3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

The composition of aviation fuels has been established by the U.S. Air Force (Air Force 1977, 1981g, 1982d, 1988a, 1989c, 1990) using specifications that are based primarily on the characteristics that give the maximum performance of the aircraft for which the fuel is used (CRC 1984). JP-4 and JP-7 were developed for use by the U.S. Air Force. JP-4 is called a wide-cut fuel because it is produced from a broad distillation temperature range and contains a wide array of carbon chain-lengths, from 4 to 16 carbons long. It was initially developed for broad availability in times of need. The composition of JP-4 is approximately 13% (v/v) aromatic hydrocarbons, 1.0% olefin hydrocarbons, and 86% saturated hydrocarbons (ITC 1985). It has a distillation temperature range of 60 to 270 °C (MacNaughton and Uddin 1984). JP-7 was developed for use in advanced supersonic aircraft because of its thermal stability and high flashpoint (CRC 1984; Dukek 1978). It has a distillation temperature range of 182 to 288 °C and contains a maximum of 5% (by volume) aromatic compounds (see Table 3-7).

Aviation fuels consist primarily of hydrocarbon compounds (paraffins, cycloparaffins or naphthenes, aromatics, and olefins) and contains additives that are determined by the specific uses of the fuel (CRC 1984; Dukek 1978; IARC 1989). Paraffins and cycloparaffins are the major components. Paraffins have a high hydrogen-to-carbon ratio, with a high heat release per unit of weight and a cleaner burn than other hydrocarbons. Cycloparaffins have a lower hydrogen-to-carbon ratio, which results in less heat released per unit of weight but increases the fuel's density. These components reduce the freezing point of the fuel. Aromatic hydrocarbons are a good energy source but produce smoke when burned; therefore, the maximum levels are restricted (20-25% by volume in JP-4, 5% by volume in JP-7). Finally, olefins are similar to the paraffins but are unsaturated with lower hydrogento- carbon ratios. They are the most reactive of the hydrocarbons and are permitted at only 5% by volume in JP-4 (CRC 1984). Benzene, present in wide-cut fuels such as JP-4, is an ineffectual contaminant usually present below 0.5% (CONCAWE 1985; IARC 1989). Nonhydrocarbon compounds such as sulfur and sulfur compounds are also found. Additives such as antioxidants, metal deactivators, fuel system icing inhibitors, corrosion inhibitors, and static dissipator additives are all present in limited quantities in jet fuels in order to improve performance (CRC 1984).

3. CHEMICAL AND PHYSICAL INFORMATION

Information regarding the chemical identity of JP-4 and JP-7 is located in Tables 3-l and 3-2, respectively.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of JP-4 and JP-7 is located in Tables 3-3 and 3-4, respectively. Information regarding the major components of JP-4 derived from petroleum and shale oil is presented in Table 3-5. Depending on the origin of the crude and the production method, there could be considerable compositional variability between fuel oils of the same grade (Air Force 1988b). This variation is reflected in the allowed military specifications (mil spec) for JP-4 and JP-7 fuel oils as shown in Tables 3-6 and 3-7, respectively, and in the compositional variability of JP-4 fuels as shown in Tables 3-5 and 3-8.

TABLE 3-1. Chemical Identity of JP-4[a]

Characteristic	Information	Reference
Chemical name	JP-4	OHM/TADS 1985
Synonym(s)	Jet fuel-4	OHM/TADS 1985
Registered trade name(s)	MIL-T-5624-L-Amd. 1 wide cut; JP-4 military (gasoline type)	Air Force 1990; Dickson and Woodward 1987; Dukek 1978; IARC 1989
Chemical formula	NA[a]	
Chemical structure[a]	NA[a]	
Identification numbers:		
CAS Registry	50815-00-4	OHM/TADS 1985
NIOSH RTECS	NY9340000	RTECS 1994a
EPA Hazardous Waste	No data	
OHM/TADS	7217071	OHM/TADS 1985
DOT/UN/NA/IMCO Shipping	1863	CHRIS 1986
HSDB	No data	
NCI	No data	

[a] JP-4 is a mixed compound composed primarily of hydrocarbons (i.e., alkanes, cycloalkanes, alkybenzenes, indan/tetralins, and naphthalenes).

