Chapter 07.00C

Physical Problem for Integration
Civil Engineering

Problem Statement
In a class X528 well in New York State, you are asked to find if the concentration of benzene is below the toxicity level of $0.5\,\text{mg/l}$ at a distance of $36\,\text{m}$ from the point of contamination. The contamination at the source is constant at $3.5\,\text{mg/l}$ for a whole year.

Solution

The equations governing transport of groundwater contaminant are quite complex. They depend on several parameters such as "the molecular diffusion of the contaminant, physical and chemical isotropy of the medium, and actual direction of the groundwater flow" [1].

Here we consider that the groundwater is flowing in one-direction, x and the aquifer has isotropic and homogeneous physical and chemical characteristics. In that case, the governing equation [2] for the concentration $c(x,t)$ of the contaminant is given by

$$\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x}=D\frac{\partial^2 c}{\partial x^2}. \tag{1}$$

where

u = velocity of ground water flow in the x-direction (m/s)

t = time (s)

x = distance from source (m)

D = dispersion coefficient (m^2).

To solve this partial differential equation (1) [3], we use Laplace transforms. Applying Laplace transform to both sides on the variable t,

$$L\left(\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x}\right)=L\left(D\frac{\partial^2 c}{\partial x^2}\right)$$

$$sC-c(x,0)+u\frac{dC}{dx}=D\frac{d^2C}{dx^2}. \tag{2}$$

where

$$L[c(x,t)]=C(x,s)$$

Since the initial concentration is zero,

$c(x,0)=0$,

Equation (2) becomes

$$sC+u\frac{dc}{dx}=D\frac{d^2C}{dx^2}$$

$$D\frac{d^2C}{dx^2}-u\frac{dC}{dx}-sC=0 \qquad (3)$$

This is a homogenous ordinary differential equation. It is linear with fixed coefficients. The characteristics equation of the above ordinary differential equation (3) is

$$Dm^2-um-s=0$$

$$m=\frac{u\pm\sqrt{u^2+4Ds}}{2D} \qquad (4)$$

The homogeneous as well as the complete solution of Equation (3) is

$$C(x,s)=A(s)e^{\frac{u+\sqrt{u^2+4Ds}}{2D}x}+B(s)e^{\frac{u-\sqrt{u^2+4Ds}}{2D}x} \qquad (5)$$

At $x=\infty$, that is far away from the source, the concentration of the pollutant is zero, that is $c(\infty,s)=0$, that is, $C(\infty,s)=0$. This forces $A(s)=0$ as the exponent of the exponential term is always positive as $u,D,s>0$. The exponent of the exponential term on the second term will be negative as $\sqrt{u^2+uDs}>u$ for all values of u,D,s as $u,D,s>0$. Equation (5) hence reduces to

$$C(x,s)=B(s)e^{\frac{u-\sqrt{u^2+4Ds}}{2D}x} \qquad (6)$$

At $x=0$, $c=c_0$ (initial concentration, c_0), then $C(0,s)=\frac{c_0}{s}$. Substituting this in equation (6) gives

$$\frac{c_o}{s}=B(s)$$

then equation (6) is

$$C(x,s)=\frac{c_0}{s}e^{\frac{u-\sqrt{u^2+4Ds}}{2D}x}$$

$$=\left(c_0e^{\frac{ux}{2D}}\right)\left(\frac{e^{-\frac{\sqrt{u^2+4Ds}}{2D}x}}{s}\right)$$

$$L^{-1}[C(x,s)]=L^{-1}\left[\left(c_0e^{\frac{ux}{2D}}\right)\left(\frac{e^{-\frac{\sqrt{u^2+4Ds}}{2D}x}}{s}\right)\right]$$

$$c(x,t)=c_0e^{\frac{ux}{2D}}L^{-1}\left(\frac{e^{-\frac{\sqrt{u^2+4Ds}}{2D}x}}{s}\right)$$

$$= C_0 e^{\frac{ux}{2D}} L^{-1}\left[\frac{e^{-\frac{x}{\sqrt{D}}\sqrt{\frac{u^2}{4D}+s}}}{S}\right] \tag{7}$$

