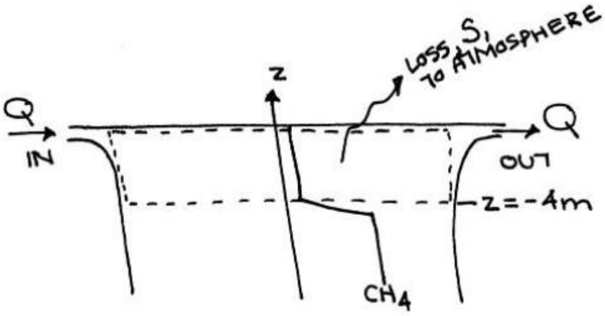
Question 1.



Define the epilimnion as the control volume of interest. The conservation of mass for this system, assuming steady state, is

(A)

$$0 = (QC)_{IN} - (QC)_{OUT} - D_Z \frac{\partial C}{\partial Z} A - S$$

given $C_{IN} = 0$. Assume epilimnion is well-mixed. $\therefore C_{OUT} = C_{EPI} = C(z = -4\,m)$. Discretize concentration gradient across thermocline,

$$\left.\frac{\partial C}{\partial Z}\right|_{z=-4} \approx \frac{[C(z=-4) - C(z=-5)]}{[-4 - -5]}$$

Then solve (A) for S,

(B)

$$\begin{aligned} S &= -QC_{EPI} - D_Z A \frac{C_{EPI} - C_{HYPO}}{1\,m} \\ &= -\left(1\,m^3/s\right)(0.4\,mg/l) - \left(2 \times 10^{-6}\,m^2 s^{-1}\right)\left(10^6\,m^2\right)\left[\frac{0.4 - 4\,mg/l}{1\,m}\right] \\ &= 6.8\,\frac{m^3}{s}\frac{mg}{l}\frac{1000\,l}{m^3} = 6.8\,g/s \end{aligned}$$

Question 2.

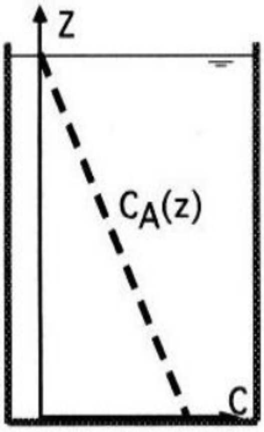
From Fick's Law, $q_z = -DA\dfrac{\partial C}{\partial Z}$.

(1) At z = 0 and z = H, $\dfrac{\partial C}{\partial Z} < 0$, $\therefore q_z > 0$, which indicates fluxes is upward at both boundaries.

(2) At steady state, $\dfrac{\partial C}{\partial t} = 0$. From 1-D conservation equation,

$$\frac{\partial C}{\partial t} = D_z \frac{\partial^2 C}{\partial Z^2}$$

$\therefore$ at steady state, $\dfrac{\partial^2 C}{\partial Z^2} = 0$. $\therefore$ $\dfrac{\partial C}{\partial Z} =$ constant. $\therefore$ linear profile indicates this system is at steady state.

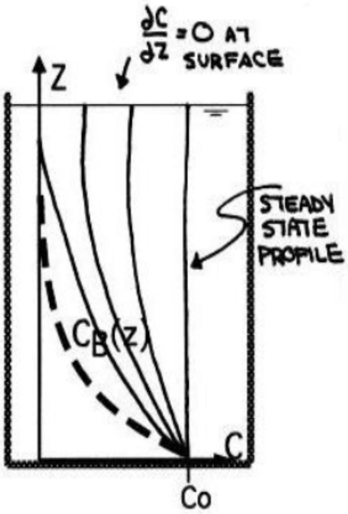


(1) $\dfrac{\partial C}{\partial Z} < 0$ at z = 0. $\therefore q_z > 0$, positive, upward. No flux at z = H.

