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Surrogate Mixtures to Represent Complex Aviation and Rocket Fuels

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Surrogate mixtures of one to 10 hydrocarbons that have similar properties to aviation fuels are desirable for experimental and computational tractability and reproducibility. However, aviation fuels, such as Jet A, JP-8, and JP-5, contain hundreds of hydrocarbons. This paper describes appropriate "surrogate" mixtures to reproduce the behavior of multicomponent aviation fuels. Surrogate mixtures from the literature and their applicability to various situations are summarized.

Introduction

MOST aviation fuels, as well as the liquid hydrocarbon rocket fuel RP-1, are mixtures of a large number of hydrocarbons (see Fig. 1 and Table 1) that meet general physical property specifications. These properties include boiling range/volatility, heat of combustion, and freeze point. The operational specifications for fuels[1] can be met by an infinite variety of hydrocarbon mixtures, although the relative proportion of the various classes of species is constrained by the property requirements. As discussed in the next section, there can be a significant variation in JP-8 properties from shipment to shipment. However, for well-controlled fundamental modeling and experimental studies a more definite chemical composition is needed for reproducibility and tractability. These mixtures can be called "surrogates" for the complex aviation and liquid hydrocarbon rocket fuels. Fuel surrogate types may be defined as follows:

1) *Physical surrogate*: a mixture that has generally the same physical properties as the aviation or rocket fuel to be studied. For example, as a first approximation, dodecane has physical properties (density, viscosity, thermal conductivity, heat capacity) similar to JP-7 over the 200–1200°F temperature range.[2] However, for studies where matching the fuel volatility/vaporization behavior is important a multicomponent surrogate will be required (e.g., Ref. 3). Often, the National Institute of Standards Supertrapp code[4] or other physical property codes are used with the surrogate composition to generate physical properties over a wide range of temperatures and pressures.

2) *Chemical surrogate*: a mixture that has generally the same chemical-class composition and average molecular weight as the aviation or rocket fuel to be studied, such as the right proportion of aromatics, naphthenes, and paraffins (Table 2)[1,3,5–10]. In theory, this surrogate would have similar gross chemical properties to the multicomponent fuel, such as combustion properties. The surrogate would not adequately simulate fuel chemistry that is dependent upon trace species. For example, fuel thermal-oxidative stability is dependent upon trace heteroatom and metal species at the ppm level, and a surrogate fuel without these species will not reproduce deposition behavior. Pollutant or soot emissions dependent upon trace fuel species will also not be reproduced by a chemical surrogate.

A number of surrogates have been proposed for the multicomponent fuels JP-4, JP-5, JP-7, JP-8 (Jet A/A-1), and RP-1[3,11–18] in a wide variety of publications. These surrogate models will be reviewed and compared to the fuel composition data, as summarized in the next section. Application of the surrogates to various fuel modeling and testing cases will be subsequently discussed.

Fuel Property Summary

A general summary of fuel property data is shown in Table 2. JP-4 is an aviation gasoline/kerosene mix used by the U.S. Air Force (USAF) until the 1980s, when it was replaced by JP-8. JP-8 is a "kerosene" fuel used by the USAF for jet aircraft. JP-8 is very similar to Jet A and A-1, which are commercial aviation kerosene fuels. JP-8 is essentially Jet A-1, with three additives: a lubricity improver/corrosion inhibitor, an antistatic additive, and a fuel system icing inhibitor. JP-5 is a high flash point kerosene used for aircraft flying from U.S. Navy ships. JP-7 is a specialty kerosene fuel used for the SR-71. RP-1 is the standard U.S. kerosene rocket propellant. The Jet A/A-1/JP-8 specifications are fairly broad, and a wide variety of hydrocarbon mixtures can meet the specification requirements. As an example of the variations encountered in practice, the variations in several JP-8 properties are shown in Figs. 2–5 (Ref. 6). By contrast, the JP-7 and RP-1 specifications are much tighter, and the distribution of properties is much smaller. Surrogates for JP-4, JP-5, JP-8/Jet A, and RP-1 will be summarized in the next section.

For broad specification aviation and rocket fuels, properties like the heat of formation are not well defined. Tabulated values generally show a lot of variation.[19–23] The heat of formation can be estimated from the measured heat of combustion data for these fuels if the fuel H/C ratio is known. Weight % hydrogen in the fuel is a specification property from which the fuel H/C ratio can be calculated. Heat of formation data is compared to the calculated values in Table 3. The calculated value was obtained using the average fuel property data from Ref. 6.