Let

$$a = \frac{x}{\sqrt{D}}$$

$$b = \frac{u}{2\sqrt{D}}$$

Then Equation (7) becomes

$$c(x,t) = c_0 e^{ab} L^{-1}\left(\frac{e^{-a\sqrt{b^2+s}}}{s}\right) \tag{8}$$

Using the formulas

$$L^{-1}(e^{-a\sqrt{s}}) = \left(\frac{a}{2\sqrt{\pi t^3}} e^{-\frac{a^2}{4t}}\right), a > 0 \text{, and}$$

$$L^{-1}(F(s+a)) = e^{-at} f(t)$$

then

$$L^{-1}\left(e^{-a\sqrt{b^2+s}}\right) = \frac{a}{2\sqrt{\pi t^3}} e^{-\frac{a^2}{4t} - b^2 t} \tag{9}$$

Then from

$$\int_0^t f(\tau) d\tau = \frac{F(s)}{s}$$

we get

$$L^{-1}\left(\frac{e^{-a\sqrt{b^2+s}}}{s}\right) = \int_0^t \frac{a}{2\sqrt{\pi\tau^3}} e^{-\frac{a^2}{4\tau}} e^{-b^2\tau} d\tau$$

$$= e^{-ab} \int_0^t \frac{a}{2\sqrt{\pi\tau^3}} e^{-\frac{(a-2b\tau)^2}{4\tau}} d\tau$$

$$= e^{-ab} \int_0^t \left(\frac{a+2b\tau}{4\sqrt{\pi\tau^3}} + \frac{a-2b\tau}{4\sqrt{\pi\tau^3}}\right) e^{-\frac{(a-2b\tau)^2}{4\tau}} d\tau$$

$$= e^{-ab} \int_0^t \frac{a+2b\tau}{4\sqrt{\pi\tau^3}} e^{-\frac{(a-2b\tau)^2}{4\tau}} d\tau + e^{-ab} \int_0^t \frac{a-2b\tau}{4\sqrt{\pi\tau^3}} e^{-\frac{(a-2b\tau)^2}{4\tau}}$$

$$= e^{-ab} \int_0^t \frac{a+2b\tau}{4\sqrt{\pi\tau^3}} e^{-\frac{(a-2b\tau)^2}{4\tau}} d\tau + e^{-ab} \int_0^t \frac{a-2b\tau}{4\sqrt{\pi\tau^3}} e^{-\frac{(a-2b\tau)^2}{4\tau} - \frac{8ab\tau}{4\tau} + \frac{8ab\tau}{4\tau}}$$

$$= e^{-ab} \int_0^t \frac{a+2b\tau}{4\sqrt{\pi\tau^3}} e^{-\frac{(a-2b\tau)^2}{4\tau}} d\tau + e^{ab} \int_0^t \frac{a-2b\tau}{4\sqrt{\pi\tau^3}} e^{-\frac{(a+2b\tau)^2}{4\tau}} d\tau$$

Let

$$p = \frac{a - 2b\tau}{\sqrt{4\tau}},$$

$$q = \frac{a + 2b\tau}{\sqrt{4\tau}}$$

then

$$L^{-1}\left(\frac{e^{-a\sqrt{b^2+s}}}{s}\right) = \frac{e^{-ab}}{\sqrt{\pi}}\int_{\infty}^{\frac{a-2bt}{\sqrt{4t}}} e^{-p^2}dp - \frac{e^{ab}}{\sqrt{\pi}}\int_{\infty}^{\frac{a+2bt}{\sqrt{4t}}} e^{-q^2}dq$$

$$= \frac{e^{-ab}}{2}erfc\left(\frac{a-2bt}{2\sqrt{t}}\right) + \frac{e^{ab}}{2}erfc\left(\frac{a+2bt}{2\sqrt{t}}\right) \quad (10)$$