(2) System is not at steady state.

$$\frac{\partial}{\partial Z}\left(\frac{\partial C}{\partial Z}\right) \neq 0, \therefore \text{ from conservation EQ, } \frac{\partial C}{\partial Z} \neq 0$$

Progression of evolving profiles shown. Note, because chemical is not volatile, surface (z = H) is a no flux boundary. $\therefore \left.\dfrac{\partial C}{\partial Z}\right|_{z=H} = 0$ so that $q_z(z = H) = 0$!

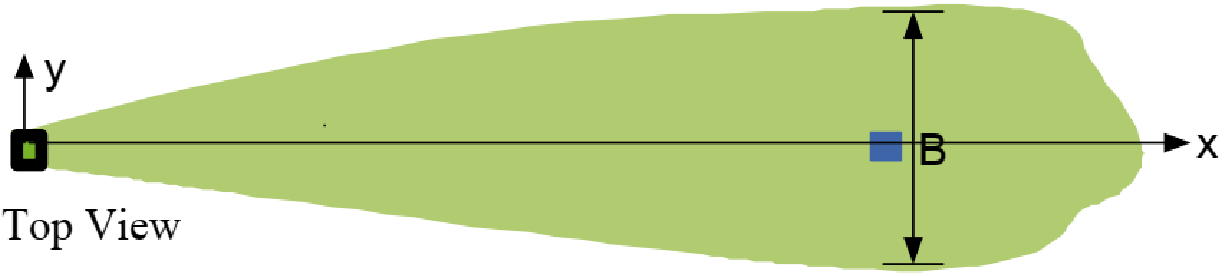


Question 3.

The release is described as continuous, and we are told that it rapidly distributes over the aquifer depth. No lateral boundaries are indicated. As a first approximation, we believe the concentration field will resemble that from a continuous release in two dimensions, (x,y), with conditions uniform in the vertical coordinate, z. No image sources are needed, because boundaries only restrict flux in the z-direction, and the concentration is already assumed to be constant in z, such that the no-flux condition, $\partial C/\partial z = 0$, is automatically satisfied. However, the source is not a point, but rather is distributed over a 5-m x 5-m square. We can treat it as a point if this area is small compared to the extent of the plume at the well (see B below), as the concentration observed at the well will then appear as if it came from a point source. We estimate the lateral dimension of the plume as $B = 4\,\sigma_y = 4\,\sqrt{(2K_y\,L/U)}$, where L = 500m is the distance to the well, and the lateral dispersivity is $K_y = 10^{-6}\ \mathrm{m^2 s^{-1}}$. Then, B = 126m. Since 5m << 126m, the concentration at the well appears as if it originated from a point source. Finally, we write the expression for brine concentration downstream of the leak.

$$C(x,y) = \frac{\dot{m}/u}{L_z\sqrt{4\pi K_y(x/u)}}\exp\left(-\frac{uy^2}{4K_y x}\right),$$

with $L_z = 2\mathrm{m}$ the thickness of the aquifer. This solution is valid for $Pe = Ux/K_x >>1$, or x >> 10m, so we may apply it at the well located at x = 500m.