The concentration of trace species, such as sulfur and metals, in fuels is important for thermal stability and emissions. As shown in Table 2, there is a wide variation in sulfur content among the various fuels. Highly refined fuels like RP-1 and JP-7 have very little sulfur, as compared to the conventional jet fuels. As shown in Fig. 4, there is a wide variation in sulfur among the JP-8 fuels delivered to the USAF with the average over the 1990–1996 period being 490 ppm (0.049 wt%), significantly less than the 0.3 wt% specification maximum. For comparison, the current average sulfur level in gasoline is 330 ppm.[24] There is significant pressure to lower the sulfur levels in fuels to the 50 ppm level or below. Metal contents in fuel are quite variable, with the most significant metal contaminant probably being copper. Especially on naval vessels, dissolved

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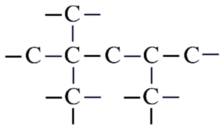
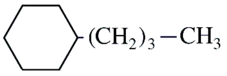
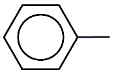
Table 1 Typical classes of hydrocarbons in aviation fuels

Compound class	Typical structure	Name
n-paraffin (*n*-alkane)	$CH_3{-}(CH_2)_{10}{-}CH_3$	*n*-dodecane
iso-paraffin		iso-octane
Naphthene (cycloparaffin)		butyl cyclohexane
Aromatic		toluene
Alkene	$CH_2{=}CH{-}CH_2{-}CH_2{-}CH_3$	1-pentene

copper concentrations in fuels can be on the order of hundreds of parts per billion, a level that significantly affects fuel thermal stability.

Surrogate Fuels

As discussed in the introduction, the type of surrogate fuel used is dependent ideally upon the fuel properties that are being simulated. For estimating heat transfer inside the fuel system, a surrogate that gives reasonable physical properties (density, specific heat, viscosity, thermal conductivity) would be adequate. For example, as a first approximation, dodecane has physical properties similar to JP-7 and JP-8/Jet A over the 200–1200°F (100–650°C) temperature range,[2,25–28] as shown in Fig. 6. For simulating fuels in situations where phase behavior is important, such as injection modeling, then the fuel boiling range/phase behavior would have to be simulated (Fig. 7).[29] For example, Wood and coworkers performed experimental combustion studies with JP-4 and JP-5 surrogates.[3,11] These surrogates, listed in Tables 4 and 5, were selected based upon five criteria: 1) limit of 10–15 hydrocarbons,

