1D Transport Equation with Analytical Solution

Initial Condition

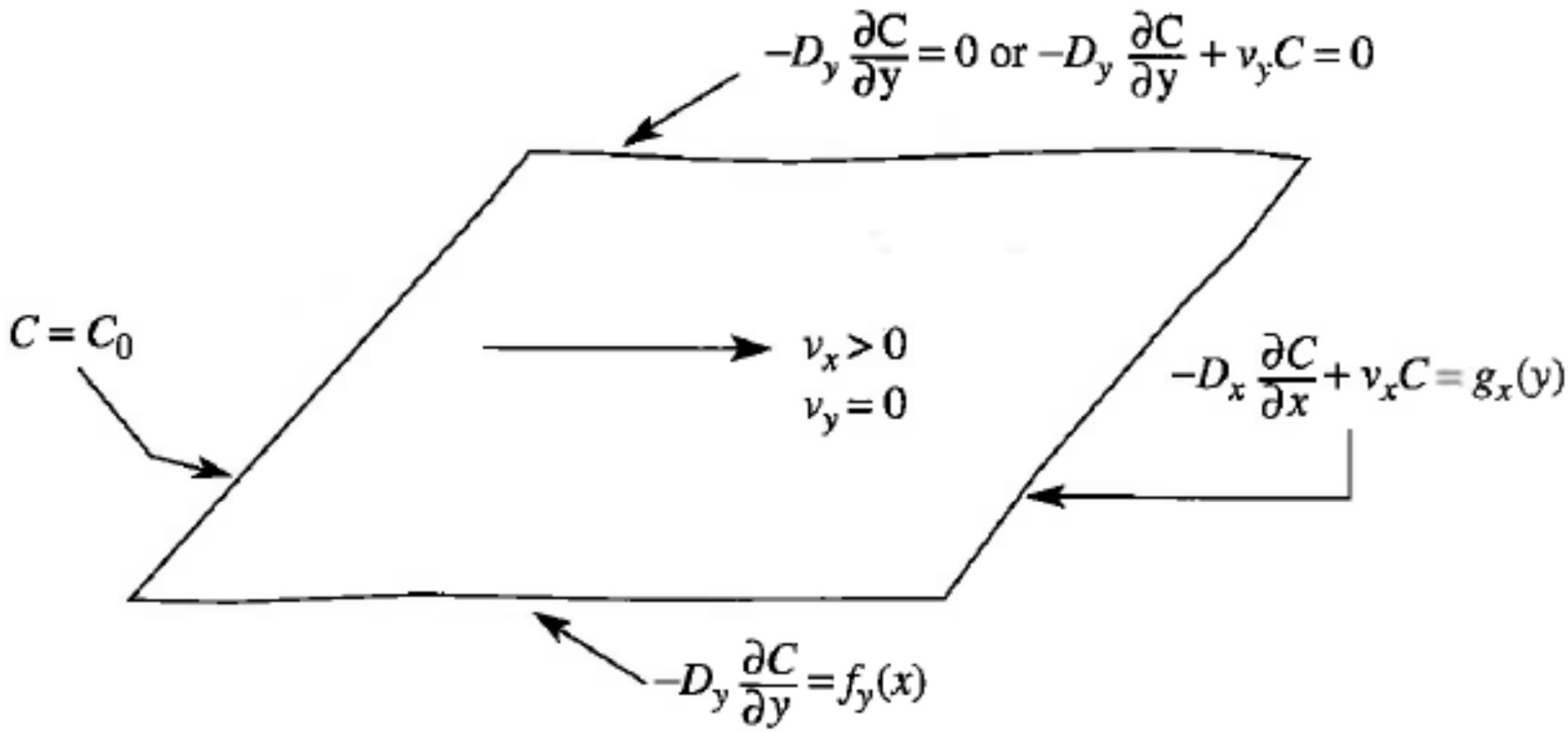
$$C(x,y,z,t)=C_0(x,y,z,t)$$

- When we do flow modeling, we always run the flow system as steady state, and use the resulting head as the initial condition.
- Can we do this for transport modeling?

