

ATRANS

**Analytical Solutions for
Three-Dimensional Solute Transport
from a Patch Source**

Appendix A: Derivations of the solutions

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1. Governing Equation

Starting from the statement of mass conservation:

$$\theta R \frac{\partial c}{\partial t} = -q \frac{\partial c}{\partial x} + \theta D_x \frac{\partial^2 c}{\partial x^2} + \theta D_y \frac{\partial^2 c}{\partial y^2} + \theta D_z \frac{\partial^2 c}{\partial z^2} - \theta R \lambda c$$

divide through by θ :

$$R \frac{\partial c}{\partial t} = -v \frac{\partial c}{\partial x} + D_x \frac{\partial^2 c}{\partial x^2} + D_y \frac{\partial^2 c}{\partial y^2} + D_z \frac{\partial^2 c}{\partial z^2} - R \lambda c$$

where: $V = \frac{q}{\theta}$ = average linear ground-water velocity

Dividing through by R yields:

$$\boxed{\frac{\partial c}{\partial t} = -v' \frac{\partial c}{\partial x} + D'_x \frac{\partial^2 c}{\partial x^2} + D'_y \frac{\partial^2 c}{\partial y^2} + D'_z \frac{\partial^2 c}{\partial z^2} - \lambda c}$$

where: $v' = \frac{v}{R}$; $D'_x = \frac{D_x}{R}$; $D'_y = \frac{D_y}{R}$; $D'_z = \frac{D_z}{R}$

Initial and Boundary Conditions

- Initial conditions: $c(x, y, z, 0) = 0.0$

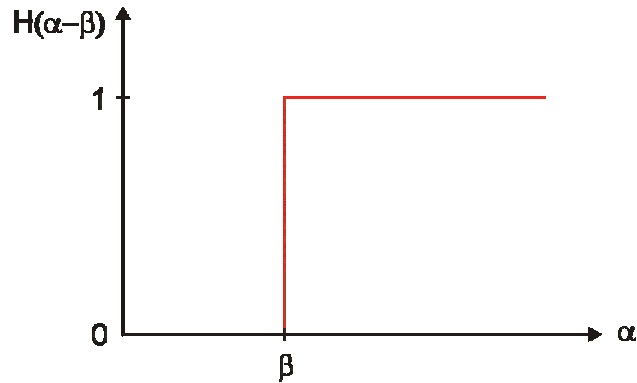
- Boundary conditions:

$$\begin{aligned} \text{i)} \quad x: & \begin{cases} c(0, y, z, t) = c_0(t) [H(y + y_0) - H(y - y_0)] [H(z - z_1) - H(z - z_2)] \\ c(\infty, y, z, t) = 0 \end{cases} \\ \text{ii)} \quad y: & \begin{cases} c(x, -\infty, z, t) = 0 \\ c(x, \infty, z, t) = 0 \end{cases} \\ \text{iii)} \quad z: & \begin{cases} \frac{\partial c}{\partial z}(x, y, 0, t) = 0 \\ \frac{\partial c}{\partial z}(x, y, B, t) = 0 \end{cases} \end{aligned}$$

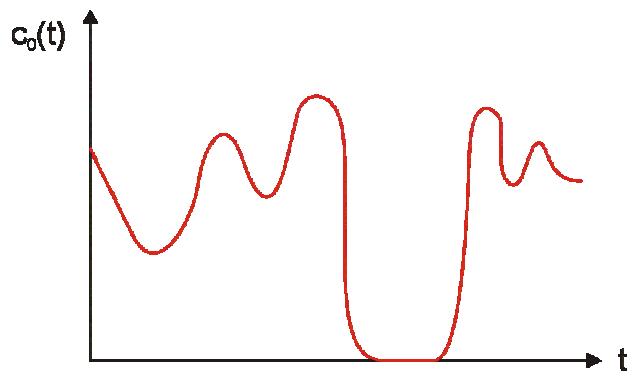
Interpretation of the inflow boundary conditions

The function $H(\alpha - \beta)$ is the Heaviside step function, defined as:

$$\begin{aligned} H(\alpha - \beta) &= 0 \text{ if } \alpha < \beta \\ &= 1 \text{ if } \alpha > \beta \end{aligned}$$



The function $c_0(t)$ represent an arbitrary time-varying concentration history at the patch on the inflow boundary.



2. Green's Function: Solution for a Point Boundary Condition of Time-Varying Concentration

The solution for a general time-varying boundary condition is derived using a Green's function approach. The general solution is expressed as:

$$c(x, y, z, t) = \int_0^t G(x, y, z, t - \tau) c_0(\tau) d\tau$$

In the general formula, G represents the Green's function, which is the solution for a pulse boundary condition..

The boundary condition for the Green's function solution is:

$$c(0, y, z, t) = c_0(t) \delta(y - y') \delta(z - z')$$

1) Applying the Laplace transform w.r.t. time:

$$\left[p\bar{c} - \cancel{c(x, y, z, 0)} \right] + v' \frac{\partial \bar{c}}{\partial x} - D_x' \frac{\partial^2 \bar{c}}{\partial x^2} - D_y' \frac{\partial^2 \bar{c}}{\partial y^2} - D_z' \frac{\partial^2 \bar{c}}{\partial z^2} + \lambda \bar{c} = 0$$

Substituting in the initial conditions:

$$p\bar{c} + v' \frac{\partial \bar{c}}{\partial x} - D_x' \frac{\partial^2 \bar{c}}{\partial x^2} - D_y' \frac{\partial^2 \bar{c}}{\partial y^2} - D_z' \frac{\partial^2 \bar{c}}{\partial z^2} + \lambda \bar{c} = 0$$

The transformed boundary conditions are:

$$\bar{c}(0, y, z, p) = \bar{c}_0(p) \delta(y - y') \delta(z - z')$$

$$\bar{c}(\infty, y, z, p) = 0$$

$$\bar{c}(x, -\infty, z, p) = 0$$

$$\bar{c}(x, \infty, z, p) = 0$$

$$\frac{\partial \bar{c}}{\partial z}(x, y, 0, p) = 0$$

$$\frac{\partial \bar{c}}{\partial z}(x, y, B, p) = 0$$

2) Applying the Fourier exponential transform w.r.t. y :

$$p\bar{c} + v' \frac{\partial \bar{c}}{\partial x} - D_x' \frac{\partial^2 \bar{c}}{\partial x^2} + D_y' \alpha_1^2 \bar{c} - D_z' \frac{\partial^2 \bar{c}}{\partial z^2} + \lambda \bar{c} = 0$$

The transformed boundary conditions are:

$$\bar{c}(0, \alpha, z, p) = \bar{c}_0(p) \exp\{-i\alpha_1 y'\} \delta(z - z')$$

$$\bar{c}(\infty, \alpha, z, p) = 0$$

$$\frac{\partial \bar{c}}{\partial z}(x, \alpha, 0, p) = 0$$

$$\frac{\partial \bar{c}}{\partial z}(x, \alpha, B, p) = 0$$

3) Applying the finite Fourier cosine transform w.r.t. z :

$$p\bar{c} + v' \frac{\partial \bar{c}}{\partial x} - D_x' \frac{\partial^2 \bar{c}}{\partial x^2} + D_y' \alpha_1^2 \bar{c} - D_z' \left[(-1)^n \frac{\partial \bar{c}}{\partial z}(0) - \frac{\partial \bar{c}}{\partial z}(B) - \frac{n^2 \pi^2}{B^2} \bar{c} \right] + \lambda \bar{c} = 0$$

Substituting in the boundary conditions:

$$p\bar{c} + v' \frac{\partial \bar{c}}{\partial x} - D_x' \frac{\partial^2 \bar{c}}{\partial x^2} + D_y' \alpha_1^2 \bar{c} + D_z' \frac{n^2 \pi^2}{B^2} \bar{c} + \lambda \bar{c} = 0$$

The transformed boundary conditions are:

$$\bar{c}(0, \alpha, n, p) = \bar{c}_0(p) \exp\{-i\alpha_1 y'\} \cos\left(\frac{n\pi z'}{B}\right)$$

$$\bar{c}(\infty, \alpha, n, p) = 0$$

4) The transformed governing equation can be written as:

$$\frac{\partial^2 \bar{c}}{\partial x^2} - \frac{v'}{D_x'} \frac{\partial \bar{c}}{\partial x} - \frac{P}{D_x'} \bar{c} = 0$$

where: $P = p + \lambda + D_y' \alpha_1^2 + D_z' \frac{n^2 \pi^2}{B^2}$

The general solution of the transformed governing equation is:

$$\bar{c} = A \exp\{r^- x\} + B \exp\{r^+ x\}$$

$$\text{where: } r^\pm = \frac{v'}{2D_x'} \pm \sqrt{\left(\frac{v'}{2D_x'}\right)^2 + \frac{P}{D_x'}} = \frac{v'}{2D_x'} \pm \frac{1}{\sqrt{D_x'}} \sqrt{\frac{v'^2}{4D_x'} + P}$$

The coefficients A and B are evaluated by considering the boundary conditions.

a. $x \rightarrow \infty$:

Since the solution is bounded, we must have:

$$B = 0$$

b. $x = 0$:

The general solution reduces to:

$$\bar{c} = A \exp\{r^- x\}$$

Evaluating the boundary condition:

$$\begin{aligned} \bar{c}(x, \alpha, n, p) &= A \exp\{r^- x\} \Big|_{x=0} \\ &= \bar{c}_0(p) \exp\{-i\alpha_1 y'\} \cos\left(\frac{n\pi z'}{B}\right) \end{aligned}$$

$$\therefore A = \bar{c}_0(p) \exp\{-i\alpha_1 y'\} \cos\left(\frac{n\pi z'}{B}\right)$$

Therefore, the transformed solution is:

$$\bar{c} = \bar{c}_0(p) \exp\{-i\alpha_1 y'\} \cos\left(\frac{n\pi z'}{B}\right) \exp\left\{\frac{v' x}{2D_x'}\right\} \exp\left\{-\left(\frac{v'^2}{4D_x'} + P\right)^{\frac{1}{2}} \frac{x}{\sqrt{D_x'}}\right\}$$

