinder research engine.** (solid line) 50% n-decane / 25% n-butylbenzene / 25% n-butylcyclohexane; (dashed line) “average” JP-8 POSF #3773; (dotted line) unreactive mixture.

80.0% N<sub>2</sub> dilution of fuel, and a residence time of 120 ms were maintained for each experiment. The proposed surrogate produced a maximum of 1070 ppm CO, as shown in Fig. 4, while JP-8 POSF #3773, of “average” composition and reactivity for JP-8, produced 650 ppm CO. Experimental error is less than 50 ppm CO. Thus, the surrogate is significantly more reactive than JP-8 at low temperatures under lean, dilute conditions.

Since the flow reactor is a fundamental experimental setup that studies the chemistry while greatly reducing the fluid mechanics and heat transfer variables of combustion, experiments were also conducted in a research engine. The proposed jet fuel surrogate and the “average” JP-8 sample were stressed to autoignition in a single cylinder research engine at Drexel University. Experiments were conducted at an inlet temperature of 500 K, compression ratio of 15, and equivalence ratio of 0.23. The proposed jet fuel surrogate had a shorter ignition delay than the “average” JP-8 sample (Fig. 5). Thus, the surrogate autoignites more easily than JP-8 in an engine at lean conditions.



**Figure 6. Variation of flame ignition temperature with fuel/N<sub>2</sub> mass ratio for an average JP-8 and several proposed surrogates.**

a twelve-component (S12)<sup>25</sup>, and (3) a two-component (S2)<sup>37</sup> that is currently under consideration in Europe and consists of 70% *n*-decane and 30% *n*-propylbenzene on a per mass basis.

### C. Experimental Results with Proposed Surrogate

The proposed jet fuel surrogate and three samples of JP-8 from were oxidized in the pressurized flow reactor at Drexel University at a constant pressure of 0.8 MPa and within the temperature range of 600-800 K. These conditions span the negative temperature coefficient region where reactivity of the fuel, as indicated by carbon monoxide (CO) production, decreases as temperature increases. An equivalence ratio of 0.30, an

80.0% N<sub>2</sub> dilution of fuel, and a residence time of 120 ms were maintained for each experiment. The proposed surrogate produced a maximum of 1070 ppm CO, as shown in Fig. 4, while JP-8 POSF #3773, of “average” composition and reactivity for JP-8, produced 650 ppm CO. Experimental error is less than 50 ppm CO. Thus, the surrogate is significantly more reactive than JP-8 at low temperatures under lean, dilute conditions.

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The proposed three-component (S3) jet fuel surrogate of 50% *n*-decane / 25% *n*-butylbenzene / 25% *n*-butylcyclohexane by liquid volume was also tested in non-premixed opposed-jet flames at the University of Southern California. Specifically, ignition and extinction limits were determined at atmospheric pressure and for fuel-stream temperatures of 110 °C similarly as in Ref. 36. The performance of the proposed jet fuel surrogate was compared against an “average” JP-8 from Wright-Patterson Air Force Base as well as against three more surrogates: (1) a six-component (S6)<sup>5</sup>, (2)

