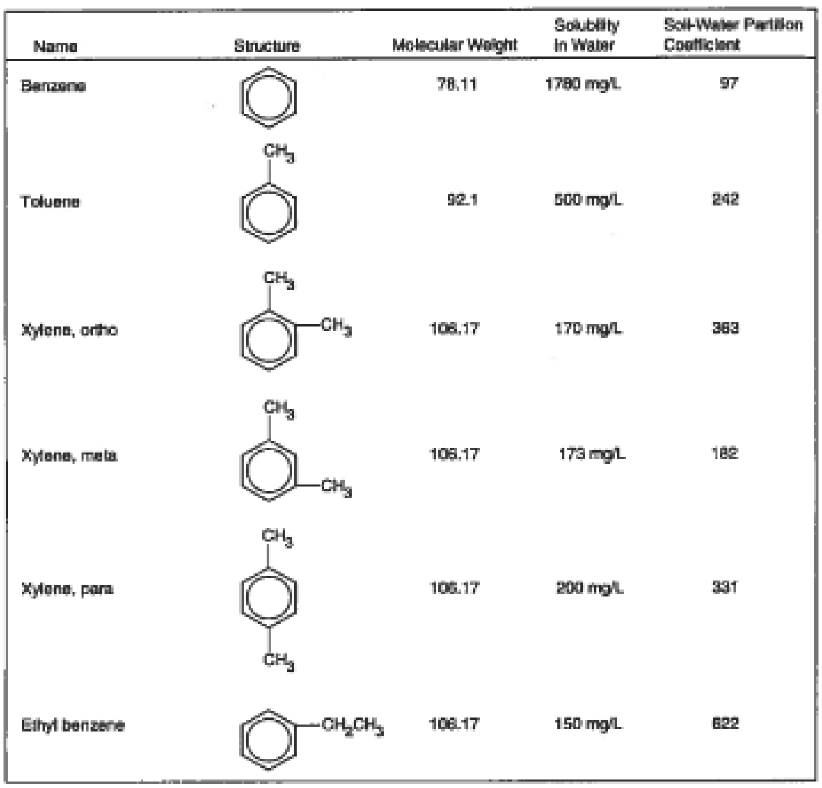
CE 5364 Groundwater Transport Phenomena
Exercise Set 3

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

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,

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	60	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

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.

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

Initial Concentration (mg/L) Date	Equilibrium Concentration (mg/L) 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:

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

4. (Data Analysis)

A batch isotherm test was performed with several 1-L solutions of the chemical of interest and one soil type, 20 g in each solution container. The initial and final solution concentrations are shown in Table 2. Fit the linear, Freundlich, and Langmuir isotherm equations to this data.

Determine:

(a) The Linear isotherm equation for these data (i.e. fit the isotherm model to the data), plot the isotherm and data

(b) The Freundlich isotherm equation for these data, plot the isotherm and data

(c) The Langmuir isotherm equation for these data, plot the isotherm and data

(d) Which isotherm model produces the best fit for these data?

Table 2: Isotherm Observations

Initial Concentration (mg/L)	Equilibrium Concentration (mg/L)
7.10	6.71
4.53	4.18
1.89	1.63
1.31	1.10
1.03	0.85

Show calculations and identify all fitted parameter values.

5. (Data Analysis)

The following table (Table 3)has data from a column test with bromide (conservative) and chromium (sorbed). The porosity of the soil was 0.485, the bulk density was 1.85 g/cc, velocity was 0.244 cm/min, and the column was 25.4 cm long with a diameter of 2.54 cm.

Table 3: Effluent Breakthrough Observations

Time (min)	Bromide $\frac{C}{Co}$	Chromium $\frac{C}{Co}$
0	0.000	0.000
15	0.000	0.000
30	0.005	0.000
45	0.003	0.000
60	0.013	0.000
75	0.075	0.000
90	0.137	0.000
105	0.530	0.000
120	0.841	0.000
135	1.000	0.000
150	1.000	0.000
165	1.000	0.009
180	1.000	0.186
195	1.000	0.595
210	1.000	0.791
225	1.000	0.875
240	1.000	0.913
255	1.000	0.946
270	1.000	0.946
285	1.000	1.000
300	1.000	1.000
315	1.000	1.000
330	1.000	1.000
345	1.000	1.000
360	1.000	1.000

Determine:

(a) Sketch the system.

(b) The dispersivity in cm

(c) The retardation coefficient for Cr.