



The ignition, oxidation, and combustion of kerosene: A review of experimental and kinetic modeling

Philippe Dagaut *, Michel Cathonnet

CNRS, Laboratoire de Combustion et Systèmes Réactifs (LCSR), UPR 4211, 1c, Avenue de la recherche scientifique, 45071 Orléans Cedex 2, France

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Abstract

For modeling the combustion of aviation fuels, consisting of very complex hydrocarbon mixtures, it is often necessary to use less complex surrogate mixtures. The various surrogates used to represent kerosene and the available kinetic data for the ignition, oxidation, and combustion of kerosene and surrogate mixtures are reviewed. Recent achievements in chemical kinetic modeling of kerosene combustion using model-fuels of variable complexity are also presented.

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1. Introduction

Until now, fossil fuels have contributed to over 80% of energy expenses, and among them, oil played the dominant role. It is expected that its use will not decline until the next two or three decades. The transportation

* Corresponding author. Tel.: +33 238 25 54 66; fax: +33 238 69 60 04.

E-mail address: dagaut@cnrs-orleans.fr (P. Dagaut).

Nomenclature

FID	flame ionization detector	PRF	primary reference fuels (<i>n</i> -heptane and <i>iso</i> -octane also called 1,2,4-trimethylpentane)
GC	gas chromatography	SI engine	spark ignition engine
JSR	jet-stirred reactor (also called continuously stirred tank reactor, CSTR)	<i>t</i>	mean residence time in the jet-stirred reactor
MS	mass spectrometry	<i>T</i>	temperature
Naphtene	also called cycloalkane	TCD	thermal conductivity detector
<i>P</i>	total pressure	ϕ	equivalence ratio ($\{[\text{fuel}]/[\text{O}_2]\}/\{[\text{fuel}]/[\text{O}_2]\}_{\text{atstoichiometry}}$; $\phi = 1$ at stoichiometry)
PAH	poly-aromatic hydrocarbon		
ppmv	part per million in volume (1 ppmv corresponds to a mol fraction of 1×10^{-6})		

sector, including aviation, an essential part of our modern society, represents the largest part of the petroleum based fuels consumption. Its importance has continuously grown at a very fast rate over the last century. Future global energy and environmental issues have imposed changes in the operating conditions of turbojet engines. As in other sectors, research is now oriented on saving energy, in parallel with enhanced protection of our environment (reduction of the emissions of pollutants and green house gases) and fuel reformulation. The detailed modeling of the combustion of jet fuels is a useful tool to solve the problem of combustion control, as well as to reduce emissions and fuel consumption. Such a modeling represents a real challenge because practical jet fuels are complex mixtures of several hundreds of hydrocarbons including alkanes, cycloalkanes, aromatics and polycyclic compounds.

In order to study the combustion behavior of commercial jet fuels, mixtures with well defined and reproducible composition are required: we call them ‘surrogates’ or ‘model-fuels’. For sake of simplicity, they should include a limited number of hydrocarbons with a well-defined composition, and show a behavior similar to that of a commercial fuel. They are of extremely high interest since they can be utilized to study the effect of chemical composition and fuel properties on the combustion process. Application of surrogates to the modeling of the ignition, oxidation, and combustion of conventional jet fuels will be discussed here, and the results of recent kinetic studies on the oxidation of surrogate kerosene mixtures will be presented. Finally, recent results concerning the reformulation of jets fuels in the context of reduced oil availability will be presented.

2. Characteristic properties of conventional jet fuels

Since the early development of the turbojet engine, the characteristics of jet fuels have evolved [1]. Initially, the turbojet engines were thought to be relatively insensitive to fuel properties. Therefore, the widely available illuminating kerosene produced for wick lamps was used. In the 1940s, ‘wide-cut’ fuel was used for availability reasons. Due to its relative high-volatility and associated evaporation and safety problems, wide-cut jet fuels (JP-4, Jet B) were replaced by kerosene-type fuel in the 1970s (Jet A, Jet A-1, and JP-8). Nowadays, there are essentially three types of conventional jet fuels [2]: (i) a kerosene type, (ii) a high-flash point kerosene, and (iii) a broad cut. Most international civilian aviation companies use the kerosene type Jet A-1 whereas some military aviation fuels are very close to Jet A-1 (TR0 in France, AVTUR in the United Kingdom, and JP-8 in the United States of America), although they include different additives [1–3]. Actually, Jet A is used in the United States and Jet A-1 is used in the rest of the world. The important difference between Jet A and Jet A-1 concerns the freezing point (-40 °C for Jet A and -47 °C for Jet A-1). All the jet fuels must meet general physical property specifications. Those for Jet A-1 (Appendix 1) were incorporated in a standard defined in 1994 as the Aviation Fuel Quality Requirement for Jointly Operated Systems (AFQRJOS) [2]. Although turbojet engines are far more fuel-tolerant than SI engines, the increased operating pressures and temperatures have rendered the modern turbojet engines fuel-sensitive [2,4]. Therefore the specifications for jet fuels represent an optimal compromise of properties for engine performances and safety aspects during storage and distribution.

Among the properties linked to the quality of combustion [2], specification requirements concern volatility, viscosity and freezing point, density, heating value, smoke point and luminosity factor, aromatic content, and thermal stability of the fuel (ASTM D 1655). Combustion in turbojet engines is characterized by the formation of soot particles which must be minimized for several reasons: (i) soot can be harmful for the engine because of carbon deposits and radiant heat loss which can lead to hot spots or to high combustor wall temperature, (ii) soot emissions from jet engines affect high altitudes atmospheric chemistry, and (iii) soot favors radar detection of military aircrafts. Fuels with high aromatics contents, especially polyaromatics, produce more soot. This is why both the total aromatic content is limited to 22–25% and the naphthalene content to 3% in volume. Practically, the aromatic content of JP-8 varies between 10 and 25% with a mean at 18% in volume [3]. However, the aromatic content of kerosene has increased since the sixties [4] for economic reasons, and the quality of kerosene is expected to deteriorate in the future with the reducing availability of light crudes.

Table 1 gives the main characteristics of JP-8 and Jet A-1 reported by several authors [3,5–7], compared with the general characteristics of kerosene from Guibet [2]. Table 1 also includes the average composition by chemical families of JP-8/Jet A-1 [3,5–7] and kerosene [2].

The average chemical formula for kerosene (Jet A, Jet A-1, TR0, JP8) differs from one source to another and ranges from $C_{10.9}H_{20.9}$ to $C_{12}H_{23}$: Gracia-Salcedo et al. [9] used $C_{12}H_{23}$, Edwards and Maurice [3] gave $C_{11}H_{21}$, Martel [6] gave $C_{11.6}H_{22}$, Guéret [10] determined $C_{11}H_{22}$, Nguyen and Ying [11] used

$C_{11}H_{23}$. Further information can be found in previous reports [12–14] whereas jet A-1 specifications are given in Appendix A. As most of the hydrocarbon mixtures used as a fuel, the composition of kerosene is subject to variations of composition. The composition varies from one source to another [15,16] and is subject to changes due to thermal instability. The specification test device for jet fuel is the thermal oxidation test as described in ASTM D3241. The thermal stability of jet fuels is improved via the use of additives. Further information can be found in [8,17,18].

3. Formulation of kerosene surrogate fuels

Since specifications on kerosene only include general physical properties, many hydrocarbon mixtures can meet these specifications, although the relative proportions of the various chemical families is constrained by the general physical properties. Because the variations in composition may be large from purchase to purchase [15], a more definite chemical composition was found necessary for modeling and experimental studies. Mixtures of a limited number of hydrocarbons have been proposed to represent commercial kerosene. These single-component or multi-component fuels are classified [3] as physical surrogates if they have the same physical properties as the real fuel, or chemical surrogates if they have the same chemical properties as the real fuel. Surrogates which have both the same physical and chemical properties as the commercial fuel are called comprehensive surrogates.

A literature survey of fuel blends and surrogates formulated to reproduce the behavior of aviation fuels was performed by Edwards and Maurice [3], yielding

Table 1
Main characteristics of kerosene jet fuel

Property	JP-8 [5]	JP-8 [6]	JP-8/Jet A-1 [3]	Jet A [6]	JP-8 [7]	Kerosene [2]
Molecular weight		152		162		
Approximate formula	–	$C_{10.9}H_{20.9}$	$C_{11}H_{21}$	$C_{11.6}H_{22}$	–	–
Number of C atoms in the fuel	–	10.9	11	11.6	–	9–13
H/C ratio	–	1.92	1.91	1.9	–	1.9–2.1
Boiling range °C	140–300	Average 204	165–265	Average 216	–	140–280
Specific gravity at 15 °C	0.81		0.81		–	0.77–0.83
Av. Composition in vol%						
Aromatics	20		18		18(monoar.)+2(diaro.)	10–20
Cycloalkanes	20		20		20	20–30
Paraffins	58		60		28(<i>n</i> -par.)+29(<i>i</i> -par.)	50–65
Olefins	2		2		–	0

recommendations for the various classes of surrogate applications. The simplest physical situation is single phase heat transfer without chemical reaction: in that case, a single component with approximately correct critical temperature can be used as surrogate. For example, *n*-dodecane has physical properties similar to JP-7 and JP-8/JetA-1 [3]. For other properties such as fuel vaporization, injection and mixing without chemical reaction, a multi-component surrogate is necessary to match distillation curve. To reproduce fuel ignition, general thermal-oxidation behavior or emissions during combustion, a chemical surrogate that matches the important chemical classes was recommended by Edwards and Maurice [3].

It is interesting to note that for gasoline, the chemical surrogates usually used to determine the resistance to knock do not reflect its chemical composition: only two hydrocarbons, a linear alkane (*n*-heptane), and a branched one (2,2,4-trimethyl pentane or '*iso*-octane') have been chosen as the components of primary reference fuels (PRF), with octane number adjusted by a linear combination of the two. More recently, other standard mixtures including toluene in addition to *n*-heptane and *iso*-octane have been adopted [2] for a better precision in the determination of gasoline octane numbers. Edwards and Maurice [3] also reported that simple two-component surrogates do not adequately reproduce the ignition behavior of real gasoline in flow reactors and engines, and that a gasoline surrogate obtained by addition of an aromatic and an alkene to the PRF mixture better reproduces the ignition behavior of this fuel. A more recent study of Lenhert et al. [19] showed

that the addition of toluene and *n*-pentene to the PRF mixture improves the accuracy with which the surrogate reproduces the low- and intermediate-temperature reactivity of industry standard fuels. Such a surrogate is more representative of the chemical composition of premium gasoline whose main constituents are monoaromatic hydrocarbons, branched alkanes, and, to a lower extent, alkenes [2].

Concerning JP-8, Edwards and Maurice [3] reported the studies of Schulz and co-workers [20,21] on the thermal and oxidative stability of this fuel and gave the composition formulated by this author for a surrogate, which could reproduce the general oxidation behavior of JP-8, but did not reproduce the deposition levels of distillate fuels. More recently, Violi et al. [7] proposed a new approach for the formulation of a JP-8 comprehensive surrogate fuel and detailed the procedure followed to match practical fuels on both physical and chemical properties: volatility, sooting tendency, and combustion property. They tested two slightly different surrogates (Table 2) reproducing very well volatility and sooting propensity of a real JP-8. The surrogate 2 was shown to better fit the distillation curve of JP-8. For comparison, we have also reported in Table 2 the composition of the JP-8 surrogate elaborated by Schulz [20,21] and the composition of a standard commercial jet fuel [2].

Table 2 shows that the chemical-class composition of the surrogate mixture #2 of Violi et al. [7] is rather different from that of the commercial fuel given by Guibet [2]. In particular, this surrogate has a higher content of dicyclic cycloalkane (decalin) than the commercial fuel, and includes no non-condensed cycloalkanes. However

Table 2
Composition of JP-8 surrogates and of a commercial jet-fuel

Composition of the surrogates in [7] (vol%)		Composition of the surrogate fuel in [20,21] (mass %)	Composition of a commercial jet-fuel from Guibet [2] (mass %)
Sur-1	Sur-2		
Isooctane 10	<i>n</i> -Octane 3.5	Isooctane 5	Paraffins 58.30
<i>n</i> -Dodecane 30	<i>n</i> -Dodecane 40	Decane 15	Non-condensed cycloalkanes 23.85
<i>n</i> -Tetradecane 20	<i>n</i> -Hexadecane 5	Dodecane 20	Dicyclic naphthenes 2.40
Methylcyclohexane 20	Xylenes 8.5	Tetradecane 15	Alkylbenzenes 13.40
<i>m</i> -Xylene 15	Decalin 35	Hexadecane 10	Indanes, tetralins 1.70
Tetralin 5	Tetralin 8	Methylcyclohexane 5	Naphthalenes 0.35
	Note: error in Table 2 of [7]	Cyclooctane 5	
		<i>m</i> -Xylene 5	
		Butylbenzene 5	
		Tetramethylbenzene 5	
		Tetralin 5	
		Methylnaphthalene 5	

Table 3
Available experimental kinetic data for the combustion of kerosene and surrogate fuels

Technique	Fuel	Conditions	Data type and comments	Reference
Flow tube	RDE/F/KER/201-206	Spray injection of the fuel <100 μ m. Ignition obtained by injection of the fuel in heated air containing 12–16% of oxygen	Ignition delays measured versus temperature (1070–1270 K) at atmospheric pressure	[22]
Flow tube	Jet A-1	Spray injection of the fuel. Ignition obtained by injection of the fuel in heated air mostly in fuel-rich conditions. Ignition delay determined by temperature rise end light emission	Ignition delays measured versus temperature (720–1070 K) at 4–11 bar, equivalence ratio in the range 0.5–7.5	[23]
Flow tube	Jet-A	Ignition measured for kerosene–air mixtures, equivalence ratio varied (0.3–1), pressure within the range 10–30 atm. Ignition obtained by injection of the fuel in heated air. Ignition delay determined by temperature rise, pressure rise, light emission	Ignition delays measured versus temperature (700–830 K). Arrhenius equation derived for the ignition delays	[24]
Flow tube	Jet-A	Fuel–air mixtures; temperature range 930–1020 K, atmospheric pressure	Ignition delays measured versus temperature at different equivalence ratios used to propose an Arrhenius expression for the delays	[25]
Shock tube	Kerosene	Kerosene–air mixtures ignited in stoichiometric conditions at 1 atm, 900–1300 K	Ignition delays measured versus temperature at one equivalence ratio	[26]
Shock tube	Jet-A	Kerosene–air mixtures ignited at ca. 8 atm, equivalence ratios of 0.5, 1, and 2, 1000–1700 K	Ignition delays measured versus temperature at three equivalence ratios. Ignition delay correlation derived from the data	[27]
Shock tube	Jet-A	Kerosene–air mixtures ignited at 10 and 20 atm, equivalence ratios of 0.5, 1, and 2, 1040–1380 K	Ignition delays measured versus temperature at three equivalence ratios. Ignition delay correlation derived from the data.	[28]
Shock tube	Jet-A and JP-8	Kerosene–air mixtures ignited in stoichiometric conditions at 30 atm, 900–1100 K	Ignition delays measured versus temperature at three equivalence ratios. Ignition delay correlation derived using these data and those from [27,28]	[29]
Flat flame burner	<i>n</i> -Decane	5.1% of fuel, 41.2% oxygen, 53.7% argon, 6 kPa, equivalence ratio of 1.9, sooting flame, velocity of the cold gas mixture at the burner exit = 18.6 cm/s, flame diameter = 9.5 cm, temperature measurement by coated (BeO/Y ₂ O ₃) Pt/Pt–Rh 10% thermocouple (S) with wires of 50 μ m	Mole fractions profiles as a function of distance to the burner, MBMS (molecular beam mass spectrometry) measurements. Profiles reported: <i>n</i> -decane, O ₂ , Ar, CO, H ₂ O, H ₂ , CO ₂ , C ₂ H ₂ , C ₂ H ₄ , CH ₄ , H, OH, CH ₂ , CH ₃ , C ₂ H ₃ , C ₂ H ₅ , C ₂ H ₆ , C ₃ H ₃ , C ₃ H ₅ , C ₃ H ₇ , C ₃ H ₈ , C ₄ H ₂ , C ₄ H ₄ , C ₄ H ₅ , C ₄ H ₆ , C ₄ H ₈ , C ₄ H ₉ , C ₆ H ₆ . Data used to propose a detailed kinetic scheme	[41]
JSR	TR0 and surrogate mixture: 79% <i>n</i> -undecane, 10% <i>n</i> -propylcyclohexane, 11% 1,2,4-trimethylbenzene	0.1% mol of fuel, diluted by nitrogen, 1 atm, variable residence time (0.1–0.22 s) and constant temperature (873–1033 K), equivalence ratio varied (0.2, 1, 1.5), temperature measurement by uncoated chromel–alumel thermocouple (K) with wires of 0.12 mm	Mole fraction profiles taken by sonic probe sampling at low pressure and analyses by GC–FID, -TCD. MS identification. Profiles reported: <i>n</i> -undecane, <i>n</i> -propylcyclohexane, 1,2,4-trimethylbenzene, CO, CO ₂ , CH ₄ , C ₂ H ₄ , C ₂ H ₆ , C ₃ H ₆ , 1-C ₄ H ₈ , 1,3-C ₄ H ₆ . Data used to propose a quasi-global kinetic scheme	[35]

Flat flame burner	<i>n</i> -Decane and TR0	(1) 8% of fuel, 56.4% oxygen, 35.6% argon, 6 kPa, equivalence ratio of 2.2, sooting flames, velocity of the cold gas mixture at the burner exit = 24 cm/s, flame diameter = 9.5 cm, temperature measurement by coated (BeO/Y ₂ O ₃) Pt/Pt-Rh 10% thermocouple (S) with wires of 50 μm. (2) Jet A-1 and <i>n</i> -decane flames: variation of the equivalence ratio (1.0–2.5) keeping the flow rate of argon and the total flow rate constant (cold gas mixture at the burner exit = 27.5 cm/s)	(1) Mole fractions profiles as a function of distance to the burner, MBMS (molecular beam mass spectrometry) measurements. Profiles reported: <i>n</i> -decane, O ₂ , Ar, CO, H ₂ O, H ₂ , CO ₂ , C ₂ H ₂ , C ₂ H ₄ , C ₄ H ₄ , C ₄ H ₅ , C ₆ H ₆ . Data used to propose a detailed kinetic scheme [30,32] (2) Signal measurements reported for C ₂ H ₂ , C ₆ H ₆ , phenylacetylene, vinylbenzene. Comparison of the formation of soot precursors in kerosene and <i>n</i> -decane flame
JSR	<i>n</i> -Decane	0.1% mol of fuel, diluted by N ₂ , 1 atm, variable residence time (0.1–0.22 s) and constant temperature (873–1033 K), equivalence ratio varied (0.2, 1, 1.5), temperature measurement by uncoated chromel–alumel thermocouple (K) with wires of 0.12 mm	Mole fraction profiles taken by sonic probe sampling at low pressure and analyses by GC–FID, -TCD. MS identification. Profiles reported: <i>n</i> -decane, CO, CO ₂ , CH ₄ , C ₂ H ₄ , C ₂ H ₆ , C ₃ H ₆ , 1-C ₄ H ₈ , 1,3-C ₄ H ₆ , 1-C ₅ H ₁₀ , 1-C ₆ H ₁₀ , 1-C ₇ H ₁₄ , 1-C ₈ H ₁₆ , 1-C ₉ H ₁₈ . Data used to propose a quasi-global kinetic scheme [42]
Jet burner	Kerosene AVTUR	Six turbulent jet flames of pre-vaporized kerosene studied in the pressure range 1–6.44 bar for several fuel and air flow rates. Reynolds number varied from 9500 to 32800. Mean temperature measured by thermocouple Pt/Pt–Rh 10% thermocouple (S) with wires of 50 μm.	Soot volume fractions measured by He–Ne laser absorption. The flame A was modeled by Wen et al. [67] [33]
JSR	<i>n</i> -Decane and TR0	0.1% mol of fuel, diluted by nitrogen, variable temperature (750–1150 K) at several fixed residence times (0.5, 1 and 2 s), equivalence ratio varied (0.5, 1, 1.5), temperature measurement by uncoated chromel–alumel thermocouple (K) with wires of 0.12 mm. Experiments reported at 10, 20 and 40 atm for kerosene and only at 10 atm for <i>n</i> -decane	Mole fraction profiles taken by sonic probe sampling at low pressure and analyses by GC–FID, -TCD. MS identification. Profiles reported: <i>n</i> -decane, O ₂ , H ₂ , CO, CO ₂ , CH ₂ O, CH ₄ , C ₂ H ₄ , C ₂ H ₆ , C ₃ H ₆ , propyne, allene, 1-C ₄ H ₈ , 1-C ₅ H ₁₀ , 1-C ₆ H ₁₀ , 1-C ₇ H ₁₄ , 1-C ₈ H ₁₆ , 1-C ₉ H ₁₈ , C ₆ H ₆ , toluene, <i>o</i> -xylene, <i>p</i> -xylene. Data used to propose a detailed kinetic scheme for <i>n</i> -decane oxidation. The kerosene model fuel is <i>n</i> -decane [36]
JSR	<i>n</i> -Decane	0.1% mol of fuel, diluted by nitrogen, 10 atm, fixed residence time (1.0 s) and variable temperature (550–1150 K), equivalence ratio varied (0.1–1.5), temperature measurement by uncoated chromel–alumel thermocouple (K) with wires of 0.12 mm. The study covers the cool flame and NTC regimes	Mole fraction profiles taken by sonic probe sampling at low pressure and analyses by GC–FID, -TCD. MS identification. Profiles reported: <i>n</i> -decane, O ₂ , H ₂ , CO, CO ₂ , CH ₂ O, CH ₃ OH, CH ₄ , C ₂ H ₄ O, CH ₃ CHO, C ₃ H ₆ O, C ₂ H ₄ , C ₂ H ₆ , C ₂ H ₅ CHO, acetone, C ₃ H ₆ , propyne, allene, 1-C ₄ H ₈ , 2-C ₄ H ₈ , 1,3-C ₄ H ₆ , 1-C ₅ H ₁₀ , 2-C ₅ H ₁₀ , 1,3-C ₅ H ₈ , C ₆ H ₆ , 1-C ₆ H ₁₀ , 1-C ₇ H ₁₄ , 1-C ₈ H ₁₆ , 1-C ₉ H ₁₈ , 1-, 2-, 3-, 4-, and 5-decenes, 2,5-dipropyltetrahydrofuran, <i>cis</i> and <i>trans</i> 2-ethyl-5-butyltetrahydrofuran, <i>trans</i> 2,5-dipropyltetrahydrofuran, <i>cis</i> and <i>trans</i> 2-methyl-5-pentyltetrahydrofuran [40]

(continued on next page)

Table 3 (continued)