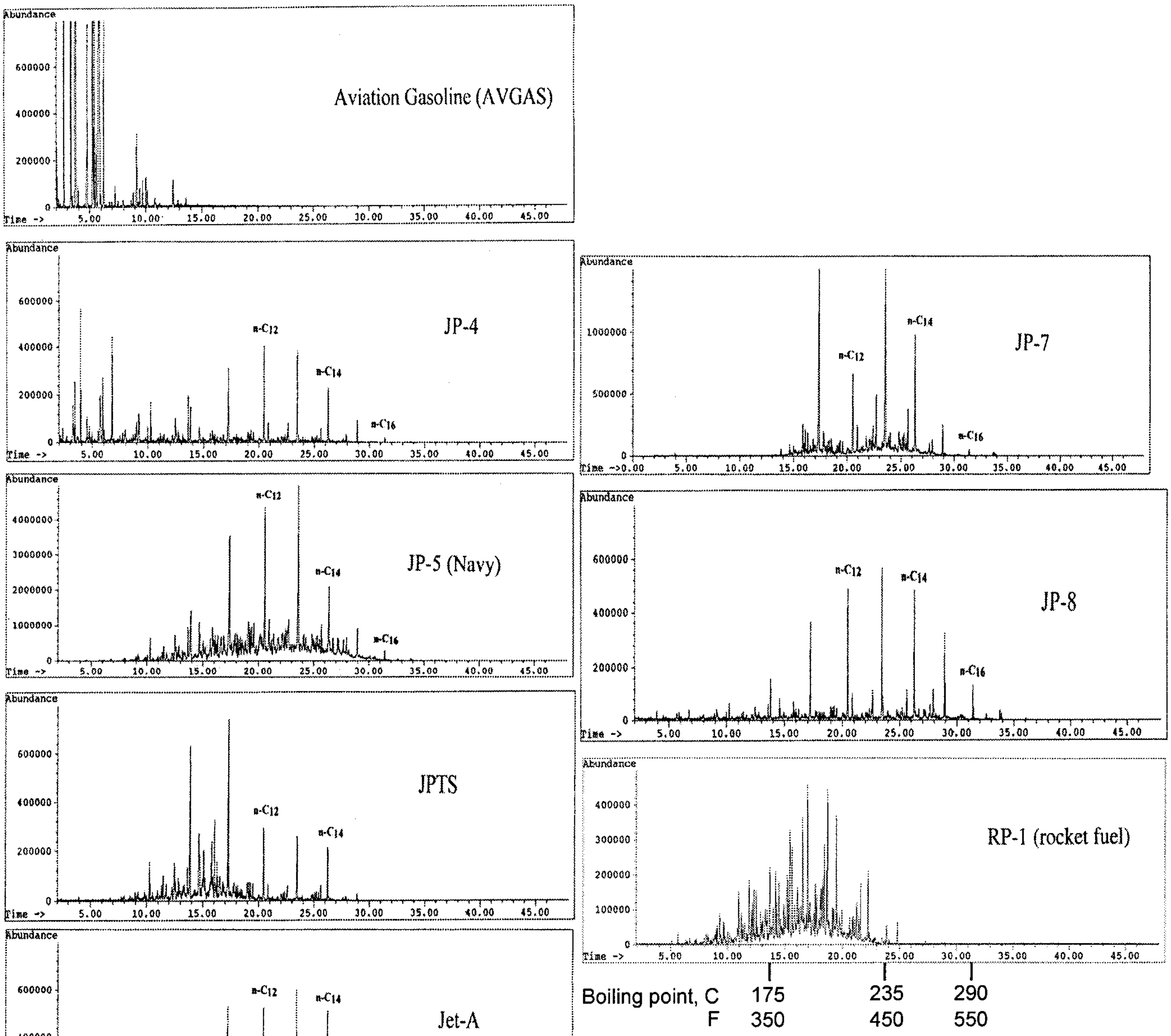


Fig. 1 Total ion chromatogram of aviation gasoline and jet and rocket fuels. The labeled peaks are *n*-alkanes.

Table 2 Typical aviation fuel properties

Property	JP-4	JP-5	JP-7	JP-8 (Jet A/A-1)	RP-1[10,23]
Approx. formula[5]	$C_{8.5}H_{17}$	$C_{12}H_{22}$	$C_{12}H_{25}$	$C_{11}H_{21}$	$C_{12}H_{24}$
H/C ratio[5]	1.99	1.87	2.02	1.91	1.98
Boiling range, F[1]	140–460	360–495	370–480	330–510	350–525
Freeze point, F[1]	−80	−57	−47	−60 JP-8/Jet A-1; −50 Jet A	−55
Flash point, F[1]	−10	147	140	127	134
Net heating value, BTU/lb[6]	18,700	18,530	18,700	18,580	18,650
Specific gravity 60 F[6]	0.76	0.81	0.79	0.81	0.81
Critical T, F[7,8]	620	750	750	770	770
Critical P, psia[7,8]	450	290	305	340	315
Avg composition[3,5,9]					
Aromatics, vol%[6]	10	19	3	18	3
Naphthenes	29	34	32	20	58
Paraffins	59	45	65	60	39
Olefins	2	2	——	2	——
Sulfur, ppm[6]	370	470	60	490	20

Table 3 Heat of formation data, in cal/g

Reference	JP-4	JP-5	JP-7	JP-8	RP-1
Harsha et al.[19]; McCoy[20]	−455 for $C_{9.5}H_{18.9}$	−410 for $C_{12}H_{24}$	−495 for $C_{12.5}H_{26}$	−475 for $C_{12}H_{23.3}$	——
Siegel and Schieder[21]	——	——	——	——	−423
Ross[22]	−437	−387	−436	——	−420
CPIA[23]	——	——	——	——	−389 to 606 avg ~ −450
Calculated from heat of combustion, %H[6,23]	−415	−355	−455	−390	−400

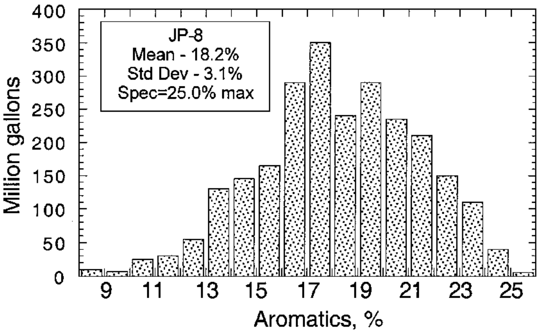


Fig. 2 Distribution of aromatics in JP-8 for 1990–1996 fuel purchases.[6]

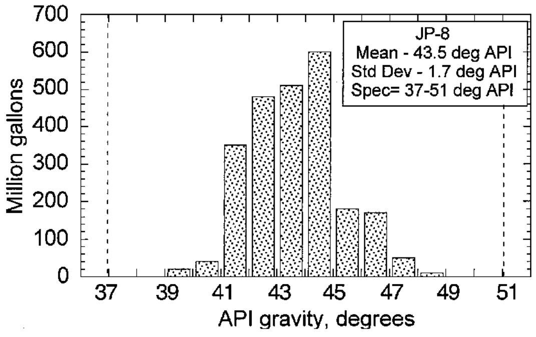


Fig. 3 Distribution of JP-8 relative density for 1990–1996 fuel purchases.[6] API gravity is deg API = (141.5/relative density at 60°F)-131.5. JP-8 spec limits of 37–51 deg API correspond to a relative density range of 0.840–0.775.

2) match compound class in fuel, 3) match distillation curve in fuel, 4) high purity, and 5) minimum cost. For example, the JP-5 surrogate blend 1 shown in Table 5 was quite expensive, hence an alternative surrogate was developed (blend 2) by replacing expensive cycloparaffins with *n*-paraffins.

Wood and co-workers[3,11] report that the physical and chemical properties of the surrogates are quite close to that of the parent fuel, except for smoke point. In cold-flow atomization tests the surrogates were indistinguishable from the corresponding distillate fuel.