Initial Condition

- For some simulation, we can use the initial condition of $C(x,y,z,t)=0$, if the concentration is zero initially, e.g., for a landfill leaching problem.
- In practice, it is always difficult to know the initial condition.
- Many methods have been developed to either estimate initial condition or correct the error in initial condition during model run (e.g., data assimilation approaches).

What are the physical explanations for the BCs below?



ADE

$$\frac{\partial c}{\partial t} = -\mathbf{v}.\nabla c + \nabla.(\mathbf{D}\nabla c)$$

$$\nabla = \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{bmatrix}$$

3D mass transport of conservative solute

$$\frac{\partial C}{\partial t} = -v_x \frac{\partial C}{\partial x} + D_L \frac{\partial^2 C}{\partial x^2}$$

$$D_L = \alpha_L v_x + D^*$$

1D Mass transport in a homogenous isotopic medium such that the average linear velocity v_x is uniform in space and D_x does not vary in space

$$\frac{\partial C}{\partial t} = -v_x \frac{\partial C}{\partial x} + D_L \frac{\partial^2 C}{\partial x^2} + D_T \frac{\partial^2 C}{\partial y^2}$$

2D flow with direction of flow parallel to x-axis

Analytical Solutions of ADE

1D step change in concentration (First-type BC)

$$\frac{\partial C}{\partial t} = -v_x \frac{\partial C}{\partial x} + D_L \frac{\partial^2 C}{\partial x^2}$$

$$C(x,0) = 0 \qquad x \ge 0 \quad \text{Initial condition}$$

$$\left.\begin{array}{ll} C(0,t) = C_0 & t \ge 0 \\ C(\infty,0) = 0 & t \ge 0 \end{array}\right\} \text{Boundary conditions}$$

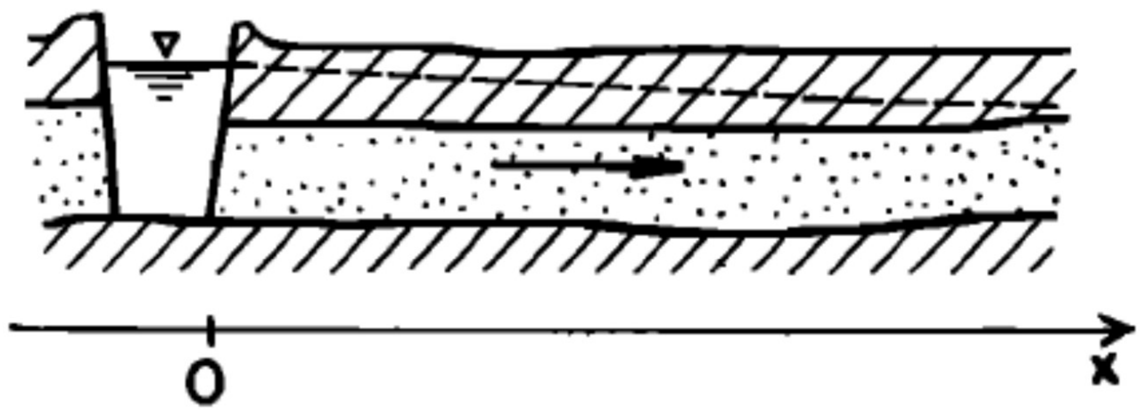


Fig. 1. Natural conditions for uniform flow in a one-dimensional semi-infinite domain. [Sauty, 1980]

Analytical Solutions of ADE

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$$\left.\begin{aligned} C(0,t) &= C_0 \qquad t \geq 0 \\ C(\infty,0) &= 0 \qquad t \geq 0 \end{aligned}\right\} \text{Boundary conditions}$$

$$C = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{L - v_x t}{2\sqrt{D_L t}}\right) + \exp\left(\frac{v_x L}{D_L}\right)\operatorname{erfc}\left(\frac{L + v_x t}{2\sqrt{D_L t}}\right)\right]$$

$$C_R(t_R, P_e) = \frac{1}{2}\left\{\operatorname{erfc}\left[\left(\frac{P_e}{4t_R}\right)^{1/2}(1 - t_R)\right] + \exp(P_e)\operatorname{erfc}\left[\left(\frac{P_e}{4t_R}\right)^{1/2}(1 + t_R)\right]\right\}$$