Technique	Fuel	Conditions	Data type and comments	Reference
JSR	<i>n</i> -Decane and TR0	0.025–0.1% mol of fuel, diluted by nitrogen, variable temperature (550–1150 K) at several fixed residence times (0.5, 1 and 2 s), equivalence ratio varied (0.1–1.5), temperature measurement by uncoated chromel–alumel thermocouple (K) with wires of 0.12 mm. Experiments reported at 10, 20 and 40 atm for kerosene and only at 10 atm for <i>n</i> -decane. The study covers the cool flame and NTC regimes	Mole fraction profiles taken by sonic probe sampling at low pressure and analyses by GC–FID, -TCD. MS identification. Profiles reported: <i>n</i> -decane, O ₂ , H ₂ , CO, CO ₂ , CH ₂ O, CH ₃ OH, CH ₄ , C ₂ H ₄ O, CH ₃ CHO, C ₃ H ₆ O, C ₂ H ₄ , C ₂ H ₆ , C ₂ H ₅ CHO, acetone, C ₃ H ₆ , propyne, allene, 1-C ₄ H ₈ , 2-C ₄ H ₈ , 1,3-C ₄ H ₆ , 1-C ₅ H ₁₀ , 2-C ₅ H ₁₀ , 1,3-C ₅ H ₈ , C ₆ H ₆ , 1-C ₆ H ₁₂ , 1-C ₇ H ₁₄ , 1-C ₈ H ₁₆ , 1-C ₉ H ₁₈ , 1-, 2-, 3-, 4-, and 5-decenes, 2,5-dipropyltetrahydrofuran, <i>cis</i> and <i>trans</i> 2-ethyl-5-butyltetrahydrofuran, <i>trans</i> 2,5-dipropyltetrahydrofuran, <i>cis</i> and <i>trans</i> 2-methyl-5-pentyltetrahydrofuran	[37]
Flat flame burner	<i>n</i> -Decane and TR0	(1) 1.15 cm ³ /s of <i>n</i> -decane, 10.3 cm ³ /s of oxygen, 24.6 cm ³ /s of nitrogen, 101 kPa, equivalence ratio of 1.7, slightly sooting flame, velocity of the cold gas mixture at the burner exit=11.7 cm/s (473 K, 1 atm), flame diameter=2.5 cm, temperature measurement by coated (BeO/Y ₂ O ₃) Pt/Pt–Rh 10% thermocouple (S) with wires of 50 μm (2) 1.06 cm ³ /s of kerosene, 10.3 cm ³ /s of oxygen, 24.6 cm ³ /s of nitrogen, 101 kPa, equivalence ratio of 1.7, slightly sooting flame, velocity of the cold gas mixture at the burner exit=11.7 cm/s (473 K, 1 atm)	Mole fraction as a function of the distance to the burner taken by sonic probe sampling at low pressure and analyses by GC–FID, -TCD. Profiles reported: <i>n</i> -decane, O ₂ , CO, H ₂ , N ₂ , H ₂ O, CO ₂ , CH ₄ , C ₂ H ₆ , C ₂ H ₄ , C ₂ H ₂ , allene, propyne, C ₄ H ₂ , 1-C ₄ H ₈ , <i>i</i> -C ₄ H ₈ , 2-C ₄ H ₈ , C ₅ H ₁₀ , C ₆ H ₆ . A detailed kinetic modeling of this flame is presented by Douté [68]	[31]
Shock tube	<i>n</i> -Decane	Mixtures of <i>n</i> -decane/air ignited at three equivalence ratios (0.5, 1.0, and 2.0) at 13 bar (700–1300 K) and $\phi=0.67$, 1.0, and 2.0 at 50 bar (650–960 K). Ignition delays based on pressure traces records	Ignition delays (first and second stage) measured over the temperature range 650–1300 K at 13 and 50 bar. Use of a heated shock tube (373 K).	[45]
Turbulent flow reactor	<i>n</i> -Decane	Pyrolysis of 1456 ppmv of <i>n</i> -decane at 1060 K investigated as a function of residence time (40–270 ms) at 1 atm. Oxidation of 1452 ppmv of <i>n</i> -decane at 1019 K as a function of residence time (10–140 ms) at 1 atm, $\phi=1$	Mole fraction profiles taken by cooled probe sampling and analyses by GC–FID, -TCD. Profiles reported: <i>n</i> -decane, O ₂ , CO, CO ₂ , CH ₄ , C ₂ H ₂ , C ₂ H ₄ , C ₂ H ₆ , C ₃ H ₆ , 1-C ₄ H ₈ , 1,3-C ₄ H ₆ , 1-C ₅ H ₁₀ , 1-C ₆ H ₁₂	[46]
Shock tube	<i>n</i> -Decane	0.49–1.5% <i>n</i> -decane and 4–23.25% O ₂ , dilution by argon. Temperature range 1239–1616 K, pressure range 1.82–10 atm	Ignition delays measured as a function of temperature used to propose an Arrhenius correlation	
JSR	TR0	0.07% mol of fuel, diluted by nitrogen, 1 atm, fixed residence time (0.07 s) and variable temperature (900–1300 K), equivalence ratio varied (0.5, 1, 1.5, 2), temperature measurement by protected (thin silica envelop) Pt/Pt–Rh 10% thermocouple (S) with wires of 0.1 mm	Mole fraction profiles taken by sonic probe sampling at low pressure and analyses by GC–FID, -TCD, on line GC–MS identification and quantification. Profiles reported: O ₂ , H ₂ , CO, CO ₂ , CH ₂ O, CH ₄ , C ₂ H ₄ , C ₂ H ₆ , C ₃ H ₆ , 1-C ₄ H ₈ , 1,3-C ₄ H ₆ , 1,3-cyclopentadiene, 1-C ₅ H ₁₀ , 2-C ₅ H ₁₀ , C ₆ H ₆ , 1-C ₆ H ₁₂ , toluene. Detailed kinetic modeling presented using the mixture 74% <i>n</i> -decane, 15% <i>n</i> -propylbenzene, 11% <i>n</i> -propylcyclohexane (mol) as model-fuel	[38]

JSR	Jet A-1	(1) at 10 atm: 0.067% mol of fuel, diluted by nitrogen, fixed residence time (0.5 s) and variable temperature (800–1200 K), equivalence ratio varied (0.25–2), temperature measurement by protected (thin silica envelop) Pt/Pt–Rh 10% thermocouple (S) with wires of 0.1 mm (2) at 20 atm: 0.05% mol of fuel, residence time 1.0 s, equivalence ratio varied (0.75–2.5), 750–1150 K (3) at 40 atm: 0.025–0.05% mol of fuel, residence time 2.0 s, equivalence ratio of 1, 750–1150 K	Mole fraction profiles taken by sonic probe sampling at low pressure and analyses by GC–FID, -TCD, on line GC–MS identification and quantification. Profiles reported: H ₂ , O ₂ , CO, CO ₂ , CH ₂ O, CH ₄ , C ₂ H ₆ , C ₂ H ₄ , C ₂ H ₂ , C ₃ H ₆ , C ₃ H ₈ , propyne, allene, 1-C ₄ H ₈ , <i>i</i> C ₄ H ₈ , <i>cis</i> 2-C ₄ H ₈ , <i>trans</i> 2-C ₄ H ₈ , 1-butyne, 1,3-butadiene, 1,3-cyclopentadiene, 1-C ₅ H ₁₀ , 1-C ₆ H ₁₂ , benzene, CH ₃ CHO, acrolein, isoprene, 1-C ₇ H ₁₄ , methylcyclohexane, toluene, 1-C ₈ H ₁₆ , ethylcyclohexane ethylbenzene, <i>m</i> + <i>p</i> -xylene, styrene, <i>o</i> -xylene, 1-C ₉ H ₁₈ , <i>n</i> -nonane, <i>n</i> -propylbenzene, 1,2,4-trimethylbenzene, <i>n</i> -decane, <i>n</i> -undecane	[39]
JSR	Surrogate mixture: <i>n</i> -decane, <i>n</i> -propylbenzene	0.076% mol of fuel (<i>n</i> -decane/ <i>n</i> -propylbenzene 80/20 and 70/30 weight), diluted by nitrogen, 10 atm, fixed residence time (0.5 s) and variable temperature (800–1100 K), equivalence ratio varied (0.75–2), temperature measurement by protected (thin silica envelop) Pt/Pt–Rh 10% thermocouple (S) with wires of 0.1 mm	Mole fraction profiles taken by sonic probe sampling at low pressure and analyses by GC–FID, -TCD, on line GC–MS identification and quantification. Profiles reported: H ₂ , O ₂ , CO, CO ₂ , CH ₂ O, CH ₄ , C ₂ H ₆ , C ₂ H ₄ , C ₂ H ₂ , C ₃ H ₆ , C ₃ H ₈ , propyne, allene, 1-C ₄ H ₈ , <i>i</i> C ₄ H ₈ , <i>cis</i> 2-C ₄ H ₈ , <i>trans</i> 2-C ₄ H ₈ , 1,3-butadiene, 1,3-cyclopentadiene, 1-C ₅ H ₁₀ , 1-C ₆ H ₁₂ , benzene, CH ₃ CHO, acrolein, 1-C ₇ H ₁₄ , toluene, 1-C ₈ H ₁₆ , ethylbenzene, styrene, <i>n</i> -propylbenzene, 1-C ₉ H ₁₈ , <i>n</i> -decane, benzaldehyde, phenol	[39]
JSR	Surrogate mixture: <i>n</i> -decane, 1,2,4-trimethylbenzene	0.075% mol of fuel (<i>n</i> -decane/1,2,4-trimethylbenzene 80/20 mol), diluted by nitrogen, 10 atm, fixed residence time (0.5 s) and variable temperature (800–1200 K), equivalence ratio varied (0.75–2), temperature measurement by protected (thin silica envelop) Pt/Pt–Rh 10% thermocouple (S) with wires of 0.1 mm	Mole fraction profiles taken by sonic probe sampling at low pressure and analyses by GC–FID, -TCD, on line GC–MS identification and quantification. Profiles reported: H ₂ , O ₂ , CO, CO ₂ , CH ₂ O, CH ₄ , C ₂ H ₆ , C ₂ H ₄ , C ₂ H ₂ , C ₃ H ₆ , propyne, allene, 1-C ₄ H ₈ , 1,3-butadiene, 1,3-cyclopentadiene, 1-C ₅ H ₁₀ , 1-C ₆ H ₁₂ , benzene, CH ₃ CHO, acrolein, isoprene, 1-C ₇ H ₁₄ , toluene, 1-C ₈ H ₁₆ , ethylbenzene, <i>m</i> + <i>p</i> -xylene, styrene, <i>o</i> -xylene, 1-C ₉ H ₁₈ , <i>n</i> -nonane, 1,2,4-trimethylbenzene, <i>n</i> -decane, <i>n</i> -undecane	[39]
Shock-tube	<i>n</i> -Decane	(i) Mixtures of <i>n</i> -decane(270–500 ppmv)/oxygen/argon ignited at high temperature (1345–1537 K) and c.a. 5–8 bar at several equivalence ratios ($\phi = 0.5, 0.8, 1$). The ignition delays were determined by monitoring the OH and CH signals. The ignition delay corresponded to the peak values of OH and CH concentrations (ii) The laminar flame speeds of <i>n</i> -decane/air mixtures were measured at 1 bar, 473 K, for equivalence ratios ranging from 0.9 to 1.3	Ignition delays of <i>n</i> -decane measured using a heated shock-tube	[34]
Bunsen burner	Jet A-1	The laminar flame speeds of Jet A-1/air mixtures were measured at 1 bar, 473 K, for equivalence ratios ranging from 0.9 to 1.4	Flame speeds measured at atmospheric pressure	[34]

(continued on next page)

Table 3 (continued)

Technique	Fuel	Conditions	Data type and comments	Reference
Bunsen burner	Surrogate mixture: <i>n</i> -decane, <i>n</i> -propylbenzene	The laminar flame speeds of a surrogate mixture (<i>n</i> -decane, <i>n</i> -propylbenzene 80/20 in weight) in air were measured at 1 bar, 473 K, for ϕ ranging from 0.9 to 1.4	Flame speeds measured at atmospheric pressure	[34]
Counterflow diffusion flame	Surrogate mixture: <i>iso</i> -octane, methylcyclohexane, <i>m</i> -xylene, <i>n</i> -dodecane, tetralin, <i>n</i> -tetradecane	The surrogate fuel composition in mol was: 10% <i>iso</i> -octane, 20% methylcyclohexane, 15% <i>m</i> -xylene, 30% <i>n</i> -dodecane, 5% tetralin, 20% <i>n</i> -tetradecane. Non-sooting counterflow diffusion flames (1.6% surrogate and 76.8% oxygen at a strain rate of 115 s^{-1} , 1.4% surrogate and 76.8% oxygen at a strain rate of 95 s^{-1}). The temperature was measurement by coated (silica) Pt/Pt–Rh 10% thermocouple (S) with wires of 190 μm , atmospheric pressure	Temperature profiles and extinction limits are reported. A semi-detailed kinetic scheme is used to simulate the experiments	[47]
Flow reactor	Surrogate mixtures: <i>n</i> -dodecane, 2,2,4,4,6,8,8-heptamethylnonane or methylcyclohexane or α -methylnaphtalene	Three mixtures used: <i>n</i> -dodecane 40%, 2,2,4,4,6,8,8-heptamethyl-nonane 60%; <i>n</i> -dodecane 37%, methylcyclohexane 63%; <i>n</i> -dodecane 51%, α -methylnaphtalene 49%. They have studied experimentally the oxidation of these binary mixtures in a pressurized flow reactor at 8 atm, equivalence ratio of 0.3, $t = 120 \text{ ms}$, 600–800 K	The formation of CO is measured by NDIR (non-dispersive infrared absorption) in the cool flame and NTC regime. Semi-detailed or lumped kinetic models were used to simulate the oxidation of the pure components and mixtures	[48]
Shock tube	<i>n</i> -Decane	0.49–1.5% <i>n</i> -decane and 4–23.25% O_2 , dilution by argon. Temperature range 1239–1616 K, pressure range 1.82–10 atm	Ignition delays measured as a function of temperature used to propose an Arrhenius correlation. Post-shock species measurements are reported for CH_4 , C_2H_4 , C_3H_6 , 1- C_4H_8 , 1- C_5H_{10} , 1- C_6H_{12} , 1- C_7H_{14} , 1- C_8H_{16} . A detailed kinetic scheme is proposed to model the results	[49]

these authors showed that another surrogate with 20% methylcyclohexane, an hydrocarbon which is more representative of the cycloalkane family in JP-8 than decalin, did not reproduce so closely the boiling-point curve of practical JP-8.

4. Experimental kinetic studies of the ignition, oxidation and combustion of kerosene and surrogates

4.1. Kerosene

The kinetics of kerosene (Jet A-1, JP-8, AVTUR, TR0) ignition, combustion, and oxidation were previously reported in the literature. Table 3 summarizes the available data for the kinetic modeling of kerosene combustion. The available data for the ignition, oxidation and combustion of a variety of surrogates, including the simplest one, *n*-decane, are also reported in Table 3.

Regarding the ignition of kerosene, a very limited database was available until recently [22–26]. The use of experimental devices more ideal than in early studies, such as heated shock-tubes operating over a wide range of temperature and pressure [27–29] recently helped complementing the early database. Borisov [26] measured the ignition delays of kerosene behind a reflected shock wave for a stoichiometric kerosene–air mixture at atmospheric pressure, over the temperature range 900–1300 K. These data are in line with the earlier measurements reported by

Mullins [22]. More recently, Dean et al. [27] measured the ignition delays of Jet-A–air mixtures at ca. 8 atm, over the temperature range 1000–1700 K, and equivalence ratios of 0.5, 1, and 2, using a heated (ca. 348–373 K) shock tube. They derived an Arrhenius expression for the ignition delays of kerosene–air mixtures. Starikowskii et al. [28] measured the ignition delays of Jet A–air mixtures at 10 and 20 atm, over the temperature range 1040–1380 K, for equivalence ratios of 0.5, 1, and 2, by means of a heated (900 K) shock tube. The measurements were done behind a reflected shock wave, recording the emission of OH* at 309 nm. An Arrhenius expression for the ignition of kerosene–air mixtures was derived from these experiments:

$$\tau/\mu\text{s} = 10^{-3}(P/\text{atm})^{-0.39} \times \phi^{-0.57} \times \exp[(14,700\text{ K})/T]$$

Davidson and Hanson [29] recently compared their ignition delay measured behind a reflected shock wave (900–1100 K, 30 atm, $\phi=1$) for Jet-A and JP-8 with the data of [27,28], showing consistency. Fig. 1 presents the ignition data available to date [22,25–29].

The flame structures database is somewhat limited [30–33] since only fuel-rich conditions were investigated in the past: to date, flame structures data for stoichiometric and fuel-lean conditions are missing and no data are available above atmospheric pressure. Therefore, new experimental work is needed, particularly under high-pressure conditions

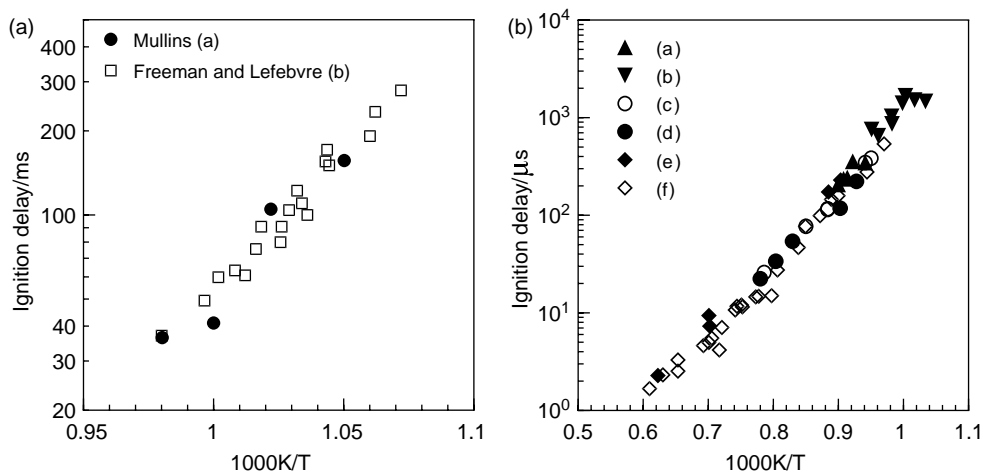


Fig. 1. Ignition delay of kerosene–air mixtures; (a): data (a) from [22], data (b) from [25]; (b) The data scaled to 20 atm [29] were taken from [29] for (a): Jet A at 30 atm), from [29] for (b): JP-8 at 30 atm), from [28] for (c): Jet A at 20 atm), from [28] for (d): jet A at 10 atm), from [27] for (e): kerosene at 10 atm), and from [27] for (f): Jet A at 10 atm).

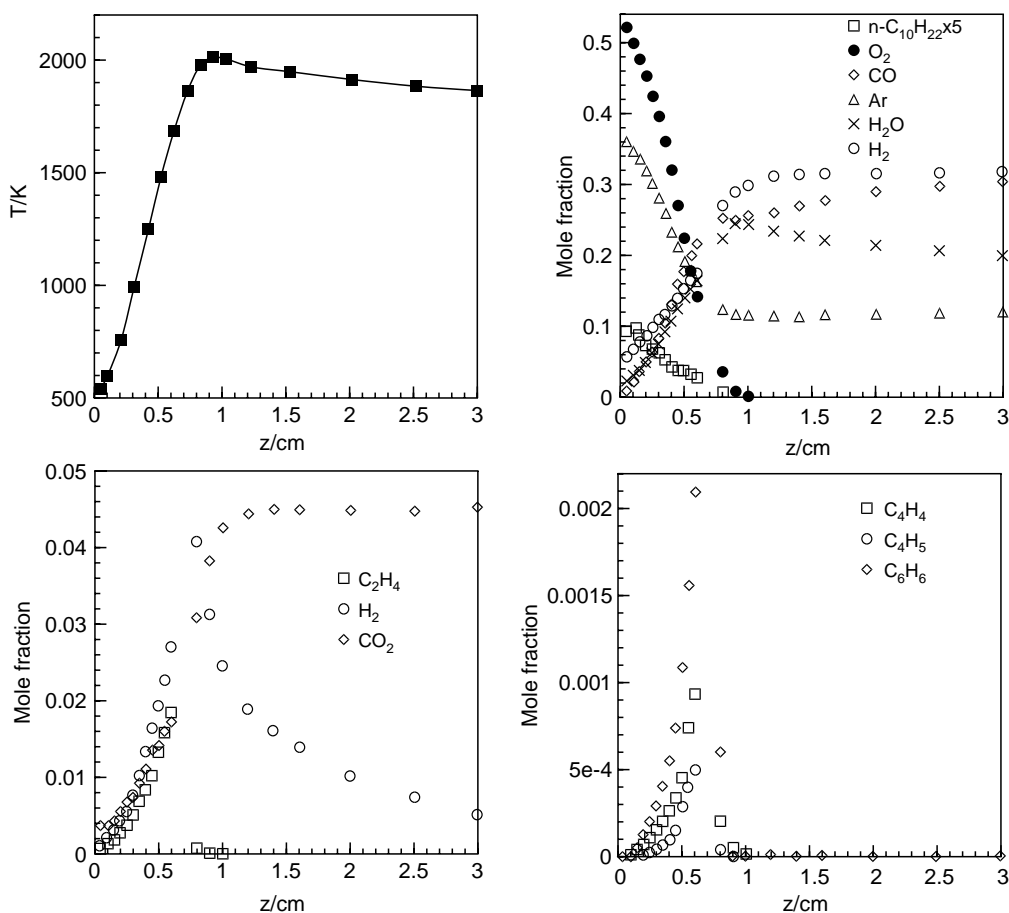


Fig. 2. Flame structure under low pressure conditions: 8% of kerosene TR0, 56.4% oxygen, 35.6% argon in mol, 6 kPa, equivalence ratio of 2.2 [30,32].

relevant to aero-jet engine operating conditions, to improve the existing database. The available flame structures at low-pressure are presented in Fig. 2 whereas Fig. 3 presents the available data at atmospheric pressure. The burning velocity of Jet A–1–air mixtures were recently measured at atmospheric pressure [34], extending the existing flame database (Fig. 4). Measurements under high-pressure conditions are missing, although they are needed to test the proposed kinetic schemes. Lots of data were obtained for the kinetics of oxidation of kerosene in diluted conditions using jet-stirred reactors (JSR) operated over a very wide range of conditions: $0.2 \leq \text{equivalence ratio} \leq 2.5$, $1 \leq P/\text{atm} \leq 40$, $550 \leq T/\text{K} \leq 1300$. The data consisted of mole fraction profiles of stable species (reactants, intermediates and products) measured as a function of residence time or temperature, by low pressure sonic probe sampling and GC analyses. The most relevant available data are presented in Figs. 5–26.

