Appendix 4A
Identification of contaminants of concern

A screening level assessment was undertaken to confirm the selection of contaminants of concern likely to be associated with the release of gasoline into the soil environment. The purpose of this assessment was to:

- confirm the indicator contaminants normally selected as the basis for the assessment of soil and groundwater contamination resulting from a gasoline release are likely to determine the risk to human health
- identify some of the compounds that may be associated with aesthetic impacts such as odour resulting from a gasoline release.

Information on the typical composition of a gasoline was obtained as shown in Table 4A1. For each constituent, or class of constituents, the following information of relevance to the fate of chemicals in the environment, their impact on human health and potential for odour impact, was sought:

- human toxicity (Slope Factor, Reference Dose or Reference Concentration)
- aquatic toxicity
- odour threshold
- solubility
- half-life in soil
- vapour pressure
- organic carbon - water partitioning coefficient
- octanol - water partitioning coefficient.

The information collected is summarised in Table 4A1. Given the screening nature of this assessment, the relative values for each of these parameters is more important than the absolute values. Therefore a rigorous assessment of the appropriateness and validity of information obtained regarding, say, the half life of a chemical in soil was not undertaken. The values listed in Table 4A1 are not used elsewhere in this document.

Information was sought from a range of sources including:

- USEPA Integrated Risk Information System database
- USEPA STF base (soil transport fate database)
- Verschueren K. (1983) *Handbook of Environmental Data on Organic Chemicals*
- American Industrial Hygiene Association (1989) *Odor Thresholds for Chemicals with Established Occupational Health Standards*.

For screening purposes, each chemical was assigned a score between 1 and 5 for the following properties:

- toxicity, expressed in terms of a tolerable dose
- abundance in fresh gasoline
- persistence (related to half-life)
- volatility

- odour index.

The basis for assigning scores to individual chemicals is presented as a note to Table 4A2.

The scores assigned to each chemical for individual properties were then combined to give an overall score reflecting the likely significance in terms of:

- **Human health**

Surface soil score = Abundance x Human Toxicity x Persistence

Depth soil score = Abundance x Toxicity x Persistence x Volatility

- **Aesthetic impact**

Overall score = Abundance x Odour Index x Persistence

The results of the screening level assessment of the chemicals of concern associated with a gasoline release are presented in Table 4A2 and are summarised as follows:

- Benzene, xylene and benzo(a)pyrene were found to be most important with respect to human health impacts associated with surface soils
- Benzene, xylene, isopentane, 2,4-dimethylhexane and n-butane were found to be most important with respect to impact on human health resulting from contaminated soil at depth. In practice the limited persistence of isopentane and n-butane means that they are rarely controlling in the case of the historical spills normally subject to a site assessment
- Xylene, trimethyl benzene and diethyl benzene were found to be most important with respect to aesthetic impacts.

The results of the screening level assessment are generally consistent with the indicator chemicals normally selected for the assessment of petroleum release sites. The indicator chemicals considered further in the derivation Tier 1 soil acceptance criteria are as follows:

- benzene, toluene, ethylbenzene and xylenes
- selected PAHs including naphthalene, pyrene (representative of non-carcinogenic PAHs) and benzo(a)pyrene.

Table 4A1 Summary of selected properties of gasoline constituents

Hydrocarbon group	Representative hydrocarbon	Selected representative hydrocarbon(%m/m)		Human toxicity[1]				Aquatic toxicity[2] (mg/L0)
				Oral		Inhalation		
		Range	Average	Slope factor 1/(mg/kg/d)	RfD (mg/kg/d)	Slope factor 1/(mg/kg/d)	RfD (mg/m^3)	
n-ALKANES		10.8-29.6	20.2			8		
C4	n-Butane	4.8-7.0	5.9			22		
C5	n-Pentane	1.9-4.5	3.2					
C6	n-Hexane	2.0-12.9	7.45		0.06		0.2	
C7	n-Heptane	0.2[-2.3	1.25					
C8	n-Octane	1.3	1.3					
C9	n-Nonane	0.4-0.8	0.6		0.6			
C10-14	n-Decane	0.2-0.8	0.5					
BRANCHED ALKANES		18.8-59.5	39.15					
C4	Isobutane	0.7-2.2	1.45					
C5	Isopentane	8.6-17.3	12.95					
C6	2-Methylpentane	4.6-9.7	7.15					
C7	2-Methylhexane	1.4-8.3	4.85					
C8	2,4-Dimethylhexane	1.8-16.7	9.25					
C9	2,4,4-Trimethylhexane	1.2-2.7	1.95					
C10-14	2,2,5,5-Tetramethylhexane	0.5-2.6	1.55					
CYCLOALKANES		3.2-13.7	8.45					
C6	Cyclohexane	0.2	0.2					
C7	Methylcyclohexane	1.0-3.9	2.45				3	
C8	1,2,4-Trimethylcyclopentane	0.2-1.4	0.8					
C9	1,1,3-Trimethylcyclohexane	9.2-0.7	0.45					
Others			4.55					
ALKENES		5.5-13.5	9.5					
C4	Butene	0.9	0.9					
	(alpha butylene)		2.3					
	(beta butylene)		1.3					
C5	1-Pentene	1.3-3.3	5					
C6	Hexene	0.8-1.8						
Others		2.5-7.5						