5) Applying the inverse Laplace transform:

$$\begin{aligned} \bar{c} &= L^{-1} \left[\bar{c} \right] \\ &= \exp \{ -i\alpha_1 y' \} \cos \left(\frac{n\pi z'}{B} \right) \exp \left\{ \frac{v'x}{2D_x'} \right\} L^{-1} \left[\bar{c}_0(p) \exp \left\{ - \left(\frac{v'^2}{4D_x'} + P \right)^{\frac{1}{2}} \frac{x}{\sqrt{D_x'}} \right\} \right] \end{aligned}$$

The inverse Laplace transform is evaluated using the convolution theorem:

$$L^{-1} \left[\bar{f}(p) \cdot \bar{g}(p) \right] = \int_0^t f(\tau) g(t-\tau) d\tau$$

Letting:

$$\begin{aligned} \bar{f}(p) &= \bar{c}_0(p) \rightarrow f(t) = c_0(t) \\ \bar{g}(p) &= \exp \left\{ - \left(\frac{v'^2}{4D_x'} + P \right)^{\frac{1}{2}} \frac{x}{\sqrt{D_x'}} \right\} \end{aligned}$$

The second inverse is evaluated using the shift theorem:

$$g(t) = \exp \left\{ - \left[\left(\lambda + D_y' \alpha_1^2 + D_z' \frac{n^2 \pi^2}{B^2} \right) + \frac{v'^2}{4D_x'} \right] t \right\} L^{-1} \left[\exp \left\{ - \sqrt{p} \frac{x}{\sqrt{D_x'}} \right\} \right]$$

The inverse Laplace transform is given by Churchill (1972) A.2 #82:

$$\begin{aligned} L^{-1} [\cdot] &= \frac{x}{2\sqrt{\pi D_x'}} t^{-\frac{3}{2}} \exp \left\{ - \frac{x^2}{4D_x' t} \right\} \\ \therefore g(t) &= \frac{x}{2\sqrt{\pi D_x'}} t^{-\frac{3}{2}} \exp \left\{ - \left[\left(\lambda + D_y' \alpha_1^2 + D_z' \frac{n^2 \pi^2}{B^2} \right) + \frac{v'^2}{4D_x'} \right] t \right\} \exp \left\{ - \frac{x^2}{4D_x' t} \right\} \end{aligned}$$

Substituting into the convolution integral yields:

$$\begin{aligned} \bar{c} &= \exp\{-i\alpha_1 y'\} \cos\left(\frac{n\pi z'}{B}\right) \exp\left\{\frac{v'x}{2D_x'}\right\} \frac{x}{2\sqrt{\pi D_x'}} \int_0^t c_0(\tau)(t-\tau)^{-\frac{3}{2}} \\ &\cdot \exp\left\{-\left[\left(\lambda + D_y'\alpha_1^2 + D_z'\frac{n^2\pi^2}{B^2}\right) + \frac{v'^2}{4D_x'}\right](t-\tau) - \frac{x^2}{4D_x'(t-\tau)}\right\} d\tau \end{aligned}$$

6) Applying the inverse Fourier exponential transform:

$$\begin{aligned} \bar{c} &= \mathfrak{F}_e^{-1}[\bar{c}] \\ &= \frac{x}{2\sqrt{\pi D_x'}} \cos\left(\frac{n\pi z'}{B}\right) \exp\left\{\frac{v'x}{2D_x'}\right\} \mathfrak{F}_e^{-1}\left[\exp\{-i\alpha_1 y'\} \int_0^t c_0(t)(t-\tau)^{-\frac{3}{2}}\right. \\ &\cdot \left.\exp\left\{-\left[\left(\lambda + D_y'\alpha_1^2 + D_z'\frac{n^2\pi^2}{B^2}\right) + \frac{v'^2}{4D_x'}\right](t-\tau) - \frac{x^2}{4D_x'(t-\tau)}\right\} d\tau\right] \end{aligned}$$

Re-arranging the order of operations we can write:

$$\begin{aligned} \bar{c} &= \frac{x}{2\sqrt{\pi D_x'}} \cos\left(\frac{n\pi z'}{B}\right) \exp\left\{\frac{v'x}{2D_x'}\right\} \int_0^t c_0(\tau)(t-\tau)^{-\frac{3}{2}} \\ &\cdot \exp\left\{-\left[\left(\lambda + D_z'\frac{n^2\pi^2}{B^2}\right) + \frac{v'^2}{4D_x'}\right](t-\tau) - \frac{x^2}{4D_x'(t-\tau)}\right\} \\ &\cdot \mathfrak{F}_e^{-1}\left[\exp\{-i\alpha_1 y'\} \exp\{-D_y'\alpha_1^2(t-\tau)\}\right] d\tau \end{aligned}$$

The inverse can be evaluated using the convolution theorem:

$$\mathfrak{F}_e^{-1}[f(\alpha_1) \cdot \bar{g}(\alpha_1)] = \int_{-\infty}^{\infty} f(\xi) g(y-\xi) d\xi$$

Let:

$$\bar{f}(\alpha_1) = \exp\{-i\alpha_1 y'\} \rightarrow f(y) = \delta(y - y')$$

$$\bar{g}(\alpha_1) = \exp\{-\alpha_1^2 D_y'(t-\tau)\} \rightarrow g(y) = \frac{1}{2\sqrt{\pi D_y'(t-\tau)}} \exp\left\{-\frac{y^2}{4D_y'(t-\tau)}\right\}$$

Therefore, the inverse is:

$$\mathfrak{F}_e^{-1}[\cdot] = \int_{-\infty}^{\infty} \delta(\xi - y') \frac{1}{2\sqrt{\pi D'_y(t-\tau)}} \exp\left\{-\frac{(y-\xi)^2}{4D'_y(t-\tau)}\right\} d\xi$$

Noting the properties of the Dirac δ function, the inverse reduces:

$$\mathfrak{F}_e^{-1}[\cdot] = \frac{1}{2\sqrt{\pi D'_y(t-\tau)}} \exp\left\{-\frac{(y-y')^2}{4D'_y(t-\tau)}\right\}$$

Finally, substituting into the solution for \bar{c} yields:

$$\begin{aligned} \bar{c} &= \frac{x}{4\pi\sqrt{D'_x D'_y}} \cos\left(\frac{n\pi z'}{B}\right) \exp\left\{\frac{v'x}{2D'_x}\right\} \int_0^t c_0(\tau) \frac{1}{(t-\tau)^2} \\ &\cdot \exp\left\{-\left[\left(\lambda + D'_z \frac{n^2\pi^2}{B^2}\right) + \frac{v'^2}{4D'_x}\right](t-\tau) - \frac{x^2}{4D'_x(t-\tau)} - \frac{(y-y')^2}{4D'_y(t-\tau)}\right\} d\tau \end{aligned}$$

7) Applying the inverse Fourier cosine transform:

$$\begin{aligned} c &= \mathfrak{F}_c^{-1}[\bar{c}] \\ &= \frac{\bar{c}(n=0)}{B} + \frac{2}{B} \sum_{n=1}^{\infty} \bar{c}(n) \cos\left(\frac{n\pi z}{B}\right) \end{aligned}$$

$$\begin{aligned} \therefore c &= \frac{x}{4\pi B\sqrt{D'_x D'_y}} \exp\left\{\frac{v'x}{2D'_x}\right\} \int_0^t c_0(\tau) \frac{1}{(t-\tau)^2} \\ &\cdot \exp\left\{-\lambda(t-\tau) - \frac{v'^2(t-\tau)}{4D'_x} - \frac{x^2}{4D'_x(t-\tau)} - \frac{(y-y')^2}{4D'_y(t-\tau)}\right\} d\tau \\ &+ \frac{x}{2\pi B\sqrt{D'_x D'_y}} \exp\left\{\frac{v'x}{2D'_x}\right\} \int_0^t c_0(\tau) \frac{1}{(t-\tau)^2} \\ &\cdot \exp\left\{-\lambda(t-\tau) - \frac{v'^2(t-\tau)}{4D'_x} - \frac{x^2}{4D'_x(t-\tau)} - \frac{(y-y')^2}{4D'_y(t-\tau)}\right\} \\ &\cdot \sum_{n=1}^{\infty} \cos\left(\frac{n\pi z'}{B}\right) \exp\left\{-D'_z \frac{n^2\pi^2}{B^2}(t-\tau)\right\} \cos\left(\frac{n\pi z}{B}\right) d\tau \end{aligned}$$

The final form of the Green's function solution is obtained by recognizing that:

$$\exp\left\{\frac{v'x}{2D'_x}\right\} \cdot \exp\left\{-\frac{v'^2(t-\tau)}{4D'_x} - \frac{x^2}{4D'_x(t-\tau)}\right\} \equiv \exp\left\{-\frac{(x-v'(t-\tau))^2}{4D'_x(t-\tau)}\right\}$$

Collecting terms and simplifying:

$$c = \frac{x}{4\pi B \sqrt{D'_x D'_y}} \int_0^t c_0(\tau) \frac{1}{(t-\tau)^2} \exp\left\{-\lambda(t-\tau) - \frac{(x-v'(t-\tau))^2}{4D'_x(t-\tau)} - \frac{(y-y')^2}{4D'_y(t-\tau)}\right\} \cdot \left[1 + 2 \sum_{n=1}^{\infty} \cos\left(\frac{n\pi z'}{B}\right) \exp\left\{-D'_z \frac{n^2 \pi^2}{B^2}(t-\tau)\right\} \cos\left(\frac{n\pi z}{B}\right)\right] d\tau$$

3. Solution for a General Time-varying Patch Boundary Condition

The patch boundary condition is derived by extending the Green's function solution from $-y_0$ to y_0 , and from z_1 to z_2 .

$$\text{i.e., } c = \int_{z_1 - y_0}^{z_2} \int_{-y_0}^{y_0} c_G(x, y; y', z; z', t) dy' dz'$$

Substituting in the Green's function solution and re-arranging yields:

$$\begin{aligned} c &= \frac{x}{4\pi B \sqrt{D'_x D'_y}} \int_{z_1 - y_0}^{z_2} \int_{-y_0}^{y_0} \int_0^t c_0(\tau) \frac{1}{(t-\tau)^2} \\ &\cdot \exp \left\{ -\lambda(t-\tau) - \frac{(x-v'(t-\tau))^2}{4D'_x(t-\tau)} - \frac{(y-y')^2}{4D'_y(t-\tau)} \right\} \\ &\cdot \left[1 + 2 \sum_{n=1}^{\infty} \cos\left(\frac{n\pi z'}{B}\right) \exp\left\{-D'_z \frac{n^2 \pi^2}{B^2}(t-\tau)\right\} \cos\left(\frac{n\pi z}{B}\right) \right] d\tau dy' dz' \end{aligned}$$