4.2. Surrogates

Several surrogate fuels have been used in order to propose detailed chemical kinetic schemes of reasonable complexity for the oxidation of kerosene. They consisted initially of *n*-decane for which many kinetic studies [30–32,35–37,40–46] appear in the literature. Most of the concentration profiles obtained from the oxidation of *n*-decane or kerosene in a JSR were very similar [36], as were the *n*-decane and kerosene flame structures [30,32]. Unfortunately, this simple surrogate showed poor predictions of benzene formation in a JSR [36] and flat flame burner experiments [30,32,44]. These findings are illustrated in Fig. 27. The higher concentration of benzene produced during the oxidation of the Jet A-1 fuel was attributed to the initial aromatic fraction present in the commercial fuel that produces benzene by oxidation. Taking into account the Jet A-1 chemical composition, Guéret et al. [35] studied the oxidation of a three-components model-fuel (79%

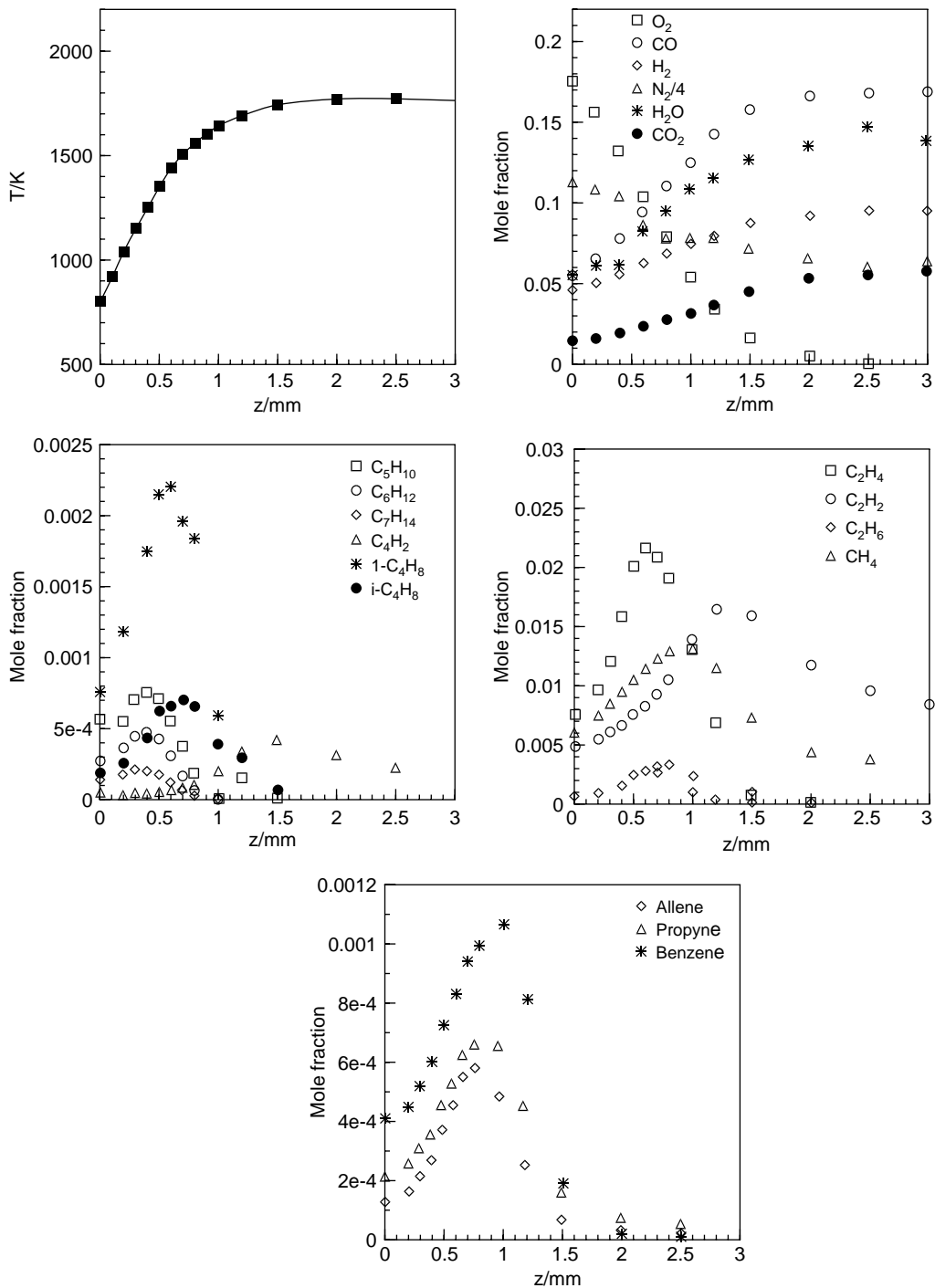


Fig. 3. Flame structure under atmospheric pressure conditions: 2.95% of kerosene TR0, 28.64% oxygen, 68.41% nitrogen in mol, equivalence ratio of 1.7 [31].

n-undecane, 10% *n*-propylcyclohexane, 11% 1,2,4-trimethylbenzene, in mol) at variable residence time and fixed temperature, in diluted conditions using an atmospheric JSR (Fig. 28). Although these data were

limited, they showed [35] a reasonable agreement between the profiles obtained from the oxidation of this surrogate and Jet A-1 for the main species. Cooke et al. [47] studied the combustion of a six-component model

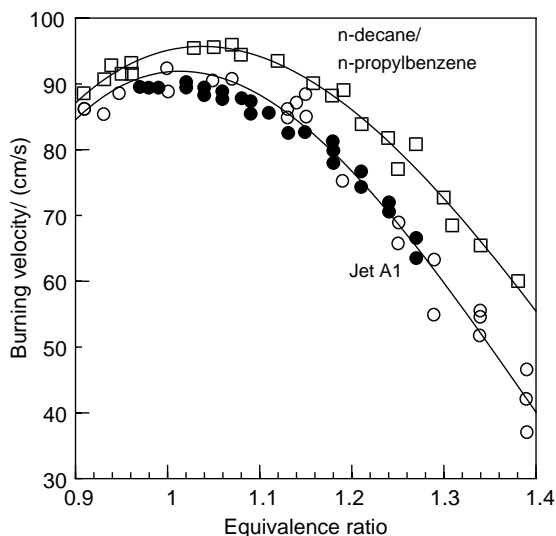


Fig. 4. Burning velocity of kerosene (Jet A-1)-air and *n*-decane/*n*-propylbenzene (80/20 wt) at atmospheric pressure and 473 K [34].

fuel (10% *iso*-octane, 20% methylcyclohexane, 15% *m*-xylene, 30% *n*-dodecane, 5% tetralin, 20% *n*-tetradecane, in mol) in non-sooting counterflow diffusion flames. The temperature profiles measured at variable distance from the fuel injection were compared for JP-8 and the surrogate mixture. They were found in close agreement, validating the selected surrogate mixture. Agosta et al. [48] studied the low-temperature oxidation of three two-components model-fuels (*n*-dodecane 40%, 2,2,4,4,6,8,8-heptamethylnonane 60%;

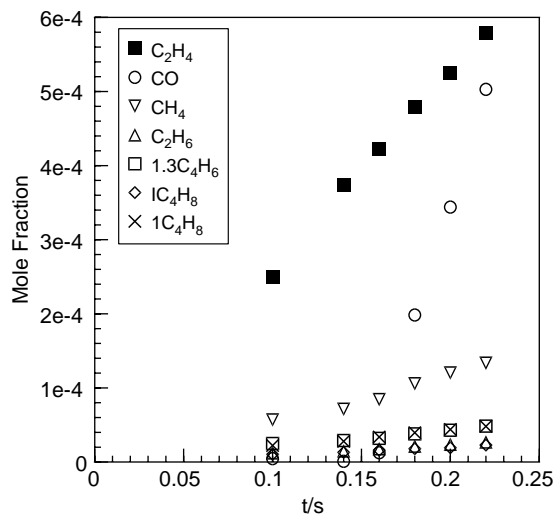


Fig. 5. Oxidation of kerosene in a JSR at 1 atm and 923 K (initial conditions: 0.1% kerosene TR0, 8.25% O₂, diluent nitrogen) [35].

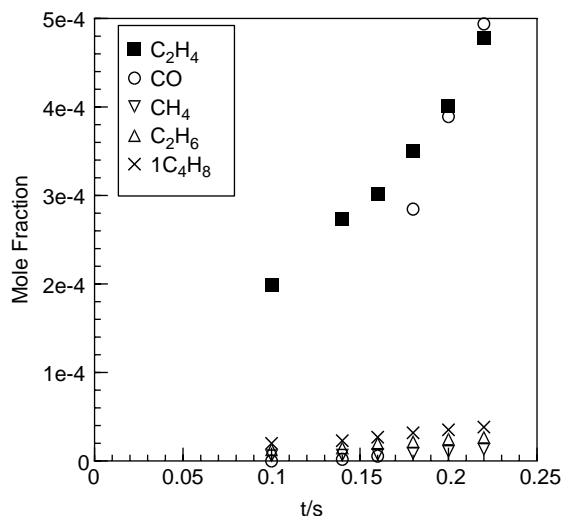


Fig. 6. Oxidation of kerosene in a JSR at 1 atm and 973 K (initial conditions: 0.1% kerosene TR0, 1.65% O₂, diluent nitrogen) [35].

n-dodecane 37%, methylcyclohexane 63%; *n*-dodecane 51%, α -methyl-naphthalene 49%, in mol). They measured the mole fractions of carbon monoxide in the cool flame regime (600–900 K) by water-cooled probe sampling and non-dispersive IR (Fig. 29). The burning velocity of *n*-decane-*n*-propylbenzene (80/20 in weight)/air mixtures were recently measured at atmospheric pressure [34] using a cone flame, extending the existing flame database. This study showed that the burning velocities of kerosene Jet A-1 are comparable but slightly lower than those of this surrogate mixture (Fig. 4).

Recently, other simple surrogates were tested. Among them, mixtures of *n*-decane and *n*-propylbenzene [34,39] and of *n*-decane and 1,2,4-trimethylbenzene [39] were tested experimentally in dilute conditions. JSR experiments performed on the oxidation of these surrogates at 10 atm have been instrumental in providing the details requested to develop a kinetic reaction scheme. The experimental set-up [40], consisted of a fused silica jet-stirred reactor equipped with an atomizer-vaporizer assembly operating at high temperatures (up to ca. 300 °C) allowing the vaporization of the heavier components of kerosene. This facility was designed to examine the low- and high-temperature chemical processes without complications due to diffusion or indeterminate reaction time-zero resulting from indeterminate nature of the mixing process which can happen in ‘plug’ flow reactors. The temperature range of emphasis was 800–1250 K, corresponding

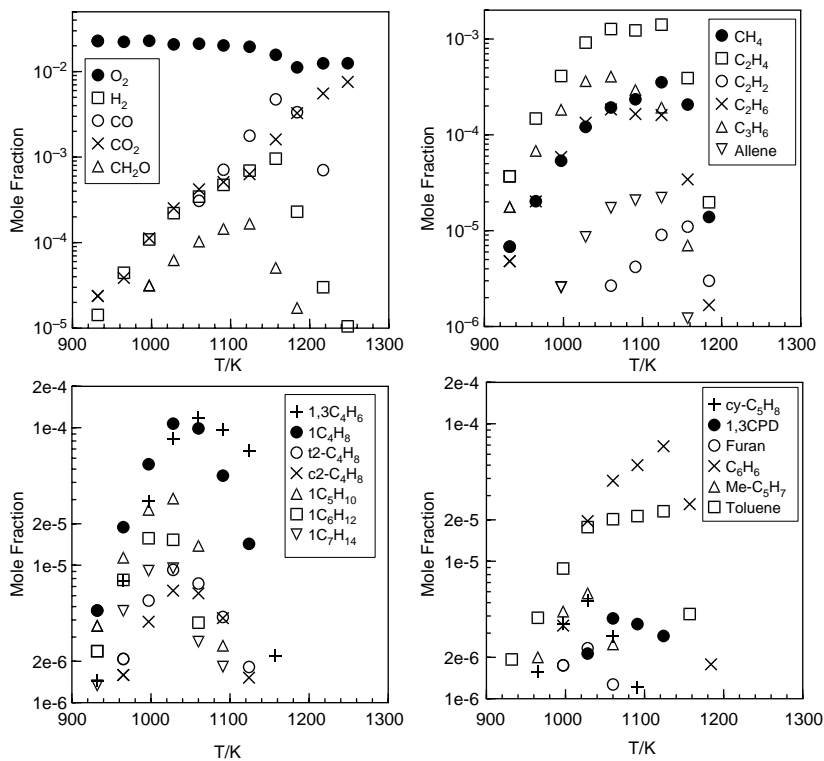


Fig. 7. Oxidation of kerosene in a JSR at 1 atm and $t=0.07$ s (initial conditions: 0.07% kerosene TR0, 2.31% O₂, diluent nitrogen) [38].

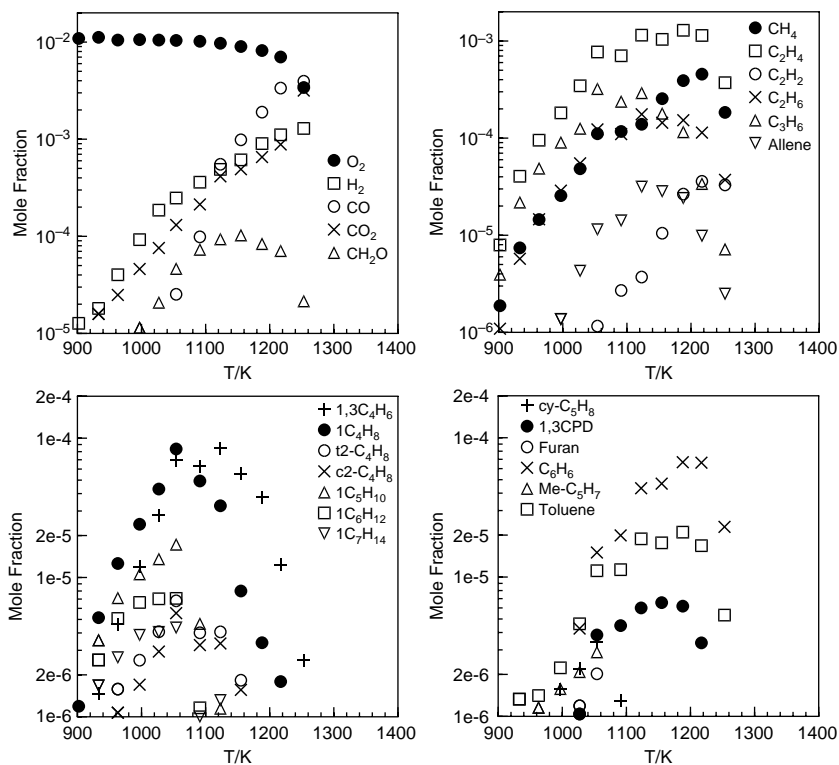


Fig. 8. Oxidation of kerosene in a JSR at 1 atm and $t=0.07$ s (initial conditions: 0.07% kerosene TR0, 1.155% O₂, diluent nitrogen) [38].

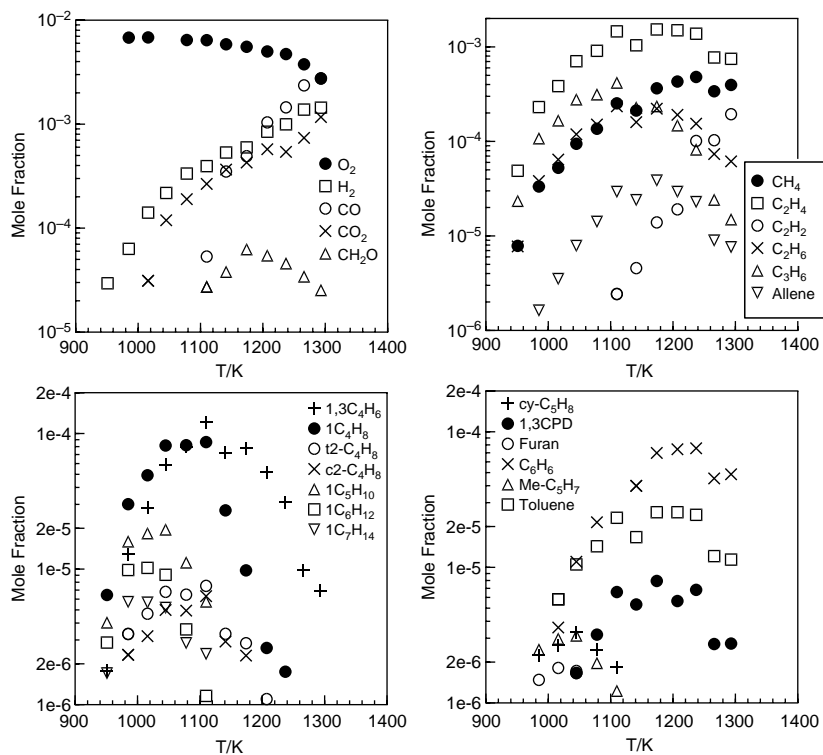


Fig. 9. Oxidation of kerosene in a JSR at 1 atm and $t=0.07$ s (initial conditions: 0.07% kerosene TR0, 0.77% O₂, diluent nitrogen) [38].

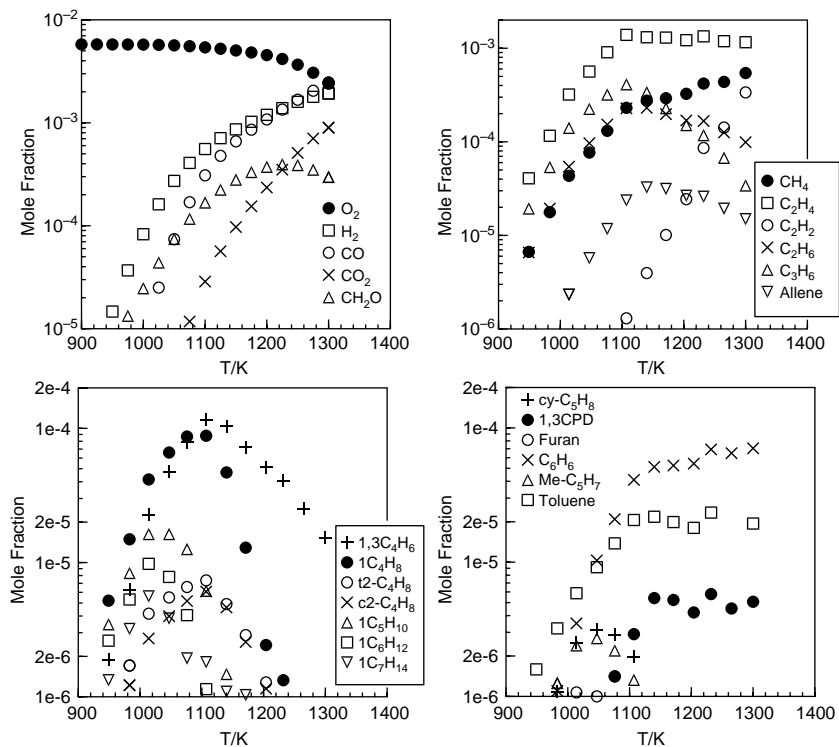


Fig. 10. Oxidation of kerosene in a JSR at 1 atm and $t=0.07$ s (initial conditions: 0.07% kerosene TR0, 0.5775% O₂, diluent nitrogen) [38].

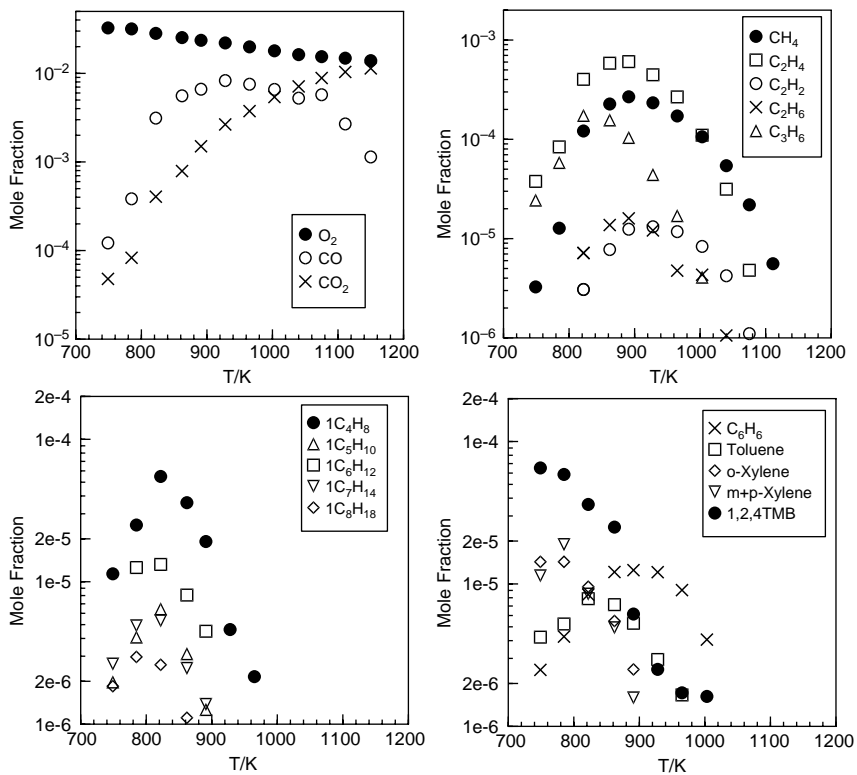


Fig. 11. Oxidation of kerosene in a JSR at 10 atm and $t=0.5$ s (initial conditions: 0.1% kerosene TR0, 3.3% O₂, diluent nitrogen) [36].

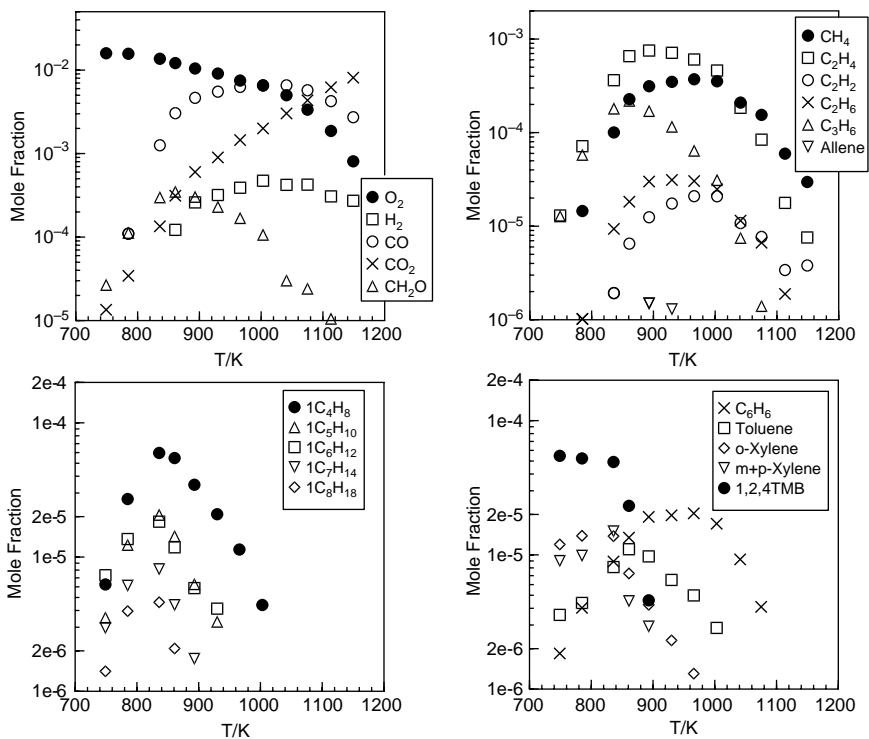


Fig. 12. Oxidation of kerosene in a JSR at 10 atm and $t=0.5$ s (initial conditions: 0.1% kerosene TR0, 1.65% O₂, diluent nitrogen) [36].

