Appendix 6A

**Composition of Crude Oil and Refined Products** 

### Appendix 6A

#### **Composition of Crude Oil and Refined Products**

Crude oils can vary greatly in composition, viscosity, density, and flammability. They can be found in a continuum ranging from highly flammable, light liquids (similar to gas condensate), to highly viscous and heavy tar-like materials. Organic compounds range from methane to extremely heavy hydrocarbon molecules with up to 80 carbon atoms. The chemical composition of crude varies between regions and even within the same geologic formation.

No two batches of crude oil are chemically identical. Crude oil is categorized based on the molecular weight distribution of their constituents, and distinctions are made between light, medium, and heavy crude oil. The EPC pipeline carried at least 22 types of crude oil during its operation between 1950 and 1995. In Table 6A-1, crude oil parameters were averaged for these 22 types based on Exxon crude oil assay sheets. No data are available on the amount of crude oils shipped, so this is not a weighted average. From the data, it appears the EPC pipeline carried mostly medium and heavy crude oil. A study done by the National Research Council in 1985 titled, *Oil in the Sea, National Academy Press* cited in Jones and Neuse (1995), was used to develop a summary compositional analysis of crude oil. This typical crude oil composition is provided in Table 6A-2.

Crude oil is composed of varying fractions of different boiling point ranges of hydrocarbon mixtures. The major fractions are defined as:

- Light ends;
- Light naphtha;
- Medium naphtha;
- Heavy naphtha;
- Kerosene;
- Light gas oil;
- PGO; and
- Residual oil.

The most flammable components are in the light ends through medium naphtha fractions, which together form a mixture somewhat similar in properties to gasoline. The heavy naphtha through residual fractions reflect properties typically perceived as those associated with oils.

The aromatic components of the crude oil, found primarily within medium to heavy naphtha fractions and gas oil fractions, include benzene, a known human carcinogen. Other aromatic compounds include toluene, ethylbenzene, and xylene. These aromatic compounds have relatively high solubilities in water, compared with other hydrocarbons. Refined products, to be carried by the Longhorn pipeline, include various gasoline grades, diesel fuel, and jet fuel. As with crude oil, gasoline is also a complex mixture of hydrocarbons. Gasoline contains more lower molecular weight hydrocarbons than crude oil, and higher fractions of both light hydrocarbons and aromatics. The hazard level of these materials must be considered on two levels: 1) their impact should they contaminate surface water or ground water, and 2) their potential to ignite and explode. To adequately model worst-case scenarios, a product most likely to rank high on both scales was selected. To accurately represent the worst-case gasoline composition that could be transported through the Longhorn pipeline, the survey composition was modified to reflect a gasoline composition containing MTBE (methyl tertiary-butyl ether).

From the point of view of toxicity and environmental impact, benzene and MTBE have greater concern. Benzene is the primary known carcinogen in gasoline. It is one of the most water-soluble hydrocarbons at 1,700 milligrams per liter (mg/L). There are also a number of hydrocarbons closely related to benzene, that have relatively high solubilities. As a result of the relatively high solubility of mono- and dialkylbenzenes, benzene-toluene-ethylbenzene-xylene (BTEX) tends to dominate the dissolved hydrocarbons in water. BTEX is readily oxidized microbiologically, provided other microbial nutrients are sufficiently available. This natural attenuation of BTEX typically constrains the extent of plume spread in contaminated water and soils, as biodegradation destroys the BTEX at the edge of the plume.

MTBE is a suspected carcinogen by some. MTBE is very mobile and has a low odor and taste threshold. This makes contaminated drinking water unpalatable at concentrations as low as 20 micrograms per liter. MTBE's mobility is due to three factors: solubility, diffusivity, and lack of biodegradability. Up to 4.8 percent MTBE dissolves in water, it adsorbs very poorly to soil, and very little biodegradation has been observed in natural conditions. As a result, MTBE usually migrates substantially ahead of a hydrocarbon plume.

In summary, MTBE and benzene are the prime water contaminants of concern for fuel hydrocarbon spills. Gasolines are the lightest, most volatile, and flammable of the products that could be carried by the Longhorn pipeline. Gasolines are the only products with the potential to contain MTBE. They also have the highest benzene content. For these reasons, gasoline was identified as the worst-case product to be carried by the pipeline.