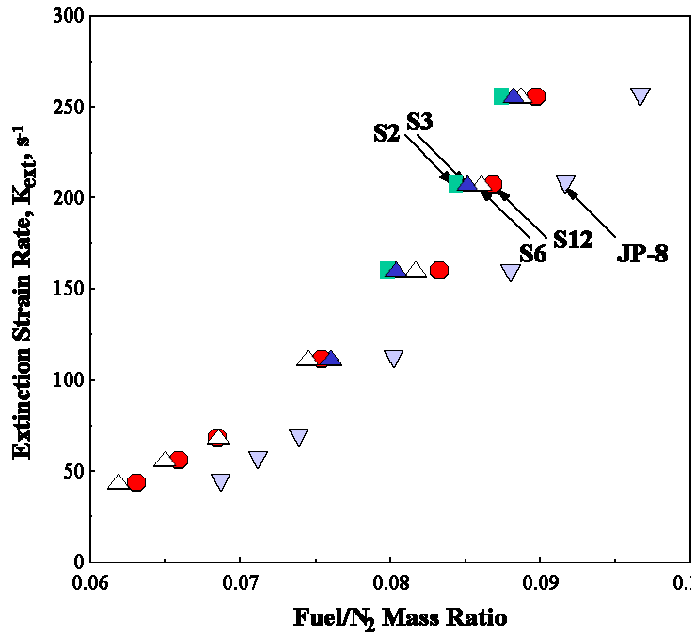


Figure 7. Variation of flame extinction strain rate with fuel/N<sub>2</sub> mass ratio for an average JP-8 and several proposed surrogates.

that all surrogates result in similar extinction response.

The proposed surrogate was also examined at the University of California, San Diego, in another opposed jet (counterflow) facility. Both extinction and ignition were examined, although a different set of experimental conditions and surrogates were considered<sup>38</sup>. A description of each of the surrogates is provided in Table 7.

Flame extinguishing experiments, shown in Fig. 8, resulted in the same qualitative results as found at the University of Southern California, that is, the preliminary surrogate suggested in this work appears to be much more reactive than is JP-8/Jet A, as the latter extinguishes at a higher fuel level than does the surrogate. Note, however, that there are several surrogates that extinguish at comparable or at yet higher levels than do the real fuels. We speculate that the iso-cetane and trimethylbenzene components contribute to these characteristics.

Table 7. Liquid volume % of surrogates tested in nonpremixed flames (Figs. 8-9).

	Surrogate C	Surrogate D*	Surrogate E	Aachen Surrogate	Modified Aachen Surrogate	Drexel Surrogate 2	Utah Surrogate
n-decane		50	34	80			
n-dodecane	60				80	43	30
n-tetradecane							20
iso-cetane						27	10
methylcyclohexane	20					15	20
o-xylene	20						15
butylcyclohexane		25	33				
butylbenzene		25	33				
trimethylbenzene				20	20		
tetralin							5
1-methylnaphthalene						15	
H/C Ratio	1.92	1.92	1.84	1.99	1.97	1.97	1.93

\* Surrogate D is the mixture specifically investigated in this work.

Figure 6 depicts the ignition limits obtained by counterflowing the heated fuel-stream against hot vitiated air and for a constant strain rate of 200 s<sup>-1</sup>. More specifically the ignition temperature, defined as the maximum temperature of the vitiated air at ignition, was determined as function of the fuel/N<sub>2</sub> mass ratio. The results indicate that for all surrogates, flame ignition is achieved more readily compared to JP-8 flames, which is in agreement with the finding in the Drexel flow reactor. The differences of the ignition behavior between the different surrogates are considered to be minor.

Figure 7 depicts the extinction limits obtained by counterflowing the heated fuel-stream against ambient-temperature O<sub>2</sub>. More specifically the extinction strain rate was determined using Digital Particle Image Velocimetry as function of the fuel/N<sub>2</sub> mass ratio. The results indicate that each of the proposed surrogate-fuel flames are more resistant to extinction compared to JP-8 flames, and

Figure 9 shows a comparison of the temperature at ignition at different strain rates for each of the surrogates and fuels. Virtually all of the surrogates (including those with iso-cetane) except the ones with trimethyl benzene ignite at temperatures lower than those for the jet fuels. The preliminary surrogate suggested in this work ignites at the lowest temperature of all the fuels tested.

As shown by the flow reactor, engine results, and both of the counterflow studies, the proposed surrogate exhibits too much reactivity to be considered an acceptable surrogate. Additionally, the work at one of the counterflow facilities has shown that (multiply) substituted methyl aromatics (particularly trimethylbenzene) may significantly alter the reactivity and ignition characteristics. Alternatively, iso-cetane and perhaps other iso-alkanes also reduce the reactivity.