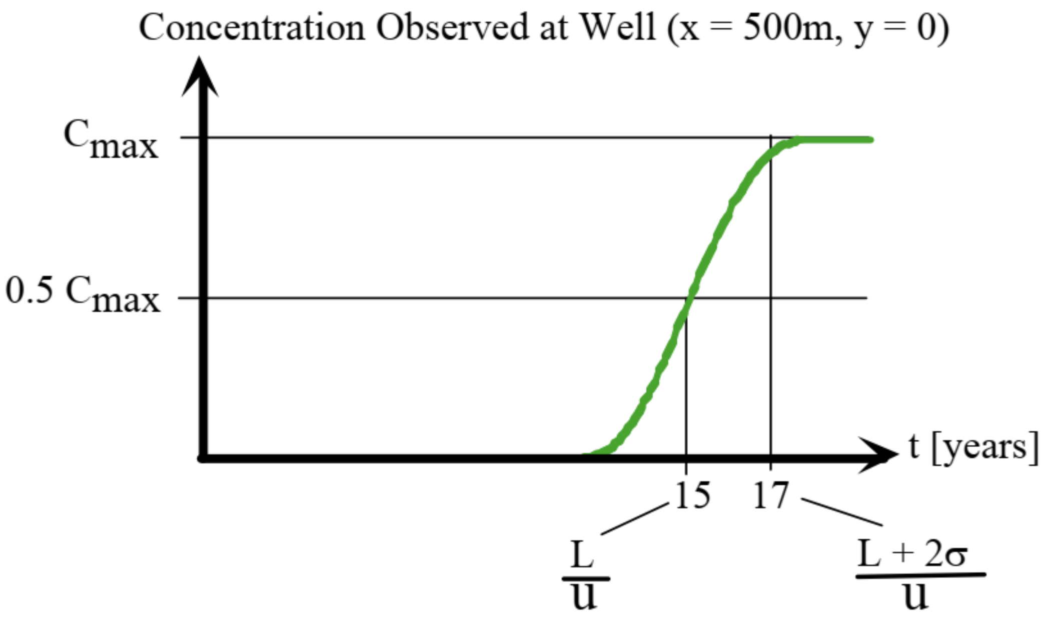


The maximum concentration at the well, C_{max}, is given by the above equation evaluated for (x=500m, y=0m).

$$C_{max} = \frac{(10\mathrm{g/l})(0.1\mathrm{m^3/week})(1\mathrm{week}/604800\mathrm{s})}{(10^{-6}\mathrm{m/s})(2\text{ - }\mathrm{m})\sqrt{4\pi(10^{-6}\mathrm{m^2/s})(500\mathrm{m}/10^{-6}\mathrm{m/s})}} = 0.011\ \mathrm{g/l} = 0.011\ \mathrm{ppt}.$$

This salinity is not detectable by the human palate. For reference, salt water is 30 ppt.

The solution above assumes that steady state has been reached at the well. The time-required for this to occur depends both on advection and longitudinal dispersion. The advection time-scale, $T_U = 500\mathrm{m}/10^{-6}\mathrm{m/s} = 5\times10^{8}\ \mathrm{s} \approx 15$ years, defines the arrival of the mid-front which will have the concentration $C_{max}/2$. The time interval Δt between the arrival of the mid-front and the end of the transient period is approximately $\Delta t = (2\sigma_x)/u$, where σ_x is estimated at the time the mid- front arrives at the well, $\sigma_x = \sqrt{(2K_xL/u)}$. So, $\Delta t = (2/10^{-6}\mathrm{ms}^{-1}) \times \sqrt{(2\times 10^{-6}\ \mathrm{m}^2\mathrm{s}^{-1} \times\ 500\mathrm{m} / 10^{-6}\mathrm{ms}^{-1})} = 6.3 \times 10^{7}\ \mathrm{s} = 2$ years. The concentration observed at the well is sketched below.



Finally, note that molecular diffusion, while present, is negligible compared to the lateral and longitudinal dispersion, and so is not considered in the plume transport calculations.