Table 4A1 (CONTINUED) Summary of selected properties of gasoline constituents

Hydrocarbon group	Representative hydrocarbon	Selected representative hydrocarbon(%m/m)		Human toxicity[1]				Aquatic toxicity[2] (mg/L0)
				Oral		Inhalation		
		Range	Average	Slope factor 1/(mg/kg/d)	RfD (mg/kg/d)	Slope factor 1/(mg/kg/d)	RfD (mg/m^3)	
MON0-AROMATICS		19.3-40.9	30.1					
	Benzene	0.9-4.4	2.65	0.029				0.3
	Toluene	4.0-6.5	5.25		0.2		0.4	0.3
	Mixed xylenes	5.6-6.8	7.2		2			
	(o-xylene)				2			
	(m-xylene)				2			
	(p-xylene)							
	Ethylbenzene	1.2-1.4	1.3		0.01		1	
C3-benzenes	1,3,5-Trimethybenzene	3.2-11.3	7.25					
C4-benzenes	1,2-Diethylbenzene	2.1-2.6	2.35					
Others		`.6-5.2	3.4					
POLY-AROMATICS								
	Benzo(a)pyrene			7.3				
	Fluorene							
	Naphthalene	0.7	0.7					
	Total PAH							0.003
CARBOXYLIC ACIDS								
	Benzoic acid				40			
UNKNOWNS		0.6-13.8	10.2					

Table 4A1 (CONTINUED) Summary of selected properties of gasoline constituents

Hydrocarbon group	Representative hydrocarbon	Geometric mean air odour threshold (ppm) [3]		Odour index[4]	Solubility (mg/L)		Persistence 1/2 life in soil[6]	Vapour pressure[5]		Koc[5]	Kow[5]
		Detection	Recognition		Water	Temp °C	days	(mmHg)	Temp °C		
n-ALKANES											
C4	n-Butane			480	61	20		1823	25		776.2
C5	n-Pentane			570	30	15		430	20		
C6	n-Hexane				9.5	20		120	20		7943
C7	n-Heptane	230	330	200	3	20		35	20		45710
C8	n-Octane	150	240	100	0.66	20		11	20		
C9	n-Nonane			9800				3.22	20		
C10-14	n-Decane							2.7	20		
BRANCHED ALKANES											
C4	Isobutane			3.00×10^6	49	20		1520	7.5		
C5	Isopentane				48	20					169.8
C6	2-Methylpentane				14	23		400	42		588.8
C7	2-Methylhexane				380	23					1995
C8	2,4-Dimethylhexane										
C9	2,4,4-Trimethylhexane										
C10-14	2,2,5,5-Tetramethylhexane	780									
CYCLOALKANES											
C6	Cyclohexane			2.03×10^5	55	20		77	20	482	2754
C7	Methylcyclohexane				45	15		144	20		724.4
C8	1,2,4-Trimethylcyclopentane				14	20					
C9	1,1,3-Tri methylcyclohexane										
Others											
ALKENES											
C4	Butene										
	(alpha butylene)			4.35×10^7				760	-6.3		
	(beta butylene)			3.33×10^6							
C5	1-Pentene			3.76×10^8	50	25		100	-18		
C6	Hexene				50	20		186	25		177.8
Others											

Table 4A1 (CONTINUED) Summary of selected properties of gasoline constituents

Hydrocarbon group	Representative hydrocarbon	Geometric mean air odour threshold (ppm) [3]		Odour index[4]	Solubility (mg/L)		Persistence 1/2 life in soil[6]	Vapour pressure[5]		Koc[5]	Kow[5]
		Detection	Recognition		Water	Temp °C	days	(mm Hg)	Temp °C		
MON0-AROMATICS											
	Benzene	61	97	300	1780	20	23	76	20	31	134.9
	Toluene	1.6		16609	515	20	5.6	22	20	95	537
	Mixed xylenes										
	(o-xylene)	5.4		300	175	20	32	5	20	129	1318
	(m-xylene)	0.62		2100	161	25	15	6	20	166	1580
	(p-xylene)	2.1		18200	198	25	17	6.5	20	260	1318
	Ethylbenzene	2.2			152	20				250	1413
C3-benzenes											
C4-benzenes											
Others											
POLY-AROMATICS											
	Benzo(a)pyrene										
	Fluorene				1.9						
	Naphthalene	0.038		2400	30	25	0.12	1	53		
	Total PAH										
CARBOXYLIC ACIDS											
	Benzoic acid	0.62			2700	18		0.0045	25	1881.9	74