The model gasoline composition for this study is provided in Table 6A-3. An existing gasoline composition (without MTBE) survey was reviewed (LUFT, 1988) and it was concluded that the hydrocarbon composition in this survey adequately represents the typical flammability range of gasolines. To accurately represent the worst-case gasoline that could be transported through the Longhorn pipeline, the survey composition was modified to reflect a gasoline composition containing MTBE.

First, the benzene concentration was adjusted. The Longhorn pipeline specifies a maximum benzene content of 4.9 percent by weight in the products carried. To properly represent a worst-case relative to benzene concentration, the LUFT survey average benzene concentration of 1.8 percent (wt) was replaced with the Longhorn pipeline product specification of 4.9 percent.

Gasoline blends may contain up to 15 percent MTBE, so this percentage was added as the worst-case. After making these two changes, the fractions of the other components were adjusted so that the total would still equal 100 percent.

Exxon PL/Longhorn	Historical Crude Assays												
			Τ	Salt Flat	Salt Flat	Salt Flat			W Texas				
		Gulf Coast	Salt	Mix	Mix	Mix	W Coast	W. Coast	Intermed.	Intermed.	Intermed.	Intermed.	Intermed.
Crude Type:	Conroe	Mix	Flat	1	2	3	Hvy	Sour	1	2	Crane	3	Monah.
API Gravity	37.4	40.3	37.0	34.2	32.6	35.5	23.2	29.0	38.0	40.5	40.9	40.3	37.2
Sulfur, wt%	0.07	0.08	0.58	0.80	1.27	0.78	1.02	0.80	0.35	0.34	0.34	0.41	0.43
H <sub>2</sub> S, ppm						60		2	1				
Light ends, Vol%													
C2-hydrocarbons	0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.06	0.00	0.04	0.05	0.05
C3- hydrocarbons	0.22	0.11	0.17		0.18	0.09	0.01	0.15	0.72	0.40	0.81	0.40	0.55
IC4 (isobutane)	0.19	0.26	0.18		0.13	0.09	0.07	0.17	0.41	0.40	0.39	0.23	0.25
NC4 (Normal butane)	0.47	1.51	0.36		0.56	0.21	0.51	0.96	2.38	1.91	1.88	1.00	1.48
IC5 (Isopentane)	0.43	1.44	0.54		0.61	0.25	1.13	1.57	1.24	1.27	1.09	0.81	0.90
NC5 (Normal Pentane)	0.48	1.83	0.50		0.81	0.32	1.29	1.79	1.94	1.95	1.89	1.52	1.61
Sum C2-C5	1.8	5.2	1.8	0.7	2.3	1.0	3.0	4.6	6.8	5.9	6.1	4.0	4.8
Light Naphthene (bp<175F)													
Volume %	4.38	8.52	3.67	2.25	4.64	2.77	5.90	8.24	7.65	9.04	8.92	7.59	7.31
Reid Vapor Pressure (psia)		10.1	8.9	7.9	9.3	8.1	10.6	10.7	10.6	9.8	9.8	9.1	9.7
Medium Naphtha (175 <bp<250f)< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></bp<250f)<>													
Volume %	9.11	10.09	6.77	4.5	5.97	5.44	5.05	6.78	8.21	10.63	11.77	11.57	8.03
Aromatics Vol.%	19.2	12.5	4.8	4.5	8.3	7.5	5.8	8.1	3.8	5.4	10.8	5.6	4.2
Naphthene Vol.%	50.3	45.3	35.9	30.4	33.9	30.5	47.7	39.6	41.5	52.2	43.0	39.9	45.7
Paraffins Vol.%													
Sum	69.5	57.8	40.7	34.9	42.2	38	53.5	47.7	45.3	57.6	53.8	45.5	49.9
Heavy Naphtha (250 <bp<375f)< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></bp<375f)<>													
Volume %	18.2	16.7	16.2	12.9	12.1	15.43	8.67	12.2	13.5	16.2	16.71	17.89	13.23
Aromatic Vol.%	35.7	19.9	11.0		11.1	11.4	13.4	15.8	8.2	12.0	16.7	11.0	8.7
Naphthenes Vol.%	31.0	38.1	38.2	33.6	33.6	35.2	52.4	39.7	43.3	43.3	39.1	36.6	45.5
Paraffins Vol.%													1
Sum	66.7	58.0	49.2	44.5	44.7	46.6	65.8	55.5	51.5	55.3	55.8	47.6	54.2
Kerosene (375 <bp<650f)< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></bp<650f)<>													
Volume %	28.68	19.63	19.84	20.07	16.95	20.19	12.02	15.31	15.62	16.88	17.26	17.38	15.23
Light Gasoil (530 <bp<650f)< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td>1</td></bp<650f)<>													1
Volume %	18.19	13.56	13.43	16.68	12.34	14.88	11.37	11.88	11.18	11.30	11.72	11.90	11.57
PGO (650 <bp<1049f)< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></bp<1049f)<>													
Volume %	19.17	23.50	30.80	31.08	30.50	33.50	31.84	26.40	29.90	24.30	23.90	24.20	32.30
Aromatics Vol.%	8.4	8.4	8.5	7.6	10.5	9.5	17.1	16.4	10.2	8.4	11.0	11.4	10.4
Naphthene Vol.%	30.5	28.2	28.2	31.5	31.9	29.8	52.1	49.2	32.5	30.1	31.2	32.2	32.1
Residual Oil (bp>1049F)													1
Volume %	1.40	6.10	8.60	12.24	16.60	7.40	24.56	17.89	10.40	9.00	6.60	7.80	10.00
Sum Volume %	100.9	103.3	101.0		101.4	100.6	102.4	103.4	103.2	103.2	103.0	102.3	102.5