$P_e = v_x L / D_L \qquad C_R = C / C_0 \qquad t_R = v_x t / L$

[Ogata and Banks, 1961]

Peclet number when flow distance *L* is chose as the reference length

Analytical Solutions of ADE

1D continuous injection into a flow field (Second-Type BC)

$$\frac{\partial C}{\partial t} = -v_x \frac{\partial C}{\partial x} + D_L \frac{\partial^2 C}{\partial x^2}$$

$C(x,0) = 0 \quad -\infty < x < +\infty$ Initial condition

$$\left.\begin{aligned} &\int_{-\infty}^{+\infty} n_e C(x,t)\,dx = C_0 n_e v_x t \quad t > 0 \\ &C(\infty,t) = 0 \quad t \geq 0 \end{aligned}\right\} \text{Boundary conditions}$$

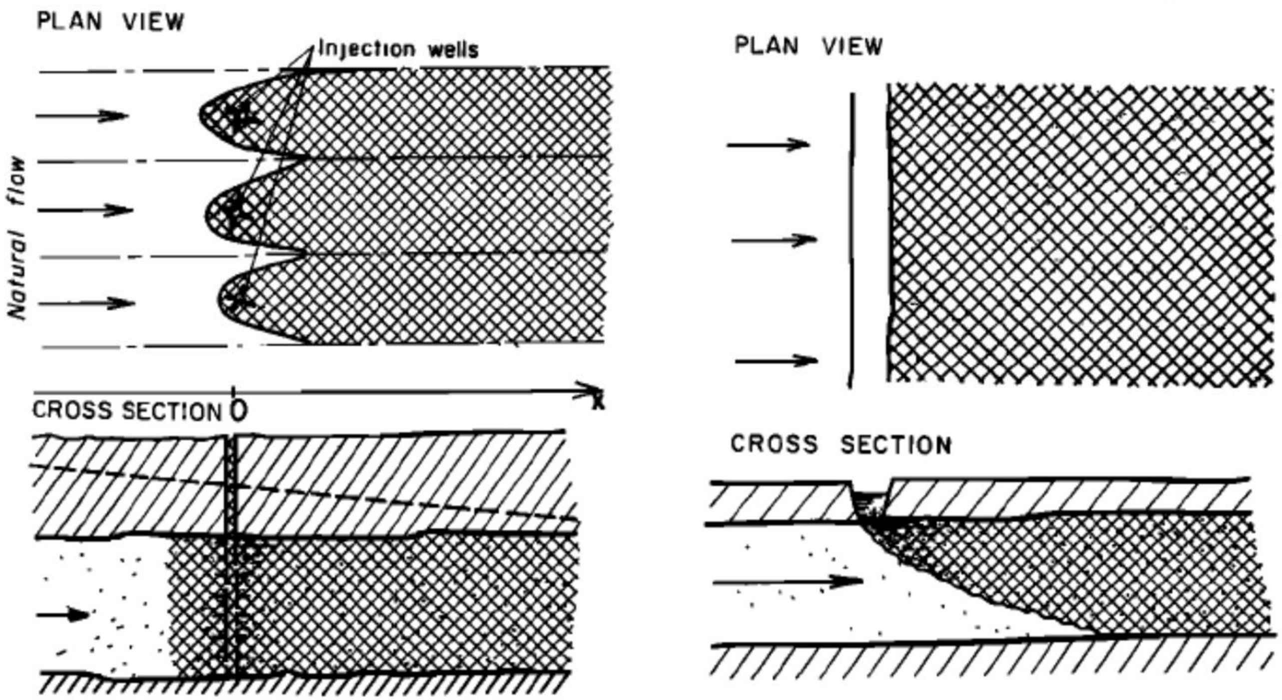

Fig. 2. Continuous injection into an aquifer from (*a*) a system of wells or (*b*) a surface canal.

