Contaminant migration through clay liner considering diffusion process

Three processes of contaminant transport in **saturated porous media:**

flux

① **Advection :** $J_A = n v_{int} C$ (1) — $v_{int}=v/n,\ v/\theta,\ v=-Ki$ — *seepage rate, leakage rate*

② **Molecular Diffusion:** $J_D = -D_m n \dfrac{\partial C}{\partial x}$ (2)

③ **Mechanical Dispersion:** $J_M = -D_L n \dfrac{\partial C}{\partial x}$ (3)

Negligible in the evaluation of contaminant transport in clay liner. why??

Advective-dispersive eq.: $R_d \dfrac{\partial C}{\partial t} = D_{hl} \dfrac{\partial^2 C}{\partial x^2} - v_{int} \dfrac{\partial C}{\partial x}$ (4)

Cof. Ret.: $R_d = 1 + \dfrac{(1-n)\rho_s K_d}{n}$

4. Transient time phenomena

Specification of liner

- clay liner with low hydraulic conductivity (ex.;10^{-9}m/s)
- under small hydraulic gradient (=1.0 ~ (0.3+0.9)/0.9=4/3)

Determine seepage rate (=advection)

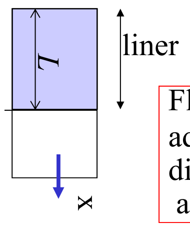
but

diffusive process dominates the contaminant transport in clay liners rather than advective process??

What is the number to show the relative importance of diffusion to advection??

time transient consideration might be necessary for the design of clay liner (ex; determining thickness).

Concentration or flux passing through at the location L (bottom of liner)

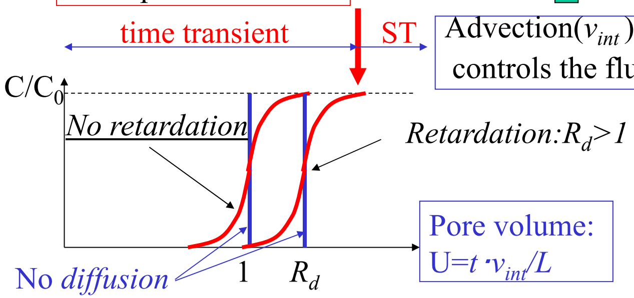


Flux depends on both advection(v_{int}), dispersion and adsorption

Hydraulic conductivity

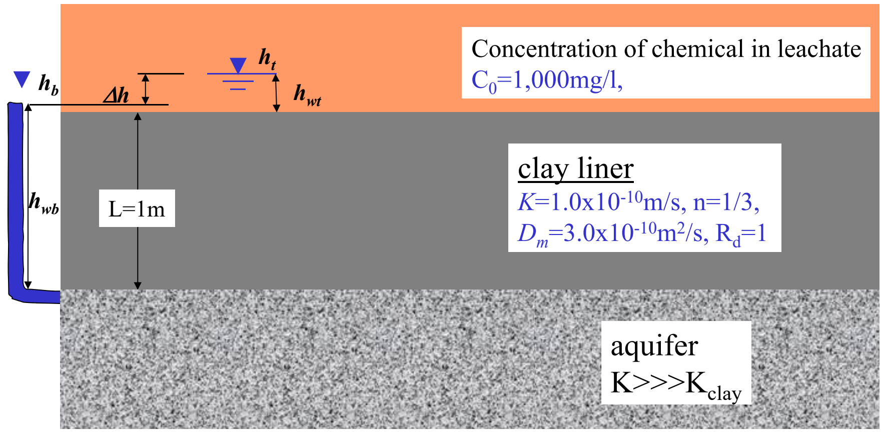
Water flow dominates the contaminant transport

Advection(v_{int}) only controls the flux



Pore volume: $U = t \cdot v_{int}/L$

Effect of molecular diffusion



No advection case: Δh=0

B.C. and I.C.