## VI. Applications to Computational Fluid Dynamics

Calculation methods for gas turbine engines have traditionally been based on the high Damköhler number assumption (characteristic mixing times  $\gg$  characteristic chemical kinetic times) combined with a presumed probably density function (e.g.,  $\beta$ -pdf) technique and with the flow field computed through Reynolds averaged based approaches<sup>39</sup>. The need to move towards a partial time resolution of the fluid motion through unsteady RANS or LES methods is in many cases obvious, but is not discussed here. However, irrespective of the choice of calculation method used to compute the turbulent flow field, the chemistry will take place on the unresolved scales and the effects of turbulence on chemistry requires modeling. A recent discussion of available techniques can be found elsewhere<sup>40</sup>. The choice of method used to account for the turbulence-chemistry interactions has a significant impact on the computational cost and, broadly, the more accurate the method, the greater the demand on the reduction process and the need for accurate, reduced models. For example, strongly chemistry influenced phenomena, such as flame extinction/re-ignition, often requires complex chemistry with the computed auto-

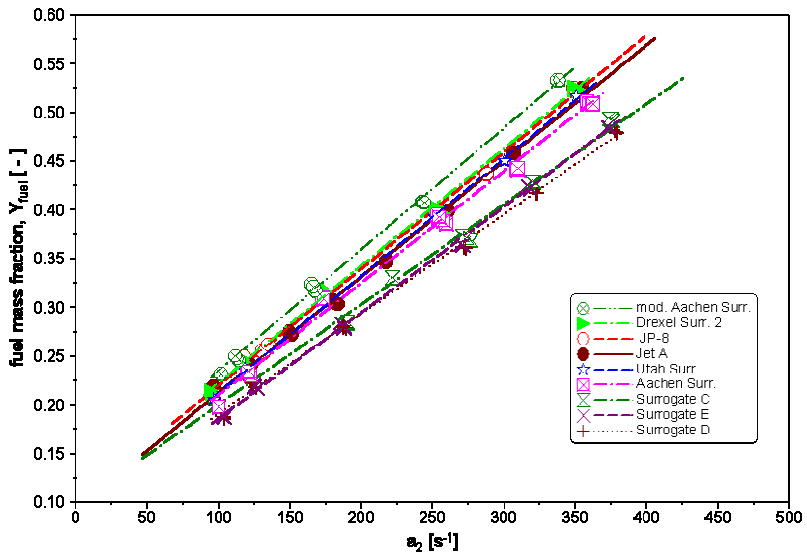


Figure 8. Relationship between fuel/N<sub>2</sub> mass ratio and flame extinction strain rate for an average JP-8 and several proposed surrogates.

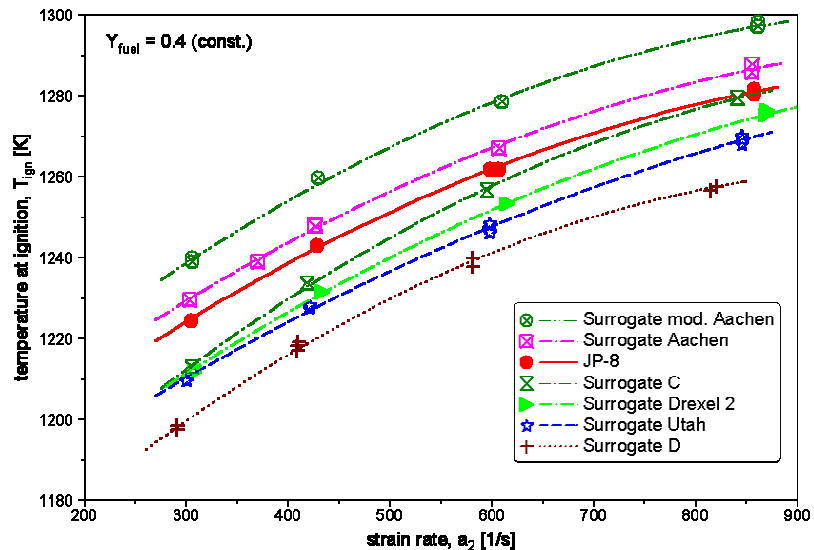


Figure 9. Relationship between temperature at ignition and flame extinction strain rate for an average JP-8 and several proposed surrogates.