Re-arranging the order of integration:

$$\begin{aligned} c &= \frac{x}{4\pi B \sqrt{D'_x D'_y}} \int_0^t c_0(\tau) \cdot \frac{1}{(t-\tau)^2} \exp \left\{ -\lambda(t-\tau) - \frac{(x-v'(t-\tau))^2}{4D'_x(t-\tau)} \right\} \\ &\cdot \int_{-y_0}^{y_0} \exp \left\{ -\frac{(y-y')^2}{4D'_y(t-\tau)} \right\} dy' \int_{z_1}^{z_2} \left[1 + 2 \sum_{n=1}^{\infty} \cos\left(\frac{n\pi z'}{B}\right) \exp\left\{-D'_z \frac{n^2 \pi^2}{B^2}(t-\tau)\right\} \cos\left(\frac{n\pi z}{B}\right) \right] dz' d\tau \end{aligned}$$

Noting the following integrals:

$$\text{i) } \int_{-y_0}^{y_0} \exp \left\{ -\frac{(y-y')^2}{4D'_y(t-\tau)} \right\} dy' = \sqrt{\pi D'_y} \sqrt{t-\tau} \left[\text{erfc} \left\{ \frac{y-y_0}{2\sqrt{D'_y(t-\tau)}} \right\} - \text{erfc} \left\{ \frac{y+y_0}{2\sqrt{D'_y(t-\tau)}} \right\} \right]$$

$$\begin{aligned} \text{ii) } &\int_{z_1}^{z_2} \left[1 + 2 \sum_{n=1}^{\infty} \cos\left(\frac{n\pi z'}{B}\right) \exp\left\{-D'_z \frac{n^2 \pi^2}{B^2}(t-\tau)\right\} \cos\left(\frac{n\pi z}{B}\right) \right] dz' \\ &= (z_2 - z_1) + \frac{2B}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \exp\left\{-D'_z \frac{n^2 \pi^2}{B^2}(t-\tau)\right\} \end{aligned}$$

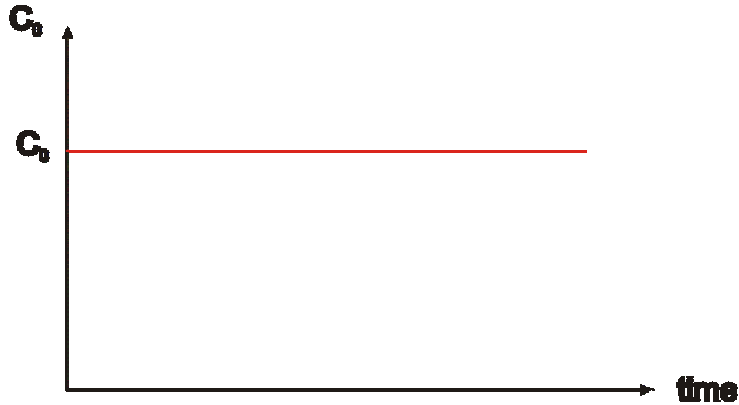
The final form of the solution becomes:

$$\begin{aligned}
 c = & \frac{x}{4\sqrt{\pi}\sqrt{D'_x}} \int_0^t c_0(\tau) \cdot \frac{1}{(t-\tau)^{\frac{3}{2}}} \exp\left\{-\lambda(t-\tau) - \frac{(x-v'(t-\tau))^2}{4D'_x(t-\tau)}\right\} \\
 & \cdot \left[\operatorname{erfc}\left\{\frac{y-y_0}{2\sqrt{D'_y(t-\tau)}}\right\} - \operatorname{erfc}\left\{\frac{y+y_0}{2\sqrt{D'_y(t-\tau)}}\right\} \right] \\
 & \cdot \left(\frac{(z_2-z_1)}{B} + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z'}{B}\right) \exp\left\{-D'_z \frac{n^2\pi^2}{B^2}(t-\tau)\right\} \right) d\tau
 \end{aligned}$$

4. Solution for Constant Inflow Concentration

A constant inflow concentration is defined as:

$$c_0(t) = C_0$$



Substituting for $C_0(t)$ in the general solution yields:

$$c = C_0 \frac{x}{4\sqrt{\pi D_x'}} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\lambda \xi - \frac{(x - v' \xi)^2}{4D_x' \xi} \right\} \left[\operatorname{erfc} \left\{ \frac{y - y_0}{2\sqrt{D_y' \xi}} \right\} - \operatorname{erfc} \left\{ \frac{y + y_0}{2\sqrt{D_y' \xi}} \right\} \right] \cdot \left(\frac{z_2 - z_1}{B} + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \cos \left(\frac{n\pi z}{B} \right) \exp \left\{ -D_z' \frac{n^2 \pi^2}{B^2} \xi \right\} \right) d\xi$$

The integral can be accelerated by scaling to the fourth power.

Defining: $\tau = \xi^{\frac{1}{4}}$
 $\rightarrow \xi = \tau^4$ and $d\xi = 4\tau^3 d\tau$

the limits of integration become:

$$\xi = 0 \rightarrow \tau = 0$$

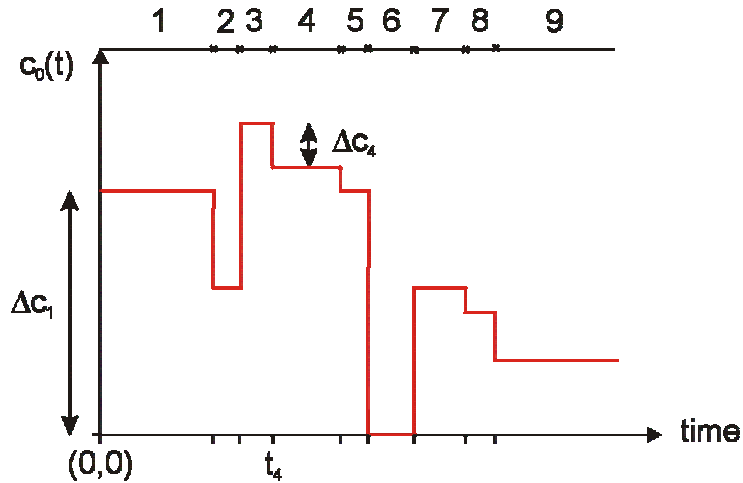
$$\xi = t \rightarrow \tau = t^{\frac{1}{4}}$$

Therefore, the solution can be rewritten as:

$$c = C_0 \frac{x}{4\sqrt{\pi D'_x}} 4 \int_0^{\frac{1}{t^4}} \frac{1}{\tau^3} \exp \left\{ -\lambda \tau^4 - \frac{(x - v' \tau^4)^2}{4D'_x \tau^4} \right\} \left[\operatorname{erfc} \left\{ \frac{y - y_0}{2\sqrt{D'_y \tau^4}} \right\} - \operatorname{erfc} \left\{ \frac{y + y_0}{2\sqrt{D'_y \tau^4}} \right\} \right] \\ \cdot \left(\frac{(z_2 - z_1)}{B} + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \cos \left(\frac{n\pi z}{B} \right) \exp \left\{ -D'_z \frac{n^2 \pi^2}{B^2} \tau^4 \right\} \right) d\tau$$

5. Solution for an Arbitrary Inflow Concentration Defined as a Set of Steps

Consider a time-varying inflow concentration defined as a set of NP steps:

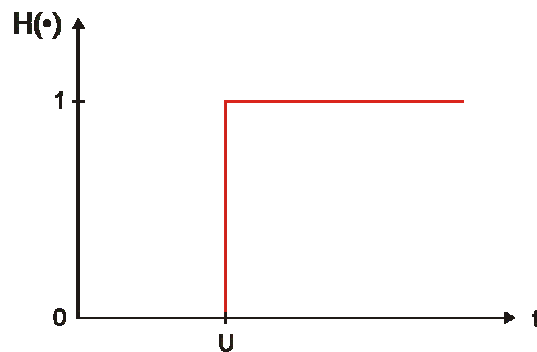


Denoting t_i as the starting time for the i^{th} step, and ΔC_i as the concentration change at the start of the i^{th} step, the inflow concentration history is defined as:

$$C_o(t) = \sum_{i=1}^{NP} \Delta C_i H(t - t_i)$$

$H(\cdot)$ is the Heaviside step function:

$$\begin{aligned} H(t - U) &= 0 \text{ if } t < U \\ &= 1 \text{ if } t > U \end{aligned}$$



Substituting for $C_0(t)$ in the solution for an arbitrary inflow concentration history:

$$c = \frac{x}{4\sqrt{\pi}\sqrt{D'_x}} \int_0^t \sum_{i=1}^{NP} \Delta C_i H(\tau - t_i) \frac{1}{(t-\tau)^{\frac{3}{2}}} \exp \left\{ -\lambda(t-\tau) - \frac{(x-v'(t-\tau))^2}{4D'_x(t-\tau)} \right\} \\ \cdot \left[\operatorname{erfc} \left\{ \frac{y-y_0}{2\sqrt{D'_y(t-\tau)}} \right\} - \operatorname{erfc} \left\{ \frac{y+y_0}{2\sqrt{D'_y(t-\tau)}} \right\} \right] \left(\frac{z_2 - z_1}{B} \right) \\ + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \cos \left(\frac{n\pi z}{B} \right) \exp \left\{ -D'_z \frac{n^2 \pi^2}{B^2} (t-\tau) \right\} d\tau$$

Making use of the properties of the Heaviside function and re-arranging:

$$c = \frac{x}{4\sqrt{\pi}\sqrt{D'_x}} \sum_{i=1}^{NP} \Delta C_i \int_{t_i}^t \frac{1}{(t-\tau)^{\frac{3}{2}}} \exp \left\{ -\lambda(t-\tau) - \frac{(x-v'(t-\tau))^2}{4D'_x(t-\tau)} \right\} \\ \cdot \left[\operatorname{erfc} \left\{ \frac{y-y_0}{2\sqrt{D'_y(t-\tau)}} \right\} - \operatorname{erfc} \left\{ \frac{y+y_0}{2\sqrt{D'_y(t-\tau)}} \right\} \right] \left(\frac{z_2 - z_1}{B} \right) \\ + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \cos \left(\frac{n\pi z}{B} \right) \exp \left\{ -D'_z \frac{n^2 \pi^2}{B^2} (t-\tau) \right\} d\tau$$

Make a change of variables:

$$\xi = t - \tau \quad \rightarrow \quad \tau = t - \xi \\ d\tau = -d\xi$$

$$\tau = t_i \quad \rightarrow \quad \xi = t - t_i \\ \tau = t \quad \rightarrow \quad \xi = 0$$

Therefore the solution becomes:

$$c = \frac{x}{4\sqrt{\pi}\sqrt{D'_x}} \sum_{i=1}^{NP} \Delta C_i \int_0^{t-t_i} \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\lambda \xi - \frac{(x-v'\xi)^2}{4D'_x \xi} \right\} \cdot \left[\operatorname{erfc} \left\{ \frac{y-y_0}{2\sqrt{D'_y \xi}} \right\} - \operatorname{erfc} \left\{ \frac{y+y_0}{2\sqrt{D'_y \xi}} \right\} \right] \left(\frac{z_2-z_1}{B} \right) + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \cos \left(\frac{n\pi z}{B} \right) \exp \left\{ -D'_z \frac{n^2 \pi^2}{B^2} \xi \right\} d\xi$$

Note:

If $NP=1$ and $t^{(1)} = 0.0$, the solution collapses to the solution for a constant patch concentration, with $C_0 = \Delta C_1 = C^{(1)}$.