## Table 6A-1. Composition of Crude Oil Carried by EPC Pipeline

 Table 6A-1. (Continued)

Exxon PL/Longhorn												
	W Texas W Texas W Texas											
	Sour	Sour	Sour		Yates	Prudhoe	Prudhoe	Prudhoe	Point		Fra	ctions
Crude Type:	Kemper	2	1	Yates	Mix	1	2	3	Arguello	Average	Vol.%, a	pprox. Cn
API Gravity	32.6	31.8	32.1	28.9	29.4	27.1	27.5	24.9	19.0	32.7		
Sulfur, wt%	1.92	2.05	1.73	1.59	1.49	1.02	0.97	1.06	4.30	1.1		
$H_2S$ , ppm				118	189				74.0			
Light ends, Vol%												
C2-hydrocarbons	0.08	0.02	0.00	0.00	0.00	0.05	0.09	0.01	0.10	0.03		
C3-hydrocarbons	0.52	0.5	0.73	0.06	0.16	0.38	0.66	0.10	0.69	0.35		
IC4 (Isobutane)	0.45	0.25	0.38	0.15	0.22	0.05	0.09	0.01	0.10	0.21		
NC4 (Normal butane)	1.35	0.86	0.94	0.42	0.54	0.30	0.43	0.08	0.45	0.85		
IC5 (Isopentane)	1.12	0.97	0.98	0.91	0.89	0.55	0.63	0.12	0.67	0.83		
NC5 (Normal pentane)	1.16	1.09	0.93	0.20	0.30	0.63	0.67	0.18	0.71	1.00		
Sum C2-C5	4.7	3.7	4.0	1.7	2.1	2.0	2.6	0.5	2.7	3.27	3.21	Light ends
Light Naphtha (bp<175F)												(C2-C5)
Volume %	6.91	6.33	6.74	3.66	3.54	3.87	4.00	1.54	3.91	5.52		
Reid Vapor Presence (psia)	9.8	9.6	9.3	9.6	10.1	9.2	9.5	7.6	9.9	9.5		
Medium Naphtha (175 <bp<250f)< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></bp<250f)<>												
Volume %	6.99	7.45	7.01	5.09	5.62	5.51	5.31	3.55	4.51	7.04		
Aromatic Vol.%	11.0	11.6	6.5	3	0.4	14.5	15.9	15.8	6.7	8.5		
Naphthnens Vol.%	40.4	34.3	49.8	42.3	44.5	25	24.2	33.2	29.9	39.07		
Paraffins Vol.%						60.4	59.9	51.0	63.4	58.7		
Sum	51.4	45.9	56.3	45.3	44.9	99.9	100.0	100.0	100.0	58.19		
Heavy Naphtha (250 <bp<375f)< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></bp<375f)<>												
Volume %	12.70	13.39	12.90	12.85	12.52	10.49	9.75	8.52	8.63	13.26	25.35	Naphta
Aromatics Vol.%	18.0	18.2	16.1	10.0	7.8	21.3	21.1	22.5	16.7	15.3		(C6-C10)
Naphthenes Vol.%	43.5	38.2	47.2	52.3	55.9	36.5	35.2	34.5	40.0	40.6		
Paraffins Vol.%						42.2	43.8	43.0	43.3	43.1		
Sum	61.5	56.4	63.3	62.3	63.7	100.0	100.1	100.0	100.0	63.8		
Kerosene (375 <bp<650f)< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></bp<650f)<>												
Volume %	16.00	15.89	15.80	16.85	16.65	16.23	16.17	16.20	11.46	17.11	16.80	Kerosene
Light Gasoil (530 <bp<650f)< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td>(C10-C12)</td></bp<650f)<>												(C10-C12)
Volume %		11.90	12.09	12.21	13.14	12.75	12.00	14.19	8.9	12.69	12.46	LtGO
PGO (650 <bp<1049f)< td=""><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td>(C12-C20)</td></bp<1049f)<>												(C12-C20)
Volume %	31.80	29.40	31.10	30.67	33.30	30.28	32.72	37.60	24.21	29.20	28.68	PGO
Aromatics Vol.%	14.7	11.9	13.6	12.8	14.6	15.2	11.7	14.0	16.3	11.9		(C20-C40)
Naphthenes Vol.%	38.4	39.5	41.7	40.9	41.3	42.3	42.0	47.2	36.9	İ		
Residual Oil (bp>1049F)												
Volume %	11.20	14.00	12.40	18.04	14.30	20.05	18.76	18.18	37.04	13.75	13.50	Resid
												(>C40)
Sum Volume %	102.3	102.1	102.0	101.1	101.2	101.1	101.3	100.3	101.4	101.8	100.00	