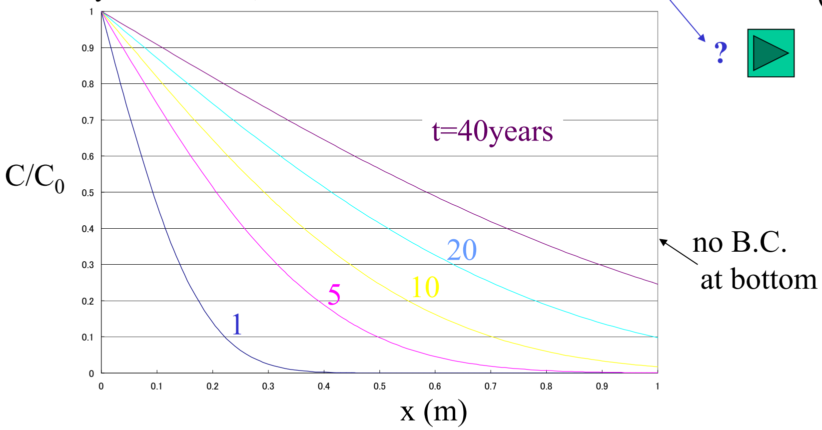
$C=C_0$ at top boundary of the clay liner

$C=0$ in clay liner at $t=0$,

$v_{int}=0$

$$C(x,t)=C_0 erfc\frac{x}{2(D_m t)^{0.5}} \quad (5)$$

?



Advection case: $\Delta h=L(i=1)$, rigorous solution, e.g., eq.(6)

same B.C. and I.C., $v_{int}=Ki/n$ = 3.0x10^{-10}m/s **why not (7)?**

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P_L?

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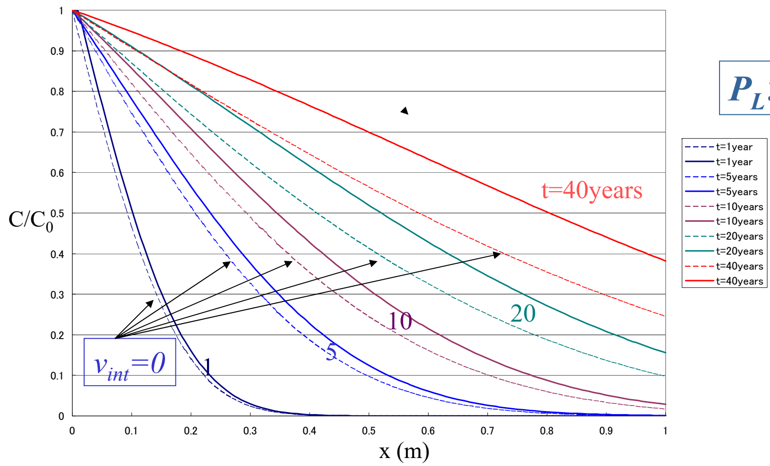


Solution of A-D equation used for estimation

step function B.C. $C(0,t)=C_0$

$C(\infty,t)=0$

I.C. $C(x,0)=0$

Ogata & Bank's

without retardation $R_d=1$

$$C(x,t)=\frac{1}{2}C_0\left[erfc\left(\frac{x-v_{int}t}{2(D_m t)^{0.5}}\right)+\exp\left(\frac{v_{int}x}{D_m}\right)erfc\left(\frac{x+v_{int}t}{2(D_m t)^{0.5}}\right)\right] \quad (6\text{-I})$$

with retardation $R_d>1$

$$\frac{C(x,t)}{C_0}=\frac{1}{2}\left[erfc(z_1)+\exp(z_2)erfc(z_3)\right] \quad (6\text{-II})$$

$$z_1=\frac{x-v_R t}{2(D_R t)^{0.5}};\quad z_2=\frac{v_R x}{D_R}=\frac{v_{int}x}{D_m};\quad z_3=\frac{x+v_R t}{2(D_R t)^{0.5}}$$

Peclet number: P_L

$$v_R=v_{int}/R_d,\quad D_R=D_m/R_d$$

$$R_d=1+\frac{(1-n)\rho_s K_d}{n}$$

Two indices as the design parameter for transient time design (1)

Specified leachate concentration

In Eq.(6-II) *C, x* and *t* are variables, but for this specification, *t* is only ***valuable*** and *C* and *x=L*(liner thickness) are *given values* in a design.

Hence the time when the concentration at the liner bottom becomes the specified value (***C_d***) can be calculated with the given conditions, *L, v_{int}, R_d, D_m*. This calculation might be iterated until the calculated time is longer than the design life of the liner (***t_d***) by changing ***L***.

