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1.061 / 1.61 Transport Processes in the Environment
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Answer 9.1

For a continuously operating smokestack and steady climatic conditions, we can assume a steady concentration field, *i.e.* $\partial C/\partial t = 0$. The wind is given as $u = 5$ m/s, implying $v = w = 0$. We are told to assume a uniform wind, *i.e.* no shear, so we neglect shear-dispersion. For the length-scale of interest, $L_x = 10,000$ m, the Peclet number is $(5\text{m/s})(10,000\text{m})/(1\text{m}^2/\text{s}) = 50,000 \gg \gg 1$. With this high value of Pe, the longitudinal diffusion term is negligible relative to longitudinal advection, and we drop it. With the above assumptions, the transport equation

$$(a) \frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} + w \frac{\partial C}{\partial z} = \frac{\partial}{\partial x} D_x \frac{\partial C}{\partial x} + \frac{\partial}{\partial y} D_y \frac{\partial C}{\partial y} + \frac{\partial}{\partial z} D_z \frac{\partial C}{\partial z} \pm S,$$

becomes

$$(b) u \frac{\partial C}{\partial x} = D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - S,$$

with $S = 0$ for Freon and $S = k_{\text{TCE}}C$ for the TCE.

For a continuous release $\dot{m} = 5$ kg/min = 83 gs^{-1} at $(x,y,z) = (0, 0, H)$, the solution to (b) is

$$(c) C(x, y, z) = \frac{\dot{m}}{4\pi\sqrt{D_y D_z} x} \exp\left(-\frac{uy^2}{4D_y x} - \frac{u(z-H)^2}{4D_z x}\right) \exp\left(-\frac{kx}{u}\right),$$

where $k = 0$ for Freon and $k = k_{\text{TCE}}$ for the TCE. To account for the no-flux boundary we add a positive image source at $(x,y,z) = (0, 0, -H)$.

$$(d) C(x, y, z) = \frac{\dot{m}}{4\pi\sqrt{D_y D_z} x} \left[\underbrace{\exp\left(-\frac{uy^2}{4D_y x} - \frac{u(z-H)^2}{4D_z x}\right) \exp\left(-\frac{kx}{u}\right)}_{\text{real source}} + \underbrace{\exp\left(-\frac{uy^2}{4D_y x} - \frac{u(z+H)^2}{4D_z x}\right) \exp\left(-\frac{kx}{u}\right)}_{\text{image source}} \right]$$

In any transverse dimension for which the plume is unbounded (here the y-direction), the maximum concentration is at the centerline of the plume (here $y = 0$). The vertical coordinate, however, is bounded by a no-flux boundary at the ground, $z = 0$. Once the plume reaches the ground, concentration will build up at the no-flux boundary. Because the upper edge of the plume is not bounded, the vertical concentration field will eventually become asymmetric with the maximum concentration at the ground. We estimate the distance at which this will occur using the time-scale for the edge of the plume (the 2σ contour) to reach the ground,

$$(e) \quad T_{2\sigma} = H^2/(8D_z) = (20\text{m})^2 / (8 \times 0.1 \text{ m}^2\text{s}^{-1}) = 500 \text{ s}.$$

Thus, for $x \gg u T_{2\sigma} = 2500 \text{ m}$, which includes the point of interest, we expect the maximum concentration to be at the ground. Therefore, the maximum concentration at $x = 10,000 \text{ m}$ will be $C_{\max} = C(x = 10000 \text{ m}, y = 0, z = 0)$. Evaluating (d) for Freon and TCE we find,

FREON:

$$C_{\max} = \frac{83 \text{gs}^{-1}}{2\pi\sqrt{(1\text{m}^2\text{s}^{-1})(0.1\text{m}^2\text{s}^{-1})} 10,000\text{m}} \exp\left(-\frac{5\text{ms}^{-1}(20\text{m})^2}{4(0.1\text{m}^2\text{s}^{-1})10,000\text{m}}\right) = 2.5 \text{ mg m}^{-3}$$

