

**Answer 9.7**

a) Write an appropriate transport equation

If Toluene is always and everywhere in equilibrium with the solid phase, its transport is described by,

$$(1) \frac{\partial C}{\partial t} + f u \frac{\partial C}{\partial x} + f v \frac{\partial C}{\partial y} + f w \frac{\partial C}{\partial z} = \frac{\partial}{\partial x} f K_x \frac{\partial C}{\partial x} + \frac{\partial}{\partial y} f K_y \frac{\partial C}{\partial y} + \frac{\partial}{\partial z} f K_z \frac{\partial C}{\partial z},$$

where C is the total concentration and f is the mobile fraction. It is given that  $v = w = 0$ , and implied that  $\partial C / \partial z = 0$ . If we also assume that K and f are homogeneous, then (1) becomes

$$(2) \frac{\partial C}{\partial t} + f u \frac{\partial C}{\partial x} = f K \frac{\partial^2 C}{\partial x^2} + f K \frac{\partial^2 C}{\partial y^2}$$

To determine f we need the bulk density, which is

$$\rho_B = \rho_S(1 - n) = 2.6 \times (1 - 0.3) = 1.82 \text{ g/mL}. \text{ Then}$$

$$f = \frac{n}{n + \rho_B K_d} = \frac{0.3}{0.3 + (1.82 \text{ g/mL})(0.5 \text{ mL/g})} = 0.25$$

Note,  $Pe = fU L / K = (0.25)(1 \text{ m d}^{-1})(1000 \text{ m}) / (0.1 \text{ m}^2 \text{ d}^{-1}) = 2500 \gg 1$ , which implies that longitudinal dispersion is small compared to advection. However, it appears likely (to be confirmed below) that the release behaves as an instantaneous release. If so, we need the longitudinal dispersion term to establish the longitudinal shape of the cloud.

b) Estimate the total concentration, C(t), at the drinking well.

To determine if the release behaves as an instantaneous point source, we estimate the transport time-scale,  $T_U = L / fU = (1000 \text{ m}) / (0.25 \times 1 \text{ m d}^{-1}) = 4000 \text{ d}$ . Since  $T_U$  is much longer than the duration of the release (2 hrs), we confirm that the release behaves as an instantaneous source. In addition, since  $T_U \gg 24 \text{ hrs}$  (time to distribute Toluene vertically), we confirm that the concentration can be assumed uniform in z. For an instantaneous source of mass, M, released at  $(x, y) = (0, 0)$ , the solution to (2) is,

$$(c) C(x, y, t) = \frac{M}{L_z 4\pi t f K} \exp\left(-\frac{(x - fut)^2 + y^2}{4 f K t}\right),$$

where  $L_z = 5 \text{ m}$  is the vertical depth of the aquifer.

c) Estimate the peak concentration in the porewater at the well and the duration of exposure.

The peak in total concentration at the well ( $x = L$ ) occurs at  $t = T_U = L/fu$  and  $y = 0$ .

$$C_{\text{peak}} = \frac{2000\text{g}}{(5\text{m}) 4\pi (4000 \text{ d}) (0.25) (0.1\text{m}^2 \text{d}^{-1})} = 0.32\text{gm}^{-3}.$$

The pore water concentration,  $C_w = (f/n) C$ . So the peak porewater concentration is,

$$C_{w,\text{peak}} = (f/n) C_{\text{peak}} = (0.25 \times 0.32 \text{ gm}^{-3}) / (0.3) = 0.26 \text{ gm}^{-3}.$$

To estimate the duration of exposure we will define the length of the Toluene cloud by  $4\sigma$ , evaluated at the peak arrival time,  $T_U$ .

$$T_{\text{exposure}} = \frac{4\sigma}{fu} = \frac{4\sqrt{2fKT_U}}{fu} = \frac{4\sqrt{2KL/u}}{fu} = \frac{4\sqrt{2(0.1\text{m}^2\text{d}^{-1})(1000\text{m})/(1\text{md}^{-1})}}{(0.25)(1\text{md}^{-1})} = 226 \text{ d}$$