Notes
1. Based on USEPA IRIS AND MDEP, 1994
2. ANZECC Guidelines 1994
3. Based on American Industrial Hygiene Association odour thresholds
4. Verschueren K 1983, Handbook of Environmental Data on Organic Chemicals
5. STFBASE - values are te first reference half-life in the database
6. Verschuerne, 1983

Table 4A2 Preliminary ranking of contaminants of concern in gasoline

Hydrocarbon group	Representative hydrocarbon	Relative concern (Score 1 to 5)							
		Abundance	Human toxicity	Odour index	Volatility	Persistence	Health		Aesthetic
							Surface	Depth	
n-ALKANES									
C4	n-Butane	4	2	1	5	1	8	40	4
C5	n-Pentane	3	2	2	4	1	6	24	6
C6	n-Hexane	4	2	1	4	1	8	32	4
C7	n-Heptane	3	2	1	3	1	6	18	3
C8	n-Octane	3	2	1	3	1	6	18	3
C9	n-Nonane	2	1	3	2	2	4	8	12
C10-14	n-Decane	2	1	3	2	2	4	8	12
BRANCHED ALKANES									
C4	Isobutane	3	2	5	5	1	6	30	15
C5	Isopentane	5	2	4	5	1	10	50	20
C6	2-Methylpentane	4	2	4	4	1	8	32	16
C7	2-Methylhexane	3	2	4	4	1	6	24	12
C8	2,4-Dimethylhexane	4	2	4	3	2	16	48	32
C9	2,4,4-Trimethylhexane	3	1	4	3	2	6	18	24
C10-14	2,2,5,5-Tetramethylhexane	3	1	4	2	2	6	12	24
CYCLOALKANES									
C6	Cyclohexane	2	2	4	3	1	4	12	8
C7	Methylcyclohexane	3	2	4	3	1	6	18	12
C8	1,2,4-Trimethylcyclopentane	2	1	4	2	2	4	8	16
C9	1,1,3-Tri methylcyclohexane	2	1	4	2	2	4	8	16
Others									
ALKENES									
C4	Butene (alpha butylene) (beta butylene)	2	2	5	5	1	4	20	10
C5	1-Pentene	3	2	5	4	1	6	24	15
C6	Hexene	3	2	5	4	1	6	24	15
Others									

Table 4A2 (CONTINUED) Preliminary ranking of contaminants of concern in gasoline

Hydrocarbon group	Representative hydrocarbon	Relative concern (Score 1 to 5)							
		Abundance	Human toxicity	Odour index	Volatility	Persistence	Health		Aesthetic
							Surface	Depth	
MON0-AROMATICS									
	Benzene	3	4	1	3	2	24	72	6
	Toluene	4	1	3	3	2	8	24	24
	Mixed xylenes	4	2	2	2	3	24	48	36
	(o-xylene)								
	(m-xylene)								
	(p-xylene)								
	Ethylbenzene	3	2	2	2	3	18	36	27
C3-benzenes		4	1	2	2	4	16	32	48
C4-benzenes		3	1	2	2	4	12	24	36
Others									
POLY-AROMATICS									
	Benzo(a)pyrene	1	5	1	1	5	25	25	5
	Fluorene	2	2	1	1	4	16	16	8
	Naphthalene	2	2	2	2	4	16	32	16
	Total PAH								
CARBOXYLIC ACIDS									
	Benzoic acid								
Prisline			1						
Pytane			1						
Waxes			1						

Notes

Determination of relative concern rankings

Dose (mg/kg/d)	Rank	Abundance	Rank	Persistence	Rank	Volatility	Rank	Odour index	Rank
10^{-4} - 10^{-5}	5	10-15%	5	B(a)P	5	>1000	5	<0.5	5
10^{-3} - 10^{-4}	4	5-10%	4	Naphthalene	4	>100	4	>0.5	4
10^{-2} - 10^{-3}	3	1-5%	3	EX	3	>10	3	>5	3
10^{-1} - 10^{-2}	2	0.1-1%	2	BT	2	>1	2	>50	2
10^{0}- 10^{-1}	1	<0.1%	1	Light alkanes	1	>0.1	1	>500	1

Surface Health rank = Abundance*Human toxicity*Persistence
Depth Health rank = Abundance*Human toxicity*Persistence*Volatility
Aesthetic rank = Abundance*Odour Index*Persiste