The integration can be accelerated by scaling the variable of integration to the 4th power:

$$\text{Let: } \tau = \xi^{\frac{1}{4}} \\ \rightarrow \xi = \tau^4 \quad ; \quad d\xi = 4\tau^3 d\tau$$

the limits of integration become:

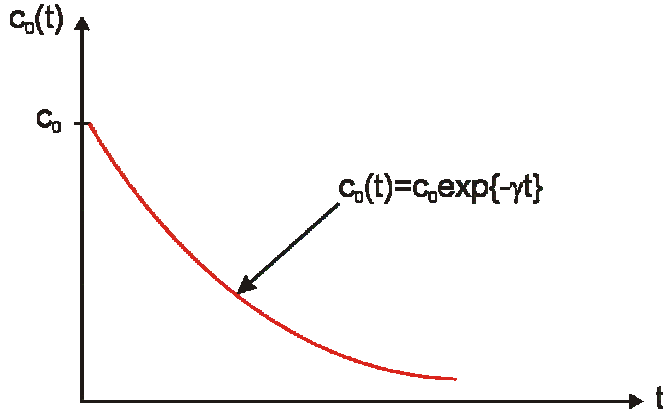
$$\xi = 0 \quad \rightarrow \tau = 0 \\ \xi = t - t_i \quad \rightarrow \tau = (t - t_i)^{\frac{1}{4}}$$

and the solution is written as:

$$c = \frac{x}{4\sqrt{\pi}\sqrt{D'_x}} \sum_{i=1}^{NP} \Delta C_i 4 \int_0^{(t-t_i)^{\frac{1}{4}}} \frac{1}{\tau^3} \exp \left\{ -\lambda \tau^4 - \frac{(x-v'\tau^4)^2}{4D'_x \tau^4} \right\} \cdot \left[\operatorname{erfc} \left\{ \frac{y-y_0}{2\sqrt{D'_y \tau^4}} \right\} - \operatorname{erfc} \left\{ \frac{y+y_0}{2\sqrt{D'_y \tau^4}} \right\} \right] \left(\frac{z_2-z_1}{B} \right) + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \cos \left(\frac{n\pi z}{B} \right) \exp \left\{ -D'_z \frac{n^2 \pi^2}{B^2} \tau^4 \right\} d\tau$$

6. Solution for an Exponentially Decaying Inflow Concentration

An exponentially-decaying concentration is defined as: $c_0(t) = c_0 \exp\{-\gamma t\}$, where γ is the “source decay constant” (units of T^{-1}).



Substituting for $c_0(t)$ in the solution for an arbitrary time-varying inflow concentration:

$$c = \frac{x}{4\sqrt{\pi D_x'}} \int_0^t c_0 \exp\{-\gamma\tau\} \frac{1}{(t-\tau)^{\frac{3}{2}}} \exp\left\{-\lambda(t-\tau) - \frac{(x-v'(t-\tau))^2}{4D_x'(t-\tau)}\right\} \\ \cdot \left[\operatorname{erfc}\left\{\frac{y-y_0}{2\sqrt{D_y'(t-\tau)}}\right\} - \operatorname{erfc}\left\{\frac{y+y_0}{2\sqrt{D_y'(t-\tau)}}\right\} \right] \left(\frac{z_2-z_1}{B}\right) \\ + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \exp\left\{-D_z' \frac{n^2 \pi^2}{B^2} (t-\tau)\right\} \right] d\tau$$

Collecting terms and re-arranging slightly:

$$c = c_0 \frac{x}{4\sqrt{\pi D_x'}} \int_0^t \frac{1}{(t-\tau)^{\frac{3}{2}}} \exp\left\{-\frac{(x-v'(t-\tau))^2}{4D_x'(t-\tau)} - \lambda(t-\tau) - \gamma\tau\right\} \\ \cdot \left[\operatorname{erfc}\left\{\frac{y-y_0}{2\sqrt{D_y'(t-\tau)}}\right\} - \operatorname{erfc}\left\{\frac{y+y_0}{2\sqrt{D_y'(t-\tau)}}\right\} \right] \left(\frac{z_2-z_1}{B}\right) \\ + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \exp\left\{-D_z' \frac{n^2 \pi^2}{B^2} (t-\tau)\right\} \right] d\tau$$

Rearranging, this can be written as:

$$\begin{aligned}
 c = c_0 & \frac{x}{4\sqrt{\pi D'_x}} \exp\{-\gamma t\} \int_0^t \frac{1}{(t-\tau)^{\frac{3}{2}}} \exp\left\{-\frac{(x-v'(t-\tau))^2}{4D'_x(t-\tau)} + (\gamma-\lambda)(t-\tau)\right\} \\
 & \cdot \left[\operatorname{erfc}\left\{\frac{y-y_0}{2\sqrt{D'_y(t-\tau)}}\right\} - \operatorname{erfc}\left\{\frac{y+y_0}{2\sqrt{D'_y(t-\tau)}}\right\} \right] \left(\frac{z_2-z_1}{B}\right) \\
 & + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \exp\left\{-D'_z \frac{n^2 \pi^2}{B^2} (t-\tau)\right\} d\tau
 \end{aligned}$$

Make a change of variables:

$$\begin{aligned}
 \text{Define: } & \xi = t - \tau \\
 \therefore & d\tau = -d\xi
 \end{aligned}$$

the limits of integration become:

$$\begin{aligned}
 \tau = 0 & \rightarrow \xi = t \\
 \tau = t & \rightarrow \xi = 0
 \end{aligned}$$

and the integral is written as:

$$\begin{aligned}
 c = c_0 & \frac{x}{4\sqrt{\pi D'_x}} \exp\{-\gamma t\} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-\frac{(x-v'\xi)^2}{4D'_x\xi} + (\gamma-\lambda)\xi\right\} \\
 & \cdot \left[\operatorname{erfc}\left\{\frac{y-y_0}{2\sqrt{D'_y\xi}}\right\} - \operatorname{erfc}\left\{\frac{y+y_0}{2\sqrt{D'_y\xi}}\right\} \right] \left(\frac{z_2-z_1}{B}\right) \\
 & + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \exp\left\{-D'_z \frac{n^2 \pi^2}{B^2} \xi\right\} d\xi
 \end{aligned}$$

Note:

The integral can be accelerated by scaling the variable of integration to the 4th power.

$$\begin{aligned} \text{Letting:} \quad \tau &= \xi^{\frac{1}{4}} \\ \rightarrow \quad \xi &= \tau^4 \quad ; \quad d\xi = 4\tau^3 d\tau \end{aligned}$$

the limits of integration become:

$$\begin{aligned} \xi = 0 &\rightarrow \tau = 0 \\ \xi = t &\rightarrow \tau = t^{\frac{1}{4}} \end{aligned}$$

The solution is written as:

$$\begin{aligned} c &= c_0 \frac{x}{4\sqrt{\pi D'_x}} \exp\{-\gamma t\} 4 \int_0^{t^{\frac{1}{4}}} \frac{1}{\tau^3} \exp\left\{-\frac{(x-v'\tau^4)^2}{4D'_x\tau^4} + (\gamma - \lambda)\tau^4\right\} \\ &\cdot \left[\operatorname{erfc}\left\{\frac{y-y_0}{2\sqrt{D'_y}\tau^4}\right\} - \operatorname{erfc}\left\{\frac{y+y_0}{2\sqrt{D'_y}\tau^4}\right\} \right] \left(\frac{z_2 - z_1}{B}\right) \\ &+ \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \exp\left\{-D'_z \frac{n^2\pi^2}{B^2} \tau^4\right\} \Big] d\tau \end{aligned}$$

Check:

The solution for a constant source concentration should be obtained if $\gamma = 0.0$.

Substituting for $\gamma = 0.0$ yields:

$$\begin{aligned} c &= c_0 \frac{x}{4\sqrt{\pi D'_x}} 4 \int_0^{t^{\frac{1}{4}}} \frac{1}{\tau^3} \exp\left\{-\frac{(x-v'\tau^4)^2}{4D'_x\tau^4} + \lambda\tau^4\right\} \left[\operatorname{erfc}\left\{\frac{y-y_0}{2\sqrt{D'_y}\tau^4}\right\} - \operatorname{erfc}\left\{\frac{y+y_0}{2\sqrt{D'_y}\tau^4}\right\} \right] \\ &\left(\frac{z_2 - z_1}{B} + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \exp\left\{-D'_z \frac{n^2\pi^2}{B^2} \tau^4\right\} \right) d\tau \end{aligned}$$

as before.