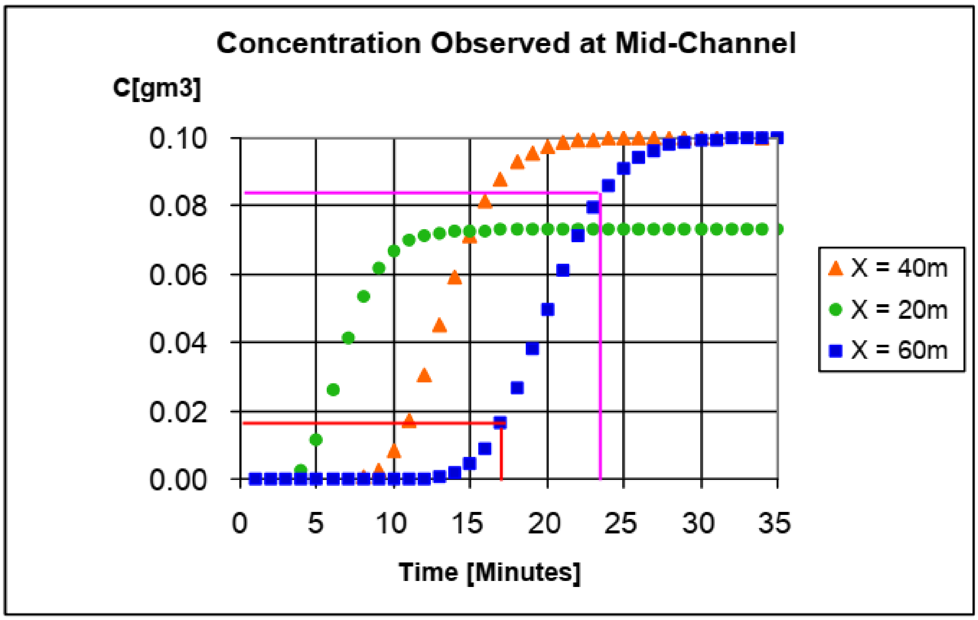
Question 4.

If the tracer is mixed over the channel area, $Q_r = Q_i C_i/C_f = \dot{m}/C_f$, where $\dot{m}$ is the tracer injection rate and C_f is the steady-state, far-field concentration. From the observed concentration, and $\dot{m} \equiv 0.01\ \mathrm{gs}^{-1}$,

X [m]	C_f [gm-3]	estimated Q_R [$\mathrm{m}^3\mathrm{s}^{-1}$]
20	0.075	0.13
40	0.1	0.10
60	0.1	0.10

The estimated river flow at the first station is higher than the later two stations. At first this suggests that flow is diverted from the channel between 20 and 40 m.

However, diversion of flow would not change the concentration, so this is implausible. Instead, we suspect that at x = 20m the tracer has not yet fully mixed within the channel, making the observed concentration lower than the steady state value. We then conclude that the flow in the channel is 0.1 m^3s^{-1}. We estimate the Lagrangian mean velocity, u, from the arrival of the mid-front. At x = L downstream of the injection, the concentration will be $0.5C_f$ at t = L/u. Using the 60-m data, C = $0.5C_f$ = 0.05 gm^{-3} at t = 20 minutes. Thus, u=(60m)/(1200s) =0.05 ms^{-1}. The mean cross-sectional area between x = 0 and x = 60-m is then, $A=Q_R/u = 2m^2$.



The coefficient of longitudinal dispersion, K_x, is estimated from the shape of the front. At $t_{0.16} = (L-\sigma_x)/u$, the concentration will be $0.16C_f$. At $t_{0.84} = (L+\sigma_x)/u$, the concentration will be $0.84C_f$. Using the concentration at x = L = 60m,

L [m]	u [m/s]	$t_{0.16}$ [min]	$\sigma_{0.16}$=L-u$t_{0.16}$ [m]	$t_{0.84}$ [min]	$\sigma_{0.84}$= u$t_{0.84}$-L [m]
60	0.05	17	9	24	12

Assuming $\sigma = 0$ at t = 0 we have two estimates for K_x

$$K_x = \frac{1}{2}\frac{\partial\sigma^2}{\partial t} = \frac{1}{2}\left(\frac{\sigma_{0.84}{}^2}{t_{0.84}}\right) = \frac{1}{2}\left(\frac{(12\text{m})^2}{24\text{min}}\right) = 3.0\ \text{m}^2\text{min}^{-1}$$

$$K_x = \frac{1}{2}\frac{\partial\sigma^2}{\partial t} = \frac{1}{2}\left(\frac{\sigma_{0.16}{}^2}{t_{0.16}}\right) = \frac{1}{2}\left(\frac{(9\text{m})^2}{17\text{min}}\right) = 2.4\ \text{m}^2\text{min}^{-1}$$

