HYDROGEOLOGICAL TRANSPORT PHENOMENA

Final Exam **29/01/2010**

Make sure to give all relevant formulas, steps of computations, and units.
No lecture notes or class notes are allowed. NOTE: The sum of all points is 110; so, you get a bonus of 10 points!
Some given parameter values may not be needed and some quantities values are not specified. In the latter case, you should assume reasonable values.

1. Governing equations for the transport of a kinetically adsorbed solute in unsaturated porous media are written as:

$$\theta \frac{\partial C}{\partial t} + v \frac{\partial C}{\partial x} = \theta D \frac{\partial^2 C}{\partial x^2} - k_{att} C + \rho^s k_{det} s - \mu^l C$$

$$\rho^s \frac{\partial s}{\partial t} = k_{att} C + \rho^s k_{det} s - \mu^s s$$

where θ is water content, C is mass concentration of solute in water, v is the average pore velocity, D is the dispersion coefficient, k_{att}, k_{det}, μ^l and μ^s are rate coefficients for adsorption, desorption, decay in water, and decay of adsorbed solutes, s is the mass fraction of adsorbed solute (mass adsorbed per unit mass of solid grains), and ρ^s is the mass density of solid grains.

a) Are these equations correct? If not, give the correct forms of these equations.
b) Give the formula for the 1-D dispersion coefficient.

(10 points)

2. A column experiment was carried out with undisturbed samples of the same sandy soil as in problem 3. The soil grain density is 2500 *g/l*. A solution containing common salt and the same adsorbing solute as in problem 3 were fed to the column continuously at a flow rate of 13.3 *ml/hr/cm²*. The breakthrough of salt and adsorbing solute were measured at a distance of 40cm from the inlet. The same relative concentrations for salt and solute are measured but at different times. The data are given in the following table.

t (hr) for salt	0.5	0.6	0.7	0.8	0.9	1.03	1.1	1.2	1.4	1.8
C/Co	0.001	0.01	0.07	0.18	0.38	0.54	0.70	0.82	0.94	0.99
t (hr) for ads. solute	3	3.6	4.2	4.8	5.4	6.18	6.6	7.2	8.4	10.8

Assuming that the solute's adsorption may be modelled as linear equilibrium, calculate the soil porosity, dispersivity, and distribution coefficient.

(15 points)

3. A shale unit, 100 meter thick, is deposited in a marine environment such that the initial pore-fluid composition is equivalent to seawater. The shale is bounded from above by a sandy layer and from below by an impermeable layer. Relatively rapidly (in a geologic sense) the entire sequence is lifted above the sea level, and the sand layer becomes filled with fresh groundwater. Assume that the sandy layer is very thick (semi-infinite for all practical purposes).

a) Assume that the transport of dissolved salts out of shale into the sand is by simple diffusion only. Give the governing equation, initial and boundary conditions, and the corresponding solution (A case in the attached set of solutions can be used with some modification here).
b) How long would it take for the salinity concentration at the bottom of the shale formation to reach one tenth of the original seawater concentration? Assume a reasonable diffusion coefficient, equal for both layers.

c) Plot qualitative curves of the concentration profile in the two layers at various times until the salt is fully distributed. *(15 points)*

4. A landfill has a clay underlining to prevent the pollution of the aquifer below the landfill. The clay has a permeability of $10^{-16}\ m^2$, a porosity of 0.385 and a thickness of one meter. Piezometric measurements show that pressure heads on top and bottom of the clay layer are $5m$ and $5.5m$, respectively. The concentration of pollutants on top of the clay lining is around 800 *mg/l* and remains constant. *Additional information:* Molecular diffusion coefficient in water, D_{mol}, $= 10^{-8}\ m^2/s$; tortuosity = 3.3; dispersivity = $0.01m$; viscosity, $\mu = 10^{-3}\ kg/m.s$; water density, $\rho = 10^3\ kg/m^3$; $g = 9.8\ m/s^2$
   a) Calculate the average pore velocity.
   b) How long does it take for the concentration of pollutants in the groundwater just below clay to reach 400 *mg/l*?
   c) Calculate the concentration under the clay layer after 20 years and 40 years.
   Hint: It's more convenient to work with year as the time unit.
   (20 points)