ignition delay times having a tendency to be very sensitive to trace amounts of radical species with corresponding demands on the accuracy of reduction and tabulation methods.

The simplest form of thermochemistry applied in design calculations follows from the assumption of full or partial (constrained) equilibrium with the chemistry of pollutants, such as NO and soot, incorporated via a perturbation technique<sup>41</sup>. Such approaches may be combined with a flamelet assumption<sup>42,43</sup> for improved accuracy with the state space typically parameterized in terms the mixture fraction and the rate of strain or scalar dissipation<sup>44</sup>. Typically, such approaches do not impose significant limitations upon the size of the mechanism that can be handled. However, the reduced correlation between any conserved scalar (e.g., mixture fraction) and species (e.g., CO and NO) or phenomena (e.g., re-light) that deviate significantly from the fast chemistry limit poses a problem for simplified approaches and two-dimensional parameterizations tend to be insufficient. Furthermore, direct coupling may occur, for example in the context of CO and residual hydrocarbon emissions close to the lean blow-out limit, and the increasing need for consideration of a range of chemical timescales is readily apparent from the examples given in Table 6.

The current trend towards increased premixing of reactants makes it necessary to consider premixed and/or partially premixed flames alongside the more traditional diffusion flame mode. Thus, at the most basic level a surrogate fuel model is required for the computation of flame properties covering a wide range of pressures, temperatures and flame types, while in general, appropriate lower dimensional parameterizations are required to accurately compute turbulence-chemistry interactions<sup>44</sup>. Practical experience suggests that around 12 independent scalars are required for simpler hydrocarbon fuels<sup>45</sup> and it may be anticipated that this number will increase by a factor 2 to 3 for a comparatively simple surrogate fuel. It is thus likely that hierarchy of computational approaches that balance the fidelity of flow field and chemistry predictions will be required for sometime.

## VII. Roadmap/Framework

An overall roadmap (schematic) of jet fuel surrogate development is shown in Fig. 10. Many of these steps should be performed in parallel. Mechanism development should follow a hierarchical approach from component to surrogate, with validation at each step by comparison to appropriate experimental data.

Key target phenomena can impose significant constraints onto the selection of surrogates. For the purpose of this study, it is assumed that all kinetically limited phenomena occurring within gas turbines are important. If this constraint were relaxed, the make-up of the surrogate fuel and its model might be significantly simplified. Furthermore, the selection of a limited number of pure compounds (<10, for example) may never simultaneously satisfy all of the target parameters for a jet fuel. Hence, it is likely that depending on the targets desired for a given simulation, different definitions of a surrogate may be appropriate.

Note that the line from the surrogate mechanism development to mechanism reduction implies a need for (or existence of) methods and procedures for developing reduced and skeletal mechanisms as well as validation of such procedures. Methods for development of such tools are not the subject of this paper.

The roadmap can be used to summarize the contributions of the present work. We have selected a palette for the surrogates, identified target parameters and ranges of interest, selected some constraints, selected one surrogate, characterized it, and compared it to reference fuel results. The results have led us back to a re-selection of the surrogate, but the studies have helped (hopefully) to select a better surrogate for future efforts.

## VIII. Recommendations

The jet fuel working group recommends that:

- 1) Researchers utilizing jet fuel surrogates should focus on the components included in the jet fuel “palette” (Table 6)
- 2) Researchers should use target conditions as defined in Table 5 for evaluations and comparison to real fuel performance.
- 3) The jet fuel research community should agree on a set of “standard” fuels to be used as common benchmarks. (The Fuels Branch of the AFRL Propulsion Directorate is willing to supply research quantities of these fuels to the community.)