We can average these to find the best estimate, $K_X = 2.7\ m^2min^{-1}$

Question 5.

a) Write an appropriate transport equation

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

$$(1)\ \frac{\partial C}{\partial t} + fu\frac{\partial C}{\partial x} + fv\frac{\partial C}{\partial y} + fw\frac{\partial C}{\partial z} = \frac{\partial}{\partial x} fK_x \frac{\partial C}{\partial x} + \frac{\partial}{\partial y} fK_y \frac{\partial C}{\partial y} + \frac{\partial}{\partial z} fK_z \frac{\partial C}{\partial z},$$

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

$$(2)\ \frac{\partial C}{\partial t} + fu\frac{\partial C}{\partial x} = fK\frac{\partial^2 C}{\partial x^2} + fK\frac{\partial^2 C}{\partial y^2}$$

To determine f we need the bulk density, which is

$\rho_B = \rho_S(1 - n) = 2.6\ \text{x}(1 - 0.3) = 1.82\ \text{g/mL}$. 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, $Pe = fU\,L / K = (0.25)(1\text{md}^{-1})(1000\text{m})/(0.1\ \text{m}^2\text{d}^{-1}) = 2500 >> 1$, 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, $T_U = L/fU = (1000\text{m})/(0.25\ \text{x}\ 1\ \text{md}^{-1}) = 4000$ 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 $T_U >> 24$ 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 $L_Z = 5$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 $y = 0$.

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

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

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

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.

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

Question 6.

Let the bubble rise velocity be w_B. A bubble requires the time $T_{rise} = h/w_B$ to reach the surface. In this time the bubble will travel a downstream distance of uT_{rise}. Thus the desired spacing scale is

(1) $L = uh/w_B$.

To find w_B we first assume creeping flow,

$$w_B = \frac{gd^2(\rho_B - \rho_W)}{18\mu_W} = \frac{9.8\text{ms}^{-2}(10^{-3}\text{ m})^2(1.4 - 998 \text{ kgm}^{-3})}{18(10^{-3}\text{kgm}^{-1}\text{s}^{-1})} = 0.54\text{ms}^{-1}$$

Check $Re_B = (0.54\text{ms}^{-1})(0.001\text{m})/(10^{-6}\text{m}^2\text{s}^{-1}) = 540 >> 1$, so creeping flow is not confirmed. We now iterate to find the bubble velocity using the relations:

$$C_D = \frac{24}{Re_B} + \frac{3}{\sqrt{Re_B}} + 0.34 \quad \text{and} \quad w_B = \left[\frac{4}{3}\,\frac{gd\,(\rho_B - \rho_F)}{\rho_F\, C_D}\right]^{1/2}.$$

Assume $Re_B = 540$

$$C_D = \frac{24}{540} + \frac{3}{\sqrt{540}} + 0.34 = 0.51$$

$$w_B = \left[\frac{4}{3}\,\frac{(9.8\text{ms}^{-1})(0.001\text{m})\,(1.4 - 998\text{kgm}^{-3})}{(998\text{kgm}^{-3})(0.51)}\right]^{1/2} = 0.16\text{m}/\text{s}$$

$Re_B = (0.16\text{ms}^{-1})(0.001\text{m})/(10^{-6}\text{m}^2\text{s}^{-1}) = 160 \neq 540$, so go around again.