[Sauty, 1980]

Analytical Solutions of ADE

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$$C_R(t_R, P_e) = \frac{1}{2}\left\{\operatorname{erfc}\left[\left(\frac{P_e}{4t_R}\right)^{1/2}(1 - t_R)\right] - \exp(P_e)\operatorname{erfc}\left[\left(\frac{P_e}{4t_R}\right)^{1/2}(1 + t_R)\right]\right\}$$

$P_e = v_x L / D_L \qquad C_R = C / C_0 \qquad t_R = v_x t / L$ [Sauty, 1980]

Peclet number when flow distance *L* is chosen as the reference length

Analytical Solutions of ADE

Approximate solution

$$C = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{L - v_x t}{2\sqrt{D_L t}}\right)\right]$$

$$C_R(t_R, P_e) = \frac{1}{2}\left\{\operatorname{erfc}\left[\left(\frac{P_e}{4t_R}\right)^{1/2}(1 - t_R)\right]\right\}$$

$$P_e = v_x L / D_L \quad C_R = C / C_0 \quad t_R = v_x t / L$$

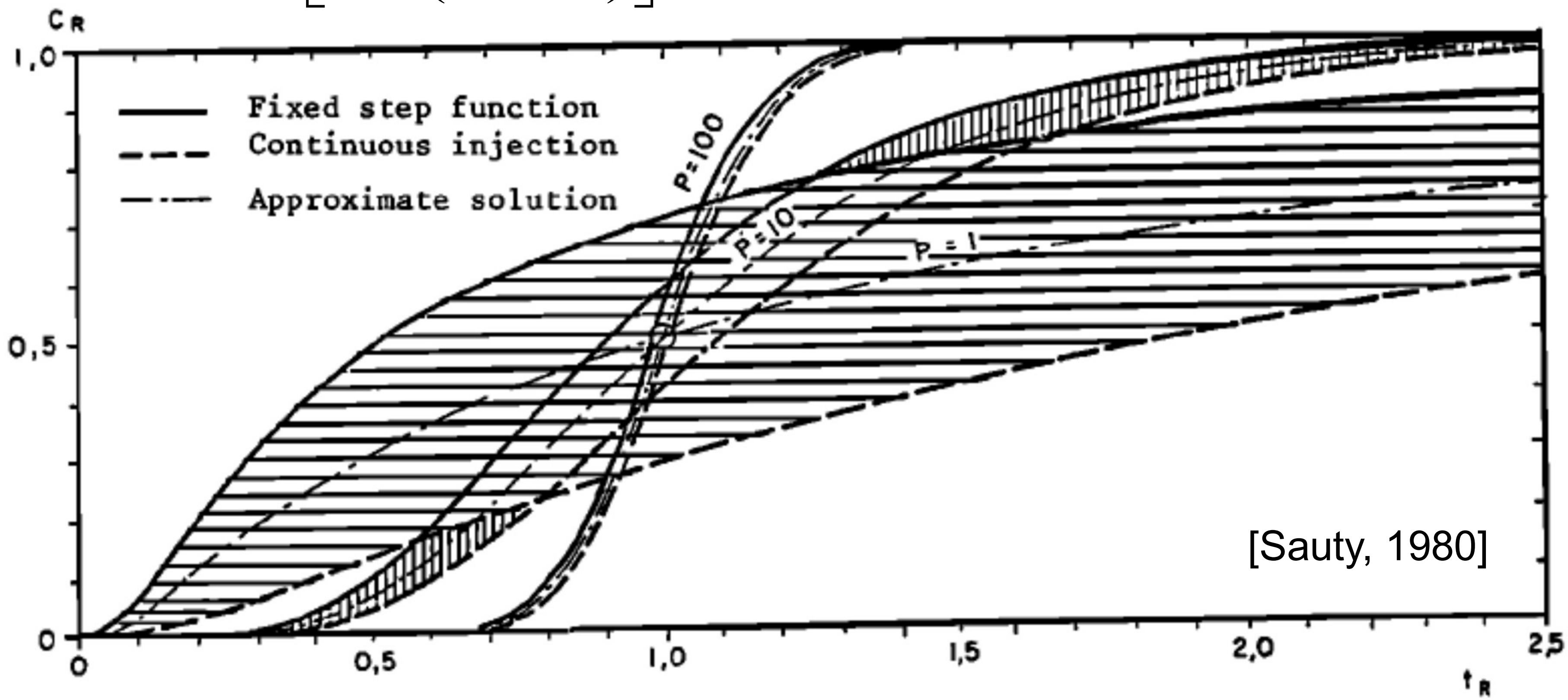

Fig. 3. Type curves for continuous tracer injection in a monodimensional uniform flow field.

Class Exercise I

The Happy Pickle Factor makes pickles in large wooden vats. One of the vats has been leaking brine directly into the water table. The concentration of chloride in the brine is 1575 mgL-1. The flow in the aquifer that receives the brine is essentially 1D with the following characteristics

Hydraulic conductivity = 2.93x10-4 m/s

Hydraulic gradient = 0.00678

Effective porosity=0.259

Estimated chloride diffusion coefficient = 2x10-9 m2/s

Calculate the concentration of chloride above any background value at a distance 125 m from the leaking vat 0.5 years after the leak began.

<u>Notes</u>

(1) You can use this equation $\alpha_L = 0.83(\log L)^{2.414}$ to estimate the longitudinal dispersivity.

(2) To evaluate the complementary error function use (i) tables (from internet, book, etc.), (ii) MATLAB or Excel *erfc*(), (iii) $erfc(B) = 1 - erf(B)$ such that $erf(B) = \sqrt{1 - \exp(-4B^2/\pi)}$ or (iv) your calculator.