7. Solutions for Degenerate Cases

7.1. 2^D Solutions

7.1.1. 2^D Areal Transport

The solution for 2^D areal transport is obtained by specifying that the patch along the inflow boundary extends over the full thickness of the aquifer.

$$\begin{array}{l} z_1 = 0 \\ z_2 = B \end{array}$$

For $z_1 = 0$ and $z_2 = B$, the general solution reduces to:

$$c = \frac{x}{4\sqrt{\pi D_x'}} \int_0^t c_0(\tau) \frac{1}{(t-\tau)^{\frac{3}{2}}} \exp \left\{ -\lambda(t-\tau) - \frac{(x-v'(t-\tau))^2}{4D_x'(t-\tau)} \right\} \left[\operatorname{erfc} \left\{ \frac{y-y_0}{2\sqrt{D_y'(t-\tau)}} \right\} - \operatorname{erfc} \left\{ \frac{y+y_0}{2\sqrt{D_y'(t-\tau)}} \right\} \right] d\tau$$

a. Solution for a Constant Patch Concentration

$$c_0(t) = c_0$$

Substituting for $c_0(t)$ in the general solution yields:

$$c = c_0 \frac{x}{4\sqrt{\pi D_x'}} \int_0^t \frac{1}{(t-\tau)^{\frac{3}{2}}} \exp \left\{ -\lambda(t-\tau) - \frac{(x-v'(t-\tau))^2}{4D_x'(t-\tau)} \right\} \left[\operatorname{erfc} \left\{ \frac{y-y_0}{2\sqrt{D_y'(t-\tau)}} \right\} - \operatorname{erfc} \left\{ \frac{y+y_0}{2\sqrt{D_y'(t-\tau)}} \right\} \right] d\tau$$

Letting $\xi = t - \tau$, the integral is written as:

$$c = c_0 \frac{x}{4\sqrt{\pi D'_x}} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\lambda \xi - \frac{(x - v' \xi)^2}{4D'_x \xi} \right\} \left[\operatorname{erfc} \left\{ \frac{y - y_0}{2\sqrt{D'_y \xi}} \right\} - \operatorname{erfc} \left\{ \frac{y + y_0}{2\sqrt{D'_y \xi}} \right\} \right] d\xi$$

b. Dicretized Inflow Concentration History

$$c = \frac{x}{4\sqrt{\pi D'_x}} \sum_{i=1}^{NP} \Delta C_i \int_0^{t-t_i} \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\lambda \xi - \frac{(x - v' \xi)^2}{4D'_x \xi} \right\} \cdot \left[\operatorname{erfc} \left\{ \frac{y - y_0}{2\sqrt{D'_y \xi}} \right\} - \operatorname{erfc} \left\{ \frac{y + y_0}{2\sqrt{D'_y \xi}} \right\} \right] d\xi$$

c. Exponentially-decaying Inflow Concentration

$$c = C_0 \frac{x}{4\sqrt{\pi D'_x}} \exp \{ -\gamma t \} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\frac{(x - v' \xi)^2}{4D'_x \xi} + (\gamma - \lambda) \xi \right\} \cdot \left[\operatorname{erfc} \left\{ \frac{y - y_0}{2\sqrt{D'_y \xi}} \right\} - \operatorname{erfc} \left\{ \frac{y + y_0}{2\sqrt{D'_y \xi}} \right\} \right] d\xi$$

7.1.2. 2^D Cross-sectional Transport

The solution for 2^D cross-sectional transport is obtained by specifying that patch is very extensive along the transverse horizontal.

$$y_0 \rightarrow \infty$$

Noting the following limits:

$$\operatorname{erfc}(-\infty) = 2$$

$$\operatorname{erfc}(\infty) = 0$$

the general solution reduces to:

$$c = \frac{x}{2\sqrt{\pi D_x'}} \int_0^t c_0(\tau) \frac{1}{(t-\tau)^{\frac{3}{2}}} \exp\left\{-\lambda(t-\tau) - \frac{(x-v'(t-\tau))^2}{4D_x'(t-\tau)}\right\} \left(\frac{z_2-z_1}{B}\right) + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \exp\left\{-D_z' \frac{n^2 \pi^2}{B^2} (t-\tau)\right\} d\tau$$

a. Constant Patch Concentration

Substituting for $c_0(t) = c_0$ in the general solution yields:

$$c = c_0 \frac{x}{2\sqrt{\pi D_x'}} \int_0^t \frac{1}{(t-\tau)^{\frac{3}{2}}} \exp\left\{-\lambda(t-\tau) - \frac{(x-v'(t-\tau))^2}{4D_x'(t-\tau)}\right\} \left(\frac{z_2-z_1}{B}\right) + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \exp\left\{-D_z' \frac{n^2 \pi^2}{B^2} (t-\tau)\right\} d\tau$$

Defining $\xi = t - \tau$, the solution can be written as:

$$c = c_0 \frac{x}{2\sqrt{\pi D_x'}} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-\lambda\xi - \frac{(x-v'\xi)^2}{4D_x'\xi}\right\} \left(\frac{z_2-z_1}{B}\right) + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \exp\left\{-D_z' \frac{n^2 \pi^2}{B^2} \xi\right\} d\xi$$

The integral can be evaluated by first splitting it into two parts:

$$I = I_1 + I_2$$

where:

$$I_1 = \frac{(z_2 - z_1)}{B} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\lambda \xi - \frac{(x - v' \xi)^2}{4D_x' \xi} \right\} d\xi$$

$$I_2 = \frac{2}{\pi} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\lambda \xi - \frac{(x - v' \xi)^2}{4D_x' \xi} \right\} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \\ \cdot \cos \left(\frac{n\pi z}{B} \right) \exp \left\{ -D_z' \frac{n^2 \pi^2}{B^2} \xi \right\} d\xi$$

(i) Evaluating the first integral:

$$I_1 = \frac{(z_2 - z_1)}{B} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\frac{(x - v' \xi)^2}{4D_x' \xi} - \lambda \xi \right\} d\xi$$

Expanding and re-arranging the exponential term:

$$\exp \{ \cdot \} = \exp \left\{ \frac{xv'}{2D_x'} \right\} \cdot \exp \left\{ - \left(\frac{v'^2}{4D_x'} + \lambda \right) \xi - \frac{x^2}{4D_x' \xi} \right\}$$

Defining:

$$a^2 = \frac{v'^2}{4D_x'} + \lambda$$

$$b^2 = \frac{x^2}{4D_x'}$$

The integral becomes:

$$I_1 = \frac{(z_2 - z_1)}{B} \exp\left\{\frac{xv'}{2D_x'}\right\} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-a^2\xi - \frac{b^2}{\xi}\right\} d\xi$$

The integral is given in S.H. Cho's table of integrals #2.9.5:

$$\begin{aligned} & \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-a^2\xi - \frac{b^2}{\xi}\right\} d\xi \\ &= \frac{\sqrt{\pi}}{2b} \left(\exp\{-2ab\} \operatorname{erfc}\left\{\frac{b}{\sqrt{t}} - a\sqrt{t}\right\} + \exp\{2ab\} \operatorname{erfc}\left\{\frac{b}{\sqrt{t}} + a\sqrt{t}\right\} \right) \end{aligned}$$

Substituting for a and b , I_1 becomes:

$$\begin{aligned} I_1 &= \frac{(z_2 - z_1)}{B} \exp\left\{\frac{xv'}{2D_x'}\right\} \frac{\sqrt{\pi D_x'}}{x} \left(\exp\left\{-\frac{x}{\sqrt{D_x'}} \left(\frac{v'^2}{4D_x'} + \lambda\right)^{\frac{1}{2}}\right\} \right. \\ &\quad \cdot \operatorname{erfc}\left\{\frac{x}{2\sqrt{D_x' t}} - \left(\frac{v'^2}{4D_x'} + \lambda\right)^{\frac{1}{2}} \sqrt{t}\right\} + \exp\left\{\frac{x}{\sqrt{D_x'}} \left(\frac{v'^2}{4D_x'} + \lambda\right)^{\frac{1}{2}}\right\} \\ &\quad \left. \cdot \operatorname{erfc}\left\{\frac{x}{2\sqrt{D_x' t}} + \left(\frac{v'^2}{4D_x'} + \lambda\right)^{\frac{1}{2}} \sqrt{t}\right\} \right) \end{aligned}$$

(ii) Evaluating the second integral:

$$\begin{aligned} I_2 &= \frac{2}{\pi} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-\frac{(x - v'\xi)^2}{4D_x'\xi} - \lambda\xi\right\} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \\ &\quad \cdot \cos\left(\frac{n\pi z}{B}\right) \exp\left\{-D_z' \frac{n^2 \pi^2}{B^2} \xi\right\} d\xi \end{aligned}$$

Re-arranging the orders of the summation and integration, collecting the exponential terms and expanding, the exponential term becomes:

$$\exp\{\cdot\} = \exp\left\{\frac{xv'}{2D'_x}\right\} \cdot \exp\left\{-\left(\frac{v'^2}{4D'_x} + \lambda + D'_z \frac{n^2\pi^2}{B^2}\right)\xi - \frac{x^2}{4D'_x\xi}\right\}$$

Defining:

$$a^2 = \frac{v'^2}{4D'_x} + \lambda + D'_z \frac{n^2\pi^2}{B^2}$$

$$b^2 = \frac{x^2}{4D'_x}$$

The integral becomes:

$$I_2 = \frac{2}{\pi} \exp\left\{\frac{xv'}{2D'_x}\right\} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-a^2\xi - \frac{b^2}{\xi}\right\} d\xi$$

Using the integral given in S.H. Cho's table (#2.9.5) again, and defining:

$$\mu_n = \left[\frac{v'^2}{4D'_x} + \lambda + D'_z \frac{n^2\pi^2}{B^2} \right]^{\frac{1}{2}}$$

and substituting for a and b , I_2 becomes:

$$I_2 = \frac{2}{\pi} \exp\left\{\frac{xv'}{2D'_x}\right\} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \frac{\sqrt{\pi D'_x}}{x} \cdot \left(\exp\left\{-\frac{x}{\sqrt{D'_x}}\mu_n\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x}t} - \mu_n\sqrt{t}\right\} + \exp\left\{\frac{x}{\sqrt{D'_x}}\mu_n\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x}t} + \mu_n\sqrt{t}\right\} \right)$$