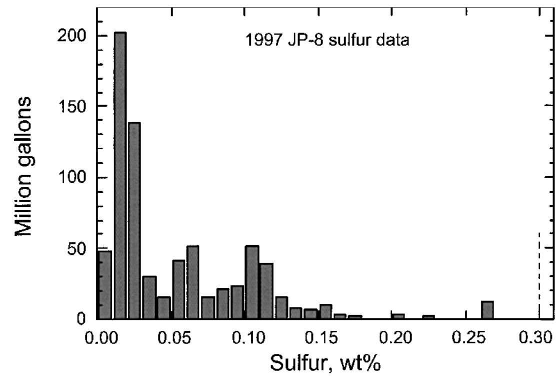


Fig. 4 JP-8 total sulfur analysis results for 1997 fuel purchases.[6]

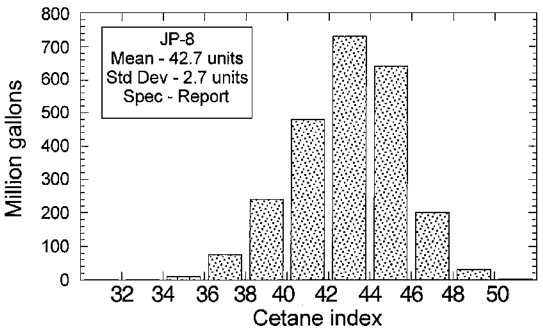


Fig. 5 Distribution of cetane index for JP-8 for 1990–1996 fuel purchases.[6]

In combustion tests in a swirl-stabilized laboratory combustor, the surrogates represented the combustion properties of the distillate fuels, including soot concentrations.[3,11] This indicates that the fuel hydrogen content, which was maintained between the surrogates and distillate fuels, is a better predictor of the soot levels in their laboratory combustor than the smoke point.

Schulz[12] also tried to match the distillation curve and compound classes in his surrogate tests with JP-8. The objective was to find

Table 4 JP-4 surrogate[2]

Compound	Vol %
n-hexane	5.5
Cyclohexane	8.0
n-heptane	8.0
Methyl cyclohexane	8.0
Toluene	8.0
n-octane	8.0
n-nonane	10.0
Cyclo-octane	8.0
n-decane	10.0
Decalin	5.0
Tetralin	1.0
n-dodecane	10.0
1-methyl naphthalene	0.5
n-tetradecane	10.0

Table 5 JP-5 surrogate[3]

Compound	Blend 1, vol %	Blend 2, vol %
n-decane	2.5	2.5
Decalin	11.5	11.5
n-undecane	0.0	5.0
n-pentylcyclohexane	11.0	0.0
1,3-diisopropylbenzene	3.0	3.0
Tetralin	9.5	9.5
n-dodecane	25.0	31.0
1-phenyl hexane	5.0	5.0
n-tridecane	10.0	15.0
n-heptylcyclohexane	11.0	0.0
1-methyl naphthalene	1.5	1.5
n-tetradecane	5.0	11.0
n-pentadecane	5.0	5.0

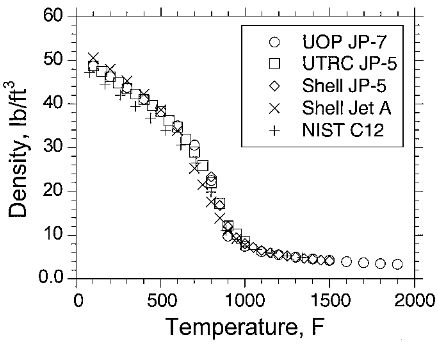


Fig. 6 Comparison of dodecane properties at 500 psia calculated with Supertrapp[2,4] **to published fuel property calculations.**[25–28]

Table 6 JP-8 surrogate[12]

Compound	Wt %
iso-octane	5.0
Methyl cyclohexane	5.0
m-xylene	5.0
Cyclooctane	5.0
Decane	15.0
Butyl benzene	5.0
1,2,4,5 tetramethyl benzene	5.0
Tetralin	5.0
Dodecane	20.0
1-methyl naphthalene	5.0
Tetradecane	15.0
Hexadecane	10.0

Table 7 RP-1 surrogate[14]

Compound	Vol %
n-undecane	4.7
n-dodecane	6.0
n-tridecane	18.8
n-tetradecane	12.5
n-hexylcyclopentane	2.7
n-heptylcyclopentane	3.6
n-octyl cyclopentane	11.2
n-nonylcyclopentane	7.5
Bicycloparaffin 1 $C_{11}H_{20}$[a]	11.3
Bicycloparaffin 2 $C_{12}H_{22}$[a]	14.7
Pentamethyl benzene	1.3
Hexamethylbenzene	1.7
Dimethylnaphthalene	4.0

[a] The identity of the bicycloparaffins is not evident.

a simpler surrogate for fuel thermal oxidation studies in a flask apparatus. The JP-8 surrogate model is listed in Table 6. The surrogate reproduced the general oxidation behavior of JP-8, but did not reproduce the deposition levels of distillate fuels. This is because of the key role that trace species, such as metals and heteroatoms, play in the deposition process.[30] Distillate fuels can be grouped into general classes by the method of processing (hydrotreatment, Merox, etc.) with the deposition generally being roughly similar for fuels produced by the same processing methods. A number of tests have been used to rank fuels by thermal stability,[31] but there is no practical method to assess the thermal stability of distillate fuels without testing the actual fuel sample under consideration.