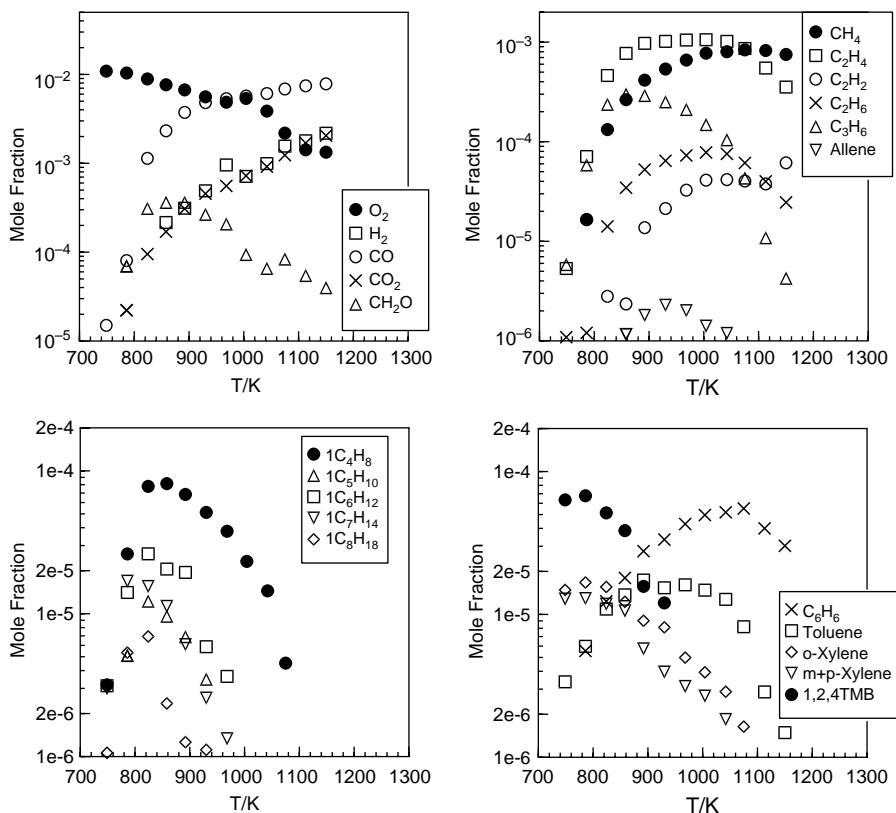


Fig. 13. Oxidation of kerosene in a JSR at 10 atm and $t=0.5$ s (initial conditions: 0.1% kerosene TR0, 1.1% O₂, diluent nitrogen) [36].

to that of the beginning reaction zone in flames where the primary fuel depletion chemistry occurs. A large set of data consisting of mole fraction profiles as a function of varied experimental conditions (temperature, initial concentration, equivalence ratio, ϕ , mean residence time, t) was obtained. The reactants, stable intermediates and products were measured after sonic quartz probe sampling by gas chromatography (GC) using several detectors (Flame ionization detector, FID; thermal conductivity detector, TCD; mass spectrometry, MS). The GC analyses involved the use of four GCs. One GC operating with nitrogen as carrier gas and TCD detection was used to measure hydrogen. The other GCs used helium as carrier gas. A multicolumn and multi-detector GC was used to measure permanent gases and simple species (O₂, CO, CO₂, CH₂O, aldehydes). Another GC equipped with a Al₂O₃-KCl column and an FID detector was used to measure hydrocarbons up to C₇ whereas hydrocarbons >C₅ were analyzed using a GC-MS operating with a DB5-ms column. PAH were analyzed on line by means of a

GC/MS: The sample is delivered to the sampling loop of the GC via a deactivated transfer heated line (300 °C). The results of this study are reported in Figs. 30–38.

The comparison of the experimental profiles obtained for the oxidation of Jet A-1 and the surrogates shows that the tested surrogates do not fully represent the oxidation of Jet A-1 although a close agreement is observed for a large variety of species (Figs. 39 and 40). The measured mole fraction profiles for hydrogen, CO, CO₂, CH₂O, CH₄, C₂H₄, C₂H₂, C₃H₆, 1-C₄H₈, 1,3-C₄H₆, and 1-C₅H₁₀ are very similar for the various surrogates used and for Jet A-1. One can interpret these results by simply saying that *n*-decane represents well the *n*-alkane fraction of Jet A-1, confirming early findings [31,36]. The main differences appear for 1,3-cyclopentadiene, benzene, toluene, and styrene. There, the experiments show that the surrogates produce less 1,3-cyclopentadiene, less benzene, and less toluene than Jet A-1 does. Regarding the formation of styrene, the surrogate mixture

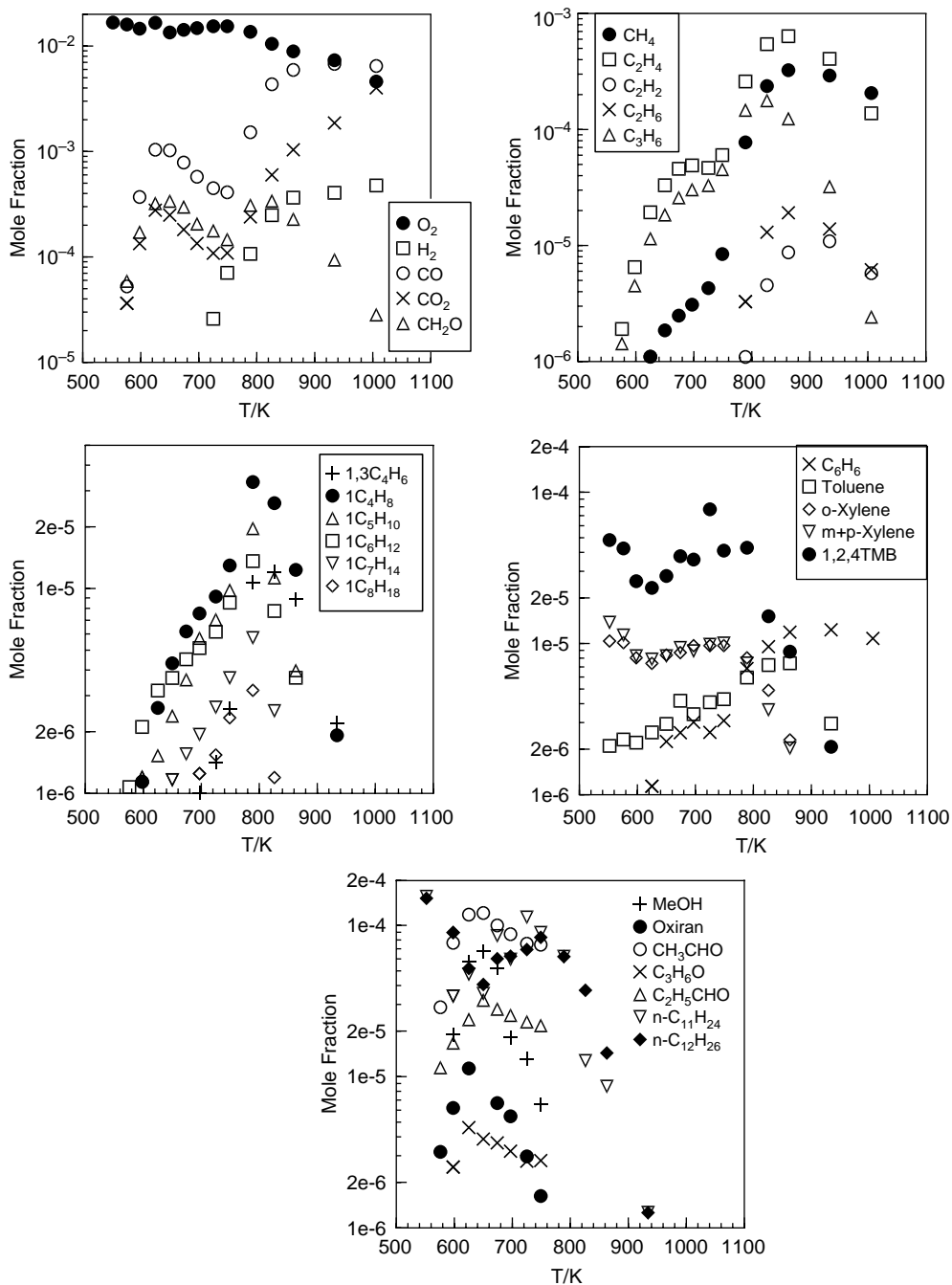
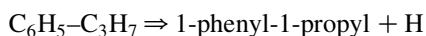
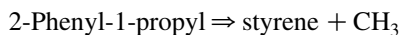
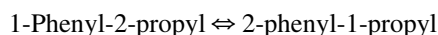


Fig. 14. Oxidation of kerosene in a JSR at 10 atm and $t = 1.0$ s (initial conditions: 0.1% kerosene TR0, 1.65% O₂, diluent nitrogen) [37].

containing 1,2,4-trimethylbenzene produces too little styrene whereas the surrogates containing *n*-propylbenzene produce too much styrene. This is due to the fact that *n*-propylbenzene oxidation yields fair amounts of styrene by oxidation of the *n*-propyl group [55], whereas 1,2,4-trimethylbenzene does not since it has only methyl groups:



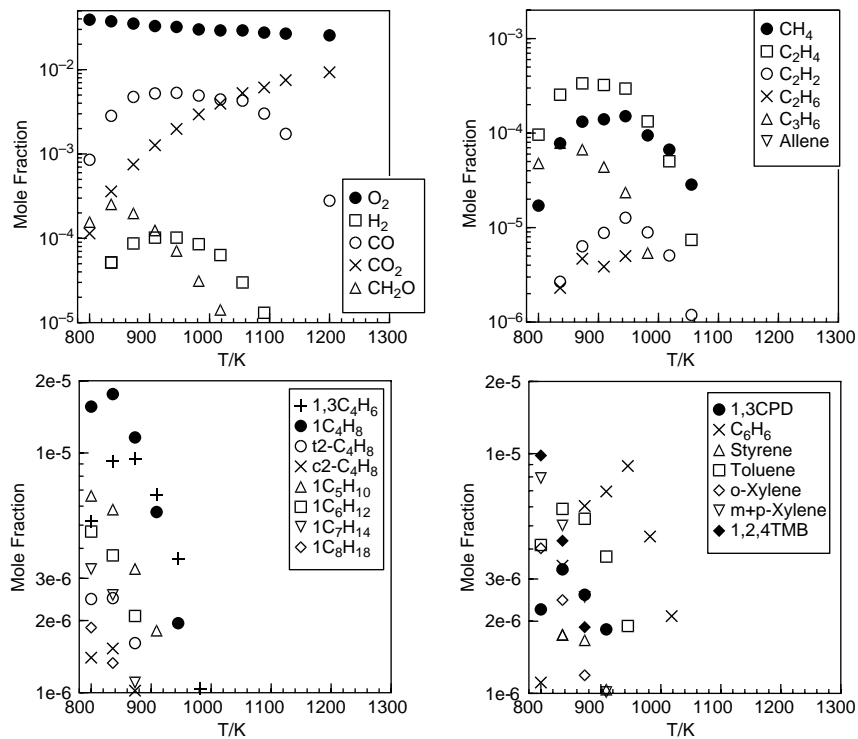


Fig. 15. Oxidation of kerosene in a JSR at 10 atm and $t=0.5$ s (initial conditions: 0.067% Jet A-1, 4.422% O_2 , diluent nitrogen) [39].

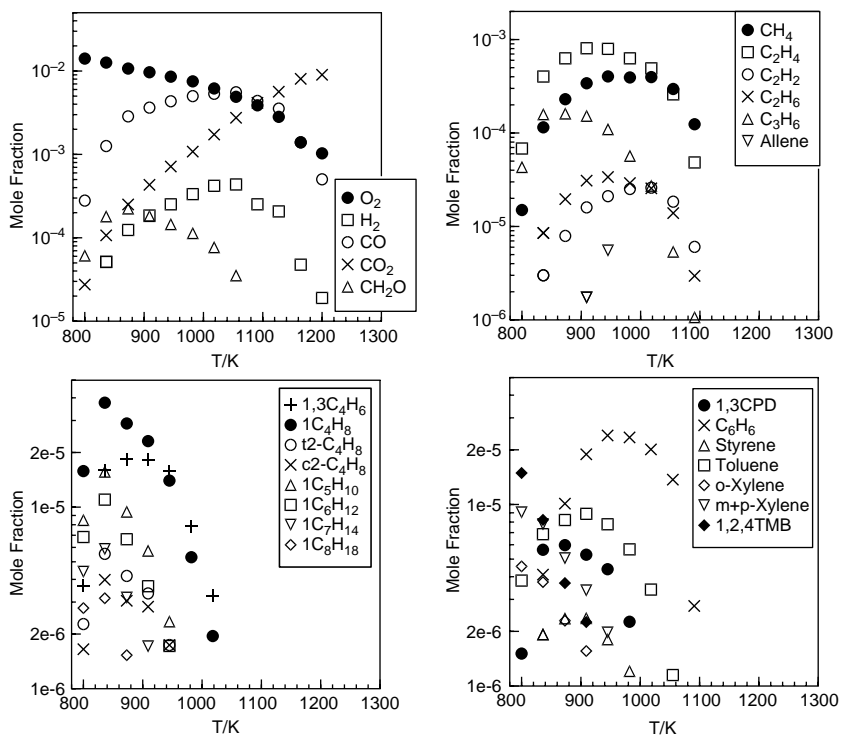


Fig. 16. Oxidation of kerosene in a JSR at 10 atm and $t=0.5$ s (initial conditions: 0.067% Jet A-1, 1.474% O_2 , diluent nitrogen) [39].

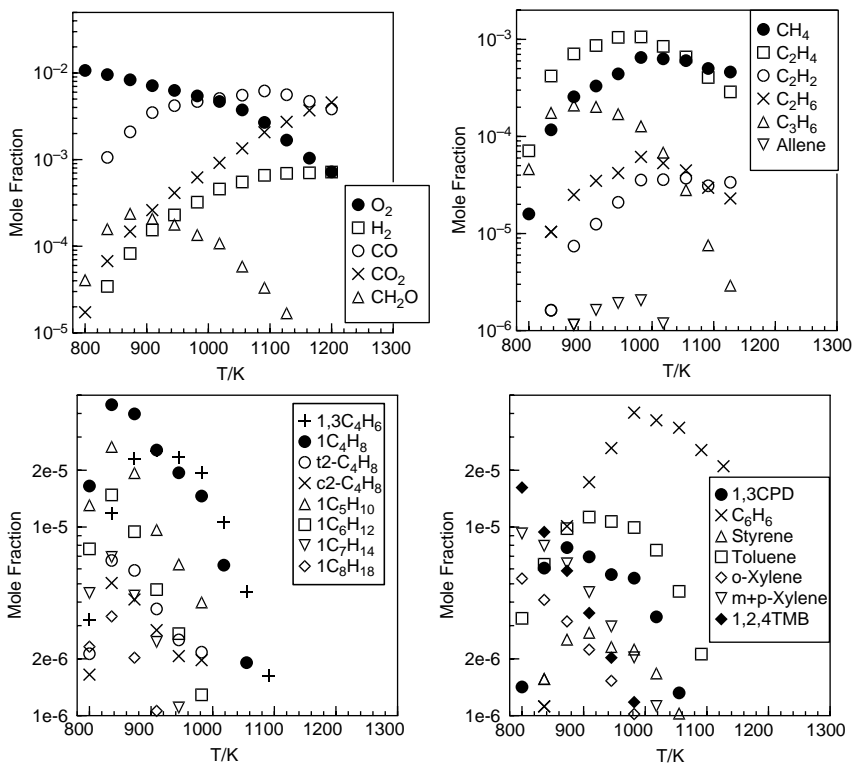


Fig. 17. Oxidation of kerosene in a JSR at 10 atm and $t=0.5$ s (initial conditions: 0.067% Jet A-1, 1.1055% O_2 , diluent nitrogen) [39].

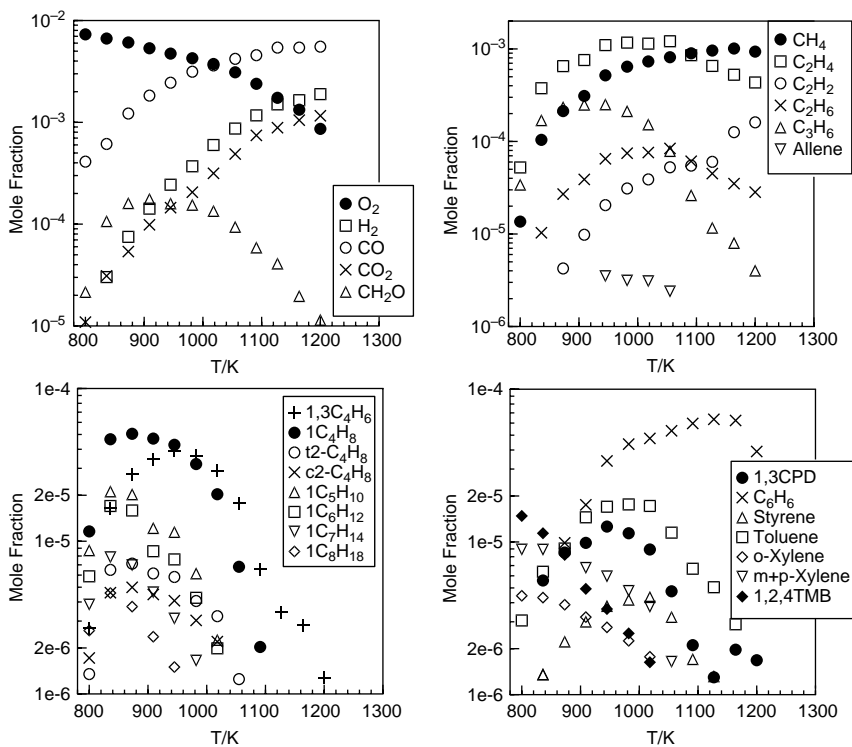


Fig. 18. Oxidation of kerosene in a JSR at 10 atm and $t=0.5$ s (initial conditions: 0.067% Jet A-1, 0.737% O_2 , diluent nitrogen) [39].

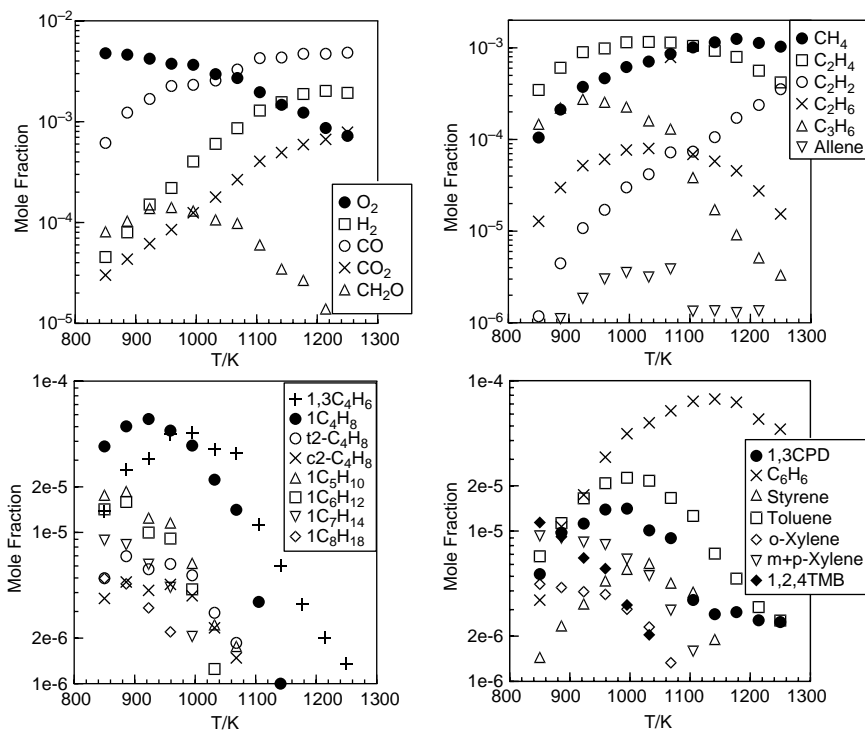


Fig. 19. Oxidation of kerosene in a JSR at 10 atm and $t=0.5$ s (initial conditions: 0.067% Jet A-1, 0.5527% O_2 , diluent nitrogen) [39].

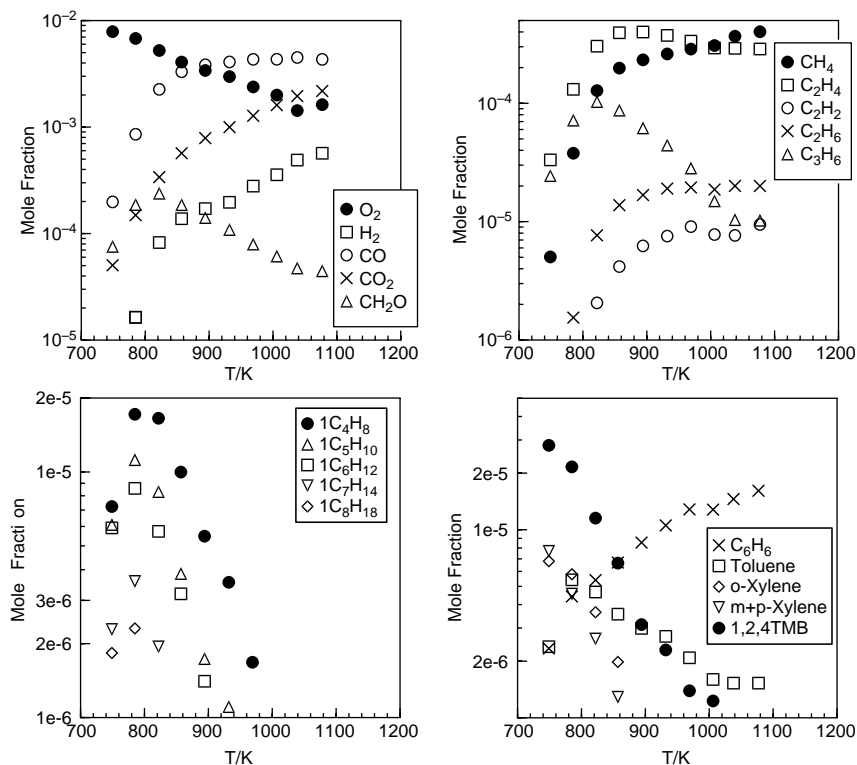


Fig. 20. Oxidation of kerosene in a JSR at 20 atm and $t=1.0$ s (initial conditions: 0.05% kerosene TR0, 0.825% O_2 , diluent nitrogen) [39].

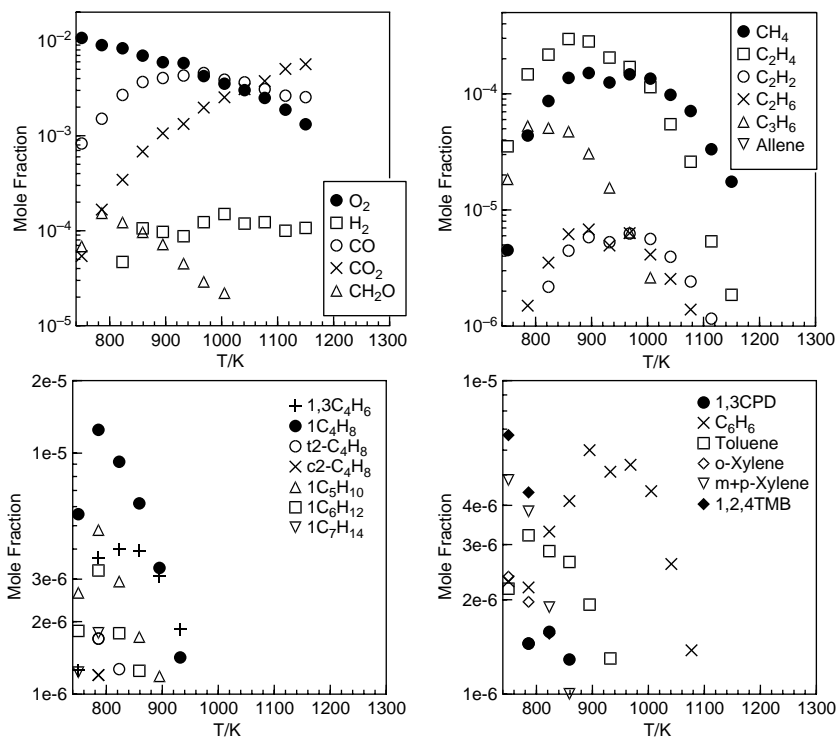


Fig. 21. Oxidation of kerosene in a JSR at 20 atm and $t = 1.0$ s (initial conditions: 0.05% Jet A-1, 1.1% O₂, diluent nitrogen) [39].