TCE:

$$C_{\max} = \frac{83 \text{gs}^{-1}}{2\pi\sqrt{(1\text{m}^2\text{s}^{-1})(0.1\text{m}^2\text{s}^{-1})} 10,000\text{m}} \exp\left(-\frac{5\text{ms}^{-1}(20\text{m})^2}{4(0.1\text{m}^2\text{s}^{-1})10,000\text{m}}\right) \exp\left(-\frac{10000\text{m}}{5\text{ms}^{-1}}(0.1\text{d}^{-1})(\text{d}/86400\text{s})\right)$$

$$= 2.5 \text{ mgm}^{-3} \times 0.998 \approx 2.5 \text{ mgm}^{-3},$$

Very little degradation of TCE occurs over the 10,000m distance.

Answer 9.2

A perfectly absorbing boundary can be treated like a dissolving boundary with $C_{eq} = 0$. The boundary is a sink rather than a source, otherwise the process of exchange between the bed and the water column is the same. Here, dye is injected as a continuous point source and the evolving plume experiences a sink at the absorbing boundary. If the system has fast mixing, then we can assume that $\partial C/\partial z = \partial C/\partial y = 0$ and use the fast-mixing model for bed-exchange. Then the effects of the boundary sink are modeled as a distributed sink S . For steady-state conditions and $Pe \gg 1$, the transport equation

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} + w \frac{\partial C}{\partial z} = \frac{\partial}{\partial x} K_x \frac{\partial C}{\partial x} + \frac{\partial}{\partial y} D_y \frac{\partial C}{\partial y} + \frac{\partial}{\partial z} D_z \frac{\partial C}{\partial z} \pm S,$$

will reduce to,

$$(1) \quad u \frac{\partial C}{\partial x} = -S.$$

However, if the dye mixes slowly over the cross-section, we cannot assume $\partial C/\partial z = \partial C/\partial y = 0$ in the channel. Under these conditions we would use the solution for a 3-D, steady, continuous release (equation 8, chapter 6), with positive image sources to account for the no-flux side-boundaries, and a negative image source to account for the perfectly absorbing bed.

Before proceeding with (1), we must check all the assumptions. First, we will determine if the flow is turbulent, and if it is we will estimate turbulent diffusivities. The hydraulic radius is $(5\text{cm} \times 10\text{cm}) / (10\text{cm} + (2 \times 5\text{cm})) = 2.5\text{ cm}$. The Reynolds number based on hydraulic radius is, $Re_H = (10\text{cm s}^{-1} \times 2.5\text{cm}) / (0.01\text{ cm}^2\text{s}^{-1}) = 2500$, which indicates the flow is likely to be turbulent. Next to each boundary there is a laminar sub-layer with thickness, $\delta_s = 5 \nu/u_*$. The friction velocity is estimated as $u_* \approx 0.1U = 1\text{ cm s}^{-1}$. This gives $\delta_s = 0.05\text{ cm}$.

Now, we estimate the coefficients of turbulent diffusion using the empirical relations for a straight channel given in Table 1 of Chapter 7.

$$D_{t,x} = 0.45 u_* h = 2.3\text{ cm}^2\text{s}^{-1}$$

$$D_{t,y} = 0.15 u_* h = 0.75\text{ cm}^2\text{s}^{-1}$$

$$D_{t,z} = 0.067 u_* h = 0.34\text{ cm}^2\text{s}^{-1}$$

Confirm Fast-Mixing Bed Exchange Model

To determine if the system will follow a fast-mixing or slow-mixing model of bed-exchange, we compare the time scale required for the channel to mix vertically with the time scale for diffusive flux to cross the laminar sub-layer.

$$\frac{T_{\delta_s}}{T_L} = \frac{\delta_s^2 / D}{h^2 / D_t} = \frac{(0.05\text{cm})^2 (0.34\text{cm}^2\text{s}^{-1})}{(5\text{cm})^2 (10^{-5}\text{cm}^2\text{s}^{-1})} = 3.4$$

To be very confident that the fast-mixing model is appropriate, we require that T_{δ_s} is an order of magnitude greater than T_L . Here the time scales only differ by a factor of three. However, the system is closer to the fast-mixing model than the slow-mixing model, so we proceed with that assumption.