Eq.(6-II) can be rewritten with ***dimensionless parameter***,

$$\frac{C(x,t)}{C_0}=\frac{1}{2}\left[erfc\left(\frac{1-T_R}{2\sqrt{T_R/P_L}}\right)+\exp(P_L)erfc\left(\frac{1+T_R}{2\sqrt{T_R/P_L}}\right)\right] \quad (6\text{-II'})$$

$$T_R=\frac{v_{int}t}{R_d x}=\frac{v_R t}{x}=\frac{v_R t}{L}\Big|_{x=L},\; P_L=\frac{v_{int}x}{D_m}=\frac{v_{int}L}{D_m}\Big|_{x=L} \quad (8)$$

For iteration

Two indices as the design parameter for transient time design (2)

Specified leachate flux

- Advective mass flux:

$$J_A = vC = KiC = n\,v_{int}\,C \quad (1)$$

(6-II)

$$J_A = \frac{1}{2} n v_{\text{int}} C_0 \left[erfc(z_1) + \exp(z_2) erfc(z_3) \right] \quad (9)$$

- Diffusive mass flux

$$J_D = -D_m n \frac{\partial C}{\partial x} \quad (2)$$

(6-II)

Two indices as the design parameter for transient time design (2) contn.1

$$\frac{\partial C}{\partial x} = \frac{1}{2} C_0 \left[\frac{-\exp(-z_1^2)}{\sqrt{\pi D_R t}} - \frac{\exp(z_2)\exp(-z_3^2)}{\sqrt{\pi D_R t}} + \frac{v_{\text{int}}}{D_m} \exp(z_2) \text{erfc}(z_3) \right] \quad (10)$$

$$\exp(z_2)\exp(-z_3^2) = \exp(-z_1^2) \quad (11)$$

$$J_D = -D_m n \frac{\partial C}{\partial x} = \frac{1}{2} D_m n C_0 \left[\frac{2\exp(-z_1^2)}{\sqrt{\pi D_R t}} - \frac{v_{\text{int}}}{D_m} \exp(z_2) erfc(z_3) \right] \quad (12)$$

Two indices as the design parameter for transient time design (2) contn.2

Using dimensionless parameters (P_L,T_R)

$$J_A = \frac{1}{2} n v_{\text{int}} C_0 \left[erfc\left(\frac{1-T_R}{2\sqrt{T_R / P_L}} \right) + \exp(P_L) erfc\left(\frac{1+T_R}{2\sqrt{T_R / P_L}} \right) \right] \quad (9')$$

$$J_D = \frac{1}{2} \frac{D_m}{L} n C_0 \left[\frac{2\exp\left[-\left(\frac{1-T_R}{2\sqrt{T_R / P_L}} \right)^2 \right]}{\sqrt{\frac{\pi T_R}{P_L}}} - P_L \exp(P_L) erfc\left(\frac{1+T_R}{2\sqrt{T_R / P_L}} \right) \right] \quad (12')$$

Two indices as the design parameter for transient time design (2) contn.3

$$J = J_A + J_D = \frac{1}{2} n v_{\text{int}} C_0 (Q_1 + Q_2) + \frac{1}{2} \frac{D_m}{L} n C_0 (Q_3 - P_L Q_2) \quad (13)$$

$$Q_1 = erfc\left(\frac{1-T_R}{2\sqrt{T_R / P_L}} \right); \quad Q_2 = \exp(P_L) erfc\left(\frac{1+T_R}{2\sqrt{T_R / P_L}} \right); \quad Q_3 = \frac{2\exp\left[-\left(\frac{1-T_R}{2\sqrt{T_R / P_L}} \right)^2 \right]}{\sqrt{\frac{\pi T_R}{P_L}}}$$

$$J = \frac{1}{2} \frac{D_m}{L} n C_0 \left[\frac{v_{\text{int}} L}{D_m} (Q_1 + Q_2) + Q_3 - P_L Q_2 \right] \quad (14)$$