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substance Data Bank; JP-4 = jet propellant-4; NA = Not Applicable; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

TABLE 3-2. Chemical Identity of JP-7[a]

Characteristic	Information	Reference
Chemical name	JP-7	RTECS 1994b
Synonym(s)	Jet fuel-7	RTECS 1994b
Registered trade name(s)	MIL-T-38219A-Amd. 2, kerosene, low volatility	IARC 1989
Chemical formula	NA[a]	
Chemical structure[a]	NA[a]	
Identification numbers:		
CAS Registry	No data	
NIOSH RTECS	SE7548500	RTECS 1994b
EPA Hazardous Waste	No data	
OHM/TADS	No data	
DOT/UN/NA/IMCO Shipping	No data	
HSDB	No data	
NCI	No data	

[a] JP-7 is a mixed compound composed primarily of hydrocarbons (i.e., alkanes, cycloalkanes, alkybenzenes, indan/tetralins, and naphthalenes).

CAS = Chemical Abstracts Services; DOT/UN/NA/IMCO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substance Data Bank; JP-7 = jet propellant-7; NA = Not Applicable; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

TABLE 3-3. Physical and Chemical Properties of JP-4[a]

Property	Information	Reference
Molecular weight	Not applicable[b]	
Color	Colorless to straw colored	CHRIS 1986; Martel 1992
Physical state	Liquid	CHRIS 1986
Melting point	-46 °C	OHM/TADS 1985
	-40–72 °C	ITC 1985
Boiling point (1 atm)	50–270 °C	Air Force 1989b
	90–300 °C	ITC 1985
	45–280 °C	Dickson and Woodward 1987
Density:		
at 15 °C	751–802 kg/m^3 (specification)	
Odor	Like gasoline and/or kerosene	
Odor threshold:		
Water	No data	
Air	1 ppm	CHRIS 1986
Solubility:		
Water at 20 °C	57 mg/L	CRC 1984
Organic solvent(s)	Since many of the components are organic solvents, the fuel is generally miscible with organic solvents	ITC 1985
Partition coefficients:		
Log K_{ow}	Major components range from 3 to 4.5	ITC 1985
Log K_{oc}	No data	
Vapor pressure at 20 °C	91 mm Hg	Air Force 1989b
Henry's law constant	$1.00x10^{-4}$-$1.00x10^{+1}$ atm-m^3/mol	Air Force 1989b
Autoignition temperature	246 °C	CRC 1984
Flashpoint	-23–1 °C	NFPA 1986
Flammability limits	1.3% lower; 8.0% upper	NFPA 1986
Explosive limits	No data	

[a]JP-4, or jet propellant-4, is a mixed compound composed primarily of hydrocarbons (i.e., alkanes, cycloalkanes, alky-benzenes, indan/tetralins, and naphthalenes).
[b]Jet fuels are blends prepared to meet certain gross property specifications. Most characteristic data only reflect gross properties covered in the specifications. Proportions and values vary with the type of crude oil from which the final fuel is derived and the refining process used.

TABLE 3-4. Physical and Chemical Properties of JP-7[a]

Property	Information	Reference
Molecular weight	Not applicable[b]	
Color	Colorless	Martel 1992
Physical state	Liquid	CHRIS 1986
Melting point	-30 °C	ITC 1985
Boiling point (1 atm)	182–288 °C (specification)	Air Force 1977; CRC 1984
	205–300 °C	ITC 1985
	150–200 °C	Dickson and Woodward 1987
Density:		
at 15 °C	779–806 kg/m^3 (specification)	Air Force 1977; CRC 1984; Dukek 1978
Odor	Like kerosene	Martel 1992
Odor threshold:		
Water	No data	
Air	No data	
Solubility:		
Water at 20 °C	38.4 mg/L	CRC 1984
Organic solvent(s)	Generally miscible with organic solvents (e.g., benzene, Freon® 113, cyclohexane)	ASTM 1982; IARC 1989
Partition coefficients:		
Log K_{ow}	No data	
Log K_{oc}	No data	
Vapor pressure;		
at 149 °C	1.55x10^2 mm Hg	Air Force 1977
at 260 °C	2.48x10^3 mm Hg	Air Force 1977
Henry's law constant	No data	
Autoignition temperature	241 °C	CRC 1984
Flashpoint	43–66 °C	NFPA 1986
	60 °C (specification)	Air Force 1977; CRC 1984
Flammability limits	0.6% lower; 4.6% upper	Dukek 1978
Explosive limits	No data	

[a]JP-7, or jet propellant-7, is a mixed compound composed primarily of hydrocarbons (i.e., alkanes, cycloalkanes, alky-benzenes, indan/tetralins, and naphthalenes).
[b]Jet fuels are blends prepared to meet certain gross property specifications. Most characteristic data only reflect gross properties covered in the specifications. Proportions and values vary with the type of crude oil from which the final fuel is derived and the refining process used.