$$C = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{L - v_x t}{2\sqrt{D_L t}}\right) - \exp\left(\frac{v_x L}{D_L}\right)\operatorname{erfc}\left(\frac{L + v_x t}{2\sqrt{D_L t}}\right)\right]$$

Class Exercise 1

(1) Calculate v_x

$$v_x = \frac{K}{n_e}\frac{dh}{dl} \qquad v_x = 7.67\times10^{-6} m/s$$

(2) Estimate the hydrodynamic dispersion coefficient

$$D_L = \alpha_L v_x + D^* \qquad \alpha_L = 0.83(\log L)^{2.414} \qquad \alpha_L = 4.96m$$

$$D_L = 3.8\times10^{-5} + 2\times10^{-9} = 3.8\times10^{-5} m^2/s$$

(3) Express time in seconds

$$0.5\times365\times24\times3600 = 1.578\times10^{7} s$$

(4) Substitute into the analytical solution

$$C = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{L - v_x t}{2\sqrt{D_L t}}\right) - \exp\left(\frac{v_x L}{D_L}\right)\operatorname{erfc}\left(\frac{L + v_x t}{2\sqrt{D_L t}}\right)\right]$$

$$C = \frac{1575}{2}\left[\operatorname{erfc}(0.0816) - \exp(25.23)\operatorname{erfc}(5.02)\right]$$

$$= \frac{1575}{2}\left[0.908 - 0.109\right] = 628.934 mg/L$$

$$C = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{L - v_x t}{2\sqrt{D_L t}}\right)\right]$$

$$C = \frac{1575}{2}\left[\operatorname{erfc}(0.0816)\right]$$

$$= \frac{1575}{2}\left[0.908\right] = 715 mg/L$$

Analytical Solutions of ADE

1D slug injection into the flow field

$$\frac{\partial C}{\partial t} = -v_x \frac{\partial C}{\partial x} + D_L \frac{\partial^2 C}{\partial x^2}$$

$$C(x,0) = M/A_e.\delta(x)$$

$\delta(x)$ Dirac function: $\delta(x) = \lim_{m\to 0} \delta m(x)$

$$\delta m(x) = 1/m \quad x \in (0,m)$$

$$\delta m(x) = 0 \qquad x > m$$

$$C(\pm\infty, t) = 0 \qquad t \geq 0$$

$$C_R(t_R, P_e) = \frac{E}{\sqrt{t_R}} \exp\left[-\frac{P_e}{4t_R}(1-t_R)^2\right]$$

$$E = \sqrt{t_{R\max}} \exp\left[\frac{P_e}{4t_{R\max}}(1-t_R \max)^2\right] \qquad t_{R\max} = \sqrt{1+P_e^{-2}} - P_e^{-1}$$

$$P_e = v_x L/D_L \qquad C_R = C/C_{\max} \qquad t_R = v_x t/L$$

[Sauty, 1980]