P_L

dimensionless flux number: F_N

$$F_N = \frac{JL}{n C_0 D_m} = \frac{1}{2} (P_L Q_1 + Q_3) \quad (15)$$

Two indices as the design parameter for transient time design (2) contn.4

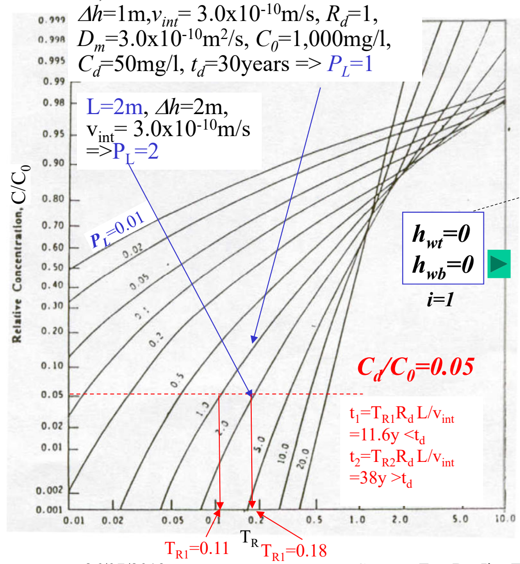
Using the same manner of specific leachate concentration, the thickness of liner can be determined **for specified flux (J_d)** and the design life of the liner (t_d) .

For iteration p15

Iteration to obtain L satisfying specified leachate concentration

ex),L=1m, K=1.0x10^{-10}m/s, n=1/3, Δh=1m,v_{int}= 3.0x10^{-10}m/s, R_d=1, D_m=3.0x10^{-10}m^2/s, C_0=1,000mg/l, C_d=50mg/l, t_d=30years => P_L=1

L=2m, Δh=2m, v_{int}= 3.0x10^{-10}m/s =>P_L=2



Given conditions: design life(t_d), specified and fill leachate concentrations (C_d, C_0), head at top and bottom of liner (h_t,h_b) and R_d, D_m and n for specific clay liner

Step1) assume thickness: L

Step2) calculate v_{int} with L and head dif. betw. top and bottom of the liner

Step3) calculate P_L= $v_{int}L/D_m$

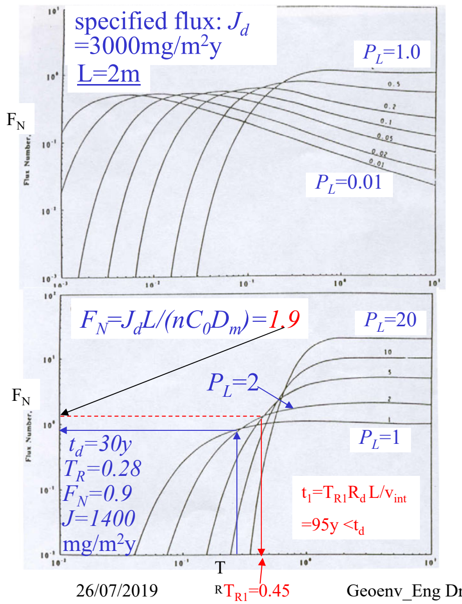
Step4) determine T_R from C_d/C_0, P_L

Step5) calculate t using eq.(8) & R_d

$t > t_d$

OK

Iteration to obtain L satisfying specified leachate flux



given condition: same for specified leachate concentration, except of specified flux: J_d

Step1) assume thickness: L

Step2) calculate v_{int} with L and head dif. betw. top and bottom of the liner

Step3) calculate P_L= $v_{int}L/D_m$ F_N=$J_dL/(nC_0D_m)$

Step4) determine T_R from F_N, P_L,

Step5) calculate t using eq.(8) & R_d

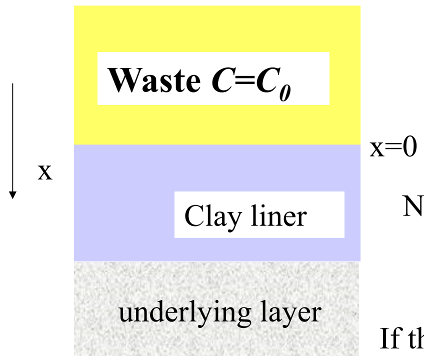
$t > t_d$ → T_R

F_N → $J < J_d$

OK

OK

Boundary Conditions



In the derivation of eq.(6) **no boundary conditions** at bottom of clay line

No effect from the layer beneath the liner

Is it realistic??

It depends on what??

If the underlying layer is high permeable aquifer with relatively high ground water velocity, what is the appropriate B.C. at the bottom?

