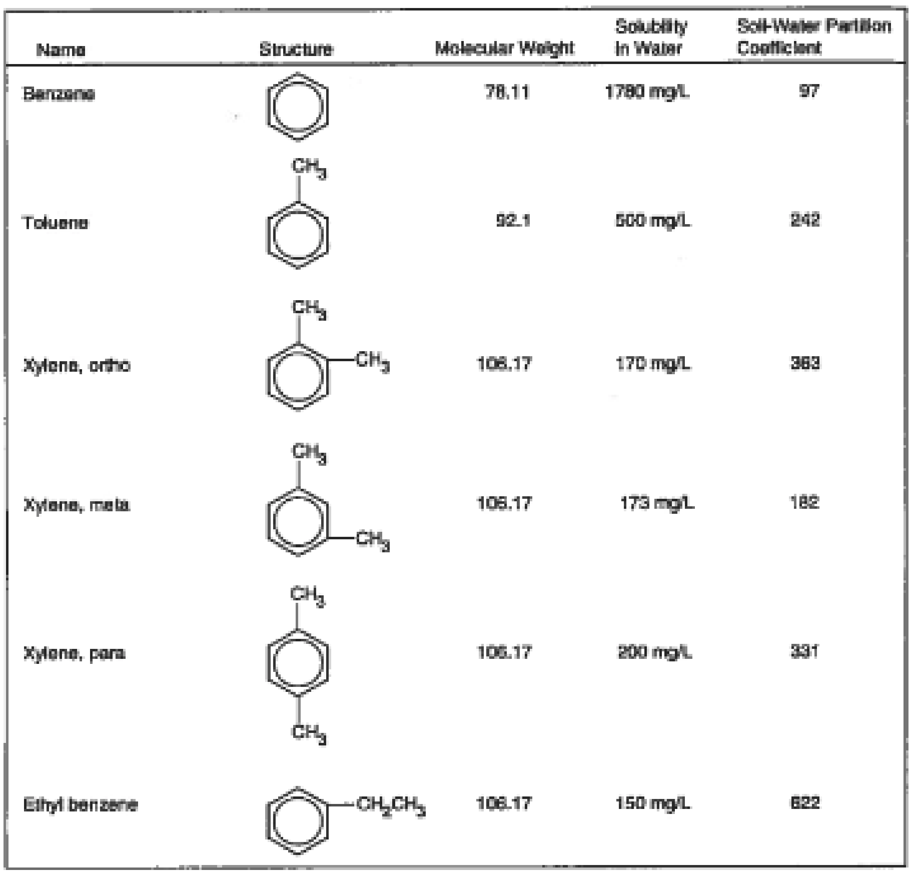
CE 5364 Groundwater Transport Phenomena
Exercise Set 3

Exercises

1. A fuel mixture of benzene, toluene, ethylbenzene at mole fractions 0.075, 0.065, and 0.035 respectively equilibrates with the atmosphere at 25^oC



Name	Structure	Molecular Weight	Solubility in Water	Soil-Water Partition Coefficient
Benzene		78.11	1780 mg/L	97
Toluene	CH_3	92.1	500 mg/L	242
Xylene, ortho	CH_3, CH_3	106.17	170 mg/L	363
Xylene, meta	CH_3, CH_3	106.17	173 mg/L	182
Xylene, para	CH_3, CH_3	106.17	200 mg/L	331
Ethyl benzene	CH_2CH_3	106.17	150 mg/L	622

Figure 4.13 Benzene related compounds.

Figure 1: Benzene Compounds - Structural diagrams and physical properties

TABLE 7.1 Properties for Selected Organic Compounds

Compound/ Family	Formula	Specific Gravity	Solubility (mg/L)	K_{ow}	Vapor Pressure (mm Hg)	Henry's Law (unitless)
			Fuels and derivatives			
Benzene	C_6H_6	0.879	1750	130	80	0.22
Ethylbenzene	C_8H_{10}	0.867	152	1400	7	0.32
Phenol	C_6H_6O	1.071	93,000	29	0.2	1.89×10^{-5}
Toluene	$C_6H_5CH_3$	0.866	535	130	22	0.26
o-Xylene	$C_6H_4(CH_3)_2$	0.880	175	890	5	0.22
			PAHs			
Acenaphthene	$C_{12}H_{10}$	1.069	3.42	10,000	0.01	0.321
Benzopyrene	$C_{20}H_{12}$	1.35	0.0012	1.15×10^6	—	5.8×10^{-8}
Benzoperylene	$C_{22}H_{12}$	—	0.0007	3.24×10^6	—	5.8×10^{-6}
Naphthalene	$C_{10}H_8$	1.145	32	2800	0.23	4.9×10^{-2}
Methyl naphthalene	$C_{10}H_7CH_3$	1.025	25.4	13,000	—	0.0164
			Ketones			
Acetone	CH_3COCH_3	0.791	inf	0.6	89	0.00104
Methyl ethyl ketone	$CH_3COCH_2CH_3$	0.805	2.68×10^5	1.8	77.5	0.00181
			Halogenated aromatics			
Chlorobenzene	C_6H_5Cl	1.106	466	690	9	0.165
2-Chlorophenol	C_6H_4ClOH	1.241	29,000	15	1.42	7.4×10^{-4}
p-Dichlorobenzene (1,4)	$C_6H_4Cl_2$	1.458	79	3900	0.6	0.067
Hexachlorobenzene	C_6Cl_6	2.044	0.006	1.7×10^5	1×10^{-5}	0.062
Pentachlorophenol	C_6OHCl_5	1.978	14	1.0×10^5	1×10^{-4}	1.5×10^{-4}
1,2,4-Trichlorobenzene	$C_6H_3Cl_3$	1.446	30	20,000	0.42	0.059
2,4,6-Trichlorophenol	$C_6H_2Cl_3OH$	1.490	800	74	0.012	—

Specific gravity at various temperatures; refer to Nyer and others (1991) for details; inf is infinite solubility
Vapor pressure about 20 °C; 1 atm = 760 mm Hg.
Modified from Nyer and others (1991). Reprinted by permission of Ground Water Monitoring Review

Figure 2: Physical properties for some organic compounds

Determine:

(a) Concentration in the gas (air) phase of the three components in $\frac{mg}{L}$

(b) Concentration in the gas (air) phase of the three components in $\frac{\mu g}{m^3}$

2. (Modified from 6.22 pg. 592)

   A well with effective diameter of 0.5 m fully penetrates an aquifer that has a uniform saturated thickness of 10 m. One hundred grams of benzene are spilled into the well, immediately dissolve, and mix into the water in the well. The seepage velocity is 30 m/yr in the x-direction, the longitudinal dispersivity is 1.0 m, and the transverse dispersivity is 0.1 m.

   The aquifer has the following characteristics:

   - Bulk density = 1.8 g/cc
   - porosity = 0.30
   - f_{oc} = 1 percent
   - K_{ow} = 135 L/kg

   Determine:

   (a) The retardation factor R for benzene in this aquifer.

   (b) The maximum benzene concentration at t = 1 yr.

   (c) The location of this maximum.

3. The following data for concentration of TCE were taken at a single monitoring well. Use the Mann-Kendall test (pp. 458-460) to determine whether the concentration has an upward or downward trend.

Table 1: TCE Observations in an Aquifer

Date	TCE (ppb)
9/92	8
12/92	19
3/93	21
6/93	13
9/93	39
12/93	24
3/94	28
6/94	25

Determine:

(a) The upward or downward concentration trend, using a Mann-Kendall test.