Longer term working group objectives (coordinated with activities by Air Force, Army, NIST<sup>1</sup> and PrIME<sup>14</sup>).

- 1) Maintain a comprehensive database of previous and ongoing jet fuel surrogate research.
- 2) Create a list of recommended surrogates and specific applications for which they could be used.
- 3) Validate detailed and reduced mechanisms for the surrogates and components

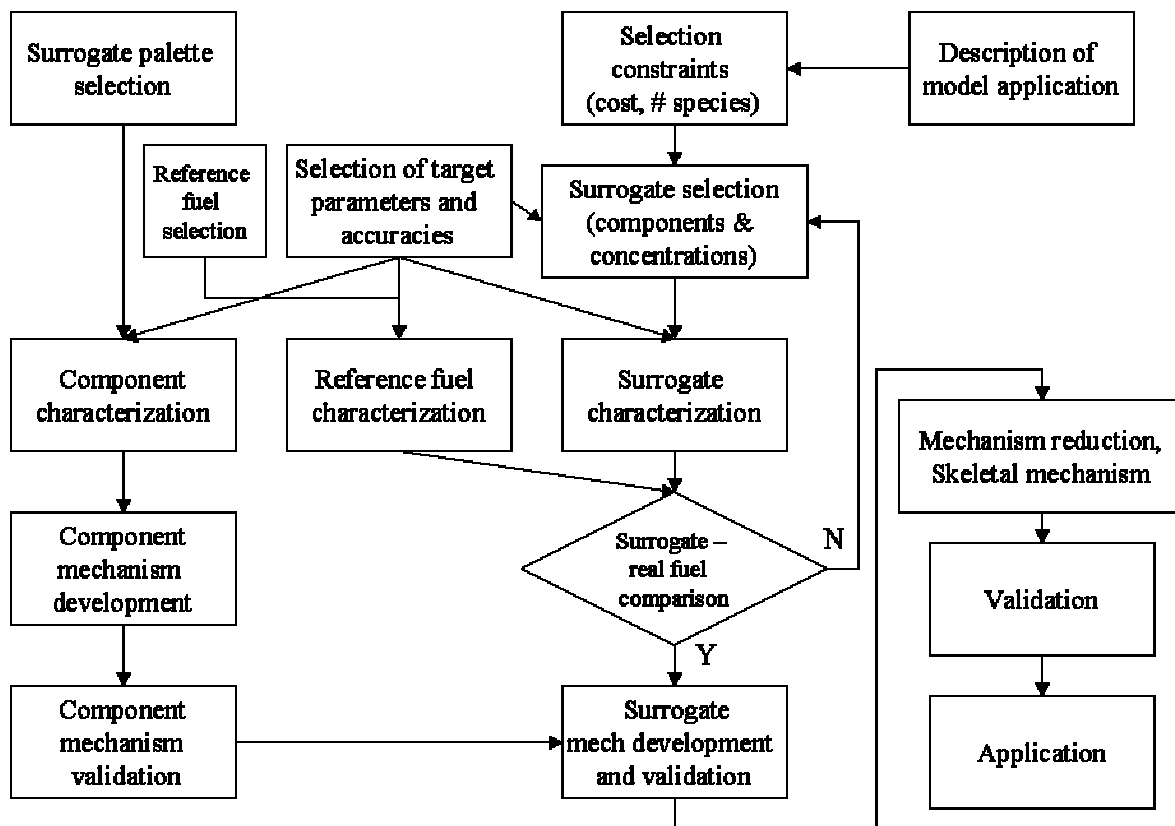


Figure 10. Proposed roadmap for development of surrogate fuels.

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## Appendix: Additional Resource Materials

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