TABLE 3-5. Composition (weight %) of Shale-Derived and Petroleum-Derived JP-4

Constituents	Shale-derived	Petroleum-derived
N-alkanes		
Heptane	4.73	15.76
Octane	7.48	6.60
Nonane	7.24	2.54
Decane	11.25	2.24
Indane	0.42	0.17
Undecane	16.62	4.17
Dodecane	11.49	5.25
Tridecane	6.07	4.71
Tetradecane	3.19	1.02
Pentadecane	0.96	1.35
Total	69.45	43.81
Monosubstituted alkanes		
3-Methyl hexane	3.05	14.39
2-Methyl heptane	3.08	6.14
3-Methyl heptane	1.64	7.19
Total	7.77	27.72
Disubstituted alkane		
2,3-Dimethyl pentane	—	—
2,5-Dimethyl pentane	0.18	1.48
2,4-Dimethyl pentane	0.63	2.52
Total	0.81	4.00
Cyclohexanes		
Cyclohexane	1.52	2.13
Methyl cyclohexane	5.68	2.17
Ethyl cyclohexane	—	—
Total	7.20	4.30
Monosubstituted aromatics		
Methyl benzene	3.77	3.41
Disubstituted aromatics (xylenes)		
m-Xylene	2.60	2.71
p-Xylene	1.70	1.63
o-Xylene	2.00	1.89
Total	6.30	6.23
Multisubstituted aromatics		
1,3,5-Trimethylbenzene	1.52	1.09
1,2,4-Trimethylbenzene	2.00	3.52
1,2,3-Trimethylbenzene	0.30	1.04
Total	3.82	5.65
Overall total	99.12	95.12

Source: Air Force 1988b

TABLE 3-6. U.S. Military Specifications for JP-4 Fuel

	Issuing agency:		USAF	
	Specification:		MIL-T-5624-N	
	Revision date:		22 March 1990	
	Grade designation:		JP-4	Test method
	Fuel type:		Wide-cut	ASTM FTMS 791
Composition	Acidity, total (mg KOH/g)	Max.	0.015	D 3242
	Aromatics (vol%)	Max.	25.0	D 1319
	Olefins (vol%)	Max.	5.0	D 1319
	Sulfur, mercaptan (wt%) (1)	Max.	0.00	D 3227
	Sulfur, total (wt%)	Max.	0.4	D 1266/D 2622/ D 3120
	Color, saybolt	Max.	Report	D 156
Volatility	Distillation			
	Temp. Init. BP (°C)	Max.	Report	D 86/D 2887
(D 2887 limits in parentheses)	Temp. 10% Rec (°C)	Max.	Report	
	20% Rec (°C)	Max.	145 (130)	
	50% Rec (°C)	Max.	190 (185)	
	90% Rec (°C)	Max.	245 (250)	
	Final BP (°C)	Max.	270 (320)	
	Residue (vol%) (for D 86)	Max.	1.5	
	Loss (vol%) (for D 86)	Max.	1.5	
	Explosiveness (%)	Max.		
	Flash point (°C)	Max.		D 93
	Gravity, °API (15 °C)	Max.	45–57	D 1298
	Density, 15 °C (kg/m^3)	Max.	751–802	D 1298
	Vapor pressure (37.8 °C) kPa (psi)		14–21 (2.03–3.0)	D 323/D 2551
Fluidity	Freezing point, °C (F)	Max.	-58 (-72)	D 2336
	Viscosity @ -20 °C (cSt)	Max.	—	D 445
Combustion	Aniline-gravity product or	Min.	5250	D 1405
	Net heat of comb., MJ/kg (Btu/lb)	Min.	42.8 (18,400)	D 2382/D 3328/ D 240
	Smoke point or	Min.	20.0	D 1322
	Hydrogen content (wt%)	Min.	13.5	D 1018/D 3343/ D 3701
Corrosion	Copper strip (2 hr @ 100 °C)	Max.	1	D 130
Stability	JFTOT ΔP (mm Hg)	Max.	25	D 3241 (5)
	JFTOT tube color code	Max.	<3	
Contaminants	Existent gum (mg/100 mL)	Max.	7	D 381
	Particulates (mg/L)	Max.	1	D 2276 (2)
	Water reaction interface	Max.	1b	D 1094
	Water separation index modified	Min.	70 (3)	D 2550
	Flitration time (minutes)	Max.	10	(2)
Additives	Anti-icing (vol%)		0.10–0.15	5330, 5340,
	Antioxidant		Required (4)	3527 FED STD 791
	Corrosion inhibitor		Required	
	Metal deactivator		Option	
	Antistatic		Required	
Other	Conductivity (pS/m) at <29.4 °C		150–600	D 2624/D 4308
	Service		All	
	NATO code No.		F-40	