The concept of surrogate fuels is also used for gasoline- and diesel-fueled engine studies (e.g., Ref. 32). Mixtures of heptane (octane number = 0) and iso-octane (octane number = 100) are used as primary reference fuels (PRF), with octane number adjusted by a linear combination of the two. However, it has been found that the simple two-component surrogates do not adequately reproduce the ignition behavior of the real multicomponent gasolines and reference fuels in flow reactors and engines.[33,34] The ignition of the PRFs occurred at a lower temperature than gasoline or standard multicomponent reference fuels. Addition of an alkene (1-pentene) and an aromatic (toluene) to the heptane/iso-octane mixture did reproduce gasoline ignition behavior.[33,34] The alkenes and aromatics acted as an ignition inhibitor. An effective gasoline surrogate for ignition studies was determined to be 31.8 vol% toluene, 4.6% 1-pentene, and 63.5% heptane+iso-octane, with research octane number adjusted by changing the ratio of the heptane and iso-octane.

An RP-1 surrogate was proposed by Farmer et al.[14] (Table 7). This surrogate was developed for modeling purposes and was derived from a detailed RP-1 analysis. The authors recognize that the aromatics content is higher than is really observed in practice (Table 2) and probably resulted from a misidentification of some of the bicycloparaffins as aromatics.[14] The authors state that the surrogate critical properties adequately match those of RP-1. An alternative to surrogate fuels consisting of specific molecules is a surrogate molecule that is just a representation of the overall stoichiometry of the distillate fuel. This surrogate would be useful for performance calculations, but not for experimental testing. A surrogate RP-1, $C_{12}H_{24}$, has been proposed.[13]

JP-5, JP-7, JP-8, Jet A, and RP-1 all belong to the general class of fuel called kerosene. Detailed kinetic modeling combustion studies of kerosene aviation fuels are generally considered prohibitive because of their inherent chemical complexity. There have been studies of surrogates for kerosene, which can serve as general examples. Aly and Salem[35] have predicted the laminar burning velocities of lean to stoichiometric laminar premixed kerosene flames using a single global kinetic step. As a first approximation, Guéret et al.[16] modeled kerosene oxidation via quasi-global models for *n*-decane, *n*-propylcyclohexane, tri-methyl benzene, xylene, toluene, and 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.[16] Dagaut et al.[17] later 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. Ranzi et al.[18] proposed a comprehensive reaction mechanism for higher-order hydrocarbon

Table 8 Recommendations on appropriate surrogate fuels

Physical situation	Minimum complexity surrogate fuel recommendation
Single phase heat transfer without chemical reaction	Single component n-paraffin with approximately correct critical temperature
Higher precision heat transfer, including enthalpy effects	Use appropriate surrogate with correct chemical compound classes and representative mixture critical temperature
Fuel vaporization/injection/mixing (multiphase, no reaction)	Use appropriate surrogate that matches distillation (boiling) curve
Fuel ignition	Use appropriate surrogate that matches the important chemical classes. If ignition-improving additives present (e.g., nitrates), then will need to include additive chemistry
Fuel heat release, flame speed	Use appropriate surrogate that matches the important compound classes
NOx emissions during fuel combustion	Use appropriate surrogate that matches the major important chemical classes
Aromatic and PAH emissions during combustion	Use appropriate surrogate that matches the major and minor important chemical classes that contribute to molecular growth
General fuel thermal-oxidation behavior (inside fuel system)	Use surrogate that matches chemical class breakdown in fuel
Pyrolytic deposition from fuels	Use appropriate surrogate that matches the major and minor important chemical classes that contribute to molecular growth
Thermal-oxidative deposition from fuels	No good surrogate—deposition levels driven by trace fuel species (heteroatomic species, dispersants)
Soot formation in combustion	No good surrogate—soot levels driven by trace fuel species (heteroatomic species, dispersants)

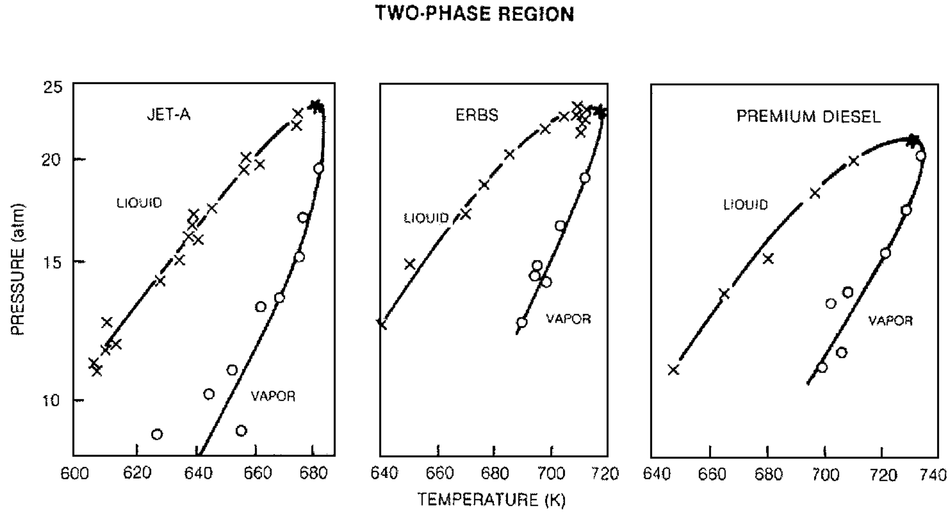


Fig. 7 Phase diagram for Jet A and diesel fuels.[29] *, critical point; ×, bubble point; and ○, dew point.