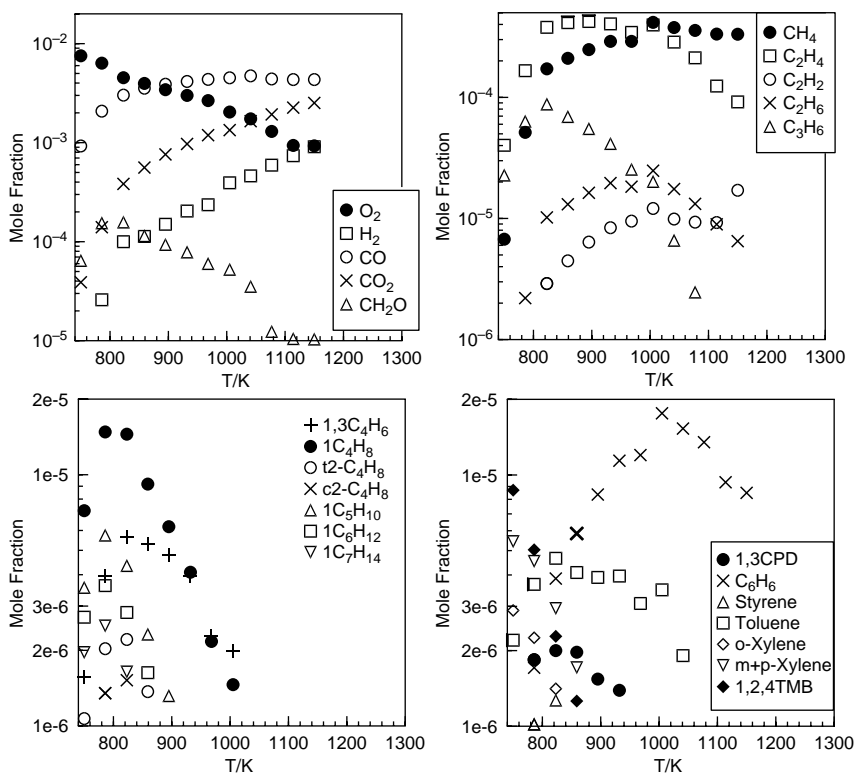


Fig. 22. Oxidation of kerosene in a JSR at 20 atm and $t = 1.0$ s (initial conditions: 0.05% Jet A-1, 0.825% O₂, diluent nitrogen) [39].

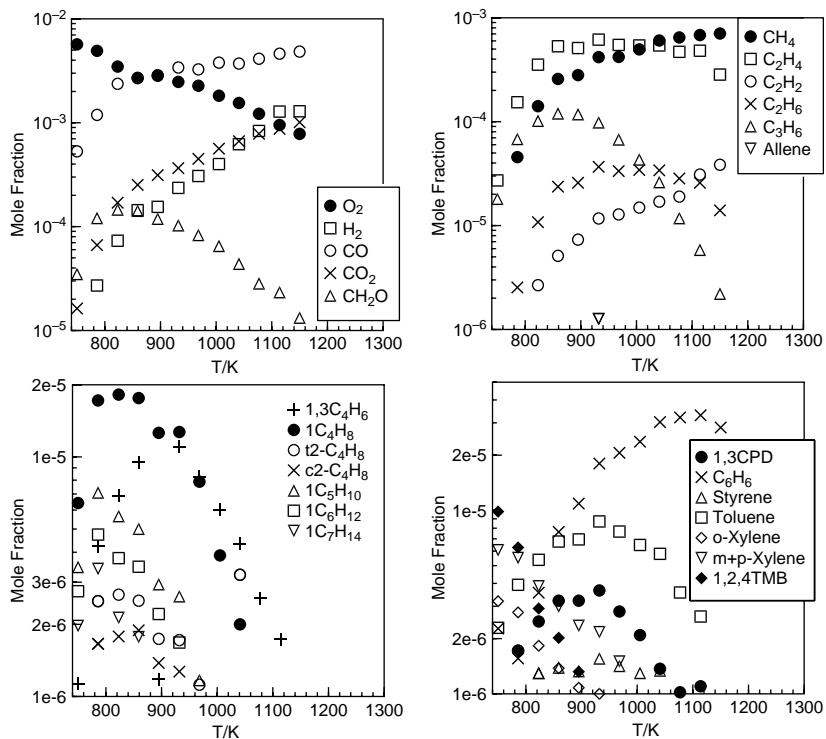


Fig. 23. Oxidation of kerosene in a JSR at 20 atm and $t = 1.0$ s (initial conditions: 0.05% Jet A-1, 0.55% O_2 , diluent nitrogen) [39].

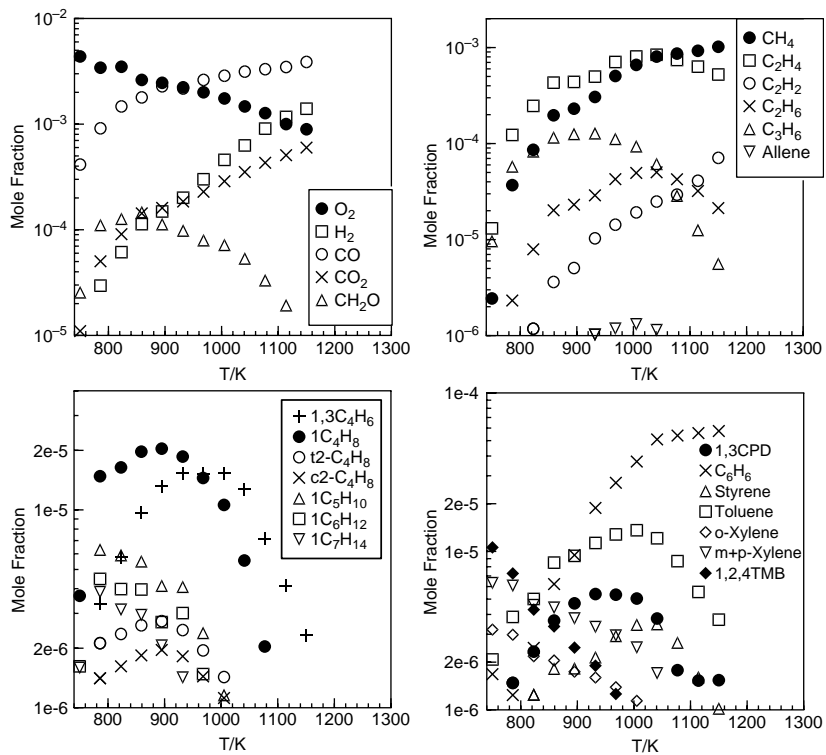


Fig. 24. Oxidation of kerosene in a JSR at 20 atm and $t = 1.0$ s (initial conditions: 0.05% Jet A-1, 1.1% O_2 , diluent nitrogen) [39].

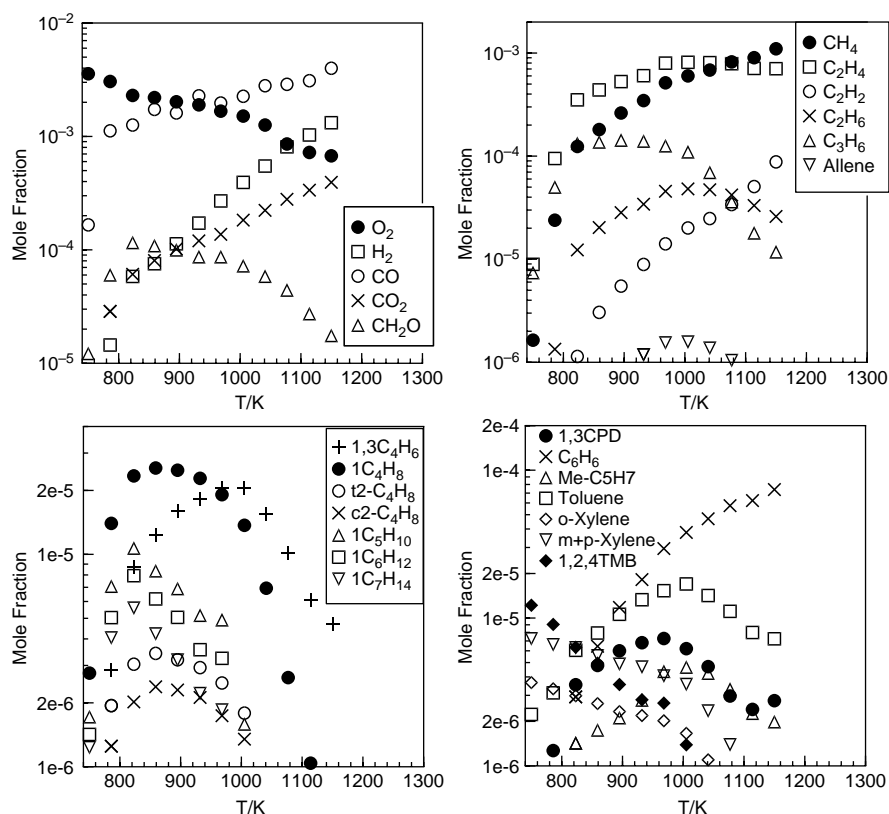
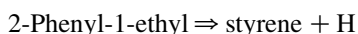
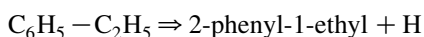
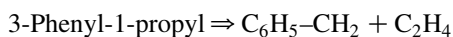
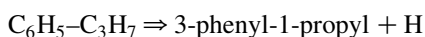
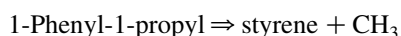


Fig. 25. Oxidation of kerosene in a JSR at 20 atm and $t=1.0$ s (initial conditions: 0.05% Jet A-1, 0.33% O₂, diluent nitrogen) [39].



The structures of the species involved in these equations are given in Table 4.

Fig. 40 shows that the increase in the initial mole fraction of *n*-propylbenzene in the surrogate mixture only moderately changes the results but those of the aromatic hydrocarbons (benzene, toluene, and styrene) for which the maximum mole fractions increase with increasing initial mole fraction of *n*-propyl benzene. These results demonstrate that it is difficult to represent the non-alkane fraction of Jet A-1 by a single

component such as *n*-propylbenzene or 1,2,4-trimethylbenzene [38].

5. Literature survey of the chemical kinetic modeling of the combustion of Jet A-1/JP-8

Table 5 summarizes the kinetic models proposed for simulating the combustion of kerosene in various conditions. The simplest published kinetic model for the combustion of kerosene is the one step reaction mechanism with a global rate expression used by Najjar and Goodger [50] to model the oxidation of this fuel. Such a rate expression was also used, after a slight modification, by Aly and Salem [51] to predict premixed laminar flame characteristics of a commercial kerosene fuel.

In an approach to elaborate more refined kinetic models, Guéret et al. [35] used quasi-global reaction mechanisms to simulate the concentration profiles of the main products of the oxidation of a TR0 (JP-8) kerosene in a jet-stirred reactor at atmospheric pressure. These mechanisms involved a global molecular

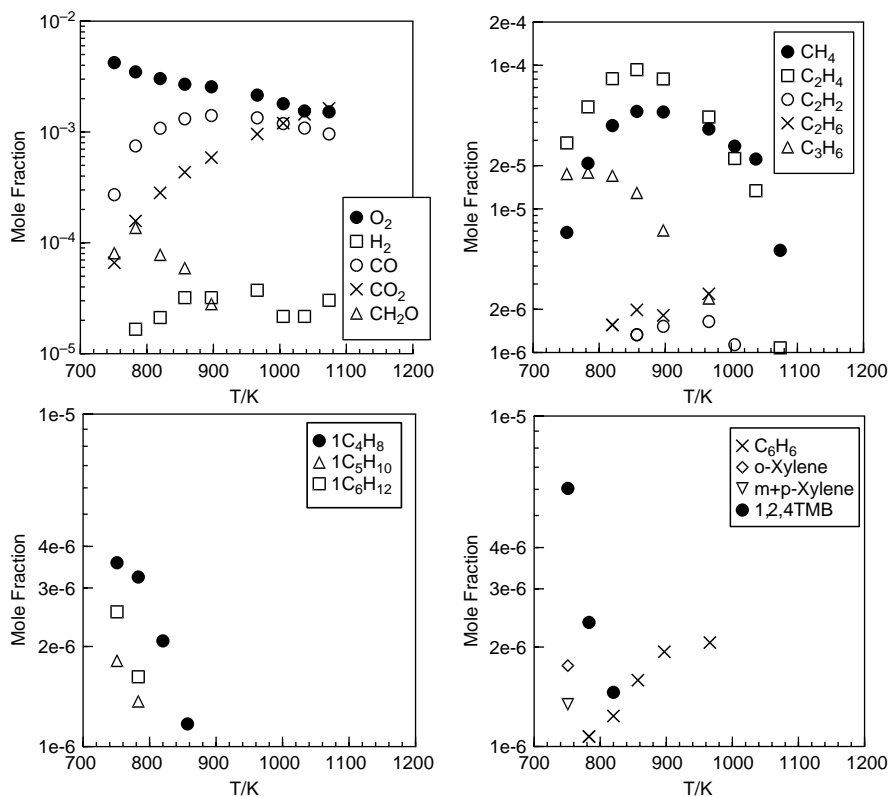


Fig. 26. Oxidation of kerosene in a JSR at 40 atm and $t=2.0$ s (initial conditions: 0.025% kerosene TR0, 0.4125% O₂, diluent nitrogen) [36].

reaction for the oxidation of the initial fuel molecules and a detailed mechanism for the oxidation of the smaller intermediate hydrocarbons. Such a semi-global mechanism was used to model the oxidation of a surrogate mixture containing *n*-undecane, *n*-propylcyclohexane and 1,2,4-trimethylbenzene. It was shown that the experimental concentration profiles of the main species measured during the oxidation of this surrogate and of a TR0 (JP-8) kerosene were very similar. The composition of the surrogate mixture, which was based on a broad chemical analysis of the kerosene, was the following (in % by mass): 79% for the alkane, 10% for the cycloalkane, and 11% for the aromatic.

Later, the experimental investigations in an atmospheric jet-stirred reactor were extended to *n*-decane, and the major products of the oxidation of this alkane were shown to follow the same evolution as those of kerosene [52]. A detailed mechanism describing the oxidation of *n*-decane was developed. It was able to predict the experimental data obtained for the oxidation of *n*-decane and kerosene [52] with reasonable accuracy.

Further oxidation experiments of kerosene TR0 and of *n*-decane were performed by Dagaut et al.

[36,37,40] in a jet-stirred reactor operating at higher pressure (10–40 atm) over an extended temperature range (550–1550 K). These experiments confirmed the strong kinetic similarity between the oxidation of *n*-decane and kerosene TR0. The detailed mechanism developed previously for the oxidation of *n*-decane in the intermediate and high temperature range (above 800 K) was adapted to the pressure range 10–40 atm giving a general good agreement with experimental data obtained for *n*-decane oxidation, and also for the major species of kerosene oxidation [36–40].

All these results indicate that the alkane portion of kerosene is the most reactive. Its relatively fast oxidation produces the necessary active species for the oxidation of the fuel mixture. The other chemical families do not have a pronounced effect on the overall oxidation kinetics of this complex mixture. However, the aromatic and the naphthenic fraction of kerosene have a few specific oxidation products: in particular, toluene, xylenes, and trimethylbenzenes were not found in the products of the oxidation of *n*-decane in a jet-stirred reactor [36,37,40], indicating that they are the products of the oxidation of the alkylbenzene family in

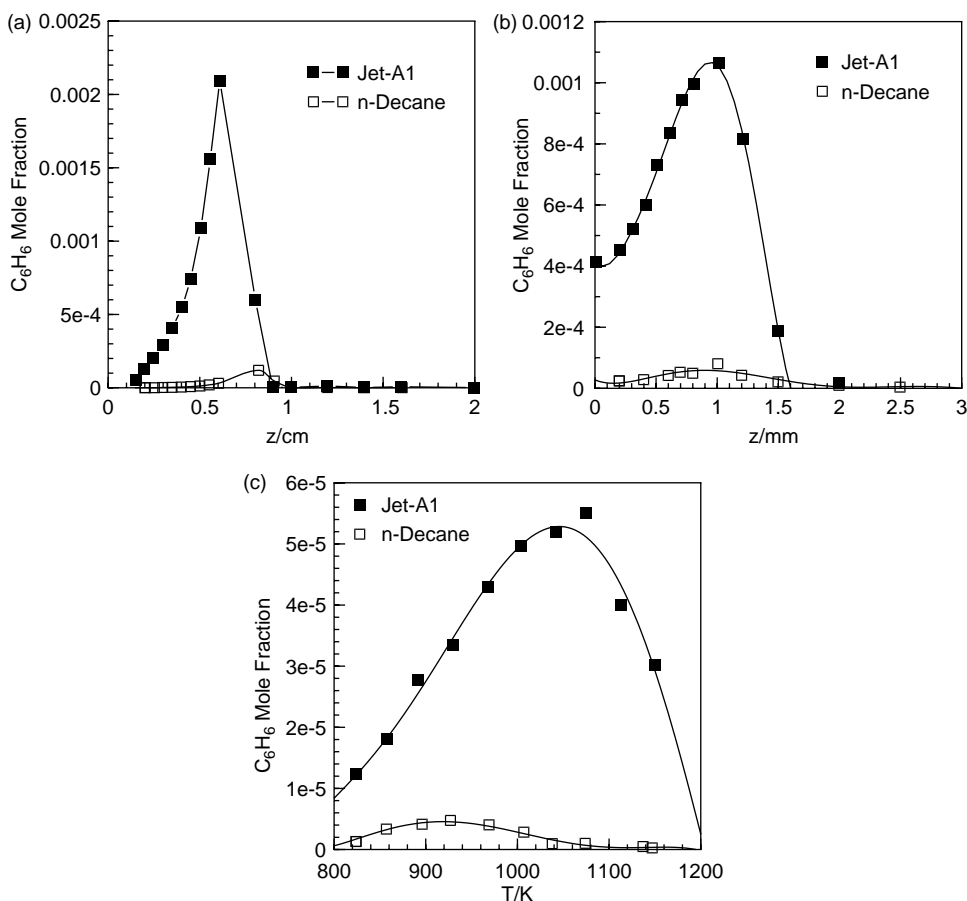


Fig. 27. Benzene experimental profiles obtained from the oxidation of Jet A-1 and *n*-decane [32,44]: (a) flat flame burner results obtained at low-pressure (6 kPa, $\Phi=2.2$, flame diameter 9.5 cm, gas velocity at burner exit 24 cm/s at 298K and 1 atm; 8.0% of *n*-decane, 56.4% of oxygen, 35.6% of argon; 7.6% of kerosene, 56.8% of oxygen, 35.6% of argon), (b) flat flame burner results [44] obtained at atmospheric pressure (101 kPa, $\Phi=1.7$, flame diameter 2.5 cm, gas velocity at burner exit 7.3 cm/s at 298 K and 1 atm; 3.2% of *n*-decane, 28.6% of oxygen, 68.2% of argon; 3.0% of kerosene, 28.6% of oxygen, 68.2% of argon), (c) JSR results [36] obtained for the oxidation of 0.1% *n*-decane (1.033% oxygen, balance nitrogen) and 0.1% kerosene (1.1% oxygen, balance nitrogen) at 1 MPa, $\Phi=1.5$, $t=0.5$ s.

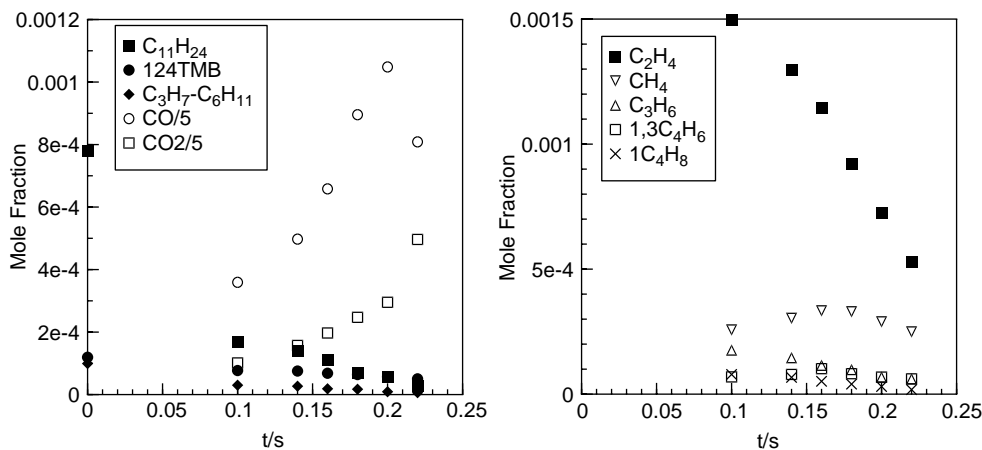


Fig. 28. Oxidation of a kerosene surrogate mixture in a JSR at 1 atm and 1023 K (initial conditions: 7900 ppmv *n*- $C_{11}H_{24}$, 1000 ppmv *n*-propylbenzene, 1100 ppmv 1,2,4-trimethylbenzene, 7.85% O_2 , diluent nitrogen) [35].

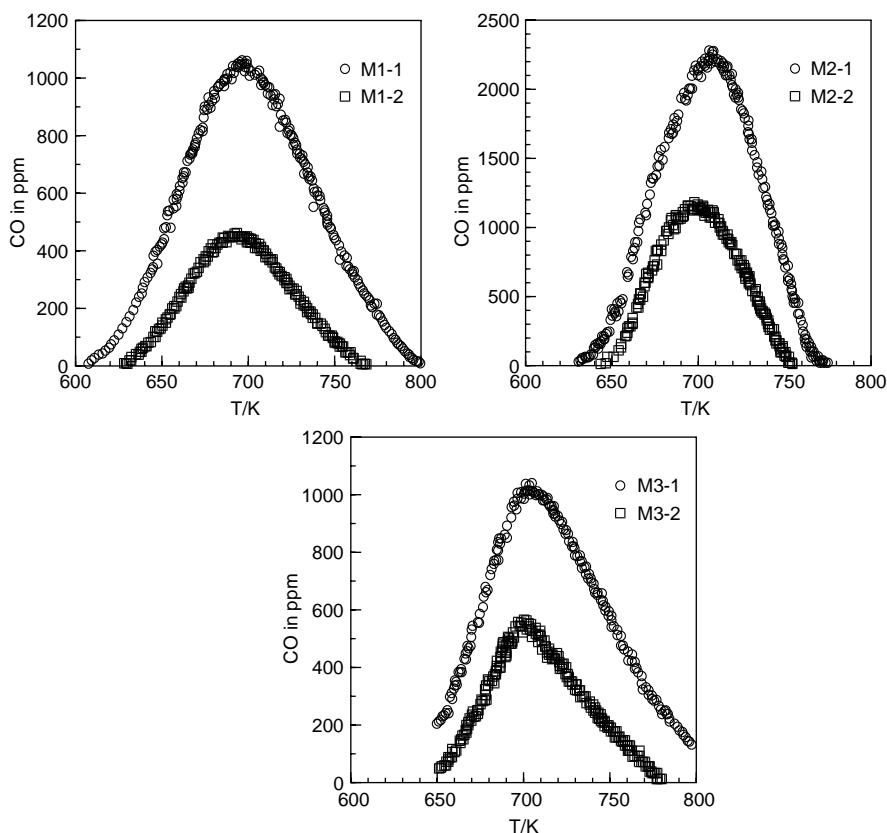


Fig. 29. CO production from the oxidation in a flow reactor at 8 atm, $\phi=0.3$, 120 ms of surrogate mixtures: M1-1, 40% *n*-dodecane and 60% 2,2,4,4,6,8,8-heptamethylnonane, 870 ppmv of fuel; M2-1, 37% *n*-dodecane and 63% methylcyclohexane, 1516 ppmv of fuel; M2-2, 37% *n*-dodecane and 63% methylcyclohexane, 1011 ppmv of fuel; M3-1, 51% *n*-dodecane and 49% α -methylnaphtalene, 1220 ppmv of fuel; M3-2, 51% *n*-dodecane and 49% α -methylnaphtalene, 814 ppmv of fuel) [48].

kerosene. It was also observed that the concentration of benzene measured during the oxidation of kerosene was significantly higher than that found among the products of *n*-decane [36,37,40]. This is not surprising since benzene is one of the products of the oxidation of toluene, xylenes and higher alkyl benzenes [53–55], which constitute the aromatic fraction of kerosene.

