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: $V = \dfrac{q}{\theta} =$ 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: $v' = \dfrac{v}{R}$; $D_x^{'} = \dfrac{D_x}{R}$; $D_y^{'} = \dfrac{D_y}{R}$; $D_z^{'} = \dfrac{D_z}{R}$

Initial and Boundary Conditions

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

i) $x: \begin{bmatrix} c(0, y, z, t) = c_0(t)\left[H(y+y_0) - H(y-y_0)\right]\left[H(z-z_1) - H(z-z_2)\right] \\ c(\infty, y, z, t) = 0 \end{bmatrix}$

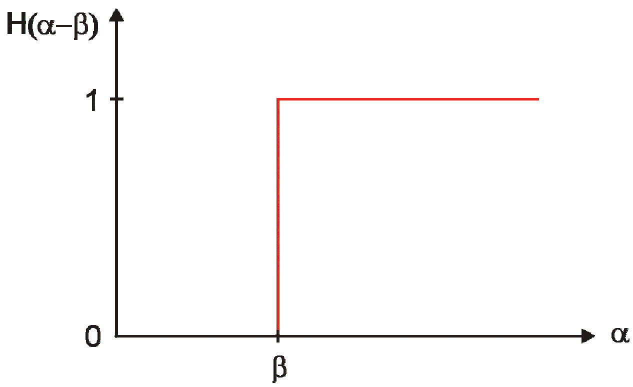
ii) $y: \begin{bmatrix} c(x, -\infty, z, t) = 0 \\ c(x, \infty, z, t) = 0 \end{bmatrix}$

iii) $z: \begin{bmatrix} \dfrac{\partial c}{\partial z}(x, y, 0, t) = 0 \\ \dfrac{\partial c}{\partial z}(x, y, B, t) = 0 \end{bmatrix}$

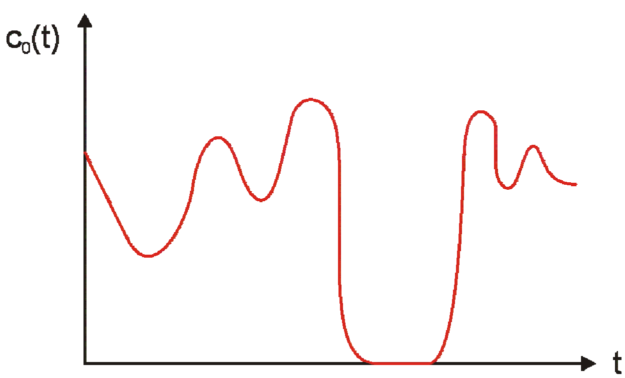
Interpretation of the inflow boundary conditions

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

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



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:

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

Substituting in the initial conditions:

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

The transformed boundary conditions are:

$$\overline{c}(0,y,z,p) = \overline{c}_0(p)\,\delta(y-y')\,\delta(z-z')$$
$$\overline{c}(\infty,y,z,p) = 0$$
$$\overline{c}(x,-\infty,z,p) = 0$$
$$\overline{c}(x,\infty,z,p) = 0$$
$$\frac{\partial \overline{c}}{\partial z}(x,y,0,p) = 0$$
$$\frac{\partial \overline{c}}{\partial z}(x,y,B,p) = 0$$

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

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

The transformed boundary conditions are:

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

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

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

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

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

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

Substituting in the boundary conditions:

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

The transformed boundary conditions are:

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

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

4) The transformed governing equation can be written as:

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

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:

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

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

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

a. $\underline{x \to \infty}$:

Since the solution is bounded, we must have:

$$B = 0$$

b. $\underline{x = 0}$:

The general solution reduces to:

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

Evaluating the boundary condition:

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

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

Therefore, the transformed solution is:

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

5) Applying the inverse Laplace transform:

$$\overline{\overline{c}} = L^{-1}\left[\overline{\overline{\overline{c}}}\right]$$

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

The inverse Laplace transform is evaluated using the convolution theorem:

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

Letting:

$$\overline{f}\left(p\right) = \overline{c}_0\left(p\right) \rightarrow f\left(t\right) = c_0\left(t\right)$$

$$\overline{g}\left(p\right) = \exp\left\{-\left(\frac{v'^2}{4D_x^{'}}+P\right)^{\frac{1}{2}}\frac{x}{\sqrt{D_x^{'}}}\right\}$$

The second inverse is evaluated using the shift theorem:

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

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

$$L^{-1}\left[\cdot\right] = \frac{x}{2\sqrt{\pi D_x^{'}}}t^{-\frac{3}{2}}\exp\left\{-\frac{x^2}{4D_x^{'}t}\right\}$$

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

Substituting into the convolution integral yields:

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

6) Applying the inverse Fourier exponential transform:

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

Re-arranging the order of operations we can write:

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

The inverse can be evaluated using the convolution theorem:

$$\Im_e^{-1}\left[\bar{f}(\alpha_1)\cdot\bar{g}(\alpha_1)\right] = \int_{-\infty}^{\infty} f(\xi)\,g(y-\xi)\,d\xi$$

Let:

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

Therefore, the inverse is:

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

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

$$\Im_e^{-1}[\cdot] = \frac{1}{2\sqrt{\pi D_y^{'}(t-\tau)}} \exp\left\{ -\frac{(y-y')^2}{4D_y^{'}(t-\tau)} \right\}$$

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

$$\overline{c} = \frac{x}{4\pi\sqrt{D_x^{'}D_y^{'}}} \cos\left(\frac{n\pi z'}{B}\right) \exp\left\{\frac{v'x}{2D_x^{'}}\right\} \int_0^t c_0(\tau) \frac{1}{(t-\tau)^2}$$
$$\cdot \exp\left\{ -\left[\left(\lambda + D_z^{'}\frac{n^2\pi^2}{B^2}\right) + \frac{v'^2}{4D_x^{'}}\right](t-\tau) - \frac{x^2}{4D_x^{'}(t-\tau)} - \frac{(y-y')^2}{4D_y^{'}(t-\tau)} \right\} d\tau$$

7) Applying the inverse Fourier cosine transform:

$$c = \Im_c^{-1}[\overline{c}]$$
$$= \frac{\overline{c}(n=0)}{B} + \frac{2}{B}\sum_{n=1}^{\infty} \overline{c}(n) \cos\left(\frac{n\pi z}{B}\right)$$

$\therefore$

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

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

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

Collecting terms and simplifying:

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

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.

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

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

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

Re-arranging the order of integration:

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

Noting the following integrals:

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

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

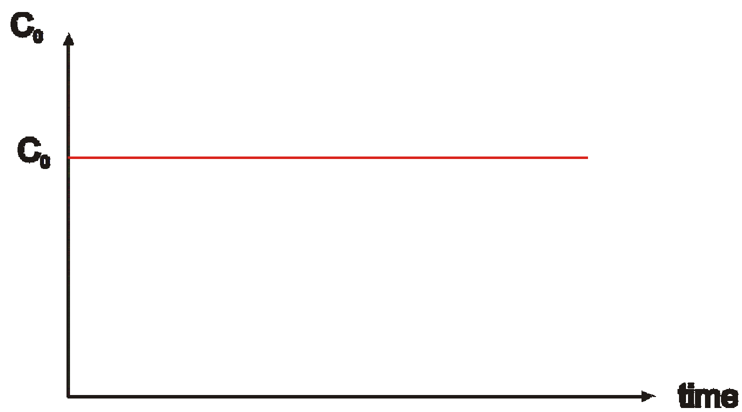
The final form of the solution becomes:

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

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:

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

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:

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

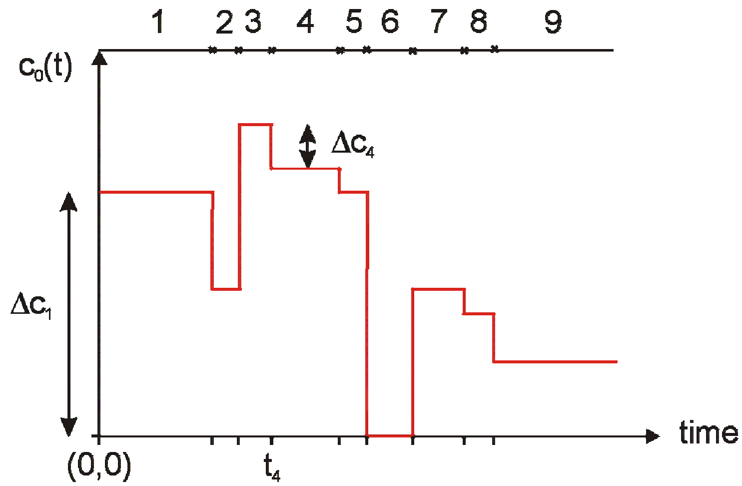
$$\xi = t \rightarrow \tau = t^{\frac{1}{4}}$$

Therefore, the solution can be rewritten as:

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

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:

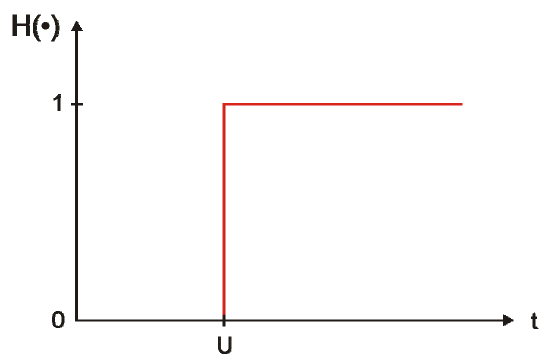


Denoting t_i as the starting time for the i^{th} step, and ΔC_i as the concentration change at the start of the i^{th} step, the inflow concentration history is defined as:

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

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

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



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

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

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

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

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:

$$\boxed{\begin{aligned} c = {} & \frac{x}{4\sqrt{\pi}\sqrt{D_x^{'}}}\sum_{i=1}^{NP}\Delta C_i \int_0^{t-t_i}\frac{1}{\xi^{\frac{3}{2}}}\exp\left\{-\lambda\xi-\frac{\left(x-v'\xi\right)^2}{4D_x^{'}\xi}\right\} \\ & \cdot\left[erfc\left\{\frac{y-y_0}{2\sqrt{D_y^{'}\xi}}\right\}-erfc\left\{\frac{y+y_0}{2\sqrt{D_y^{'}\xi}}\right\}\right]\left(\frac{\left(z_2-z_1\right)}{B}\right. \\ & \left.+\frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\left[\sin\left(\frac{n\pi z_2}{B}\right)-\sin\left(\frac{n\pi z_1}{B}\right)\right]\cos\left(\frac{n\pi z}{B}\right)\exp\left\{-D_z^{'}\frac{n^2\pi^2}{B^2}\xi\right\}\right)d\xi \end{aligned}}$$

<u>Note</u>:

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:

Let: $\tau = \xi^{\frac{1}{4}}$

$\rightarrow\ \xi = \tau^4 \qquad ;\ d\xi = 4\tau^3 d\tau$

the limits of integration become:

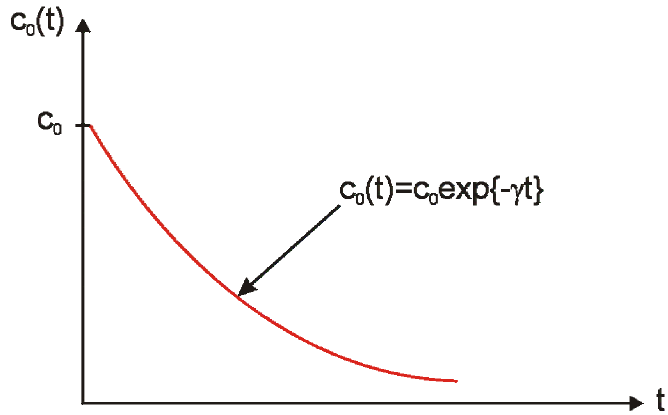
$$\begin{aligned} \xi &= 0 && \rightarrow \tau = 0 \\ \xi &= t-t_i && \rightarrow \tau = \left(t-t_i\right)^{\frac{1}{4}} \end{aligned}$$

and the solution is written as:

$$\begin{aligned} c = {} & \frac{x}{4\sqrt{\pi}\sqrt{D_x^{'}}}\sum_{i=1}^{NP}\Delta C_i 4\int_0^{(t-t_i)^{\frac{1}{4}}}\frac{1}{\tau^3}\exp\left\{-\lambda\tau^4-\frac{\left(x-v'\tau^4\right)^2}{4D_x^{'}\tau^4}\right\} \\ & \cdot\left[erfc\left\{\frac{y-y_0}{2\sqrt{D_y^{'}\tau^4}}\right\}-erfc\left\{\frac{y+y_0}{2\sqrt{D_y^{'}\tau^4}}\right\}\right]\left(\frac{\left(z_2-z_1\right)}{B}\right. \\ & \left.+\frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\left[\sin\left(\frac{n\pi z_2}{B}\right)-\sin\left(\frac{n\pi z_1}{B}\right)\right]\cos\left(\frac{n\pi z}{B}\right)\exp\left\{-D_z^{'}\frac{n^2\pi^2}{B^2}\tau^4\right\}\right)d\tau \end{aligned}$$

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:

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

$$\cdot \left[erfc\left\{ \frac{y-y_0}{2\sqrt{D_y^{'}(t-\tau)}} \right\} - erfc\left\{ \frac{y+y_0}{2\sqrt{D_y^{'}(t-\tau)}} \right\} \right] \left(\frac{(z_2 - z_1)}{B} \right.$$

$$\left. + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \exp\left\{ -D_z^{'} \frac{n^2\pi^2}{B^2}(t-\tau) \right\} \right) d\tau$$

Collecting terms and re-arranging slightly:

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

$$\cdot \left[erfc\left\{ \frac{y-y_0}{2\sqrt{D_y^{'}(t-\tau)}} \right\} - erfc\left\{ \frac{y+y_0}{2\sqrt{D_y^{'}(t-\tau)}} \right\} \right] \left(\frac{(z_2 - z_1)}{B} \right.$$

$$\left. + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right) \right] \cos\left(\frac{n\pi z}{B}\right) \exp\left\{ -D_z^{'} \frac{n^2\pi^2}{B^2}(t-\tau) \right\} \right) d\tau$$