fuels, which only considers benzene in a semi-empirical manner. By contrast, Foelsche et al.[36] modeled the efflux composition of a rich JP-7/toluene-fueled gas generator operating at intermediate temperatures (900–1300 K) using the toluene oxidation kinetic model of Emdee et al.[37] to describe the aromatic constituents; a surrogate could not represent the soot formation process. Vovelle et al.[38] studied low-pressure kerosene flames and modeled the aromatic component with a simplified toluene mechanism. Discrepancies between computations and experimental observations were attributed to uncertainties in the aromatic model. Leung[39] studied kerosene diffusion flames and modeled the aliphatic component with a quasi-global undecane submechanism while assuming the aromatic component to be benzene. The preceding studies recognize the need to include an aromatic submechanism, preferably considering monosubstituted aromatic molecules, in detailed kerosene kinetic modeling. Maurice[40] used a surrogate model of 89 mole% decane and 11 mole% of various aromatic surrogates: benzene, toluene, ethylbenzene, and ethylbenzene/naphthalene as an input to a detailed chemical kinetic model, which was compared to a number of experimental data sets for species profiles in kerosene flames. The n-decane/benzene surrogate captured major species profiles, but failed to predict benzene concentrations. By contrast, the major characteristics of the kerosene flame, including benzene profiles, were predicted accurately using n-decane/alkyl-substituted aromatic surrogate blends. No differences were noted amongs the various alkylbenzene surrogates. Addition of naphthalene did not affect major characteristics of the flame. However, if aromatics are used as inputs to soot formation model (e.g., Ref. 41) individual aromatic concentrations in the parent fuel must be considered.

An outgrowth of the work of Lindsted and Maurice[15,40,41] was the comparison between nitrogen oxides (NOx) and CO emissions from combustion of Jet A in a well-stirred reactor and model predictions using a surrogate model of 78% n-decane and 22% ethylbenzene.[42] The comparison was generally good. A general conclusion from this work was that a detailed aromatic component needed to be added to the two-component surrogate model to properly predict molecular growth.

Summary and Recommendations

This paper has briefly reviewed several surrogate fuels. If care is taken, the use of these surrogates can dramatically simplify experimental and modeling efforts. The authors take the bold step of suggesting some guidelines for the various classes of surrogate applications, as listed in Table 8.

In our opinion, the only physical situation that can be represented with a single-component surrogate is single-phase heat transfer. Fuel vaporization, injection, and mixing without chemical reaction may have to be represented by a multicomponent surrogate. The former surrogate need only capture the correct critical temperature, whereas the latter must match the distillation (boiling) curve.

Higher precision heat transfer, fuel heat release and flame speed, fuel ignition, and general fuel thermal-oxidation behavior inside the fuel system can be captured with surrogate fuels, which match the correct major chemical classes. However, if additives such as ignition-enhancers additives are used it is critical to include the additives in the surrogate model.

NOx emissions during fuel combustion can be captured with a surrogate that matches important chemical classes that drive temperature. However, capturing aromatic and polycyclic aromatic hydrocarbon (PAH) emissions during combustion and pyrolytic deposition from fuels requires surrogates that match the major and minor important chemical classes that contribute to molecular growth.

Finally, capturing thermal deposition from fuels and soot formation from combustion is in our opinion not viable with a surrogate fuel. The physical processes are driven by trace fuel species (e.g., heteroatomic species and dispersants), which cannot be accurately captured by a surrogate.

References

[1] "Handbook of Aviation Fuel Properties," Coordinating Research Council Rept. 530, Coordinating Research Council, Atlanta, GA, 1983.

[2] Edwards, T., "USAF Supercritical Hydrocarbon Fuels Interests," AIAA Paper 93-0807, Jan. 1993.

[3] Wood, C. P., McDonell, V. G., Smith, R. A., and Samuelson, G. S., "Development and Application of a Surrogate Distillate Fuel," *Journal of Propulsion and Power*, Vol. 5, No. 4, 1989, pp. 399–405.

[4] Ely, J. F., and Huber, M. L., "NIST Standard Reference Database 4—NIST Thermophysical Properties of Hydrocarbon Mixtures," National Inst. of Standards, Gaithersburg, MD, Feb. 1990.

[5] Martel, C. R., "Molecular Weight and Average Composition of JP-4, JP-5, JP-8, and Jet A," Chemical Propulsion Information Agency Airbreathing Propulsion Manual CPIA/M6, Units 8 (JP-7) and 11 (JP-8), Columbia, MD, Sept. 2000.