Studies performed on rich premixed flames of *n*-decane and TR0 kerosene, stabilized on a flat flame burner at pressure lower [30] or equal to 1 atm [31], showed similar results: a close similarity was observed for the mole fraction profiles of major species and main intermediates measured in both flames, except for benzene which was found at a much higher concentration in kerosene flames [32]. These experimental observations lead Vovelle et al. [30] to use a mechanism involving an aromatic (toluene) in addition to *n*-decane to model their low-pressure kerosene flame.

Later, the 1 atm rich flame of Douté et al. [31] was modeled by Lindstedt and Maurice [56] using a detailed mechanism for a kerosene model fuel containing *n*-decane, to represent the paraffin component, and various aromatic components. A reasonable agreement between the modeling and the data was obtained by the authors for the major species. The different surrogate fuel blends used in the modeling were made of 89 mol% *n*-decane and 11 mol% benzene, or toluene, or ethylbenzene or ethylbenzene/naphthalene. This modeling study showed that benzene cannot represent the aromatic component in kerosene fuels and that the inclusion of a higher aromatic is necessary. Surrogates incorporating toluene or ethylbenzene could reproduce with a good accuracy the concentrations of benzene in the kerosene laminar flame of Douté et al. [31].

Wang [57] proposed a quasi-global reaction scheme for kerosene combustion using a model-fuel of global

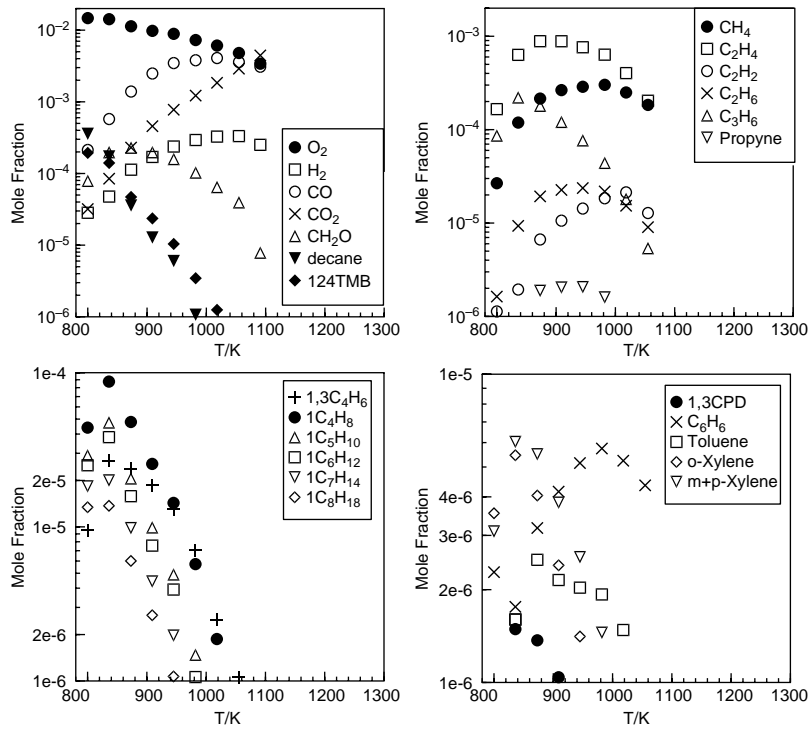


Fig. 30. Oxidation of a kerosene surrogate mixture in a JSR at 10 atm and $t=0.5$ s (initial conditions: 600 ppmv n -C₁₀H₂₂, 150 ppmv 1,2,4-trimethylbenzene, 1.48% O₂, diluent nitrogen) [39].

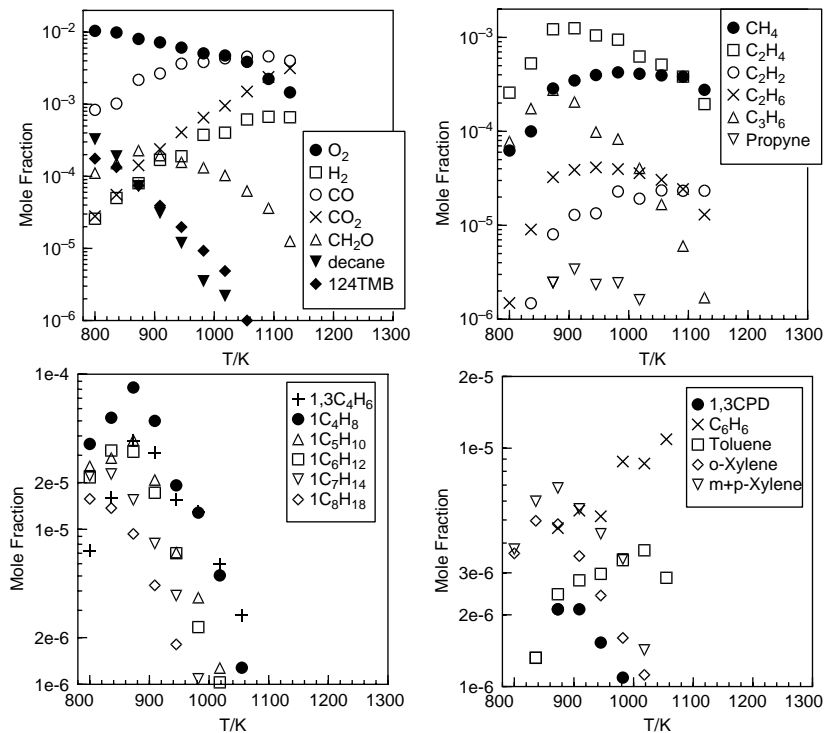


Fig. 31. Oxidation of a kerosene surrogate mixture in a JSR at 10 atm and $t=0.5$ s (initial conditions: 600 ppmv n -C₁₀H₂₂, 150 ppmv 1,2,4-trimethylbenzene, 1.11% O₂, diluent nitrogen) [39].

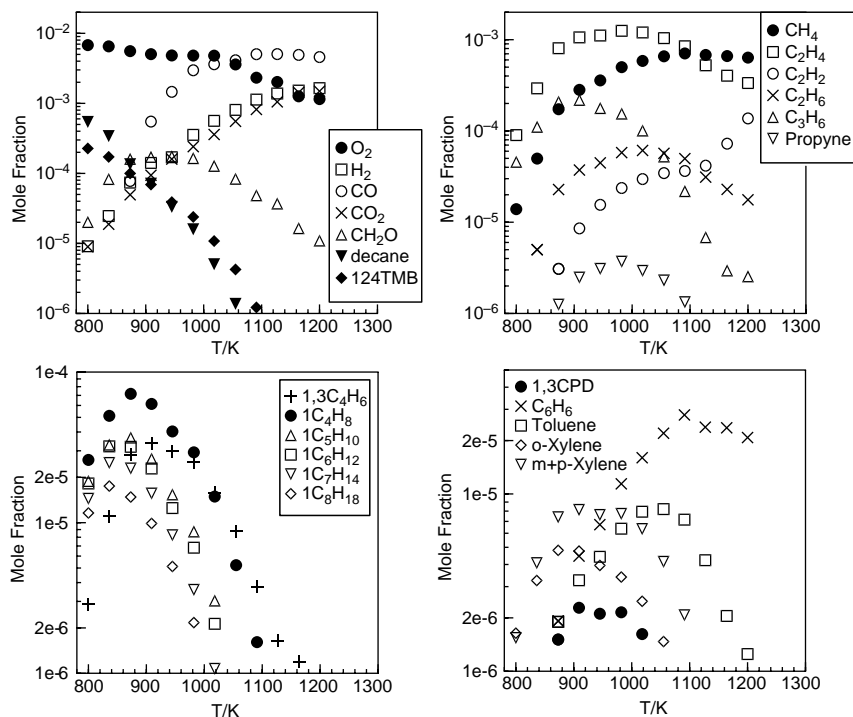


Fig. 32. Oxidation of a kerosene surrogate mixture in a JSR at 10 atm and $t=0.5$ s (initial conditions: 600 ppmv n - $C_{10}H_{22}$, 150 ppmv 1,2,4-trimethylbenzene, 0.74% O_2 , diluent nitrogen) [39].

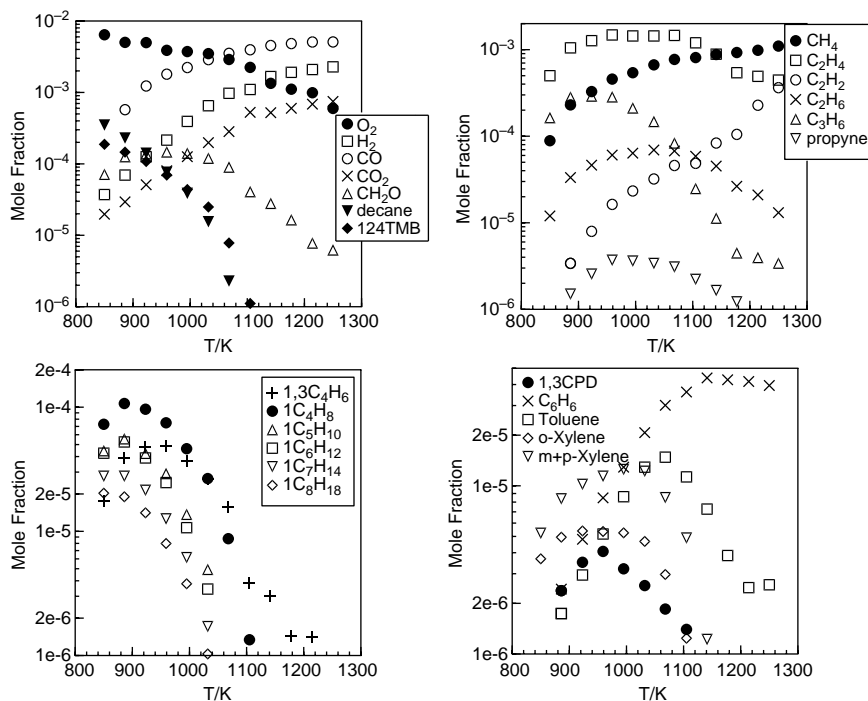


Fig. 33. Oxidation of a kerosene surrogate mixture in a JSR at 10 atm and $t=0.5$ s (initial conditions: 600 ppmv n - $C_{10}H_{22}$, 150 ppmv 1,2,4-trimethylbenzene, 0.555% O_2 , diluent nitrogen) [39].

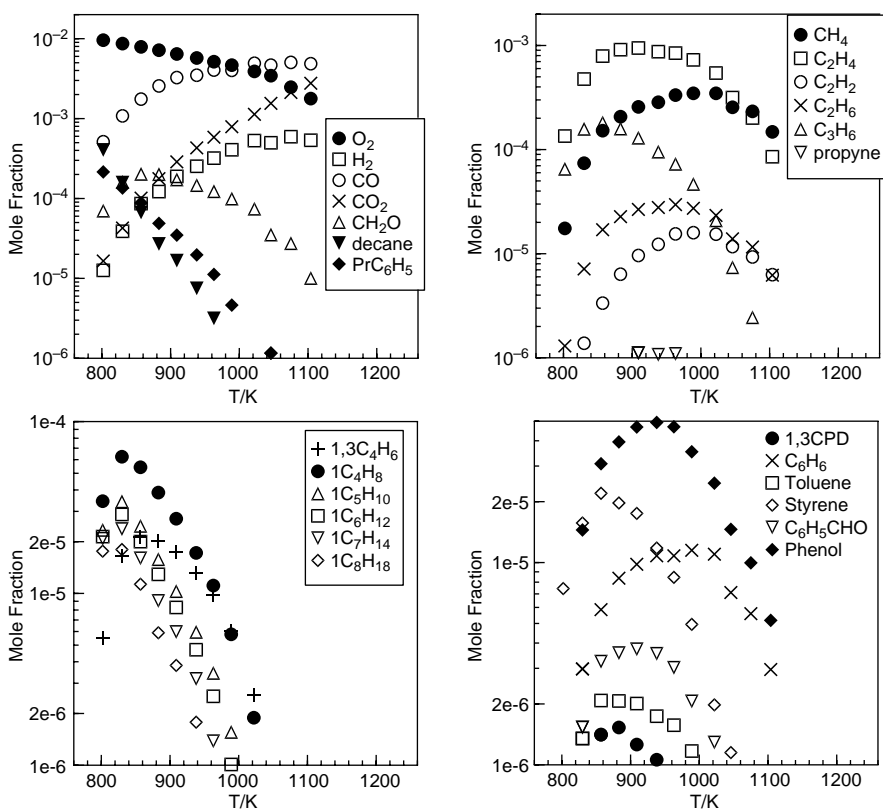


Fig. 34. Oxidation of a kerosene surrogate mixture in a JSR at 10 atm and $t=0.5$ s (initial conditions: 579 ppmv n -C₁₀H₂₂, 171 ppmv n -propylbenzene, 1.103% O₂, diluent nitrogen) [39].

formula C₁₂H₂₄ representing a mixture of a paraffin and a cycloalkane. It included global steps for soot formation (one reaction) and oxidation (two reactions), two global reactions for the oxidation of the fuel to CO and H₂ (one for the paraffin fraction and one for the cycloalkane), and a H₂–CO–O₂ reaction sub-mechanism (12 reactions). The kinetic scheme was used in a CFD code to model the combustion in kerosene-fueled rocket engines.

In another computational study, Patterson et al. [58] used a semi-detailed mechanism for the combustion of a mixture of 89% n -decane and 11% toluene to reproduce the jet-stirred reactor data at 10 and 40 atm [37] and the structure of the 1 atm fuel-rich flame [31]. The initial steps in their n -decane mechanism involve 14 global reactions to break down the parent molecule into smaller alkyl radicals and olefins. The complete mechanism gives a reasonable agreement between computation and experimental data from both experiments and was also used to predict the structure of a counterflow kerosene/air diffusion flame [58].

Riesmeier et al. [59] modeled the combustion and pollutants formation, nitrogen oxides and soot, in a gas turbine combustion chamber using a flamelet model including detailed kinetics. The model-fuel consisted of a mixture of n -decane (80% wt) and 1,2,4-trimethylbenzene (20% wt). The model was initially validated against the flame structures of Douté et al. [31].

However, several recent modeling studies of the oxidation of kerosene aviation fuels [7,38,60] have included cycloalkanes in the jet A-1/JP-8 surrogate to represent the naphthenic family in this fuel. This class of hydrocarbons is probably involved in the formation of soot since the sooting tendency of cycloalkanes is intermediate between that of alkanes and monoaromatics [61]. Cycloalkanes are also suspected to increase PAH and soot emissions in diesel engines, and finally cyclohexane has been shown to produce significant amounts of air toxics, namely 1,3-butadiene and benzene within a gasoline single cylinder engine [62].

In order to develop chemical mechanisms for the oxidation of these hydrocarbons, two cycloalkanes

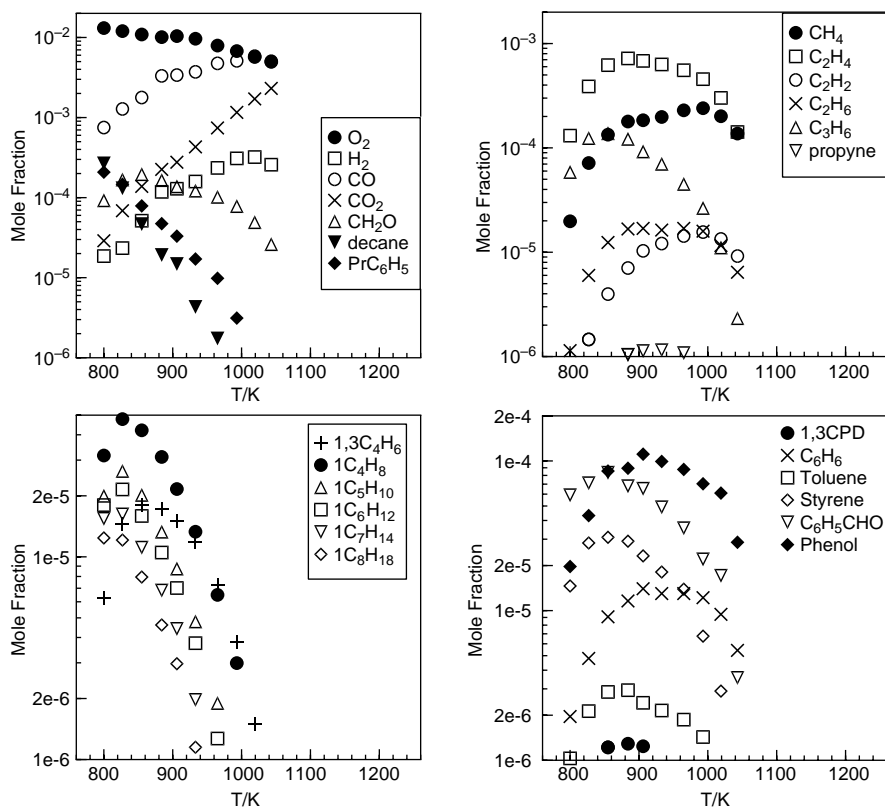


Fig. 35. Oxidation of a kerosene surrogate mixture in a JSR at 10 atm and $t=0.5$ s (initial conditions: 504 ppmv n -C₁₀H₂₂, 256 ppmv n -propylbenzene, 1.45% O₂, diluent nitrogen) [39].

were studied in a jet-stirred reactor at various pressures ranging from 1 to 10 atm: cyclohexane [63,64] and n -propylcyclohexane [65]. Detailed chemical mechanisms have been developed and refined to reproduce these experimental data [38,63–65].

In a first study using detailed mechanisms to model the oxidation of a three component jet-fuel surrogate in a jet-stirred reactor, a mixture of 78% n -decane, 9.8% cyclohexane and 12.2% toluene by volume was used [60]. Comparison with the previous modeling study based on a single component, n -decane [37] showed that the inclusion of a cycloalkane and an aromatic improved considerably the prediction of benzene in the oxidation of kerosene TR0 from 10 to 40 atm and for equivalence ratios between 0.5 and 2.

An improvement of the formulation of a surrogate mixture for kerosene TR0 was more recently provided by the modeling study of Dagaut [38]. He used a surrogate mixture of 74% n -decane, 11% n -propylcyclohexane and 15% n -propylbenzene by volume to

reproduce the oxidation of kerosene TR0 in a jet-stirred reactor at atmospheric pressure. Propylcyclohexane and propylbenzene are more representative of the naphthenic and aromatic family of kerosene than cyclohexane and toluene used before [60]. The neat oxidation of these hydrocarbons has been studied experimentally [55,65] in a jet-stirred reactor and detailed mechanisms have been elaborated to predict the experimental data [38,55,65]. The mechanism established for the ternary blend gave a good agreement between the computed and the experimental mole fractions of most of the species, including benzene, toluene and 1,3-cyclopentadiene [38].

Violi et al. [7], have also formulated a JP-8 surrogate containing a cycloalkane in addition to alkanes and aromatics to reproduce the structure of the flame of Douté et al. [31]. This surrogate contains 73.5% n -dodecane, 5.5% *iso*-octane, 10% methylcyclohexane, 1% benzene and 10% toluene by volume and fits reasonably well the boiling-point curve of a commercial JP-8 kerosene. The combustion of this mixture was

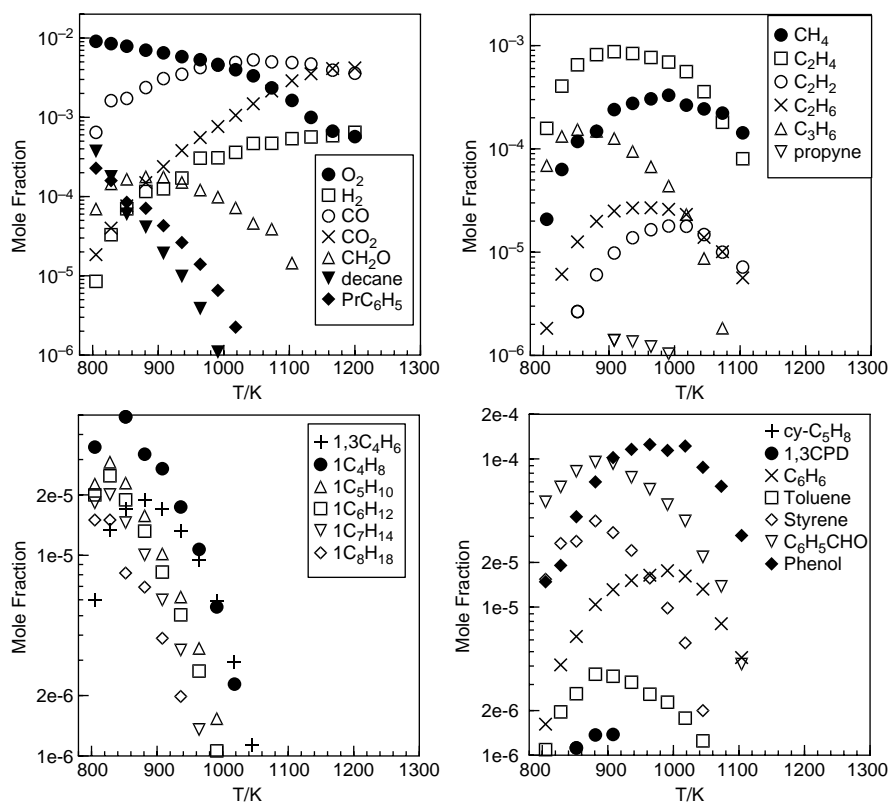


Fig. 36. Oxidation of a kerosene surrogate mixture in a JSR at 10 atm and $t=0.5$ s (initial conditions: 504 ppmv n -C₁₀H₂₂, 256 ppmv n -propylbenzene, 1.09% O₂, diluent nitrogen) [39].

modeled using a semi-detailed kinetic scheme and the computed profiles fit the experimental results with a precision compatible with the experimental uncertainties [7].

A four-species surrogate mixture was used by Montgomery et al. [66] for the validation of detailed and reduced chemical kinetic mechanisms for JP-8 combustion based on the scheme of [36,38]. This mixture contains by mole 32.6% n -decane, 34.7% n -dodecane, 16.7% methylcyclohexane, and 16.0% n -butylbenzene. The reduced mechanism generated in that study reproduces reasonably ignition delay measurements for JP-8.