Based on Historical Crude Assays								
				F	ractions			
					Name &			
	High	Low	Average	Vol.%	Approx.			
General								
API Gravity	40.9	19.0	32.7		C-range			
Sulfur, wt%	4.3	0.1	1.1					
H2S, ppm <sup>1</sup>	189.0	1.0	74.0					
Light ends, Vol%								
C2 – hydrocarbons	0.10	0.00	0.03					
C3 – hydrocarbons	0.81	0.01	0.35					
iC4 (Isobutane)	0.45	0.01	0.21					
nC4 (Normal butane)	2.38	0.08	0.85					
iC5 (Isopentane)	1.57	0.12	0.83					
nC5 (Normal pentane)	1.95	0.18	1.00					
Sum C2-C5	6.75	0.50	3.27	3.21	Light ends			
Light Naphtha (bp<175F)					(C2-C5)			
Volume %	9.0	1.5	5.5					
Reid Vapor Pressure (psia)	10.7	7.6	9.5					
Medium Naphtha (175 <bp<250f)< td=""><td></td><td></td><td></td><td></td><td></td></bp<250f)<>								
Volume %	11.8	3.6	7.0					
Aromatics Vol.%	19.2	0.4	8.5					
Naphthenes Vol.%	52.2	24.2	39.1					
Paraffins Vol.% <sup>1</sup>	63.4	51.0						
Heavy Naphtha (250 <bp<375f)< td=""><td></td><td></td><td></td><td></td><td></td></bp<375f)<>								
Volume %	18.2	8.5	13.3	25.35	Naphta			
Aromatics Vol.%	35.7	7.8			(C6-C10)			
Naphthenes Vol.%	55.9	31.0			()			
Paraffins Vol.% <sup>1</sup>	43.8	42.2	43.1					
Kerosene (375 <bp<650f)< td=""><td></td><td></td><td></td><td></td><td></td></bp<650f)<>								
Volume %	28.7	11.5	17.1	16.80	Kerosene			
Light Gasoil (530 <bp<650f)< td=""><td></td><td></td><td></td><td> •</td><td>(C10-C12)</td></bp<650f)<>				•	(C10-C12)			
Volume %	18.2	8.9	12.7	12.46	LtGO			
PGO (650 <bp<1049f)< td=""><td></td><td></td><td></td><td></td><td>(C12-C20)</td></bp<1049f)<>					(C12-C20)			
Volume %	37.6	19.2	29.2	28.68	PGO			
Aromatics Vol.%	17.1	7.6			(C20-C40)			
Naphthenes Vol.%	52.1	28.2			( 0.0)			
Residual Oil (bp>1049F)		_0.2	20.7					
Volume %	37.0	1.4	13.8	13.50	Resid			
	57.0	1.7	15.0	10.00	(>C40)			