[6] "Survey of Jet Fuels (1990-1997)," Defense Energy Supply Center, Ft Belvoir, VA, June 1998 (annual updates thereafter).

[7] Yu, J., and Eser, S., "Determination of Critical Properties (T_c, P_c) of Some Jet Fuels," *Industrial and Engineering Chemistry Research*, Vol. 34, No. 1, 1995, pp. 404–409.

[8] Martel, C. R., "Air Force Aviation Fuel Thermal Oxidation Stability R&D," *Jet Fuel Thermal Stability*, edited by W. F. Taylor, NASA TM 79231, National Aeronautics and Space Administration, Cleveland, OH, Nov. 1978.

[9] Sobel, D. R., and Spadaccini, L. J., "Hydrocarbon Fuel Cooling Technologies for Advanced Propulsion," *American Society of Mechanical Engineers Journal of Engineering for Gas Turbines and Power*, Vol. 119, No. 2, April 1997, pp. 344–351.

[10] Mehta, G., Stone, W., Ingram, C., Bai, S., and Sanders, T., "Comparative Testing of Russian Kerosene and RP-1," AIAA Paper 95-2962, July 1995.

[11] Wood, C. P., "The Development and Application of Surrogate Blends in Simulating the Combustion Performance of Distillate Aviation Fuels," M.S. Thesis, Dept. of Mechanical Engineering, Univ. of California, Irvine, 1989.

[12] Schulz, W. D., "Oxidation Products of a Surrogate JP-8 Fuel," *ACS Petroleum Chemistry Division Preprints*, Vol. 37, No. 2, 1991, pp. 383–392; also, *Journal of Propulsion and Power*, Vol. 9, No. 1, 1993, pp. 5–9.

[13] Wang, T.-S., "Thermo-Kinetics Characterization of Kerosene/RP-1 Combustion for Tri-Propellant Engine Design Calculations," JANNAF Combustion Meeting, CPIA Publ. 631, Vol. II, Chemical Propulsion Information Agency, Columbia, MD, Oct. 1995, pp. 355–363.

[14] Farmer, R. C., Anderson, P. G., Cheng, G. C., Myruski, B. L., and Pike, R. W., "Propulsion Chemistry for CFD Applications," Final Rept. on Contract NAS8-40574, National Aeronautics and Space Administration, Marshall Space Flight Center, AL, Sept. 1997.

[15] Lindstedt, R. P., and Maurice, L. Q., "A Detailed Chemical Kinetic Model for Practical Aviation Fuels," *Journal of Propulsion and Power*, Vol. 16, No. 2, 2000, pp. 187–195.

[16] Guerèt, C., Cathonnet, M., Boettner, J. C., and Gaillard, F., "Experimental Study and Modeling of Kerosene Oxidation in a Jet-Stirred Flow Reactor," *Proceedings of the Twenty-Third Symposium (International) on Combustion*, Combustion Inst., Pittsburgh, PA, 1990, p. 211.

[17] Dagaut, P., Reuillon, M., Boettner, J. C., and Cathonnet, M., "Kerosene Combustion at Pressures up to 40 Atm: Experimental Study and Detailed Chemical Kinetic Modeling," *Proceedings of the Twenty-Fifth Symposium (International) on Combustion*, Combustion Inst., Pittsburgh, PA, 1994, pp. 919–926.

[18] Ranzi, E., Sogaro, A., Gaffuri, P., Pennati, G., Westbrook, C. K., and Pitz, W. J., "A New Comprehensive Reaction Mechanism for Hydrocarbon Fuels," *Combustion and Flame*, Vol. 99, No. 2, 1994, pp. 201–211.

[19] Harsha, P. T., Edelman, R. B., and Farmer, R. C., "Fundamental Combustion Technology for Ramjet Applications," Vol. II, CPIA Publ. 363, Chemical Propulsion Information Agency, Columbia, MD, Sept. 1982, pp. 2-1–2-63.

[20] McCoy, J. R., "Liquid Airbreathing Missile Fuels: An Overview of Properties and Applications," *Proceedings of the 1980 JANNAF Propulsion Meeting*, CPIA Publ. 315, Vol. V, Chemical Propulsion Information Agency, Columbia, MD, 1980, pp. 613–620.

[21] Siegel, B., and Schieler, L., *Energetics of Propellant Chemistry*, Wiley, New York, 1964, p. 176.

[22] Ross, J. L., "A Fuel Data Standardization Study for JP-4, JP-5, JP-7, and RJ-5 Combusted in Air," AFAPL-TR-74-22, Air Force Aero Propulsion Lab., Wright–Patterson AFB, OH, March 1974.

[23] Chemical Propulsion Information Agency Liquid Propellant Manual CPIA/M4 Unit 20a (RP-1), Chemical Propulsion Information Agency, Columbia, MD, Sept. 1997.

[24] "BP Amoco Will Offer Cleaner Fuels," *Chemical and Engineering News*, Vol. 77, No. 5, 1999, p. 22.

