3. CHEMICAL AND PHYSICAL INFORMATION

3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of fuel oils is located in Table 3-l. Information on the composition of selected fuel oils, specifically fuel oil no. 2 and kerosene, is presented in Table 3-2.

All of the fuel oil classes discussed in this Profile are refined from crude petroleum and may be categorized as either a distillate fuel or a residual fuel depending on the method of production. Fuel oils no. 1 and no. 2 are distillate fuels which consist of distilled process streams. Residual fuel oils such as fuel oil no. 4 are residues remaining after distillation or cracking, or blends of such residues with distillates (IARC 1989). Diesel fuels are approximately similar to fuel oils used for heating (fuel oils no. 1, no. 2, and no. 4). All fuel oils consist of complex mixtures of aliphatic and aromatic hydrocarbons. The aliphatic alkanes (paraffins) and cycloalkanes (naphthenes) are hydrogen saturated and compose approximately 80-90% of the fuel oils. Aromatics (e.g., benzene) and olefins (e.g., styrene and indene) compose 10-20% and l%, respectively, of the fuel oils. Fuel oil no. 1 (straightrun kerosene) is a light distillate which consists primarily of hydrocarbons in the C_9—C_{16} range; fuel oil no. 2 is a heavier, usually blended, distillate with hydrocarbons in the C_{11}-C_{20} range. Straight-run distillates may also be used to produce fuel oil no. 1 and diesel fuel oil no. 1. Diesel fuel no. 1 and no. 2 are similar in chemical composition to fuel oil no. 1 and fuel oil no. 2, respectively, with the exception of the additives. Diesel fuels predominantly contain a mixture of C_{10} through C_{19} hydrocarbons, which include approximately 64% aliphatic hydrocarbons, l-2% olefinic hydrocarbons, and 35% aromatic hydrocarbons (Air Force 1989). Jet fuels are based primarily on straight-run kerosene, as well as additives. All of the above fuel oils contain less than 5% polycyclic aromatic hydrocarbons. Fuel no. 4 (marine diesel fuel) is less volatile than diesel fuel no. 2 and may contain up to 15% residual process streams, in addition to more than 5% polycyclic aromatic hydrocarbons (IARC 1989). Residual fuel oils are generally more complex in composition and impurities than distillate fuel oils; therefore, a specific composition cannot be determined (Air Force 1989). Sulfur content in residual fuel oils has been reported to be from 0.18% to 4.36% by weight.

TABLE 3-1. Chemical Identity of Fuel Oils

Characteristic	Fuel oil no. 1	Fuel oil no. 1-D	Fuel oil no. 2	Fuel oil no. 2-D	Fuel oil no. 4	Fuel oil UNSP
Synonym(s)	Kerosene; coal oil; kerosine; range oil; straight run kerosene; distillate fuel oils, light; furnace oil no. 1; Deobase®; JP-5; JP-1; range oil[a,b,c]	Diesel fuel; diesel fuel oil no. 1; diesel oil no. 1; no. 1 diesel; diesel oil (light); Arctic diesel[a,d,e]	API no. 2 fuel oil; gas oil; home heating oil no. 2; number 2 burner oil; diesel fuel; furnace oil no. 2[b]	Diesel fuel; diesel fuel oil no. 2; diesel oil no. 2; no. 2 diesel; diesel oil (medium)[a,d,e]	Oil, fuel, no. 4; residual fuel oil no. 4; no. 4 fuel oil; residual fuel oil; marine boiler fuel; marine diesel fuel; diesel fuel no. 4; grade 4[a,d,e]	No data
Registered trade name(s)	Deobase®[c]	No data	No data	No data	No data	No data
Chemical formula[f]	No data	No data	No data	No data	No data	No data
Chemical structure[f]	No data	No data	No data	No data	No data	No data
Identification numbers:						
CAS registry	8008-20-6[c]/70892-10-3[e]	No data	68476-30-2[d]	68476-34-6[a]	68476-31-3[b]	No data
NIOSH RTECS	OA5500000[c]	No data	HZ1800000[d]	No data	No data	LS8950000[d]
EPA hazardous waste	No data	No data	No data	No data	No data	No data
OHM/TADS	7217063[e]	No data	No data	No data	7217065[e]	No data
DOT/UN/NA/IMCO shipping	UN 1223; IMO 3.3[c]	No data	No data	No data	No data	No data
HSDB	632[c]	No data	No data	No data	No data	No data
NCI	No data	No data	C54795[g]	No data	No data	No data

[a]IARC 1989
[b]RTECS 1991
[c]HSDB 1991
[d]Air Force 1989
[e]OHM/TADS 1985
[f]Fuel oils are mixtures of various hydrocarbons designed to meet specifications set forth by the American Society for Testing and Materials (IARC 1989); therefore, chemical structure, chemical formula, and molecular weight cannot be determined.
[g]Sax and Lewis 1989