Class Exercise 2

- For 1D slug injection into the flow field

  What will happen to (i) peak concentration C_{max} and (ii) break through curve when we
  (1) increase the Peclet number? (Try Pe=1,10 and 100)
  (2) use a non-conservative tracer? (Try R=1.1)

$$C_R(t_R, P_e) = \frac{E}{\sqrt{t_R}} \exp\left[-\frac{P_e}{4t_R}(1 - t_R)^2 \right]$$

$$E = \sqrt{t_{R\max}} \exp\left[\frac{P_e}{4t_{R\max}}(1 - t_R \max)^2 \right] \qquad t_{R\max} = \sqrt{1 + P_e^{-2}} - P_e^{-1}$$

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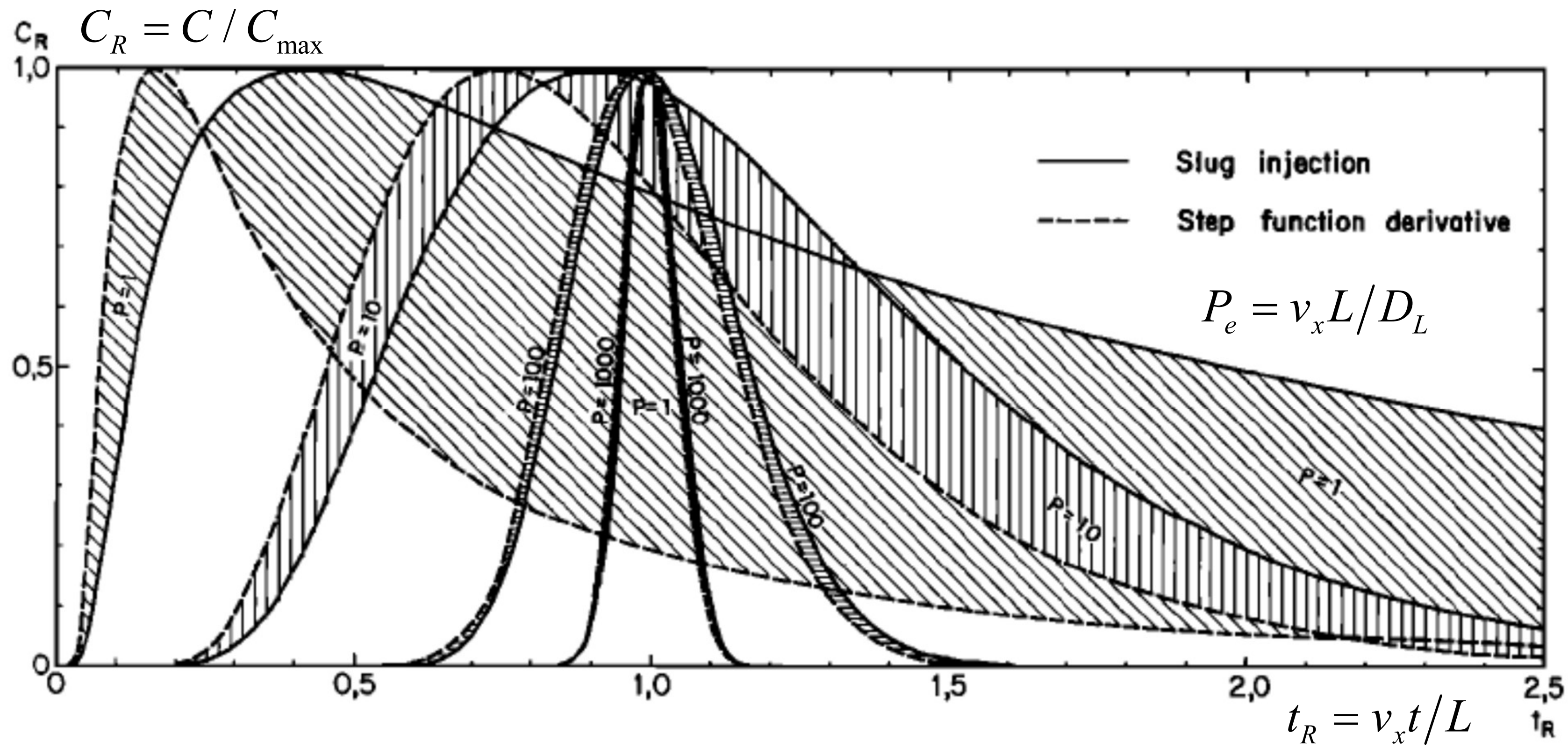