[25] Faith, L. E., Ackerman, G. H., and Henderson, H. T., "Heat Sink Capabilities of Jet A Fuel: Heat Transfer and Coking Studies," NASA CR-72951, National Aeronautics and Space Administration, Cleveland, OH, July 1971.

[26] TeVelde, J. A., and Glickstein, M. R., "Heat Transfer and Thermal Stability of Alternative Aircraft Fuels," Naval Air Propulsion Center Rept. NAPC-PE-87C (AD 137404), Naval Air Propulsion Center, Trenton, NJ, Nov. 1983.

[27] Nixon, A. C., Ackerman, G. H., Faith, L. E., Henderson, H. T., Ritchie, A. W., Ryland, L. B., and Shryne, T. M., "Vaporizing and Endothermic Fuels for Advanced Engine Applications: Part III: Studies of Thermal and Catalytic Reactions, Thermal Stabilities, and Combustion Properties of Advanced Fuels," AFAPL-TR-67-114, Part III, Vol. 1, Air Force Aero Propulsion Lab., Wright–Patterson AFB, OH, Feb. 1970.

[28] MacFarlane, W. R., and Wiese, D. E., "Fuel Options for High Mach Propulsion, Vol. II, Fuel Properties," WRDC-TR-90-2090, Air Force Wright Research and Development Center, Wright–Patterson AFB, OH, Oct. 1990.

[29] Szetela, E. J., and TeVelde, J. A., "External Fuel Vaporization Study," NASA CR 165513, National Aeronautics and Space Administration, Cleveland, OH, Nov. 1981; also American Society of Mechanical Engineers, Paper 82-GT-59, 1982.

[30] Hazlett, R. N., "Thermal Oxidation Stability of Aviation Turbine Fuels," American Society for Testing and Materials, ASTM Monograph 1, Philadelphia, PA, 1991.

[31] Heneghan, S. P., and Kauffman, R. E., "Analytic Tests and Their Relation to Jet Fuel Thermal Stability," *5th International Conference on Stability and Handling of Liquid Fuels*, DOE/CONF 941022, U.S. Dept. of Energy, Washington, DC, 1994, pp. 29–42.

[32] Curran, H. J., Pitz, W. J., Westbrook, C. K., Callahan, C. V., and Dryer, F. L., "Oxidation of Automotive Primary Reference Fuels at Elevated Pressures," *Proceedings from the 27th Symposium (International) on Combustion*, Combustion Inst., Pittsburgh, PA, 1998, pp. 379–387.

[33] Khan, A. R., "Oxidation of Industry Standard Fuels and Blends of Primary Reference Fuels in the Low Temperature and Negative Temperature Coefficient Regions," M.S. Thesis, Dept. of Mechanical Engineering and Mechanics, Drexel Univ., Philadelphia, PA, June 1998.

[34] Prabhu, S. K., "Pre and Post-Combustion Hydrocarbon Oxidation Studies Related to Engine Knock and Emissions," Ph.D. Dissertation, Dept. of Mechanical Engineering and Mechanics, Drexel Univ., Philadelphia, PA, 1997.

[35] Aly, S. L., and Salem, H., "Prediction of Premixed Laminar Flame Characteristics of Commercial Kerosene Fuel," *Fuel*, Vol. 68, 1989, p. 1203.

[36] Foelsche, R. O., Keen, J. M., Solomom, W. C., Buckley, P. L., and Corporan, E., "Non-Equilibrium Combustion Models for Fuel-Rich Gas Generators," *Journal of Propulsion and Power*, Vol. 10, No. 4, 1994, p. 461.

[37] Emdee, J. L., Brezinsky, K., and Glassman, I., "A Kinetic Model for the Oxidation of Toluene Near 1200 K," *Journal of Physical Chemistry*, Vol. 96, No. 5, 1992, pp. 2151–2161.

[38] Vovelle, C., Delfau, J. L., and Reuillion, M., "Formation of Aromatic Hydrocarbons in Decane and Kerosene Flames at Reduced Pressures," *Soot Formation in Combustion: Mechanisms and Models*, edited by H. Bockhorn, Springer-Verlag, 1994.

[39] Leung, K. M., "Kinetic Modelling of Hydrocarbon Flames Using Detailed and Systematically Reduced Chemistry," Ph.D. Dissertation, Mechanical Engineering Dept., Imperial College, Univ. of London, 1996.

[40] Maurice, L. Q., "Detailed Chemical Kinetic Models for Aviation Fuels," Ph.D. Dissertation, Mechanical Engineering Dept., Imperial College, Univ. of London, Dec. 1996.

[41] Lindstedt, R. P., and Maurice, L. Q., "Detailed Chemical Kinetic Modelling of Toluene Combustion," *Combustion Science and Technology*, Vol. 120, 1996, pp. 119–167.

[42] Maurice, L. Q., Blust, J. W., Leung, K. M., and Lindstedt, R. P., "Emissions from Combustion of Hydrocarbons in a Well-Stirred Reactor," AIAA Paper 99-1038, Jan. 1999.