Confirm well-mixed conditions ($\partial C/\partial y = \partial C/\partial z = 0$) for plume evolution.

To use (1) to describe plume evolution, we must confirm that the plume rapidly mixes over the channel cross-section. We need to find the distance from the source at which the plume is uniform in y and z . These distances are,

$$X_{\text{mix},y} = b^2 u / (4 D_{t,y}) = (10\text{cm} \times 10\text{cm} \times 10 \text{cm}^2\text{s}^{-1}) / (4 \times 0.75 \text{cm}^2\text{s}^{-1}) = 333 \text{ cm}$$

$$X_{\text{mix},z} = h^2 u / (4 D_{t,z}) = (5\text{cm} \times 5\text{cm} \times 10 \text{cm}^2\text{s}^{-1}) / (4 \times 0.34 \text{cm}^2\text{s}^{-1}) = 183 \text{ cm}.$$

This indicates that for distances greater than 333 cm from the source, the plume will be uniform in y and z . We are interested in the position $x = 2000$ cm, so we can model the concentration as if it originated from a one-dimensional source at $x = 0$. That is, we can assume $\partial C/\partial y = \partial C/\partial z = 0$.

Confirm assumption of $Pe \gg 1$

If $Pe = UL_x/K_x \gg 1$, we can neglect longitudinal dispersion relative to longitudinal advection. The relevant length-scale is the distance at which we want to predict the concentration, $L = 2000$ cm. The longitudinal dispersion is $K_x = 5.9u \cdot h = 30 \text{cm}^2\text{s}^{-1}$. Then, $Pe = (10 \text{cm s}^{-1} \times 2000 \text{cm}) / (30 \text{cm}^2\text{s}^{-1}) = 666 \gg 1$. So, this assumption is confirmed.

We have confirmed the assumptions that led to (1). Now, we can replace the sink term, S , in (1) with the form given in equation (16) in Chapter 9. That is,

$$(2) \quad S = - \left[\frac{D_m A}{V \delta_s} \right] (C - C_{eq}) = -k(C - C_{eq}).$$

With $V/A = h$, we estimate the bed-exchange rate constant $k = 10^{-5} \text{cm}^2\text{s}^{-1} / (5\text{cm} \times 0.05\text{cm}) = 4 \times 10^{-5} \text{s}^{-1}$. In this system $C_{eq} = 0$, such that (1) becomes

$$(3) \quad u \frac{\partial C}{\partial x} = -kC$$

As shown in Chapter (6), leading to and including equation 13, the initial concentration at the source will be $C(x = 0) = \dot{m}/ubh$. With this initial condition, the solution to (3) is.

$$(4) \quad C(x) = \frac{\dot{m}}{ubh} \exp\left(-\frac{kx}{u}\right)$$

Note, a generic form of equation (4) was also given for a 1-D, steady, continuous release with first-order reaction in equation (11) of chapter 9.

Using (4) we find the concentration at $x = 2000$ cm to be,

$$C(x = 2000 \text{ cm}) = \frac{1 \text{ gs}^{-1}}{(10 \text{ cms}^{-1})(10 \text{ cm})(5 \text{ cm})} \exp\left(-\frac{(4 \times 10^{-5} \text{ s}^{-1})(2000 \text{ cm})}{10 \text{ cms}^{-1}}\right) = 0.00198 \text{ gcm}^{-3}$$

In fact, the boundary sink does not make a significant contribution between $x = 0$ and 2000 cm, as the initial concentration is 0.002 gcm^{-3} . Barely 1 percent of the dye has been lost to the bed.