Notes: (1) The mercaptan sulfur determination may be waived if fuel "Doctor Sweet."
(2) Minimum one-gallon sample. Filtration time in accordance with D 2276 particulate.
(3) With all additives except electrical conductivity additive.
(4) If hydrogen treated blend stocks used—optional if no hydrotreating used.
(5) Test at 260 °C tube temperature.

Source: Air Force 1990; CRC 1984.

TABLE 3-7. U.S. Military Specifications for JP-7 Fuel

	Issuing agency:		USAF	
	Specification:		MILT-38219A - Amd. 2	
	Revision date:		26 January 1981	
	Grade designation:		JP-7	Test method
	Fuel type:		Low volatility	ASTM
Composition	Acidity, total (mg KOH/g)	Max.		D 3242
	Aromatics (vol%)	Max.	5	D 1319
	Olefins (vol%)	Max.		D 1319
	Sulfur, mercaptan (wt%)	Max.	0.001	D 3227
	or			
	Doctor test, N = negative	Max.	N	D 1266, D 2622 or
	Sulfur, total (wt%)		0.1	D 3120
Volatility	Distillation			
	Temp. Init. BP (°C)		182 min.	D 86 or D 2887
	10% Rec (°C)		196 min.	
	20% Rec (°C)		206 min.	
	50% Rec (°C)		Report	
	90% Rec (°C)		260 max.	
	Final BP (°C)		288 max.	
	Residue (vol%)		1.5 max.	D 86
	Loss (vol%)		1.5 max.	D 86
	Flash point (°C)		60 min.	D 56 or D 93
	Gravity, °API (15 °C)		44–50	D 1298
	Density, 15 °C (kg/m^3)		779–806	D 1298
	Vapor pressure @ 149° (kPa)	Max.	20.7 (1)	
	Vapor pressure @ 260° (kPa)	Max.	331 (1)	
Fluidity	Freezing point, (°C)	Max.	-43.5	D 2386
	Viscosity @ -40 °C (cSt)	Max.		D 445
	Viscosity @ -34.5 °C (cSt)	Max.	15.0	
Combustion	Net heat of comb., MJ/kg	Min.	43.5	D 240, D 2382, or D 3338
	Luminometer No.	Min.	75 (2)	D 1740
	Smoke point	Min.		D 1322
	Hydrogen content (wt%)	Min.	(2)	D 3343
Corrosion	Copper strip (2hrs @ 100 °C)	Max.	1b	D 130
Thermal stability	(JFTOT or coker)			
	JFTOT TDR	Max.	12 (3)	D 3241
	JFTOT (mm Hg pressure diff.)	Max.	25 (3)	D 3241
	Coker, tube deposit		<3 (4)	D 1660 (TS only)
	Coker (mm Hg pressure diff.)	Max.	76 (4)	D 1660 (TS only)
Contaminants	Existent gum (mg/100 mL)	Max.	5.0	D 381
	Particulate matter (mg/L)			D 2776
	FOB origin deliveries	Max.	.3	(5)
	FOB destination deliveries	Max.	.5	
	WSIM	Min.	85	D 2550 or D 3948
Additives	JFA-5 (mg/L)			
	Anti-icing (vol%)		0.10 to 0.15	FTMS 791, 5327, or
	Antioxidant		Option	5340
	Metal deactivator		Option	
	Lubricity (ppm)		200–250	
Other	Thermal precipitation rating	Max.	B-2 (6)	

Notes: (1) Vapor pressure test in accordance with Appendix C, MIL-T-38219A.
(2) If luminometer No. between 70 and 75, fuel acceptable—if hydrogen content is not less than 14.4 wt% as calculated by ASTM D 3343.
(3) Test by D 3241—conditions as specified in MIL-T-38219A Amd. 2 and tube rating in Appendix D.
(4) Research fuel coker—conditions as specified in MIL-T-38219A Amd. 2
(5) Minimum sample size of 3.785 L (1 gal) shall be filtered.
(6) Test by Appendix B. MIL-T-38219A.