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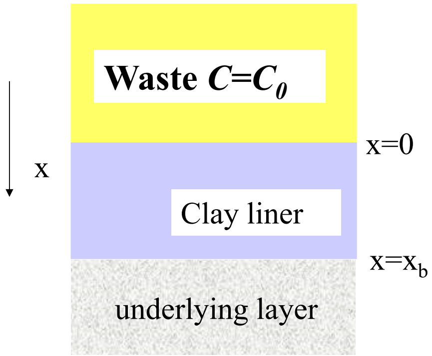
Boundary condition at bottom of clay liner

(1)Fixed concentration

$$C = 0 \ \Big|_{x=x_b}$$

(2)Fixed gradient

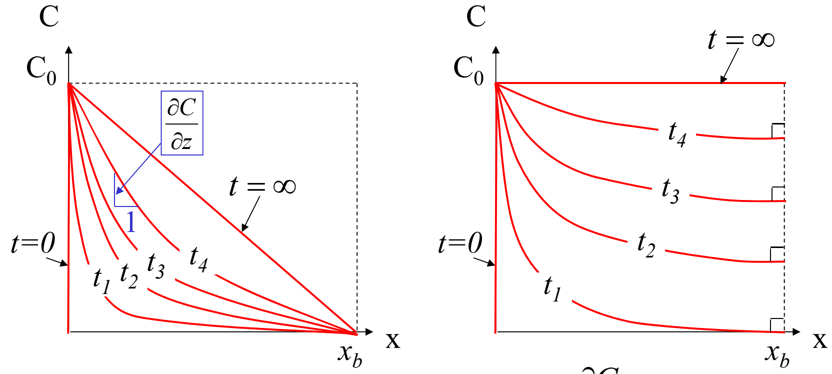
$$\frac{\partial C}{\partial z} = 0 \ \Big|_{x=x_b}$$



Solution of eq. (16) (diffusive equation) for the two B.C.s at base with the common conditions; by separation of variables

$$\frac{\partial C}{\partial t} = D_m \frac{\partial^2 C}{\partial x^2} \quad (16)$$

Variation of concentration profiles for two B.C.s at base of liner



$$C = 0 \ \Big|_{x=x_b} \qquad \frac{\partial C}{\partial z} = 0 \ \Big|_{x=x_b}$$

Which does give higher mass flux at $x=x_b$?

Comparison between two boundary conditions

For diffusion case where v_{int}=0m/s,

Which B.C. does give higher diffusive mass flux at $x=x_b$?

How about advective mass flux?

For A-D case where v_{int}= Ki/n=3x10^{-9}m/s,

Which B.C. gives higher diffusive mass flux at $x=x_b$?

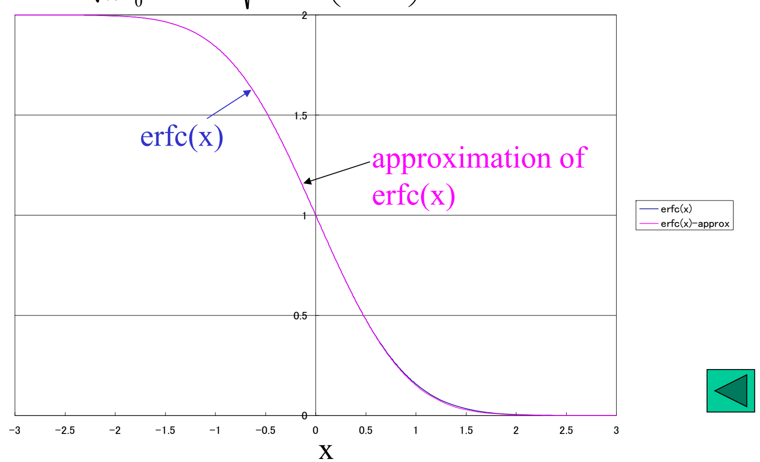
Which B.C. gives higher advective mass flux at $x=x_b$?

Which B.C. gives higher total mass flux at $x=x_b$ at steady state($t=\infty$)?