Answer 9.3

We are interested in the vertical diffusion of PCE from its source at $z = 0$ upward into the aquifer. The groundwater is given to be stagnant, so that $u = v = w = 0$. In addition, all groundwater is laminar, so we will use the laminar (slow mixing) model of dissolution. That is, the boundary source is modeled by a fixed concentration boundary condition. We assume that the DNAPL pool is large in lateral extent and uniform in concentration, so that the lateral gradients of PCE are negligible ($\partial C/\partial x = \partial C/\partial y = 0$). No additional sources or sinks are named, so that $S = 0$. The system cannot be in steady state, because there is a source at the lower boundary and no sink, so that $\partial M/\partial t > 0$ within the aquifer. Directly at the boundary, $z = 0$, the concentration is assumed to be at the solubility concentration, $C_o = 150 \text{ mg l}^{-1} = 150 \text{ ppm}$. We assume that the total PCE in the DNAPL pool is sufficiently large that C_o remains constant, even as PCE dissolves out of the pool. With these assumptions we may write the transport equation and boundary conditions,

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial z^2},$$

$$C = 0, \text{ for all } z, \text{ at } t < 0$$

$$C = C_o = 150 \text{ ppm at } z = 0 \text{ for } t \geq 0.$$

The PCE concentration profile evolves according to,

$$C(z, t) = C_o \operatorname{erfc}\left(\frac{z}{2\sqrt{Dt}}\right).$$

The maximum concentration in the aquifer will be at the source ($z = 0$) and the minimum concentration at $z = 2\text{m}$, until a uniform concentration is reached throughout the aquifer. Thus, to find $C > 5 \text{ ppb}$ throughout the aquifer, we need only find when $C(z=2 \text{ m}) = 5 \text{ ppb}$. From the above equation, we need to find when

$$\operatorname{erfc}\left(\frac{z}{2\sqrt{Dt}}\right) = \frac{0.005}{150} = 0.000033.$$

Interpolating from the table at the end of chapter 9,

$$\operatorname{erfc}(2.94) \approx 0.000033$$

$$\frac{2\text{m}}{2\sqrt{(4.4 \times 10^{-9} \text{ m}^2\text{s}^{-1})t}} = 2.94$$

$$t = 2.6 \times 10^7 \text{ s} = 304 \text{ days}$$

Answer 9.4

Since Propane and TCE are both water-side controlled [$H \gg 0.01$], from Chapter 9 we expect the rate constants describing their exchange with the atmosphere to have the following ratios:

Thin-Film Model, Water-Side Control

$$\frac{K_{\text{TCE}}}{K_{\text{Propane}}} = \frac{D_{\text{wTCE}}}{D_{\text{wPropane}}}$$

Surface Renewal Model, Water-Side Control

$$\frac{K_{\text{TCE}}}{K_{\text{Propane}}} = \sqrt{\frac{D_{\text{wTCE}}}{D_{\text{wPropane}}}}$$

The channel Reynolds number based on hydraulic radius is $Re_{RH}=13,000$, indicating that the flow is turbulent. As described in the text, empirical evidence suggests that the surface renewal model is more appropriate for turbulent flows. Using this model, $K_{\text{TCE}} = 1.1 \times 10^{-4} \text{ s}^{-1}$.

Given that the atmospheric concentration of TCE is negligible, the flux of TCE to the atmosphere can be represented by the first-order sink, $S = -K_{\text{TCE}}C$, in the mass balance equation for the stream. As a first guess, we assume that this is the only source/sink of TCE along the stream. Assume that the cross-section has uniform concentration, *i.e.* with rapid mixing, $\partial C/\partial y = \partial C/\partial z = 0$. Assume the system is at steady-state ($\partial C/\partial t = 0$). Then, the mass balance equation is $u\partial C/\partial x = -K_{\text{TCE}}C$. With an upstream boundary condition, $C = C_0 = 10 \text{ ppb}$ at $x = 0$, the concentration downstream of the source will be

$$C(x) = C_0 \exp(-K_{\text{TCE}}x/u).$$

Evaluating this at $x = 2000\text{m}$,

$$C(x = 2\text{km}) = 10\text{ppb} \exp(-(1.1 \times 10^{-4} \text{ s}^{-1})(2000\text{m})/(0.1\text{ms}^{-1})) = 1.1 \text{ ppb}.$$

The estimated concentration is much less than the measured concentration at this position ($C = 5 \text{ ppb}$). This suggests that there is another source of TCE between $x = 0$ and 2 km .