Substituting for I_1 and I_2 :

$$\begin{aligned}
c &= \frac{x}{2\sqrt{\pi D'_x}} [I_1 + I_2] \\
&= \frac{x}{2\sqrt{\pi D'_x}} \left\| \left[\frac{(z_2 - z_1)}{B} \exp \left\{ \frac{xv'}{2D'_x} \right\} \frac{\sqrt{\pi D'_x}}{x} \right. \right. \\
&\quad \left. \left(\exp \left\{ -\frac{x}{\sqrt{D'_x}} \left(\frac{v'^2}{4D'_x} + \lambda \right)^{\frac{1}{2}} \right\} \operatorname{erfc} \left\{ \frac{x}{2\sqrt{D'_x t}} - \left(\frac{v'^2}{4D'_x} + \lambda \right)^{\frac{1}{2}} \sqrt{t} \right\} \right. \right. \\
&\quad \left. \left. + \exp \left\{ \frac{x}{\sqrt{D'_x}} \left(\frac{v'^2}{4D'_x} + \lambda \right)^{\frac{1}{2}} \right\} \operatorname{erfc} \left\{ \frac{x}{2\sqrt{D'_x t}} + \left(\frac{v'^2}{4D'_x} + \lambda \right)^{\frac{1}{2}} \sqrt{t} \right\} \right) \right. \\
&\quad \left. + \frac{2}{\pi} \exp \left\{ \frac{xv'}{2D'_x} \right\} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \cos \left(\frac{n\pi z}{B} \right) \right. \\
&\quad \left. \cdot \frac{\sqrt{\pi D'_x}}{x} \left(\exp \left\{ -\frac{x}{\sqrt{D'_x}} \mu_n \right\} \operatorname{erfc} \left\{ \frac{x}{2\sqrt{D'_x t}} - \mu_n \sqrt{t} \right\} \right. \right. \\
&\quad \left. \left. + \exp \left\{ \frac{x}{\sqrt{D'_x}} \mu_n \right\} \operatorname{erfc} \left\{ \frac{x}{2\sqrt{D'_x t}} + \mu_n \sqrt{t} \right\} \right) \right] \right\|
\end{aligned}$$

Simplifying:

$$\begin{aligned}
 c = & \frac{c_0}{2} \exp\left\{\frac{xv'}{2D'_x}\right\} \left\| \left[\frac{(z_2 - z_1)}{B} \right. \right. \\
 & \cdot \left. \left. \exp\left\{-\frac{x}{\sqrt{D'_x}} \left(\frac{v'^2}{4D'_x} + \lambda\right)^{\frac{1}{2}}\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x t}} - \left(\frac{v'^2}{4D'_x} + \lambda\right)^{\frac{1}{2}} \sqrt{t}\right\} \right. \right. \\
 & + \left. \left. \exp\left\{\frac{x}{\sqrt{D'_x}} \left(\frac{v'^2}{4D'_x} + \lambda\right)^{\frac{1}{2}}\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x t}} + \left(\frac{v'^2}{4D'_x} + \lambda\right)^{\frac{1}{2}} \sqrt{t}\right\} \right] \right\} \\
 & + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \\
 & \cdot \left. \left. \exp\left\{-\frac{x}{\sqrt{D'_x}} \mu_n\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x t}} - \mu_n \sqrt{t}\right\} \right. \right. \\
 & + \left. \left. \exp\left\{\frac{x}{\sqrt{D'_x}} \mu_n\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x t}} + \mu_n \sqrt{t}\right\} \right] \right\|
 \end{aligned}$$

b. Discretized Inflow Concentration History

$$\begin{aligned}
 c = & \frac{x}{2\sqrt{\pi D'_x}} \sum_{i=1}^{NP} \Delta C_i \int_0^{t-t_i} \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-\lambda\xi - \frac{(x-v'\xi)^2}{4D'_x\xi}\right\} \left(\frac{(z_2 - z_1)}{B}\right) \\
 & + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \exp\left\{-D'_z \frac{n^2\pi^2}{B^2} \xi\right\} d\xi
 \end{aligned}$$

Defining the integral as:

$$\begin{aligned}
 I = & \int_0^{t-t_i} \left[\frac{(z_2 - z_1)}{B} \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-\lambda\xi - \frac{(x-v'\xi)^2}{4D'_x\xi}\right\} \right] + \left[\frac{2}{\pi} \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-\lambda\xi - \frac{(x-v'\xi)^2}{4D'_x\xi}\right\} \right. \\
 & \cdot \left. \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \exp\left\{-D'_z \frac{n^2\pi^2}{B^2} \xi\right\} \right] d\xi
 \end{aligned}$$

The integral can be evaluated by first splitting it into two parts:

$$I = I_1 + I_2$$

where:

$$I_1 = \frac{(z_2 - z_1)}{B} \int_0^{t-t_i} \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\lambda \xi - \frac{(x - v' \xi)^2}{4D'_x \xi} \right\} d\xi$$

$$I_2 = \frac{2}{\pi} \int_0^{t-t_i} \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\lambda \xi - \frac{(x - v' \xi)^2}{4D'_x \xi} \right\} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \cdot \cos \left(\frac{n\pi z}{B} \right) \exp \left\{ -D'_z \frac{n^2 \pi^2}{B^2} \xi \right\} d\xi$$

(i) Evaluating the first integral:

$$I_1 = \frac{(z_2 - z_1)}{B} \int_0^{t-t_i} \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\frac{(x - v' \xi)^2}{4D'_x \xi} - \lambda \xi \right\} d\xi$$

Expanding and re-arranging the exponential term:

$$\exp \{ \cdot \} = \exp \left\{ \frac{xv'}{2D'_x} \right\} \cdot \exp \left\{ - \left(\frac{v'}{4D'_x} + \lambda \right) \xi - \frac{x^2}{4D'_x \xi} \right\}$$

Defining:

$$a^2 = \frac{v'^2}{4D'_x} + \lambda$$

$$b^2 = \frac{x^2}{4D'_x}$$

The integral becomes:

$$I_1 = \frac{(z_2 - z_1)}{B} \exp \left\{ \frac{xv'}{2D'_x} \right\} \int_0^{t-t_i} \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -a^2 \xi - \frac{b^2}{\xi} \right\} d\xi$$

The integral is given in S.H. Cho's table of integrals #2.9.5:

$$\int_0^{t-t_i} \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-a^2\xi - \frac{b^2}{\xi}\right\} d\xi = \frac{\sqrt{\pi}}{2b} \left(\exp\{-2ab\} \operatorname{erfc}\left\{\frac{b}{\sqrt{t-t_i}} - a\sqrt{t-t_i}\right\} \right. \\ \left. + \exp\{2ab\} \operatorname{erfc}\left\{\frac{b}{\sqrt{t-t_i}} + a\sqrt{t-t_i}\right\} \right)$$

Substituting for a and b , I_1 becomes:

$$I_1 = \frac{(z_2 - z_1)}{B} \exp\left\{\frac{xv'}{2D_x'}\right\} \frac{\sqrt{\pi D_x'}}{x} \\ \cdot \left(\exp\left\{-\frac{x}{\sqrt{D_x'}} \left(\frac{v'^2}{4D_x'} + \lambda\right)^{\frac{1}{2}}\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D_x'}(t-t_i)} - \left(\frac{v'^2}{4D_x'} + \lambda\right)^{\frac{1}{2}} \sqrt{t-t_i}\right\} \right. \\ \left. + \exp\left\{\frac{x}{\sqrt{D_x'}} \left(\frac{v'^2}{4D_x'} + \lambda\right)^{\frac{1}{2}}\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D_x'}(t-t_i)} + \left(\frac{v'^2}{4D_x'} + \lambda\right)^{\frac{1}{2}} \sqrt{t-t_i}\right\} \right)$$

(ii) Evaluating the second integral:

$$I_2 = \frac{2}{\pi} \int_0^{t-t_i} \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-\frac{(x-v'\xi)^2}{4D_x'\xi} - \lambda\xi\right\} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \\ \cdot \cos\left(\frac{n\pi z}{B}\right) \exp\left\{-D_z' \frac{n^2\pi^2}{B^2} \xi\right\} d\xi$$

Re-arranging the orders of the summation and integration, collecting the exponential terms and expanding, the exponential term becomes:

$$\exp\{\cdot\} = \exp\left\{\frac{xv'}{2D_x'}\right\} \cdot \exp\left\{-\left(\frac{v'^2}{4D_x'} + \lambda + D_z' \frac{n^2\pi^2}{B^2}\right)\xi - \frac{x^2}{4D_x'\xi}\right\}$$

Defining:

$$a^2 = \frac{v'^2}{4D'_x} + \lambda + D'_z \frac{n^2 \pi^2}{B^2}$$

$$b^2 = \frac{x^2}{4D'_x}$$

The integral becomes:

$$I_2 = \frac{2}{\pi} \exp\left\{\frac{xv'}{2D'_x}\right\} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \\ \int_0^{t-t_i} \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-a^2 \xi - \frac{b^2}{\xi}\right\} d\xi$$

Using the integral given in S.H. Cho's table (#2.9.5) again, and defining:

$$\mu_n = \left[\frac{v'^2}{4D'_x} + \lambda + D'_z \frac{n^2 \pi^2}{B^2} \right]^{\frac{1}{2}}$$

and substituting for a and b , I_2 becomes:

$$I_2 = \frac{2}{\pi} \exp\left\{\frac{xv'}{2D'_x}\right\} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \frac{\sqrt{\pi D'_x}}{x} \\ \cdot \left(\exp\left\{-\frac{x}{\sqrt{D'_x}} \mu_n\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x}(t-t_i)} - \mu_n \sqrt{t-t_i}\right\} \right. \\ \left. + \exp\left\{\frac{x}{\sqrt{D'_x}} \mu_n\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x}(t-t_i)} + \mu_n \sqrt{t-t_i}\right\} \right)$$