Fig. 4. Type curves for slug injection compared with the derivative of the fixed step function solution.

Analytical Solutions of ADE

2D slug injection into a uniform 2D flow field

Tracer with concentration C_0 is 2D flow field over area A at point (x_0,y_0) the concentration at a point (x,y) at time t after the injection is

$$C(x,y,t) = \frac{C_0 A}{4\pi t\sqrt{D_L D_T}} \exp\left[-\frac{((x-x_0)-v_x t)^2}{4D_L t} - \frac{(y-y_0)^2}{4D_T t} \right]$$

[Fetter, 1993]

The maximum concentration of contaminant is found at the center of the plume (center of mass)

$$C_{\max} = \frac{C_0 A}{4\pi t\sqrt{D_L D_T}}$$

and the distribution of the plume follow a normal distribution such that

$$\sigma_x = \sqrt{2D_L t} \qquad \sigma_y = \sqrt{2D_T t}$$

By definition 99.7% of the mass will be contained within the 3σ area away from the center of mass of the plume. Thus the plume can be defined by the location of the center of mass, $3\sigma_x$ and $3\sigma_y$

Class Exercise 3

A truck carrying a dilute brine with 2130 mg/L chloride (from a cleanup of a pond containing waste from a producing oil well) overturns and spills the dilute brine over area of 455 square feet. The underlying thin aquifer has an average linear groundwater velocity of 1.23 ft/day.

- Where would the center of mass of the plume be in 133 day?
- What would be the maximum concentration?
- How far beyond and to the side of the center of mass would the plume spread?

$$C_{\max} = \frac{C_0 A}{4\pi t\sqrt{D_L D_T}} \qquad \sigma_x = \sqrt{2D_L t} \qquad \sigma_y = \sqrt{2D_T t}$$

$$\alpha_L = 0.83(\log L)^{2.414}$$

$$D_L = \alpha_L v_x + D^*$$

Class Exercise 3

(1) The plume will be advected by the flowing groundwater so the center of the mass would be at:

$$x = v_x t \qquad x = 1.23\,ft/d \times 133d = 164\,ft$$

(2) The maximum contraction of the center of mass

$$\alpha_L = 0.83(\log L)^{2.414} = 5.66\,ft \qquad D_L = \alpha_L v_x = 6.96\,ft^2/d$$

and we can assume D_T to be 10% of D_L

$$D_T = 0.696\,ft^2/d$$

and then substitute to get the maximum concentration

$$C_{\max} = \frac{C_0 A}{4\pi t\sqrt{D_L D_T}} = \frac{2130mg/L \times 455\,ft^2}{4\pi \times 133d\sqrt{6.96\,ft^2/d \times 0.696\,ft^2/d}} = 263mg/L$$

(3) The size of the plume can be determined from the standard deviations

$$\sigma_x = \sqrt{2D_L t} = 43\,ft \qquad \sigma_y = \sqrt{2D_L t} = 13.6\,ft$$

The leading edge is $3\sigma_x$ feet ahead of the center of mass (129 feet) and the plume has spread out $3\sigma_y$ feet on either side of the center of mass (40.8 feet)