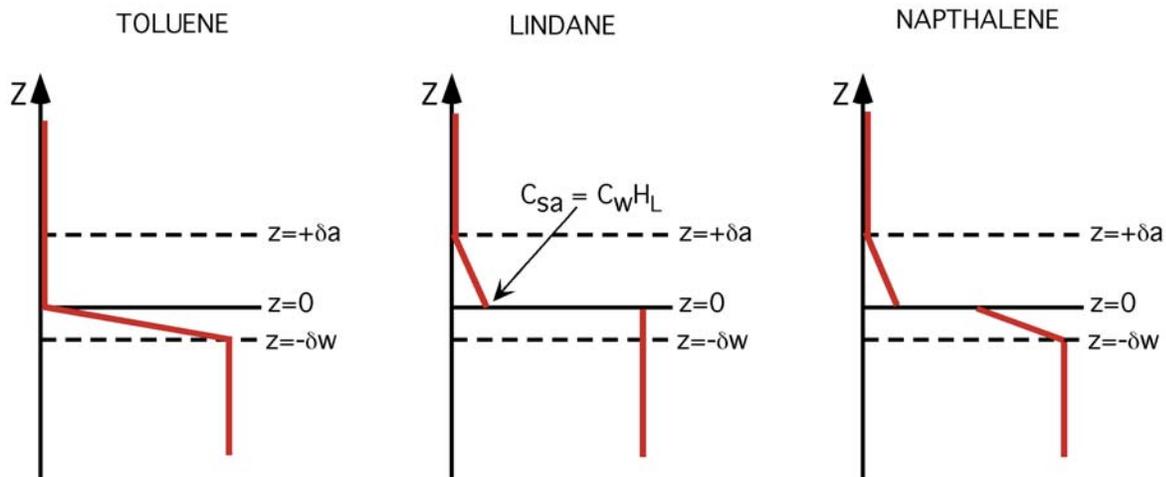
Answer 9.5

Toluene [$H_T = 0.28 \gg 0.01$] is waterside controlled

Lindane [$H_L = 2.2 \times 10^{-5} \ll 0.01$] is airside controlled

Napthalene [$H_N = 0.04 \approx 0.01$] is controlled by both air and water side conditions.

(a) Sketch the profile of $C(z)$ for each chemical



b) Write an equation for the mass flux at the air-water interface for each chemical.

c) For each chemical determine the time at which only 5% of the original mass remains.

TOLUENE	LINDANE	NAPHTHALENE
$\dot{m} = D_w A \frac{C_w}{\delta_w}$	$\dot{m} = D_a A \frac{C_w H_L}{\delta_a}$	$\dot{m} = A \frac{C_w}{\left[(\delta_w / D_w) + \delta_a / (H_N D_a) \right]}$
$\frac{\partial C_w}{\partial t} = - \left[\frac{D_w}{\delta_w h} \right] C_w$	$\frac{\partial C_w}{\partial t} = - \left[\frac{D_a H_L}{\delta_a h} \right] C_w$	$\frac{\partial C_w}{\partial t} = - \frac{C_w / h}{\left(\delta_w / D_w \right) + \delta_a / (H_N D_a)}$
$C_w(t) = C_o \exp \left(- \frac{D_w}{\delta_w h} t \right)$	$C_w(t) = C_o \exp \left(- \frac{D_a H_L}{\delta_a h} t \right)$	$C_w = C_o \exp \left(- \frac{t}{\left[\frac{\delta_w}{D_w} + \frac{\delta_a}{H_N D_a} \right] h} \right)$
$T_{5\%} = \frac{3 \delta_w h}{D_w} = 3 \times 10^5 \text{ s}$	$T_{5\%} = 3 \frac{\delta_a h}{D_a H_L} = 1.4 \times 10^8 \text{ s}$	$T_{5\%} = 3h \left[\frac{\delta_w}{D_w} + \frac{\delta_a}{H_N D_a} \right]$ $= 3.8 \times 10^5 \text{ s}$

d) For which chemicals is the assumption of a uniform concentration within the bulk fluid appropriate?