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 Substances Data Bank; 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. Analysis of Fuel Oils[a]

Hydrocarbon type	Volume %	
	Fuel oil no. 1	Fuel oil no. 2
Paraffins (*n*- and iso-)	52.4	41.3
Monocycloparaffins	21.3	22.1
Bicycloparaffins	5.1	9.6
Tricycloparaffins	0.8	2.3
Total saturated hydrocarbons	79.7	75.3
Olefins	No data	No data
Alkylbenzenes	13.5	5.9
Indans/tetralins	3.3	4.1
Dinaphthenobenzenes/indenes	0.9	1.8
Naphthalenes	2.8	8.2
Biphenyls/acenaphthenes	0.4	2.6
Fluorenes/acenaphthylenes	No data	1.4
Phenanthrenes	No data	0.7
Total aromatic hydrocarbons	23.6	24.7

[a]Derived from IARC 1989; provided by the American Petroleum Institute

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of fuel oils is located in Table 3-3.

TABLE 3-3. Physical and Chemical Properties of Fuel Oils[a]

Characteristic	Fuel oil no. 1	Fuel oil no. 1-D	Fuel oil no. 2	Fuel oil no. 2-D	Fuel oil no. 4	Fuel oil no. UNSP
Molecular weight	No data	No data	No data	No data	No data	No data
Color	Pale yellow[b]; Colorless to brown[c,d]	Colorless to brown[c]	Colorless to brown[c]	Colorless to brown[c]	Colorless to brown[c]	Colorless to brown[c]
Physical state	Liquid[c]	Liquid[c]	Liquid[c]	Liquid[c]	Liquid[c]	Liquid[c]
Melting point	-45.6°C[d]	-34°C[d]	-29°C[d]	18°C[d]	-29°C to -9°C[d]; -46°C[e]	-48°C–18°C[c]
Boiling point	175–325°C[b]; 200–260°C[d]	193–293°C[d]	160–360°C[f] 282–338°C[d]	282–338°C[d]	101–588°C[d]	151–>588°C[c]
Density:						
At 15°C	0.810–0.9360 g/mL[c]	0.810–0.9360 g/mL[c]	No data	No data	0.810–0.9360 g/mL[c]	No data
At 20°C	0.80 g/mL[e,f]	No data	0.8700–0.9500[e]	0.8700–0.9500 g/mL[c]	1 g/mL[e]	No data
Odor	Kerosene-like[c]	Kerosene-like[c]	Kerosene-like[c]	Kerosene-like[c]	Kerosene-like[c]	Kerosene-like[c]
Odor threshold (ppm)	0.082[f]; 1[d]	0.7[d]	No data	No data	0.5[e]	No data
Solubility						
Water at 20°C	≈5 mg/L[c]	≈5 mg/L[c]	≈5 mg/L[c]	≈5 mg/L[c]	≈5 mg/L[c]	≈5 mg/L[c]
Organic solvent(s)	Miscible with other petroleum solvents[b]	No data	No data	No data	No data	No data
Partition coefficients:						
Log K_{ow}	3.3–7.06[c]	3.3–7.06[c]	3.3–7.06[c]	3.3–7.06[c]	3.3–7.06[c]	3.3–7.06[c]
Log K_{oc}	3.0–6.7[c]	3.0–6.7[c]	3.0–5.7[c]	3.0–6.7[c]	3.0–6.7[c]	3.0–6.7[c]
Vapor pressure at 21°C	2.12–26.4 mmHg[c]	2.12–26.4 mmHg[c]	2.12–26.4 mmHg[c]	2.12–26.4 mmHg[c]	2.12–26.4 mmHg[c]	2.12–26.4 mmHg[c]
Henry's law constant at 20°C - atm-m^3/mol	5.9 x 10^{-5}–7.4[c]	5.9 x 10^{-5}–7.4[c]	5.9 x 10^{-5}–7.4[c]	5.9 x 10^{-5}–7.4[c]	5.9 x 10^{-5}–7.4[c]	5.9 x 10^{-5}–7.4[c]
Autoignition temperature	229°C[d]	177.0–329.0°C[d]	257°C[d]	254–285°C[d]	263°C[d]	No data
Flashpoint (close cup)	38°C[c,d]	38°C[d,f]	58°C[d]	52°C[d,f]	55°C[f];>54°C[d]	No data
Flammability limits (% volume in air)	0.7%–5%[d]	1.3–6.0%[d]	0.6–7.5%[d]	1.3–6.0%[d]	1.0–5.0%[d]	No data
Conversion factors	No data	No data	No data	No data	No data	No data
Explosive limits	0.7%–5%[b]	No data	No data	No data	No data	No data

[a]Values listed are specifications required or general characteristics of each class of fuel oils.
[b]HSDB 1991
[c]Air Force 1989
[e]OHM/TADs 1985
[d]Coast Guard 1985
[f]IARC 1989