Using Equation (10), Equation (8) becomes

$$c(x,t) = c_0 e^{ab}\left[\frac{e^{-ab}}{2}erfc\left(\frac{a-2bt}{2\sqrt{t}}\right) + \frac{e^{ab}}{2}erfc\left(\frac{a+2bt}{2\sqrt{t}}\right)\right]$$

$$= \frac{c_0}{2}\left[erfc\left(\frac{a-2bt}{2\sqrt{t}}\right) + \frac{e^{2ab}}{2}erfc\left(\frac{a+2bt}{2\sqrt{t}}\right)\right] \quad (11)$$

Substituting back

$$a = -\frac{x}{\sqrt{D}},$$

$$b = \frac{u}{2\sqrt{D}}$$

$$c(x,t) = \frac{c_0}{2}\left[erfc\left(\frac{x-ut}{2\sqrt{Dt}}\right) + e^{\frac{ux}{D}}erfc\left(\frac{x+ut}{2\sqrt{Dt}}\right)\right] \quad (12)$$

The velocity of the ground flow, u is given by

$$u = \frac{k}{n_{ed}}\frac{dh}{d\ell} \quad (13)$$

where

n_{ed} = effective Darcian porosity,

K = permeability,

$\frac{dh}{dl}$ = ground water gradient.

Assuming

$n_{ed} = 22\% = 0.22$

$K = 0.002 \ \frac{\text{cm}}{\text{s}}$

$\frac{dh}{dl} = 0.01\frac{\text{cm}}{\text{cm}}$.

Then from Equation (13),

$$u = \frac{0.002}{0.22}(0.01)$$

$$= 9.091 \times 10^{-5}\ \frac{\text{cm}}{\text{s}}.$$

So in the formula for concentration given by Equation (12), substituting

$$D = 0.01\frac{\text{cm}^2}{\text{s}}$$

$$c_0 = 3.5\frac{\text{mg}}{\text{L}}$$

$$x = 36\,\text{m}$$

$$t = 1\ \text{year} = 3.15 \times 10^7\ \text{s}$$

the concentration of benzene after 1 year at a distance of $36\,\text{m}$ is

$$c = \frac{3.5}{2}\left[erfc\left(\frac{3.6 - (9.091 \times 10^{-5})(3.15 \times 10^7)}{2\sqrt{(0.01)(3.15 \times 10^7)}} \right) + e^{\frac{(9.091\text{x}10^{-5})(36)}{0.01}} erfc\left(\frac{36 + (9.091 \times 10^{-5})(3.15 \times 10^7)}{2\sqrt{(0.01)(3.15 \times 10^7)}} \right) \right]$$

$$= 1.75[erfc(0.6560) + e^{32.73} erfc(5.758)] \quad (14)$$

As you can see to calculate the concentration of benzene at $x = 36\,\text{m}$, we need to calculate $erfc(0.6560)$ and $erfc(5.758)$. How is $erfc(x)$ defined?

$$erfc(x) = \int_{\infty}^{x} e^{-z^2} dz$$

So

$$erfc(0.6560) = \int_{\infty}^{0.6560} e^{-z^2} dz$$

Since e^{-z^2} decays rapidly as $z \to \infty$, we will approximate

$$erfc(0.6560) = \int_{5}^{0.6560} e^{-z^2} dz$$

So to find whether the concentration of benzene is below toxicity level, we need to find the integral numerically.

QUESTIONS

1. What is the concentration of benzene after 2 years?
2. After 1 year, at what distance does the concentration go below the toxicity level of 0.5 mg/L?

REFERENCES

1. EPA Region 5 Water Draft UIC Class IV and V Site Assessment Guidelines, http://www.epa.gov/R5water/uic/r5guid/siteasst.htm, last accessed July 2004.
2. Fetter, C.W., Jr., Applied Hydrology, Merill Publishing Co, Columbus, 1980.

3. Li, W., Differential Equations of Hydraulic Transients, Dispersion, and Groundwater Flow, Prentice Hall, Englewood Cliffs, NJ, 1972

Topic	INTEGRATION
Sub Topic	Physical problem
Summary	Find if the concentration of benzene is above or below the toxicity limit at a critical distance from its source.
Authors	Autar Kaw
Last Revised	December 7, 2008
Web Site	http://numericalmethods.eng.usf.edu