The mixing time is, $T_D = h^2 / (4D_t) = (1\text{m})^2 / (4 \times 0.001 \text{ m}^2 \text{ s}^{-1}) = 250 \text{ s}$. For every chemical $T_D \ll T_{5\%}$, so the assumption of well-mixed conditions in the lake are appropriate for each chemical.

Answer 9.6

Chemical 1 is a conservative tracer that does not react or degrade.

The peak of the non-adsorbing, non-degrading chemical will arrive soonest and with the highest concentration. This corresponds to the red curve. From the peak arrival time we can estimate the velocity, $u = 8\text{m}/4\text{day} = 2 \text{ md}^{-1}$.

Chemical 2 does not adsorb, but is degraded by microbes living in the aquifer.

This chemical does not adsorb, and so has no retardation. Its peak will arrive with that of chemical 1, but with a diminished concentration. This corresponds to the green curve.

Specifically, $C_2(t) = C_1(t) \exp(-kt)$. Using the peak values at $T_{1,2} = 4$ days, $C_{2\text{peak}}/C_{1\text{peak}} = (10.5/15.8) = \exp(-kt)$, from which

$$k_2 = -\ln(C_2/C_1)/t = -\ln(10.5/15.8) / (4 \text{ days}) = 0.1 \text{ d}^{-1}.$$

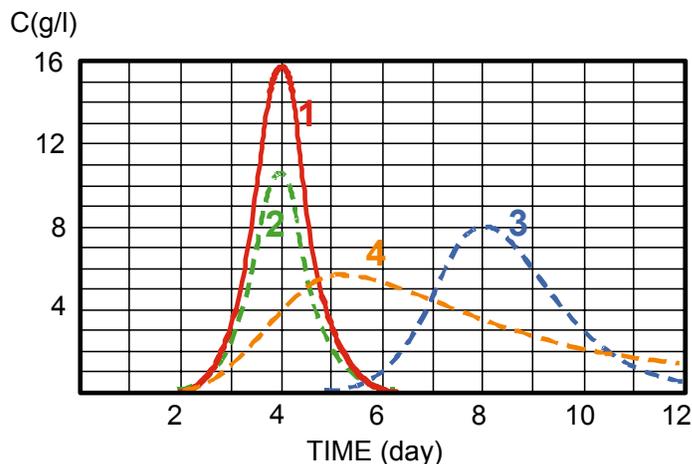
Both Chemical 3 and 4 adsorb to the soil matrix, and so experience some retardation, as seen in the orange and blue curves. However, Chemical 4 has a slow adsorption process, and so will not be in equilibrium. Slow sorption leads to additional dispersion. This is consistent with the orange curve. Chemical 3 therefore corresponds to the blue curve.

Chemical 3 adsorbs rapidly and the partitioning is always at equilibrium.

Blue Curve. The transport of this plume is slowed because at any time only the fraction f of the mass is in the dissolved phase and subject to fluid transport. Specifically, the plume advects at the speed fu rather than u . We can estimate f by comparing the peak arrival time with that of the non-adsorbing chemical. Specifically, $T_{1,2} = L/u$ and $T_3 = L/(fu)$, so that $f = T_{1,2} / T_3 = 4 \text{ d} / 8 \text{ d} = 0.5$.

Chemical 4 adsorbs so that the partitioning is not at equilibrium.

From the discussion above, this corresponds to the orange curve. The rate of sorption/desorption must be slow compared to the transport time scales. Using the observed transport scale, $k_4^{-1} \gg 5 \text{ d}$, or $k_4 \ll 0.2 \text{ d}^{-1}$.



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 4σ , evaluated at the peak arrival time, T_U .

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