In a more recent study, Cooke et al. [47] studied experimentally and computationally counter flow diffusion flames using JP-8, the JP-8 surrogate 2 of Violi et al. [7] (see Table 2), and individual components of this surrogate. Good agreement was obtained between predicted and measured temperature profiles and extinction limits in surrogate and JP-8 flames.

In addition to the surrogates proposed recently by Violi et al. [7] and Montgomery et al. [66], Agosta et al.

[48] have selected the following possible reference components for JP-8 in the following concentrations (in volume): n -dodecane 26%, 2,2,4,4,6,8,8-heptamethylnonane 36%, methylcyclohexane 14%, decalin 6% and α -methylnaphtalene 18%. They have studied experimentally the oxidation of these components and of several binary mixtures in a pressurized flow reactor. Semi-detailed or lumped kinetic models were used to simulate the oxidation of pure components and general agreement was found with the experimental measurements.

Wen et al. [67] modeled the formation of soot from kerosene flames in the experimental conditions of [33] in confined co-flowing kerosene/air jet flame configuration. The turbulent flame was contained within a borosilicate glass tube of 155 mm diameter, mounted in a pressure-resistant housing. The burner consisted of a 1.5 mm diameter cylindrical nozzle, surrounded by a coaxial annulus, 0.25 mm wide, on which is burnt a rich ethylene/oxygen laminar premixed flame to rim-stabilize the turbulent kerosene jet flame. A kerosene AVTUR having a H/C

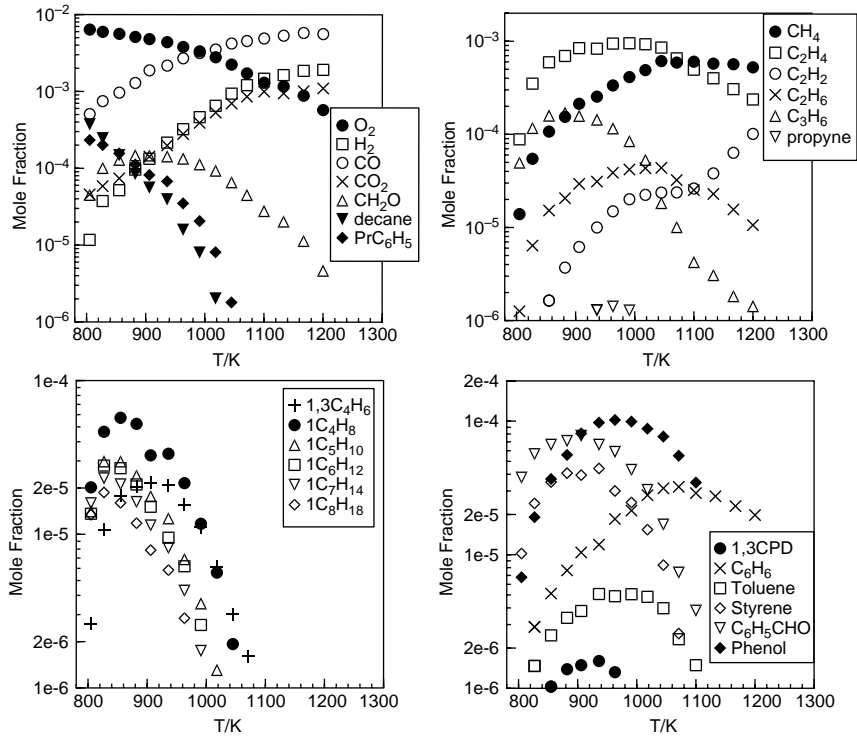


Fig. 37. Oxidation of a kerosene surrogate mixture in a JSR at 10 atm and $t=0.5$ s (initial conditions: 504 ppmv n -C₁₀H₂₂, 256 ppmv n -propylbenzene, 0.73% O₂, diluent nitrogen) [39].

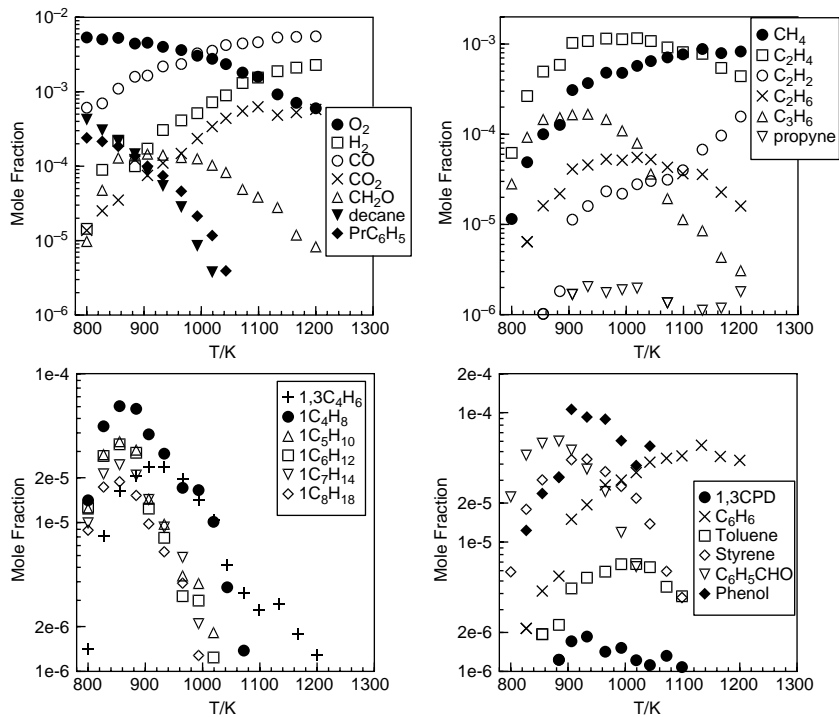


Fig. 38. Oxidation of a kerosene surrogate mixture in a JSR at 10 atm and $t=0.5$ s (initial conditions: 504 ppmv n -C₁₀H₂₂, 256 ppmv n -propylbenzene, 0.54% O₂, diluent nitrogen) [39].

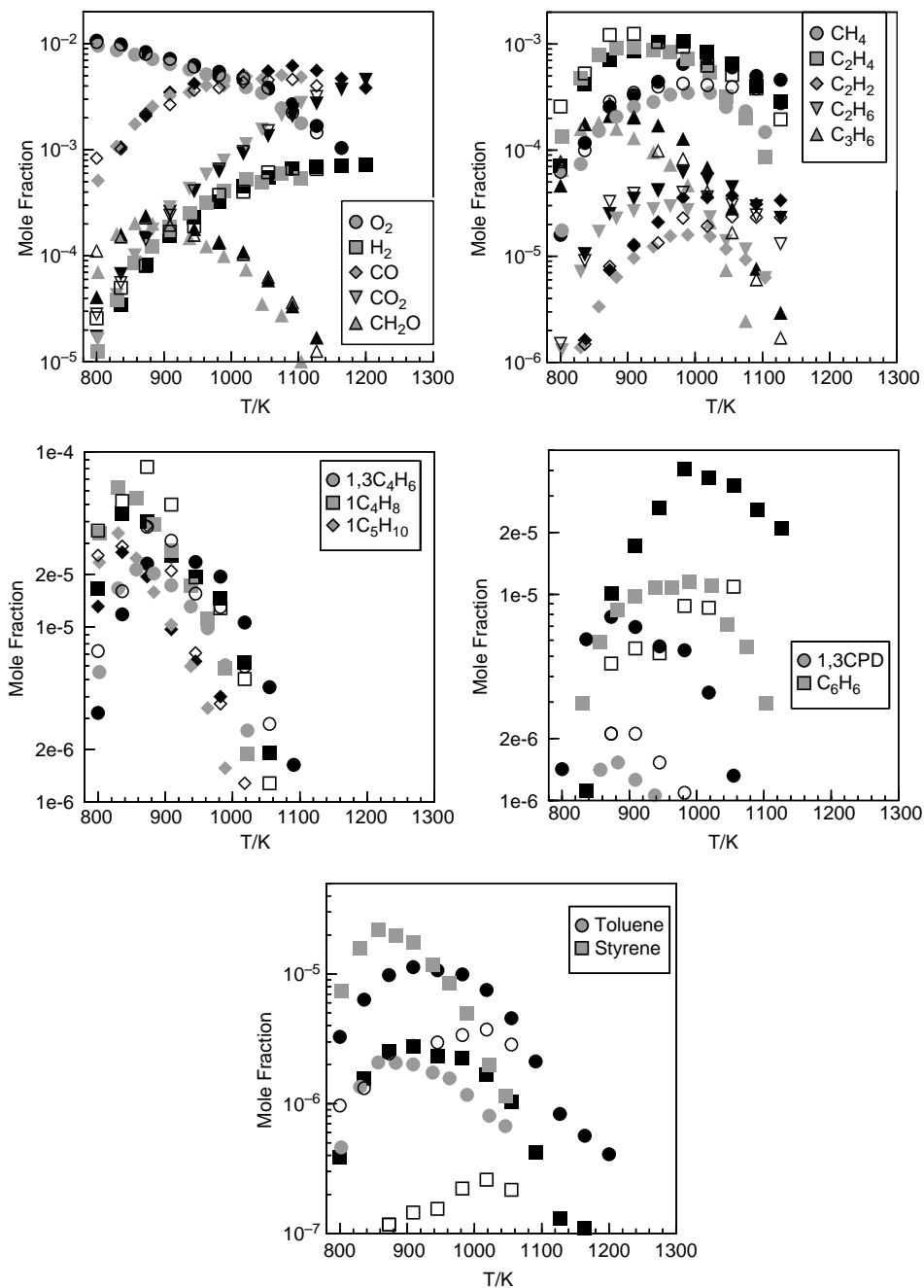


Fig. 39. Comparison of the oxidation of three fuels in a JSR at 10 atm, $\phi=1$, and $t=0.5$ s (initial conditions: 670 ppmv Jet A-1: filled black symbols; 579 ppmv n -C₁₀H₂₂ and 171 ppmv n -propylbenzene: filled grey symbols; 600 ppmv n -C₁₀H₂₂ and 150 ppmv 1,2,4-trimethylbenzene: open symbols; diluent nitrogen) [39].

ratio of 0.51, encompassing 14% H by mass and 20% aromatic content by volume was used. Three key scalar variables, the soot volume fraction, the temperature, and the mixture fraction were measured. Using the detailed chemical scheme of [38], Wen

et al. modeled these variables. Their model fuel was a mixture of 20% toluene and 80% n -decane by volume (H/C ratio of 0.49).

Luche et al. [69] used an early version of the detailed kinetic scheme of [38] involving 134 species

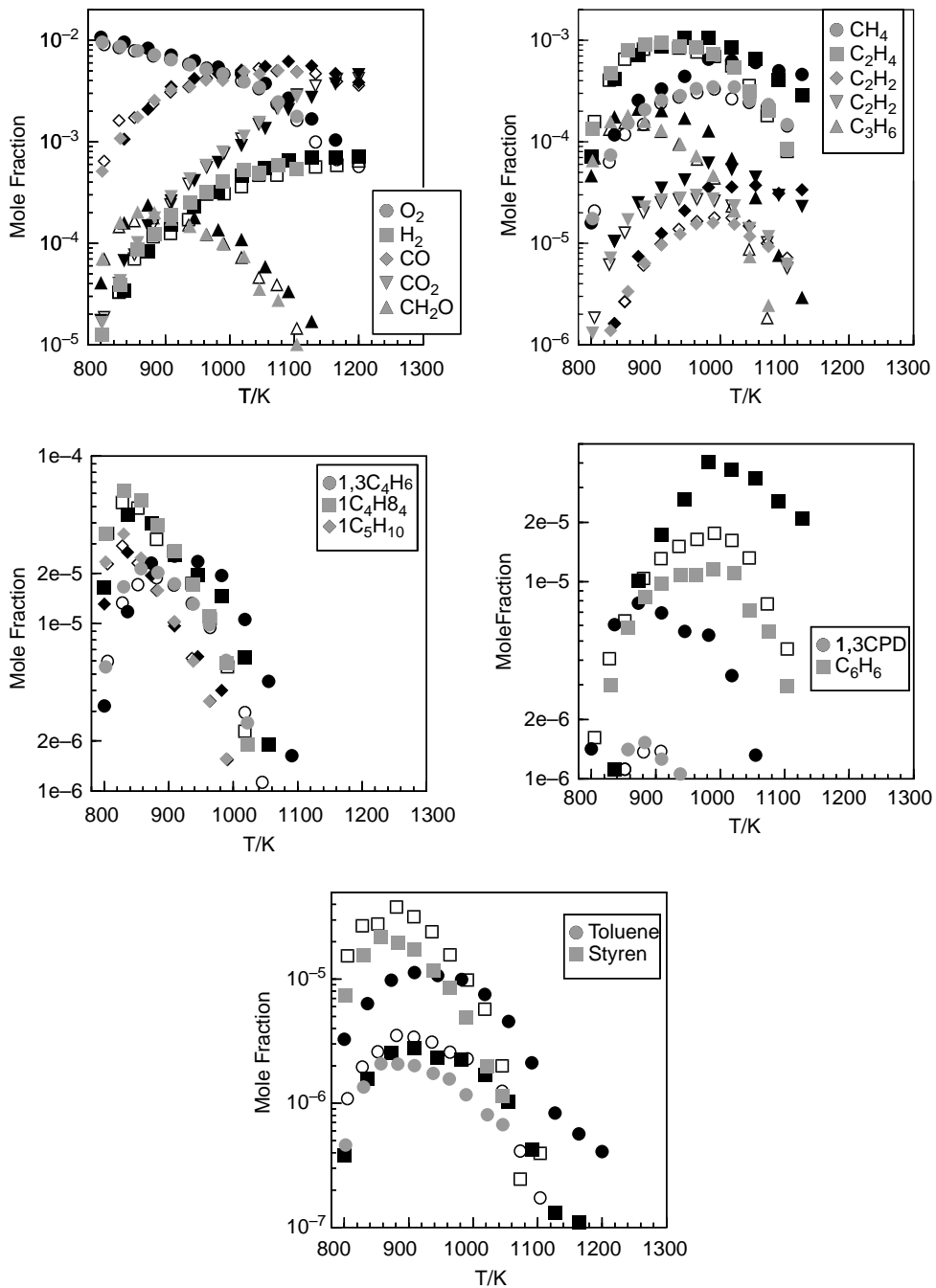
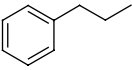
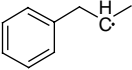
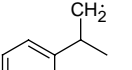
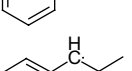
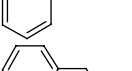
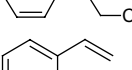
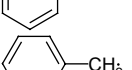
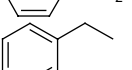
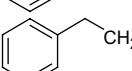


Fig. 40. Comparison of the oxidation of three fuels in a JSR at 10 atm, $\phi=1$, and $t=0.5$ s (initial conditions: 670 ppmv Jet A-1: filled black symbols; 579 ppmv *n*-C₁₀H₂₂ and 171 ppmv *n*-propylbenzene: filled grey symbols; 504 ppmv *n*-C₁₀H₂₂ and 256 ppmv *n*-propylbenzene: open symbols; diluent nitrogen) [39].

and 3493 reactions to derive a skeletal kinetic mechanism (134 species and 1220 reactions) and two reduced kinetic schemes (involving 40 or 33 species) to simulate the combustion of kerosene in a

JSR. Elliott et al. [70,71] also proposed an optimized reduced kinetic scheme to simulate kerosene combustion in flames and JSR. The degree of agreement achieved by the authors using this scheme is similar

Table 4
Species and their structure

Species	Formula
<i>n</i> -Propylbenzene	
1-Phenyl-2-propyl	
2-Phenyl-1-propyl	
1-Phenyl-1-propyl	
3-Phenyl-1-propyl	
Styrene	
Benzyl, C ₆ H ₅ -CH ₂	
Ethylbenzene, C ₆ H ₅ -C ₂ H ₅	
2-Phenyl-1-ethyl	

to that obtained using the scheme of Kyne et al. [72] (167 reactions, 63 species).

Mawid et al. [73] studied the effect of the composition of the model-fuel on the model predictions (1330 reversible reactions vs. 202 species). Two model-fuels were used: (i) a four-components model-fuel: 45% *n*-dodecane, 20% *n*-decane, 25% *n*-butylbenzene, 10% methyl-cyclohexane; (ii) a 12-components model-fuel: 20% *n*-dodecane, 15% *n*-decane, 15% *n*-tetradecane, 10% *n*-hexadecane, 5% *iso*-octane, 5% methylcyclohexane, 5% *cyclo*-octane, 5% butylbenzene, 5% *m*-xylene, 5% 1,2,4-trimethylbenzene, 5% tetraline, 5% 1-methylnaphtalene. A reasonable agreement between the ignition data [22,25] and the modeling was reported although the predicted activation energy was lower than measured. Better predictions were obtained using the 12-components model-fuel. Mawid et al. [74] further studied the effect of the model-fuel composition on the model predictions, concentrating on the aromatic contents. Five compositions of a 14-components model-fuel were considered by the authors. The constituents of the model-fuels were: *n*-dodecane, *n*-decane,

n-hexadecane, *n*-tetradecane, *iso*-octane, *cyclo*-octane, methylcyclohexane, 1-methylnaphtalene, tetralin, 1,2,4,5-tetramethylbenzene, butylbenzene, *m*-xylene, benzene, toluene. The kinetic scheme consisted of 1484 reversible reactions vs. 222 species. A reasonable agreement between the ignition data [22,25] and the predictions was obtained although the predicted activation energy is lower than measured. In a more recent study, Mawid et al. [75] studied the effect of the model-fuel composition on the model predictions in the same conditions as before [73,74]. Three compositions of a 13-components model-fuel were used. The model-fuels included 12 or 6 compounds among *n*-dodecane, *n*-decane, *n*-tetradecane, *n*-hexadecane, *iso*-octane, methylcyclohexane, *cyclo*-octane, *n*-butylbenzene, *m*-xylene, 1,2,4-trimethylbenzene, tetralin, 1-methylnaphtalene. The kinetic mechanism they used consisted of 1500 reversible reactions vs. 223 species. Better predictions with the 12-components model-fuel were obtained, although the predicted activation energy was still lower than measured [22,25].

6. New kinetic modeling of kerosene oxidation and combustion

In the present paper, the modeling approach of Dagaut [38] was extended to the oxidation of Jet A-1 under high pressure. This kinetic mechanism is available from the authors upon request (dagaut@cns-orleans.fr). Examples of the modeling results are presented below using the computer program from the Chemkin package [76–78]. As before, a preliminary validation of the kinetic scheme for the oxidation of the pure components of the surrogate mixture (*n*-decane, *n*-propylbenzene, and *n*-propylcyclohexane [38,79] was performed. The kerosene kinetic model used here consisted of 209 species and 1673 reversible reactions. The model-fuel molar composition used in this modeling is that used previously [38]: 74% *n*-decane, 15% *n*-propylbenzene, and 11% *n*-propylcyclohexane. The computed ignition delays are in reasonable agreement with the literature data [22,25,27–29] obtained for an equivalence ratio of 0.5 (Fig. 41). As can be seen from Figs. 42–44, the proposed kerosene kinetic oxidation scheme represents fairly well the experimental results obtained in JSR conditions at 1, 10 and 40 atm. From these figures, it is clear that the kinetic model presently used still needs improvements under high-pressure conditions. A good agreement with

Table 5
Kinetic schemes used for simulating the ignition, oxidation, or combustion of kerosene

Scheme type	Fuel	Conditions	Comments	Ref.
Global	Kerosene	Combustion rig 0.3–1 MPa	Modeling of soot formation. Two Arrhenius equations used: one for the fuel consumption, one for the formation of soot	Najar, Goodger [50]
One step	Commercial kerosene	Combustion in a duct of parallel plates	Global Arrhenius equation scheme used to simulate flame speed, flame temperature, and heat release	Aly, Salem [51]
Quasi global	Kerosene TR0	JSR at atmospheric pressure	Concentration profiles versus time were modeled. The major species were simulated correctly. Model fuel: 79% <i>n</i> -undecane, 10% <i>n</i> -propylcyclohexane, 11% 1,2,4-trimethylbenzene (by wt)	Gueret et al. [35]
Detailed	Kerosene TR0	JSR at atmospheric pressure	Concentration profiles versus time were modeled. The major species were simulated correctly. Model fuel: <i>n</i> -decane. 603 reversible reactions and 78 species	Cathonnet et al. [52]
Detailed	Kerosene TR0	JSR at 10–40 atm	Concentration profiles versus temperature were modeled. The major species were simulated correctly. Model fuel: <i>n</i> -decane. 573 reversible reactions and 90 species.	Dagaut et al. [36,37]
Detailed	Kerosene TR0	Premixed flat flame burner at 6 kPa. Equivalence ratio:2.2	Concentration profiles versus distance to the burner were modeled. Major and minor species simulated correctly. Model-fuel: 90% <i>n</i> -decane, 10% toluene (vol). 207 reversible reactions and 39 species	Vovelle et al. [30]
Detailed	Kerosene TR0	Premixed flat flame burner at 6 kPa. Equivalence ratio:2.2 [30]	Concentration profiles versus distance to the burner were modeled. Major and minor species simulated correctly. Model-fuels: <i>n</i> -decane + benzene or toluene, or ethylbenzene, or ethylbenzene–naphtalene. 1085 reversible reactions and 193 species	Lindstedt and Maurice [56]
Quasi-global	Kerosene	Combustion chamber at c.a. 35 atm	CFD computations, soot predictions. Model-fuel: C ₁₂ H ₂₄ . Five global reactions, 12 reversible reactions and 10 species including soot	Wang [57]
Semi-detailed	Kerosene	JSR data from [37] at 10–40 atm, and premixed flat flame burner at 1 atm, data of [31]	Major species correctly predicted. Model-fuel: 89% <i>n</i> -decane, 11% toluene (vol). 440 reversible reactions and 84 species	Patterson et al. [58]
Detailed	Kerosene	Gas turbine, premixed flat flame burner data of [31]	Flamelet modeling including NO _x and soot formation. Validation against the premixed flat flame burner data of [31]. Model-fuel: <i>n</i> -decane-1,2,4-trimethylbenzene. The size of the kinetic scheme is not specified	Riesmeier et al. [59]
Detailed	Kerosene TR0	JSR data of [37] 10–40 atm	Concentration profiles versus temperature were modeled. The major and minor species were simulated correctly. Benzene formation was under predicted. Model fuel: 78% <i>n</i> -decane, 9.8% cyclohexane, 12.2% toluene (vol). 1463 reversible reactions and 188 species	Cathonnet et al. [60]
Detailed	Kerosene TR0	JSR data of [38] 1 atm	Concentration profiles versus temperature were modeled. The major and minor species were simulated correctly. Benzene and toluene formation was well predicted. Model fuel: 74% <i>n</i> -decane, 11% <i>n</i> -propylcyclohexane, 15% <i>n</i> -propylbenzene (vol). 1592 reversible reactions, 207 species	Dagaut [38]
Semi-detailed	JP-8 and kerosene TR0	Premixed flat flame burner data of [31]	Concentration profiles versus distance to the burner were modeled. Major and minor species simulated correctly. Acetylene and benzene mole fractions were under-predicted. Model-fuel: 73.5% <i>n</i> -dodecane, 5.5% <i>iso</i> -octane, 10% methylcyclohexane, 10% benzene, 1% toluene (vol). The size of the kinetic scheme is not specified	Violi et al. [7]