Source: CRC 1984.

TABLE 3-8. Typical Hydrocarbon Composition of JP-4 Fuel[a]

Compound	JP-4[b]
N-alkanes	
Butane	0.12
Pentane	1.06
Hexane	2.21
Heptane	3.67
Octane	3.80
Nonane	2.25
Decane	2.16
Undecane	2.32
Dodecane	2.00
Tridecane	1.52
Tetradecane	0.73
Pentadecane	—
Hexadecane	—
Heptadecane	—
Octadecane	—
Isoalkanes	
Isobutane	0.66
2,2-Dimethylbutane	0.10
2-Methylpentane	1.28
3-Methylpentane	0.89
2,2-Dimethylpentane	0.25
2-Methylhexane	2.35
3-Methylhexane	1.97
2,2,3,3-Tetramethylbutane	0.24
2,5-Dimethylhexane	0.37
2,4-Dimethylhexane	0.58
3,3-Dimethylhexane	0.26
2,2-Dimethylhexane	0.71
2-Methylheptane	2.70
4-Methylheptane	0.92
3-Methylheptane	3.04
2,5-Dimethylheptane	0.52
2,4-Dimethylheptane	0.43
4-Ethylheptane	0.18
4-Methyloctane	0.86
2-Methyloctane	0.88
3-Methyloctane	0.79

TABLE 3-8. Typical Hydrocarbon Composition of JP-4 Jet Fuel[a] *(continued)*

Compound	JP-4[b]
2-Methylundecane	0.64
2,6-Dimethylundecane	0.71
2,4,6-Trimethylheptane	—
4-Methyldecane	—
2-Methyldecane	—
2,6-Dimethyldecane	—
2-Methylundecane	—
2,6-Dimethylundecane	—
Cycloparaffins	
Methylcyclopentane	1.16
Cyclohexane	1.24
t-1,3,-Dimethylcyclopentane	0.36
c-1,3,-Dimethylcyclopentane	0.34
c-1,2-Dimethylcyclopentane	0.54
Methylcyclohexane	2.27
Ethylcyclopentane	0.26
1,2,4-Trimethylcyclopentane	0.25
1,2,3-Trimethylcyclopentane	0.25
c-1,3-Dimethylcyclohexane	0.42
1-Methyl-3-ethylcyclohexane	0.17
1-Methyl-2-ethylcyclohexane	0.39
Dimethylcyclohexane	0.43
1,3,5-Trimethylcyclohexane	0.99
1,1,3-Trimethylcyclohexane	0.48
1-Methyl-4-ethylcyclohexane	0.48
n-Butylcyclohexane	0.70
Propylcyclohexane	—
Hexylcyclohexane	—
Heptylcyclohexane	—
Aromatic hydrocarbons	
Benzene	0.50
Toluene	1.33
Ethylbenzene	0.37
m-Xylene	0.96
p-Xylene	0.35
o-Xylene	1.01
Isopropylbenzene	0.30

TABLE 3-8. Typical Hydrocarbon Composition of JP-4 Jet Fuel[a] *(continued)*

Compound	JP-4[b]
n-Propylbenzene	0.71
1-Methyl-3-ethylbenzene	0.49
1-Methyl-4-ethylbenzene	0.43
1,3,5-Trimethylbenzene	0.42
1-Methyl-2-ethylbenzene	0.23
1,2,4-Trimethylbenzene	1.01
1,3-Diethylbenzene	0.46
1,4-Diethylbenzene	—
1-Methyl-4-propylbenzene	0.40
1,3-Dimethyl-5-ethylbenzene	0.61
1-Methyl-2-isopropylbenzene	0.29
1,4-Dimethyl-2-ethylbenzene	0.70
1,2-Dimethyl-4-ethylbenzene	0.77
1,2,3,4-Titramethylbenzene	0.75
1-Ethylpropylbenzene	—
1,2,4-Triethylbenzene	—
1,3,5-Triethylbenzene	—
Phenylcyclohexane	—
1-t-Butyl-3,4,5-trimethylbenzene	—
n-Heptylbenzene	—
Naphthalene	0.50
2-Methylnaphthalene	0.56
1-Methylnaphthalene	0.78
2,6-Dimethylnaphthalene	0.25
Biphenyl	—
1-Ethylnaphthalene	—
2,3-Dimethylnaphthalene	—
n-Octylbenzene	—

[a]Smith et al. 1981
[b]Concentrations in weight percent