Assembling the final solution and simplifying:

$$\begin{aligned}
 c = & \frac{1}{2} \exp \left\{ \frac{xv'}{2D'_x} \right\} \sum_{n=1}^{NP} \Delta C_i \left\| \left[\frac{(z_2 - z_1)}{B} \right. \right. \\
 & \cdot \left. \left. \exp \left\{ -\frac{x}{\sqrt{D'_x}} \left(\frac{v'^2}{4D'_x} + \lambda \right)^{\frac{1}{2}} \right\} \operatorname{erfc} \left\{ \frac{x}{2\sqrt{D'_x}(t-t_i)} - \left(\frac{v'^2}{4D'_x} + \lambda \right)^{\frac{1}{2}} \sqrt{t-t_i} \right\} \right. \right. \\
 & + \left. \left. \exp \left\{ \frac{x}{\sqrt{D'_x}} \left(\frac{v'^2}{4D'_x} + \lambda \right)^{\frac{1}{2}} \right\} \operatorname{erfc} \left\{ \frac{x}{2\sqrt{D'_x}(t-t_i)} + \left(\frac{v'^2}{4D'_x} + \lambda \right)^{\frac{1}{2}} \sqrt{t-t_i} \right\} \right] \right. \\
 & + \left. \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \cos \left(\frac{n\pi z}{B} \right) \right. \\
 & \cdot \left. \left. \exp \left\{ -\frac{x}{\sqrt{D'_x}} \mu_n \right\} \operatorname{erfc} \left\{ \frac{x}{2\sqrt{D'_x}(t-t_i)} - \mu_n \sqrt{t-t_i} \right\} \right. \right. \\
 & + \left. \left. \exp \left\{ \frac{x}{\sqrt{D'_x}} \mu_n \right\} \operatorname{erfc} \left\{ \frac{x}{2\sqrt{D'_x}(t-t_i)} + \mu_n \sqrt{t-t_i} \right\} \right] \right\|
 \end{aligned}$$

c. Exponentially-decaying Inflow Concentration

- General solution:

$$\begin{aligned}
 c = & c_0 \frac{x}{2\sqrt{\pi D'_x}} \exp \{ -\gamma t \} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\frac{(x-v'\xi)^2}{4D'_x \xi} + (\gamma - \lambda) \xi \right\} \left(\frac{z_2 - z_1}{B} \right. \\
 & + \left. \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \cos \left(\frac{n\pi z}{B} \right) \exp \left\{ -D'_z \frac{n^2 \pi^2}{B^2} \xi \right\} \right) d\xi
 \end{aligned}$$

Alternative Solution Valid for $\frac{v'^2}{4D'_x} > (\gamma - \lambda)$:

The solution can be re-written in an alternative form by splitting the integral into two parts:

$$\begin{aligned}
 I &= (z_2 - z_1) \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\frac{(x - v'\xi)^2}{4D'_x \xi} + (\gamma - \lambda)\xi \right\} d\xi + \frac{2B}{\pi} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \\
 &\cdot \exp \left\{ -\frac{(x - v'\xi)^2}{4D'_x \xi} + (\gamma - \lambda)\xi \right\} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \\
 &\cdot \cos \left(\frac{n\pi z}{B} \right) \exp \left\{ -D'_z \frac{n^2 \pi^2}{B^2} \xi \right\} d\xi \\
 &= I_1 + I_2
 \end{aligned}$$

where: $I_1 = (z_2 - z_1) \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\frac{(x - v'\xi)^2}{4D'_x \xi} + (\gamma - \lambda)\xi \right\} d\xi$

and: $I_2 = \frac{2B}{\pi} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\frac{(x - v'\xi)^2}{4D'_x \xi} + (\gamma - \lambda)\xi \right\} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \cos \left(\frac{n\pi z}{B} \right) \exp \left\{ -D'_z \frac{n^2 \pi^2}{B^2} \xi \right\} d\xi$

(i) Evaluating the first integral:

$$I_1 = (z_2 - z_1) \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\frac{(x - v'\xi)^2}{4D'_x \xi} + (\gamma - \lambda)\xi \right\} d\xi$$

Expanding and re-arranging the exponential term:

$$\exp \{ \cdot \} = \exp \left\{ \frac{xv'}{2D'_x} \right\} \cdot \exp \left\{ -\left(\frac{v'^2}{4D'_x} + (\gamma - \lambda) \right) \xi - \frac{x^2}{4D'_x \xi} \right\}$$

Defining:

$$a^2 = \frac{v'^2}{4D'_x} - (\gamma - \lambda) \quad \text{this is a valid expression if } a^2 > 0$$

$$b^2 = \frac{x^2}{4D'_x}$$

The integral becomes:

$$I_1 = (z_2 - z_1) \exp\left\{\frac{xv'}{2D'_x}\right\} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-a^2\xi - \frac{b^2}{\xi}\right\} d\xi$$

The integral is given in S.H. Cho's table of integrals #2.9.5:

$$\int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-a^2\xi - \frac{b^2}{\xi}\right\} d\xi = \frac{\sqrt{\pi}}{2b} \left(\exp\{-2ab\} \operatorname{erfc}\left\{\frac{b}{\sqrt{t}} - a\sqrt{t}\right\} + \exp\{2ab\} \operatorname{erfc}\left\{\frac{b}{\sqrt{t}} + a\sqrt{t}\right\} \right)$$

Substituting for a and b , I_1 becomes:

$$I_1 = (z_2 - z_1) \exp\left\{\frac{xv'}{2D'_x}\right\} \frac{\sqrt{\pi D'_x}}{x} \cdot \left(\exp\left\{-\frac{x}{\sqrt{D'_x}} \left(\frac{v'^2}{4D'_x} - (\gamma - \lambda)\right)^{\frac{1}{2}}\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x t}} - \left(\frac{v'^2}{4D'_x} - (\gamma - \lambda)\right)^{\frac{1}{2}} \sqrt{t}\right\} + \exp\left\{\frac{x}{\sqrt{D'_x}} \left(\frac{v'^2}{4D'_x} - (\gamma - \lambda)\right)^{\frac{1}{2}}\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x t}} + \left(\frac{v'^2}{4D'_x} - (\gamma - \lambda)\right)^{\frac{1}{2}} \sqrt{t}\right\} \right)$$

(ii) Evaluating the second integral:

$$I_2 = \frac{2B}{\pi} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-\frac{(x - v'\xi)^2}{4D'_x \xi} + (\gamma - \lambda)\xi\right\} \cdot \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \exp\left\{-D'_z \frac{n^2 \pi^2}{B^2} \xi\right\} d\xi$$

Re-arranging the orders of the summation and integration, collecting the exponential terms and expanding, the exponential term becomes:

$$\exp\{\cdot\} = \exp\left\{\frac{xv'}{2D'_x}\right\} \cdot \exp\left\{-\left(\frac{v'^2}{4D'_x} - (\gamma - \lambda) + D'_z \frac{n^2\pi^2}{B^2}\right)\xi - \frac{x^2}{4D'_x\xi}\right\}$$

Defining:

$$a^2 = \frac{v'^2}{4D'_x} - (\gamma - \lambda) + D'_z \frac{n^2\pi^2}{B^2}$$

$$b^2 = \frac{x^2}{4D'_x}$$

The integral becomes:

$$I_2 = \frac{2B}{\pi} \exp\left\{\frac{xv'}{2D'_x}\right\} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-a^2\xi - \frac{b^2}{\xi}\right\} d\xi$$

Using the integral given in S.H. Cho's table (#2.9.5) again, and defining:

$$\mu_n = \left[\frac{v'^2}{4D'_x} + (\gamma - \lambda) + D'_z \frac{n^2\pi^2}{B^2} \right]^{\frac{1}{2}}$$

and substituting for a and b , I_2 becomes:

$$I_2 = \frac{2B}{\pi} \exp\left\{\frac{xv'}{2D'_x}\right\} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \frac{\sqrt{\pi D'_x}}{x} \cdot \left(\exp\left\{-\frac{x}{\sqrt{D'_x}}\mu_n\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x}t} - \mu_n\sqrt{t}\right\} + \exp\left\{\frac{x}{\sqrt{D'_x}}\mu_n\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x}t} + \mu_n\sqrt{t}\right\} \right)$$

Substituting for I_1 and I_2 :

$$\begin{aligned}
c = & \frac{x}{2\sqrt{\pi D'_x}} \sum_{i=1}^{NP} \Delta c_i \left\| \left[\frac{(z_2 - z_1)}{B} \exp\left\{\frac{xv'}{2D'_x}\right\} \frac{\sqrt{\pi D'_x}}{x} \right. \right. \\
& \cdot \left. \left. \left(\exp\left\{-\frac{x}{\sqrt{D'_x}} \left(\frac{v'^2}{4D'_x} + \lambda\right)^{\frac{1}{2}}\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x t}} - \left(\frac{v'^2}{4D'_x} + \lambda\right)^{\frac{1}{2}} \sqrt{t}\right\} \right. \right. \right. \\
& + \left. \left. \left. \exp\left\{\frac{x}{\sqrt{D'_x}} \left(\frac{v'^2}{4D'_x} + \lambda\right)^{\frac{1}{2}}\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x t}} + \left(\frac{v'^2}{4D'_x} + \lambda\right)^{\frac{1}{2}} \sqrt{t}\right\} \right] \right. \right. \\
& + \left. \left. \frac{2}{\pi} \exp\left\{\frac{xv'}{2D'_x}\right\} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \frac{\sqrt{\pi D'_x}}{x} \right. \right. \\
& \cdot \left. \left. \left(\exp\left\{-\frac{x}{\sqrt{D'_x}} \mu_n\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x t}} - \mu_n \sqrt{t}\right\} \right. \right. \right. \\
& + \left. \left. \left. \exp\left\{\frac{x}{\sqrt{D'_x}} \mu_n\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x t}} + \mu_n \sqrt{t}\right\} \right) \right] \right\|
\end{aligned}$$

Simplifying yields the final form of the solution:

$$\begin{aligned}
 c = & \frac{c_0}{2} \exp \left\{ -\gamma t + \frac{xv'}{2D_x'} \right\} \left\| \left(\frac{z_2 - z_1}{B} \right. \right. \\
 & \cdot \left. \left. \exp \left\{ -\frac{x}{\sqrt{D_x'}} \left(\frac{v'^2}{4D_x'} - (\gamma - \lambda) \right)^{\frac{1}{2}} \right\} \operatorname{erfc} \left\{ \frac{x}{2\sqrt{D_x' t}} - \left(\frac{v'^2}{4D_x'} - (\gamma - \lambda) \right)^{\frac{1}{2}} \sqrt{t} \right\} \right. \right. \\
 & + \left. \left. \exp \left\{ \frac{x}{\sqrt{D_x'}} \left(\frac{v'^2}{4D_x'} - (\gamma - \lambda) \right)^{\frac{1}{2}} \right\} \operatorname{erfc} \left\{ \frac{x}{2\sqrt{D_x' t}} + \left(\frac{v'^2}{4D_x'} - (\gamma - \lambda) \right)^{\frac{1}{2}} \sqrt{t} \right\} \right) \right\} \\
 & + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin \left(\frac{n\pi z_2}{B} \right) - \sin \left(\frac{n\pi z_1}{B} \right) \right] \cos \left(\frac{n\pi z}{B} \right) \\
 & \cdot \left(\exp \left\{ -\frac{x}{\sqrt{D_x'}} \mu_n \right\} \operatorname{erfc} \left\{ \frac{x}{2\sqrt{D_x' t}} - \mu_n \sqrt{t} \right\} \right. \\
 & \left. \left. + \exp \left\{ \frac{x}{\sqrt{D_x'}} \mu_n \right\} \operatorname{erfc} \left\{ \frac{x}{2\sqrt{D_x' t}} + \mu_n \sqrt{t} \right\} \right) \right\| \left\| \right.
 \end{aligned}$$