Detailed and reduced	JP-8	Ignition delays at 1 atm from Mullins [22] and Freeman and Lefebvre [25]	Reasonable agreement with the data. Good agreement between the reduced and detailed scheme (1162 reversible reactions and 164 species). Model-fuel: 32.6% <i>n</i> -decane, 34.7% <i>n</i> -dodecane, 16.7% methylcyclohexane, 16% <i>n</i> -butylbenzene (vol)	Montgomery et al. [66]
Semi-detailed	JP-8	Counter-flow diffusion flame	Modeling of the temperature profiles and extinction limits. Model-fuel: <i>n</i> -octane, <i>n</i> -dodecane, <i>n</i> -hexadecane, xylenes, decaline, tetraline [7]. 5032 reversible reactions, 221 species	Cooke et al. [47]
Semi-detailed, lumped reactions	JP-8	Flow reactor at 8 atm	Modeling of CO concentration profiles measured versus temperature. Model-fuels: <i>n</i> -dodecane, heptamethylnonane, methylcyclohexane, decaline, 1-methylnaphtalene with variable composition. The size of the kinetic scheme is not specified	Agosta et al. [48]
Detailed	Kerosene AVTUR	Co-flowing kerosene-air jet flames of [33]	Modeling of soot volume fraction, temperature, mixture fraction. Model-fuel <i>n</i> -decane, toluene. 1592 reversible reactions and 207 species	Wen et al. [67]
Reduced	Kerosene TR0	JSR conditions [37]	Reduction of a detailed scheme (225 species, 34993 irreversible reactions). Good agreement between the detailed and reduced schemes. Model-fuel: <i>n</i> -decane, <i>n</i> -propylbenzene, <i>n</i> -propylcyclohexane	Luche et al [69]
Detailed and reduced	Kerosene TR0	Premixed flat flame burner data of [31]	Concentration profiles versus distance to the burner were modeled. Major and minor species simulated correctly. Acetylene and benzene mole fractions were under-predicted. Model-fuel: 89% <i>n</i> -decane, 11% toluene (vol). A 165 reaction versus 60 species was obtained by reduction of a 440 reactions versus 84 species scheme. Flame speeds as a function of equivalence ratio and initial temperature were predicted	Kyne et al. [72]
Reduced optimized	Kerosene TR0	JSR conditions of [37] and premixed flat flame burner experiments of [31]	An optimized reduced scheme was proposed base on the scheme of Kyne et al. [72]. The same degree of agreement between the reduced and original schemes was obtained	Elliott et al. [70,71]
Detailed	JP-8	Plug flow ignition using the data from Mullins [22] and Freeman and Lefebvre [25]	Study of the effect of the model-fuel composition on the model predictions. Two model-fuels were used: (i) a four-components model-fuel: 45% <i>n</i> -dodecane, 20% <i>n</i> -decane, 25% <i>n</i> -butylbenzene, 10% methylcyclohexane; (ii) a 12-components model-fuel: 20% <i>n</i> -dodecane, 15% <i>n</i> -decane, 15% <i>n</i> -tetradecane, 10% <i>n</i> -hexadecane, 5% <i>iso</i> -octane, 5% methylcyclohexane, 5% <i>cyclo</i> -octane, 5% butylbenzene, 5% <i>m</i> -xylene, 5% 1,2,4-trimethylbenzene, 5% tetraline, 5% 1-methylnaphtalene. 1330 reactions vs. 202 species. Reasonable agreement between the data and the predictions. Better predictions with the 12-components model-fuel. The predicted activation energy is lower than measured	Mawid et al. [73]
Detailed	JP-8	Plug flow ignition using the data from Mullins [22] and Freeman and Lefebvre [25]	Study of the effect of the model-fuel composition, aromatic contents, on the model predictions. Five compositions of a 14-components model-fuel were used. Model-fuel: <i>n</i> -dodecane, <i>n</i> -decane, <i>n</i> -hexadecane, <i>n</i> -tetradecane, <i>iso</i> -octane, <i>cyclo</i> -octane, methylcyclohexane, 1-methylnaphtalene, tetralin, 1,2,4,5-tetramethylbenzene, butylbenzene, <i>m</i> -xylene, benzene, toluene. 1484 reactions vresus 222 species. Reasonable agreement between the data and the predictions. The predicted activation energy is lower than measured	Mawid et al. [74]

(continued on next page)

Table 5 (continued)

Scheme type	Fuel	Conditions	Comments	Ref.
Detailed	JP-8	Plug flow ignition using the data from Mullins [22] and Freeman and Lefebvre [25]	Study of the effect of the model-fuel composition on the model predictions. Three compositions of a 13-components model-fuel were used, consisting of 12 or six compounds among <i>n</i> -dodecane, <i>n</i> -decane, <i>n</i> -tetradecane, <i>n</i> -hexadecane, <i>iso</i> -octane, methylcyclohexane, <i>cyclo</i> -octane, <i>n</i> -butylbenzene, <i>m</i> -xylene, 1,2,4-trimethylbenzene, tetralin, 1-methyl-naphthalene. 1500 reversible reactions versus 223 species. Reasonable agreement between the data and the predictions. Better predictions with the 12-components model-fuel. The predicted activation energy is lower than measured	Mawid et al. [75]

the kerosene flame data from [31] was also obtained with this model, as depicted on Fig. 45.

According to kinetic model, the fuel oxidation is driven by the oxidation of *n*-decane. The oxidation of this *n*-alkane produces C₁₀ alkyl radicals. Via their decomposition, 1-C₄H₉ is produced. The decomposition of this radical is the major source of ethyl radicals (60% at 900 K in the conditions of Fig. 41). Ethyl is also produced in these conditions by decomposition of 3-C₁₀H₂₁ (15%), and by decomposition of *n*-propylbenzene. Ethyl radicals react with molecular oxygen yielding HO₂. The recombination of HO₂ and the reactions of HO₂ with the fuel yield H₂O₂. The decomposition of this intermediate produces OH radicals that, in turn, oxidize the fuel.

7. Reformulated jet-fuels

Although the price of crude oil is expected to still further increase making alternative fuels economically viable, mostly for safety reasons, the aviation industry is resistant to new or reformulated fuels. Therefore, it is foreseen that non-renewable kerosene should still be used by aviation for the next ten years whereas renewable alternatives such as biodiesel should be further applied to ground transportation. Biodiesel produced from crops (soya, rapeseed, sunflower,...) can be blended with kerosene for use in aero-jet engines with the advantage of reducing greenhouse emissions [80]. However, such blends have less performance under cold temperatures conditions, with potential fuel lines or filter blockage [81]. Fischer–Tropsch [82–86] synthetic kerosene can be produced from a wide variety of sources including renewable (crops, wood, straw, animal fat, waste,...) and fossil (coal, natural gas, methane hydrates) sources. They are obtained by catalytic conversion of CO/H₂ mixtures yielding liquid hydrocarbons, primary straight-chain paraffins, and alternatively, after further process, branched paraffins and cyclic hydrocarbons, more suitable for kerosene blending. Such Fischer–Tropsch kerosenes currently produced in South Africa and extensively tested [84–86] might spread over the World in the near future based on their encouraging test results.

8. Concluding remarks

A large data set of experimental data is available for the combustion of kerosene. However, more data are still necessary in flame conditions (high pressure

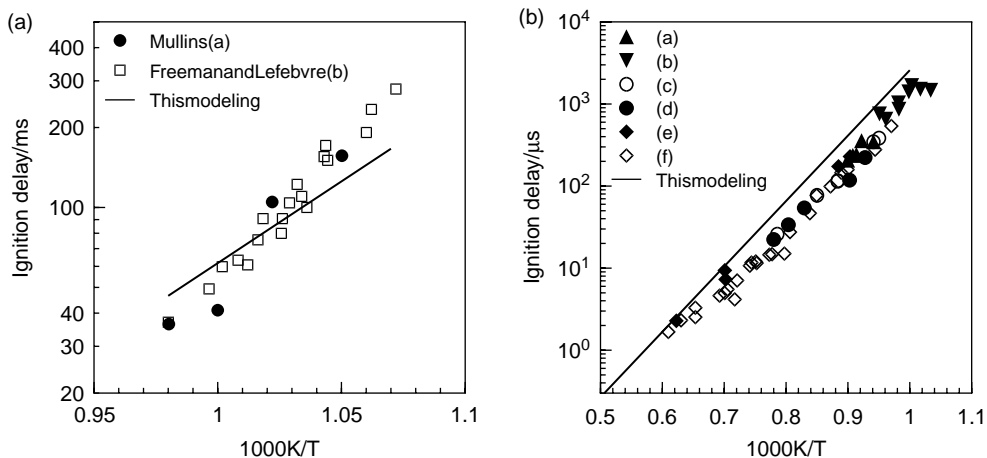


Fig. 41. Ignition delay of kerosene/air mixtures at 1 atm (a) and 20 atm (b). (a) The data were taken from [22] for (a) and from [25] for (b). (b) The data were taken from [29] for (a) and (b), from [28] for (c) and (d), from [27] for (e) and (f). The modeling results are presented as lines.

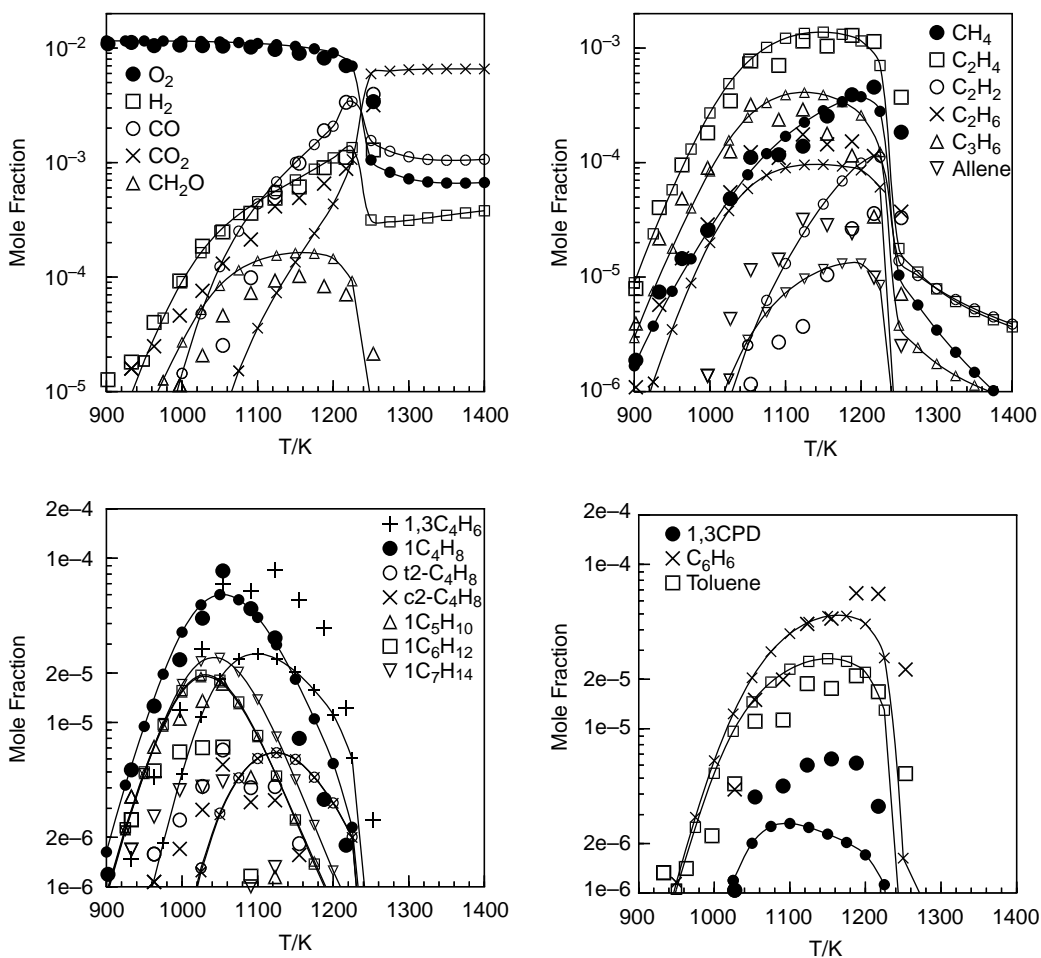


Fig. 42. Oxidation of kerosene in a JSR at 1 atm and $t=0.07$ s (initial conditions: 0.07% kerosene TR0, 1.155% O₂, diluent nitrogen) [48]. Comparison between experimental results (large symbols) and modeling (small symbols and lines).

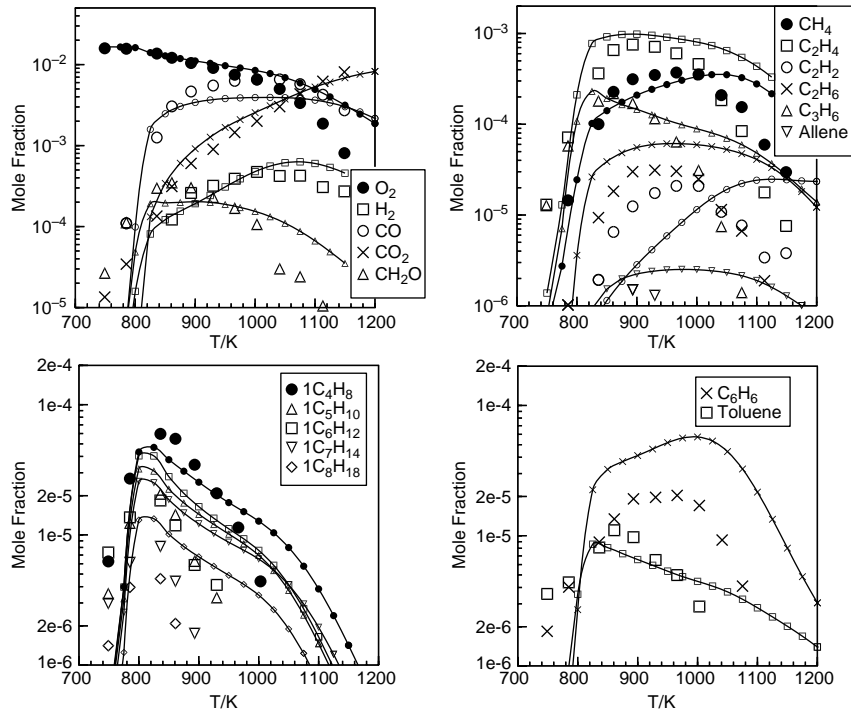


Fig. 43. Oxidation of kerosene in a JSR at 10 atm and $t=0.5$ s (initial conditions: 0.1% kerosene TR0, 1.65% O_2 , diluent nitrogen) [36]. Comparison between experimental results (large symbols) and modeling (small symbols and lines).

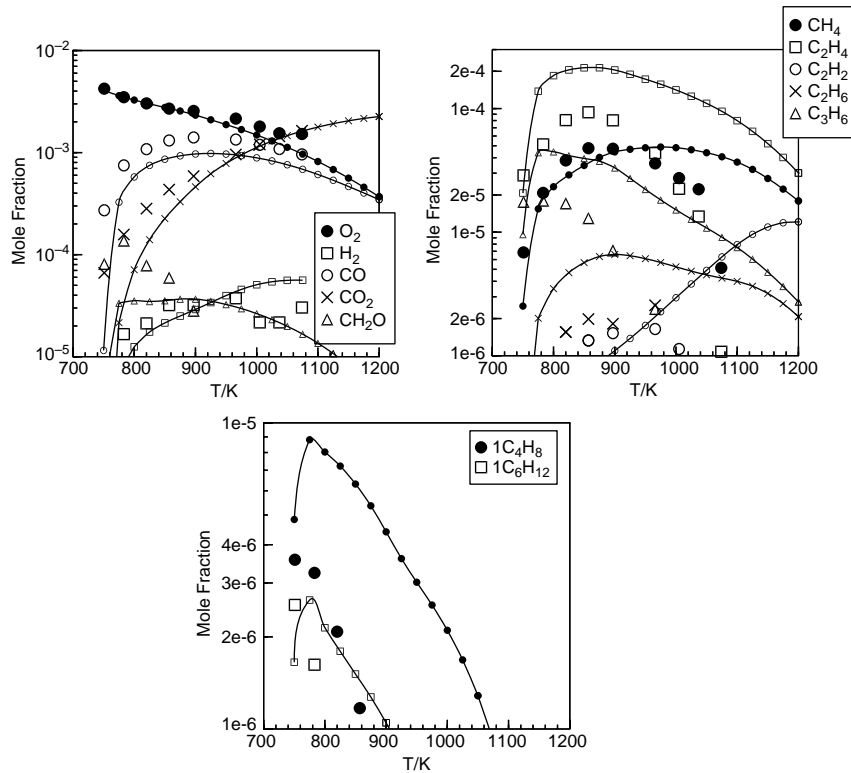


Fig. 44. Oxidation of kerosene in a JSR at 40 atm and $t=2.0$ s (initial conditions: 0.025% kerosene TR0, 0.4125% O_2 , diluent nitrogen) [36]. Comparison between experimental results (large symbols) and modeling (small symbols and lines).

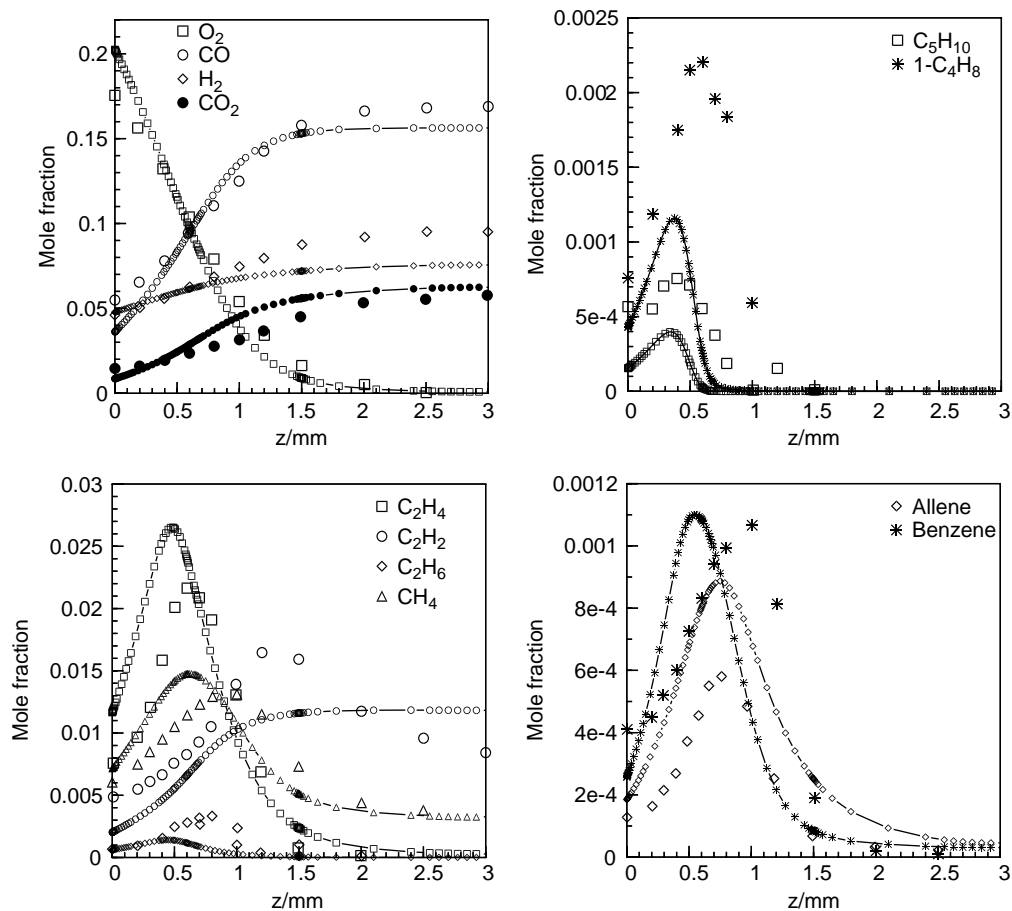


Fig. 45. Flame structure under atmospheric pressure conditions: 2.95% of kerosene TR0, 28.64% oxygen, 68.41% nitrogen in mol, equivalence ratio of 1.7 [31]. Comparison between experimental results (large symbols) and modeling (small symbols and lines).

and fuel-lean conditions) to further test the models. New measurements for the ignition of kerosene would be useful too. Further improvements of the existing kinetic models are still necessary although lots of progress was made in the recent years. Such work is currently undertaken through a collaborative effort between CNRS and the DLR-Stuttgart.

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Appendix A

Properties of aviation jet turbine fuel (Jet A-1) produced from crude oil straight distillation with hydroprocessing of the kerosene fraction. The fuel is 100% hydroprocessed kerosene fraction with antioxidant and static dissipator additives.

Properties	Values	Test method
Appearance	Clear, bright and visually free from solid matter and insoluble water at ambient temperature	Visual
Composition		
Total acidity, mg KOH/g, not more than	0.015	ASTM D 3242
Aromatics, vol%, not more than	25.0	ASTM D 1319

(continued on next page)

Properties	Values	Test method
Total sulfur, wt%, not more than	0.30	ASTM D 4294
Mercaptan sulfur, wt%, not more than	0.0030	ASTM D 3227
or Doctor test	Negative	ASTM D 4952
Hydroprocessed components in batch, %	Negative, incl. 'nil' or 100%	
Volatility		
Distillation range		ASTM D 86
Initial boiling point, °C	Report	
Recovered at temperature		
10% vol, °C, not higher than	205	
50% vol, °C, not higher than	Report	
90% vol, °C, not higher than	Report	ASTM D 3828
End boiling point, °C, not higher than	300	ASTM D 1298
Residue, vol%, not more than	1.5	
Loss, vol%, not more than	1.5	
Flash point, °C, not lower than	40	
Specific density at 15 °C, kg/m ³	775–840	
Fluidity		
Freezing point, °C, not higher than	–47	ASTM D 5972
Viscosity at –20 °C, mm ² /s, not more than	8.0	ASTM D 445
Combustion		
Specific energy, MJ/kg, not less than	42.8	ASTM D 4529
Smoke point, mm, not less than	25	ASTM D 1322
Or Smoke Point, mm, not less than	19	ASTM D 1322
And naphthalenes, vol%, not more than	3.0	ASTM D 1840
Corrosion		
Copper strip, 2 h at 100 °C, class, not higher than	1	ASTM D 131
Stability		
Thermal stability	25.0	ASTM D 3241
JETOT at 260 °C		
Fiker pressure differential, mmHg, not higher than	3	
Tube deposits rating (visual), not higher than	Without peacock or abnormal color deposits	
Contaminants		
Existent gums, mg/100 cm ³ , not more than	7	ASTM D 381

Properties	Values	Test method
Water separation characteristics: Water reaction interface rating, not higher than	1b	ASTM D 1094
Microseparator, at point of manufacture, MSEP		
Fuel with static dissipator, not less than	70	ASTM D 3948
Fuel without static dissipator, not less than	85	
Conductivity		
Specific electrical conductivity, pS/m at time and temperature of custody	50–450	ASTM D 2624
Lubricity		
BOCLE wear scar diameter, not more than	0.85	ASTM D 5001
Additives		
Antioxidant in hydroprocessed fuels, mg/dm ³ , (Mandatory)	17–24	
Static dissipation, mg/dm ³ :	Mandatory	
First doping, Stadis 450 max	3	
Icing inhibitor, % vol, by agreement, not more than.	0.15	ASTM D 5006

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