5. A solvent contains the following components (collectively called BTEX):

	Weight (%)	Molecular Wt. (g/mole)	Vapor Pressure (mm *Hg*)	Solubility (mg/L) at 25°C
Benzene	33 %	78	95.2	1800
Toluene	24 %	92	28.4	470
Ethylbenzene	24 %	106	9.5	140
Xylene	19 %	106	6.6	213

15 grams of this solvent is put inside a glass vial containing 10 mL of water. The remaining volume of the vial is 10 mL, which is filled with air. The vial is put on a shaker and gently shaken for a few hours until equilibrium with air and water is reached. The air pressure remains at one atmosphere (100 kPa or 760 mm Hg). The universal gas constant is equal to 8.3144 J/□K mole. Assume that the dissolution and volatilization of BTEX does not change its the composition.
a) Determine whether any BTEX remains in the vial as a separate phase. If yes, determine the mass remaining.
b) In any case, determine the concentrations of BTEX components in water?
(20 points)

6. A series of batch experiments have been carried out to study the sorption of phosphorous to a glacial outwash. Nine suspensions were prepared in nine different flasks, each containing 10 *g* of dried sediment and 100 *mL* of water with dissolved disodium phosphate in concentrations ranging from 0.85 *mg/l* to 14.6 *mg/l*, as given in the table below. The flasks were shaken for 4 days on an autoshaker. The samples were then filtered and the filtrate (i.e. water) was analyzed for phosphate. The equilibrium concentrations of phosphate for the flasks are also given below.

Solution conc. (*mg/l*)	0.85	1.95	3.25	3.85	5.65	7.1	9.8	12.4	14.6
Equilibrium conc. (*mg/l*)	0.75	1.25	2.05	2.45	3.85	5.1	7.5	10.0	12.1

It was known that the sediments already had some adsorbed phosphate in their natural state. Thus, a solution of HCl was used to extract the adsorbed phosphate and it was found that the amount of phosphorus sorbed to the sediment prior to the test was 16 $\mu g/g$.
Assume that the adsorption follows Langmuir isotherm. Give the corresponding adsorption formula and calculate the adsorption parameters. *(30 points)*

Tables of Error Function and Complementary Error Function

$(erfc(-\beta) = 2 - erfc(\beta))$

β	erf (β)	erfc (β)
0	0	1.0
0.05	0.056372	0.943628
0.1	0.112463	0.887537
0.15	0.167996	0.832004
0.2	0.222703	0.777297
0.25	0.276326	0.723674
0.3	0.328627	0.671373
0.35	0.379382	0.620618
0.4	0.428392	0.571608
0.45	0.475482	0.524518
0.5	0.520500	0.479500
0.55	0.563323	0.436677
0.6	0.603856	0.396144
0.65	0.642029	0.357971
0.7	0.677801	0.322199
0.75	0.711156	0.288844
0.8	0.742101	0.257899
0.85	0.770668	0.229332
0.9	0.796908	0.203092
0.95	0.820891	0.179109
1.0	0.842701	0.157299
1.1	0.880205	0.119795
1.2	0.910314	0.089686
1.3	0.934008	0.065992
1.4	0.952285	0.047715
1.5	0.966105	0.033895
1.6	0.976348	0.023652
1.7	0.983790	0.016210
1.8	0.989091	0.010909
1.9	0.992790	0.007210
2.0	0.995322	0.004678
2.1	0.997021	0.002979
2.2	0.998137	0.001863
2.3	0.998857	0.001143
2.4	0.999311	0.000689
2.5	0.999593	0.000407
2.6	0.999764	0.000236
2.7	0.999866	0.000134
2.8	0.999925	0.000075
2.9	0.999959	0.000041
3.0	0.999978	0.000022