7.2. 1^D Transport

The solution for 1^D transport is obtained by specifying that the patch along the inflow boundary both penetrates the aquifer completely, and is laterally extensive:

i.e.,

$$\begin{cases} z_1 = 0 \\ z_2 = B \\ y_0 \rightarrow \infty \end{cases}$$

For this case the general solution reduces to:

$$c = \frac{x}{2\sqrt{\pi D_x'}} \int_0^t \frac{c_0(\tau)}{(t-\tau)^{\frac{3}{2}}} \exp \left\{ -\lambda(t-\tau) - \frac{(x-v'(t-\tau))^2}{4D_x'(t-\tau)} \right\} d\tau$$

a. Constant Inflow Concentration

Substituting $c_0(t) = c_0$ in the general solution yields:

$$c = c_0 \frac{x}{2\sqrt{\pi D_x'}} \int_0^t \frac{1}{(t-\tau)^{\frac{3}{2}}} \exp \left\{ -\lambda(t-\tau) - \frac{(x-v'(t-\tau))^2}{4D_x'(t-\tau)} \right\} d\tau$$

Defining $\xi = t - \tau$, the solution is written as:

$$c = c_0 \frac{x}{2\sqrt{\pi D_x'}} \int_{\xi}^t \frac{1}{\xi^{\frac{3}{2}}} \exp \left\{ -\lambda\xi - \frac{(x-v'\xi)^2}{4D_x'\xi} \right\} d\xi$$

Expanding the exponential term in the integrand:

$$\begin{aligned} \exp\{\cdot\} &= \exp \left\{ -\lambda\xi - \frac{x^2 - 2xv'\xi + (v'\xi)^2}{4D_x'\xi} \right\} \\ &= \exp \left\{ -\frac{xv'}{4D_x'} \right\} \exp \left\{ -\frac{x^2}{4D_x'\xi} - \left(\frac{v'^2}{4D_x'} + \lambda \right) \xi \right\} \end{aligned}$$

Letting: $a^2 = \frac{v'^2}{4D'_x} + \lambda$

$$b^2 = \frac{x^2}{4D'_x}$$

The solution is written as:

$$c = c_0 \frac{x}{2\sqrt{\pi D'_x}} \exp\left\{-\frac{xv'}{4D'_x}\right\} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-\frac{b^2}{\xi} - a^2\xi\right\} d\xi$$

The integral is given by S.H. Cho #2.9.5:

$$I = \frac{\sqrt{\pi}}{2b} \left(\exp\{-2ab\} \operatorname{erfc}\left\{\frac{b}{\sqrt{t}} - a\sqrt{t}\right\} + \exp\{2ab\} \operatorname{erfc}\left\{\frac{b}{\sqrt{t}} + a\sqrt{t}\right\} \right)$$

Substituting for a and b :

$$ab = \left(\frac{v'^2}{4D'_x} + \lambda\right)^{\frac{1}{2}} \left(\frac{x^2}{4D'_x}\right)^{\frac{1}{2}} = \frac{x}{2\sqrt{D'_x}} \left(\frac{v'^2}{4D'_x} + \lambda\right)^{\frac{1}{2}}$$

$$b - at = \left(\frac{x^2}{4D'_x}\right)^{\frac{1}{2}} - \left(\frac{v'^2}{4D'_x} + \lambda\right)^{\frac{1}{2}} t$$

$$b + at = \left(\frac{x^2}{4D'_x}\right)^{\frac{1}{2}} + \left(\frac{v'^2}{4D'_x} + \lambda\right)^{\frac{1}{2}} t$$

$$\begin{aligned} \therefore I &= \frac{\sqrt{\pi D'_x}}{x} \left\{ \exp\left\{-\frac{x}{\sqrt{D'_x}} \left(\frac{v'^2}{4D'_x} + \lambda\right)^{\frac{1}{2}}\right\} \operatorname{erfc}\left\{\frac{1}{\sqrt{t}} \left[\left(\frac{x^2}{4D'_x}\right)^{\frac{1}{2}} - \left(\frac{v'^2}{4D'_x} + \lambda\right)^{\frac{1}{2}} t\right]\right\} \right\} \\ &+ \exp\left\{\frac{x}{\sqrt{D'_x}} \left(\frac{v'^2}{4D'_x} + \lambda\right)^{\frac{1}{2}}\right\} \operatorname{erfc}\left\{\frac{1}{\sqrt{t}} \left[\left(\frac{x^2}{4D'_x}\right)^{\frac{1}{2}} + \left(\frac{v'^2}{4D'_x} + \lambda\right)^{\frac{1}{2}} t\right]\right\} \end{aligned}$$

Defining $\mu = \left(\frac{v'^2}{4D'_x} + \lambda \right)^{\frac{1}{2}}$, the solution becomes:

$$c = c_0 \frac{x}{2\sqrt{\pi D'_x}} \exp\left\{-\frac{xv'}{4D'_x}\right\} \frac{\sqrt{\pi D'_x}}{x} \cdot \left(\exp\left\{-\frac{x\mu}{\sqrt{D'_x}}\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x t}} - \mu\sqrt{t}\right\} + \exp\left\{\frac{x\mu}{\sqrt{D'_x}}\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x t}} + \mu\sqrt{t}\right\} \right)$$

Simplifying:

$$c = c_0 \frac{1}{2} \exp\left\{-\frac{xv'}{4D'_x}\right\} \cdot \left(\exp\left\{-\frac{x\mu}{\sqrt{D'_x}}\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x t}} - \mu\sqrt{t}\right\} + \exp\left\{\frac{x\mu}{\sqrt{D'_x}}\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x t}} + \mu\sqrt{t}\right\} \right)$$

b. Discretized Inflow Concentration History

$$c = \frac{x}{2\sqrt{\pi D'_x}} \sum_{i=1}^{NP} \Delta c_i \int_0^{t-t_i} \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-\lambda\xi - \frac{(x-v'\xi)^2}{4D'_x\xi}\right\} d\xi$$

Making use of the integral:

$$\int_0^U \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-a^2\xi - \frac{b^2}{\xi}\right\} d\xi = \frac{\sqrt{\pi}}{2b} \left(\exp\{-2ab\} \operatorname{erfc}\left\{\frac{b}{\sqrt{U}} - a\sqrt{U}\right\} + \exp\{2ab\} \operatorname{erfc}\left\{\frac{b}{\sqrt{U}} + a\sqrt{U}\right\} \right)$$

the solution becomes:

$$c = \frac{1}{2} \exp\left\{\frac{xv'}{4D'_x}\right\} \sum_{i=1}^{NP} \Delta c_i \left(\exp\left\{-\frac{x\mu}{\sqrt{D'_x}}\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x}(t-t_i)} - \mu\sqrt{t-t_i}\right\} \right. \\ \left. + \exp\left\{\frac{x\mu}{\sqrt{D'_x}}\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x}(t-t_i)} + \mu\sqrt{t-t_i}\right\} \right)$$

where: $\mu = \left(\frac{v'^2}{4D'_x} + \lambda\right)^{\frac{1}{2}}$.

c. Exponentially-decaying Inflow Concentration

- General solution:

$$c = c_0 \frac{x}{2\sqrt{\pi D'_x}} \exp\{-\gamma t\} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-\frac{(x-v'\xi)^2}{4D'_x\xi} + (\gamma-\lambda)\xi\right\} d\xi$$

An alternative form of this situation is written by expanding the exponential term in the integrand:

$$\exp\left\{-\frac{(x-v'\xi)^2}{4D'_x\xi} + (\gamma-\lambda)\xi\right\} \\ = \exp\left\{-\frac{x^2 + 2xv'\xi - v'^2\xi^2}{4D'_x\xi} + (\gamma-\lambda)\xi\right\} \\ = \exp\left\{\frac{xv'}{2D'_x}\right\} \exp\left\{-\frac{x^2}{4D'_x\xi} - \left(\frac{v'^2\xi}{4D'_x} - (\gamma-\lambda)\right)\xi\right\}$$

Substituting into the solution yields:

$$c = c_0 \frac{x}{2\sqrt{\pi D'_x}} \exp\left\{-\gamma t + \frac{xv'}{2D'_x}\right\} \int_0^t \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-\frac{x^2}{4D'_x\xi} - \left(\frac{v'^2\xi}{4D'_x} - (\gamma-\lambda)\right)\xi\right\} d\xi$$

Alternative solution:

For the case of $\frac{v'^2}{4D'_x} \geq \gamma - \lambda$, we can make use of the integral:

$$\int_0^U \frac{1}{\xi^{\frac{3}{2}}} \exp\left\{-a^2\xi - \frac{b^2}{\xi}\right\} d\xi$$
$$= \frac{\sqrt{\pi}}{2b} \left(\exp\{-2ab\} \operatorname{erfc}\left\{\frac{b}{\sqrt{U}} - a\sqrt{U}\right\} + \exp\{2ab\} \operatorname{erfc}\left\{\frac{b}{\sqrt{U}} + a\sqrt{U}\right\} \right)$$

and the alternate solution can be written as:

$$c = \frac{c_0}{2} \exp\left\{-\gamma t + \frac{xv'}{2D'_x}\right\} \left(\exp\left\{-\frac{x\mu}{\sqrt{D'_x}}\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x t}} - \mu\sqrt{t}\right\} \right.$$
$$\left. + \exp\left\{\frac{x\mu}{\sqrt{D'_x}}\right\} \operatorname{erfc}\left\{\frac{x}{2\sqrt{D'_x t}} + \mu\sqrt{t}\right\} \right)$$

where: $\mu = \left(\frac{v'^2}{4D'_x} - (\gamma - \lambda)\right)^{\frac{1}{2}}$.