Assume $Re_B = 160$

$$C_D = \frac{24}{160} + \frac{3}{\sqrt{160}} + 0.34 = 0.73$$

$$w_B = \left[\frac{4}{3}\frac{(9.8\text{ms}^{-1})(0.001\text{m})\,(1.4 - 998\text{kgm}^{-3})}{(998\text{kgm}^{-3})(0.73)}\right]^{1/2} = 0.13\text{m/s}$$

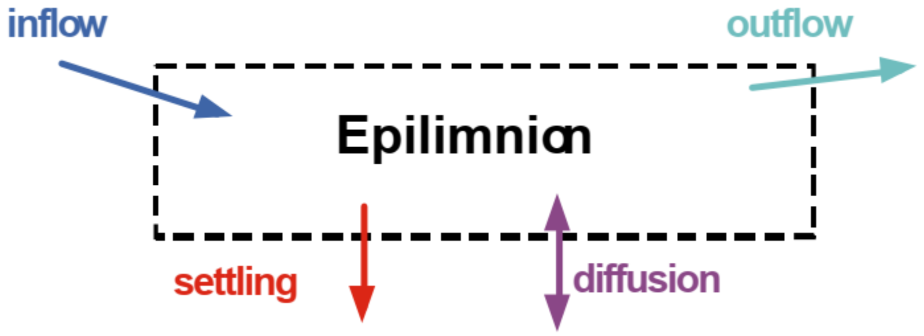
$Re_B = (0.13\text{ms}^{-1})(0.001\text{m})/(10^{-6}\text{m}^2\text{s}^{-1}) = 130 \approx 160$, we are close enough to stop.

Now, returning to (1),

$L = uh/w_B = (1\text{ms}^{-1})(1\text{m})/(0.13\text{ms}^{-1}) = 7.6$ m

Question 7.

To estimate whether phosphorus mass in the epilimnion will change in the near future, we consider a mass balance for this region. There are four fluxes contributing to and/or removing phosphorus from the epilimnion volume.



Inflow Flux = $Q_I C_I = (0.1\ \text{m}^3\text{s}^{-1})(100\mu\text{gL}^{-1})(1000\text{Lm}^{-3}) = 10\ \text{mgs}^{-1}$.

Outflow Flux = $Q_O C_O = (0.1\ \text{m}^3\text{s}^{-1})(50\mu\text{gL}^{-1})(1000\text{Lm}^{-3}) = 5\ \text{mgs}^{-1}$.

The settling flux occurs across the base of the epilimnion control volume. From the graph, this is located at 4m depth at which point $C_{4m} = 40\ \mu\text{gL}^{-1}$. If we assume a cylindrical lake basin, the area at the base of the epilimnion is the same as the water surface area, A. Then,

Settling Flux = $w_P A C = (2.0 \times 10^{-6}\ \text{ms}^{-1})(2 \times 10^4\ \text{m}^2)(40\mu\text{gL}^{-1})(1000\text{Lm}^{-3}) = 1.6\ \text{mgs}^{-1}$.

The diffusive flux also occurs across the base of the epiliminion. We need to estimate the gradient of concentration at the base. For this we can use a central difference z = 4m,

$(\partial C/\partial z)_{4m} = (C_{3m} - C_{5m})/(3 - 5\text{ m}) = (50\text{-}30\ \mu gL^{-1})/(3\text{-}5m) = -10\mu gL^{-1}m^{-1}$.

Diffusive Flux =

$- D_t\, A\, \partial C/\partial z = -(2x10^{-6}m^2s^{-1})(2x10^4m^2)(-10\mu gL^{-1}m^{-1})(1000Lm^{-3}) = +\ 0.4\ mgs^{-1}$.

The positive sign indicates that the diffusive flux is directed downward, along the positive z axis. This flux is a loss for the control volume.

The sum of these fluxes gives the rate of change of phosphorus mass in the epilimnion,

$\partial M/\partial t = +$ Inflow - Outflow - Settling - Diffusive Flux $= (+10 - 5 - 1.6 - 0.4) = +3mgs^{-1}$.

With $\partial M/\partial t > 0$, the phosphorus levels in the epilimnion will continue to increase.