# Table 6A-2. Representative Characteristics of Crude Oil Carriedby the EPC Pipeline

<sup>1</sup> Not available for most crudes carried.

			Properties					
Carbon Number	Compound	Mass %	Solubility (mg/L)	Vapor Pressure (atm)	Henry's Law Coefficient			
	chain Alkanes			· · · ·				
4	C4 (Butanes)	3.67	61.4	2.4	38.7			
5	C5 (Pentanes)	7.08	38.5	0.675	51.7			
6	C6 (Hexanes)	1.59	9.5	0.199	73.9			
7	C7 (Heptanes)	0.96	2.93	0.0603				
8	C8 (Octanes)	0.76	0.66	0.0178				
	Subtotal	14.07						
Branche	d Alkanes							
6	2,3-Dimethyl butanes	0.91	19.1	31.6	58.3			
5	Isopentanes	6.90	13.8	0.904				
6	2-Methyl pentanes	2.87	13.8	0.278				
6	3- Methyl Pentanes	2.04	12.8	0.25	68.7			
7	2,4-Dimethyl Pentanes	0.82	4.06	0.129				
7	2,3-Dimethyl Pentanes	1.91	5.25	0.0906				
8	2,2,4-Trimethyl Pentanes	2.08	2.44	0.0647	124			
8	2,3,3-Trimethyl pentanes	0.99		0.00017				
8	2,3,4-Trimethyl Pentanes	1.24	2	0.0355	83			
7	2-Methyl hexanes	0.78	2.54	0.0867	140			
7	3-Methyl hexanes	0.88	3.3	0.081	101			
9	2,2,5-Trimethyl hexanes	2.58	1.15	0.0218				
9	2,3,5-Trimethyl hexanes	0.48	1.10	0.0210	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,			
8	2-Methyl heptanes	0.65	0.85	0.0257	141			
8	3-Methyl heptanes	0.92	0.792	0.0258				
10	2,2,4-Trimethyl heptanes	0.77	0.772	0.0200				
10	Subtotal	26.83						
	Subtotal	20.05						
Branche	d Alkenes							
6	2-Methyl-2-butene	0.95						
	Subtotal	0.95						
Alkyl Be	nzenes							
6	Benzene	4.90	1,780	0.125	0.225			
7	Toluene	10.43	515	0.0375	0.274			
8	otho-xylene	1.37	220	0.0115	0.228			
8	meta-xylene	1.50	160	0.0109	0.295			
8	para-xylene	2.40	215	0.0115	0.233			
8	Ethylbenzene	0.99	152	0.0125	0.358			
9	1-Methyl-4-Ethylbenzene	0.50	95	0.0039	0.202			
9	1-Methyl-3-Ethylbenzene	1.35		0.00386				
9	1,2,4-Trimethylbenzene	1.68	57	0.00266				
	Subtotal	26.18						

 Table 6A-3. Model Gasoline Composition <sup>1</sup>

			Properties				
Carbon Number	Compound	Mass %	Solubility (mg/L)	Vapor Pressure (atm)	Henry's Law Coefficient		
	Benzo(a)pyrene	1.27E-04	3.80E-03	2.10E-10	1.86E-05		
	Subtotal	1.27E-04					
	MTBE	15.00	48,000	0.309			
	Other	16.97					
	Total	100.00					

## Table 6A-3. (Continued)

<sup>1</sup> 15 percent MTBE, 4.9 percent Benzene, according to Longhorn product specs (RAD 05138-05155)

Source: LUFT 1988