6. Instantaneous pulse injection within a strip of width $2h$ in an infinite domain with $q = 0$ and $\mu = 0$.

Initial conditions:

$$C = C_0 \qquad -h < x < h$$
$$C = 0 \qquad x < -h \quad \text{and} \quad x > h$$

Boundary conditions:

$$C = 0 \qquad x = -\infty$$
$$C = 0 \qquad x = \infty$$

Solution:

$$C(x,t) = \frac{1}{2}C_0 \left\{ \text{erf}\left[\frac{h-x}{\sqrt{4Dt/R}}\right] + \text{erf}\left[\frac{x+h}{\sqrt{4Dt/R}}\right] \right\}$$

7. Instantaneous pulse injection within a strip of width h in a semi–infinite domain with $q = 0$ and $\mu = 0$.

Initial conditions:

$$C = C_0 \qquad 0 \leq x < h$$
$$C = 0 \qquad x > h$$

Boundary conditions:

$$\frac{\partial C}{\partial x} = 0 \qquad x = 0$$
$$C = 0 \qquad x = \infty$$

Solution:

$$C(x,t) = \frac{1}{2}C_0 \left\{ \text{erf}\left[\frac{h-x}{\sqrt{4Dt/R}}\right] + \text{erf}\left[\frac{x+h}{\sqrt{4Dt/R}}\right] \right\}$$

8. An infinite column of porous medium with a constant continuous injection of a tracer at $x = 0$. The mass of tracer material injected during Δt at time t is given by $C_0(q/Rn)\Delta t$. The boundary conditions read

$$\lim_{x \to \pm\infty} C(x,t) = 0,$$

and the solution is given by

$$C(x,t) = \frac{C_0 q/Rn}{\sqrt{4\pi D}} \exp\left[\frac{qx}{2Dn}\right] \int_0^{\tau = t/R} \frac{1}{\sqrt{\tau}} \exp\left[-\frac{x^2}{4D\tau} - \left(\frac{q^2}{4Dn^2} + \mu\right)\tau\right] d\tau.$$

9. A semi–infinite column of porous medium, $x > 0$, with no decay, $\mu = 0$.
Initial conditions:

$$C = 0 \qquad x \geq 0.$$

Boundary conditions:

$$C = C_0 \qquad x = 0,$$
$$C = 0 \qquad x = \infty.$$

The solution reads

$$C(x,t) = \frac{1}{2}C_0 \left\{ \text{erfc}\left[\frac{x-(qt/Rn)}{\sqrt{4Dt/R}}\right] + \exp\left[\frac{xq}{nD}\right] \text{erfc}\left[\frac{x+(qt/Rn)}{\sqrt{4Dt/R}}\right]\right\}.$$

If $q = 0$, this solution reduces to solution number 5 with $\mu = 0$.

10. Semi–infinite column of porous media, $x > 0$ with decay.
Initial conditions:

$$C = 0 \qquad x \geq 0.$$

Boundary conditions:

$$C = C_0 \qquad x = 0,$$
$$C = 0 \qquad x = \infty.$$

Solution for constant q:

$$C(x,t) = \frac{1}{2}C_0 \exp\left[\frac{qx}{2Dn}\right] \left\{ \exp\left[-x\beta\right] \text{erfc}\left[\frac{x - \left((q/n)^2 + 4\mu D\right)^{1/2} t/R}{\sqrt{4Dt/R}}\right] + \exp\left[x\beta\right] \text{erfc}\left[\frac{x + \left((q/n)^2 + 4\mu D\right)^{1/2} t/R}{\sqrt{4Dt/R}}\right]\right\},$$

with $\beta^2 = (q/2Dn)^2 + \mu/D$. If $\mu = 0$, this solution reduces to solution 9.

11. A semi–infinite column of porous media, $x > 0$, $\mu = 0$, and a total flux boundary condition.
Initial conditions:

$$C = 0 \qquad x \geq 0.$$

Boundary conditions:

$$-D\frac{\partial C}{\partial x} + (q/Rn)C = (q/Rn)C_0 \qquad x = 0,$$
$$\frac{\partial C}{\partial x} \text{ is finite at } \qquad x = \infty.$$