Complementary error function

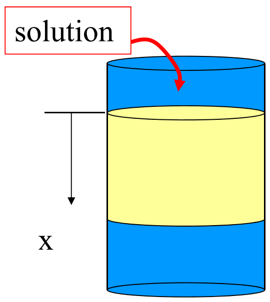
$$erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt \approx \sqrt{1 - \exp\left(\frac{-4x^2}{\pi}\right)}$$

$$erfc(x) = 1 + erf(x) \quad x \le 0$$
$$erfc(x) = 1 - erf(x) \quad x \succ 0$$



Approximate solution for A-D eq.

Column test

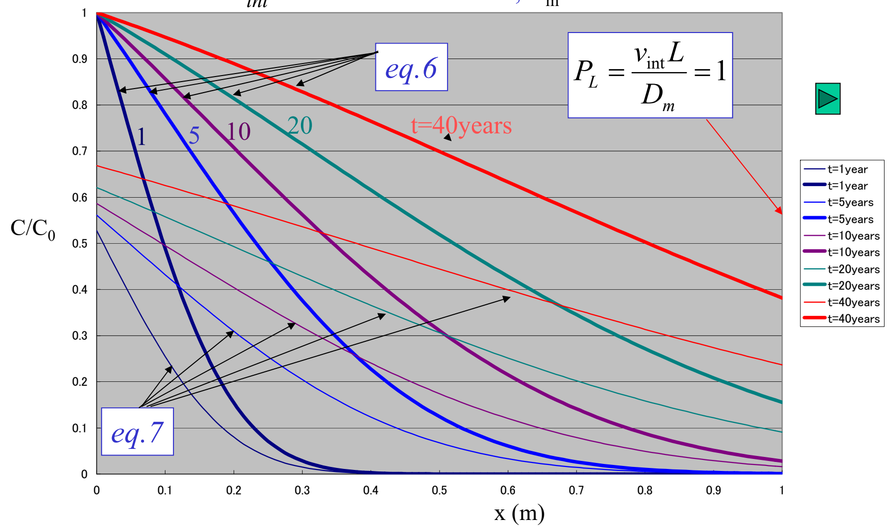


$$C(x,t)=\frac{1}{2}C_0 erfc\left(\frac{R_d x - v_{\text{int}} t}{2(R_d D_{hl} t)^{0.5}}\right) \quad (7)$$

$v = v_{int} \cdot n$

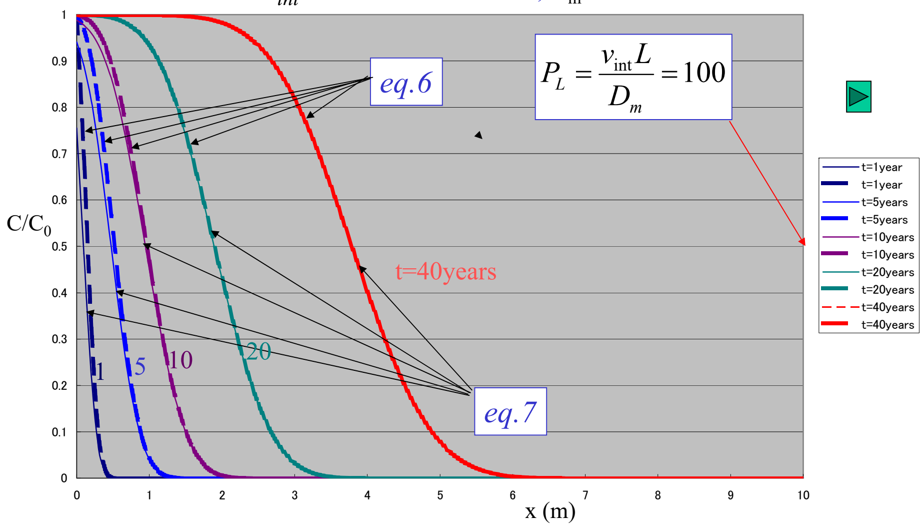
comparison of eqs. (6) and (7): *Δh=L(i=1)*,

L=1m $v_{int} = Ki/n$ = 3.0x10^{-10}m/s, D_m= 3.0x10^{-10}m/s



comparison of eqs. (6) and (7): *Δh=L(i=1)*,

L=10m $v_{int} = Ki/n$ = 3.0x10^{-9}m/s, D_m= 3.0x10^{-10}m/s



Effect of seepage flow in aquifer underneath clay liner

Rowe et al. (1995)

2D analysis using **PLLUTE**.