Rearranging, this can be written as:

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

Make a change of variables:

Define: $\xi = t - \tau$

$\therefore$ $d\tau = -d\xi$

the limits of integration become:

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

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

and the integral is written as:

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

Note:

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

Letting: $\tau = \xi^{\frac{1}{4}}$

$\rightarrow \quad \xi = \tau^4 \qquad ; \; d\xi = 4\tau^3 d\tau$

the limits of integration become:

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

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

The solution is written as:

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

Check:

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

Substituting for $\gamma = 0.0$ yields:

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

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.

$$\boxed{\begin{aligned} z_1 &= 0 \\ z_2 &= B \end{aligned}}$$

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

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

a. Solution for a Constant Patch Concentration

$$c_0(t) = c_0$$

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

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

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

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

b. <u>Dicretized Inflow Concentration History</u>

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

c. <u>Exponentially-decaying Inflow Concentration</u>

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

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.

$$\boxed{y_0 \to \infty}$$

Noting the following limits:

$$erfc(-\infty) = 2$$
$$erfc(\infty) = 0$$

the general solution reduces to:

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

a. Constant Patch Concentration

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

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

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

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

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:

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

Substituting for *a* and *b*, I_1 becomes:

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

(ii) Evaluating the second integral:

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

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:

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

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:

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

Substituting for I_1 and I_2:

$$c = \frac{x}{2\sqrt{\pi D_x^{'}}}\left[I_1 + I_2\right]$$

$$= \frac{x}{2\sqrt{\pi D_x^{'}}}\left[\!\left[\frac{(z_2 - z_1)}{B}\exp\left\{\frac{xv'}{2D_x^{'}}\right\}\frac{\sqrt{\pi D_x^{'}}}{x}\right.\right.$$

$$\left(\exp\left\{-\frac{x}{\sqrt{D_x^{'}}}\left(\frac{v'^2}{4D_x^{'}} + \lambda\right)^{\frac{1}{2}}\right\}erfc\left\{\frac{x}{2\sqrt{D_x^{'}t}} - \left(\frac{v'^2}{4D_x^{'}} + \lambda\right)^{\frac{1}{2}}\sqrt{t}\right\}\right.$$

$$\left. + \exp\left\{\frac{x}{\sqrt{D_x^{'}}}\left(\frac{v'^2}{4D_x^{'}} + \lambda\right)^{\frac{1}{2}}\right\}erfc\left\{\frac{x}{2\sqrt{D_x^{'}t}} + \left(\frac{v'^2}{4D_x^{'}} + \lambda\right)^{\frac{1}{2}}\sqrt{t}\right\}\right)$$

$$+ \frac{2}{\pi}\exp\left\{\frac{xv'}{2D_x^{'}}\right\}\sum_{n=1}^{\infty}\frac{1}{n}\left[\sin\left(\frac{n\pi z_2}{B}\right) - \sin\left(\frac{n\pi z_1}{B}\right)\right]\cos\left(\frac{n\pi z}{B}\right)$$

$$\cdot\frac{\sqrt{\pi D_x^{'}}}{x}\left(\exp\left\{-\frac{x}{\sqrt{D_x^{'}}}\mu_n\right\}erfc\left\{\frac{x}{2\sqrt{D_x^{'}t}} - \mu_n\sqrt{t}\right\}\right.$$

$$\left.\left.\left. + \exp\left\{\frac{x}{\sqrt{D_x^{'}}}\mu_n\right\}erfc\left\{\frac{x}{2\sqrt{D_x^{'}t}} + \mu_n\sqrt{t}\right\}\right)\right]\!\right]$$

Simplifying:

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

b. Discretized Inflow Concentration History

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

Defining the integral as:

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

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:

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

Substituting for *a* and *b*, I_1 becomes:

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

(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:

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

Assembling the final solution and simplifying:

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

c. <u>Exponentially-decaying Inflow Concentration</u>

- General solution:

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

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

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

(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:

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

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

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:

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

Substituting for *a* and *b*, I_1 becomes:

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

(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:

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

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:

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

Substituting for I_1 and I_2:

$$c = \frac{x}{2\sqrt{\pi D_x^{'}}} \sum_{i=1}^{NP} \Delta c_i \left[\!\!\left[\frac{\left(z_2 - z_1\right)}{B} \exp\left\{ \frac{xv'}{2D_x^{'}} \right\} \frac{\sqrt{\pi D_x^{'}}}{x} \right.\right.$$

$$\cdot \left(\exp\left\{ -\frac{x}{\sqrt{D_x^{'}}} \left(\frac{v'^2}{4D_x^{'}} + \lambda \right)^{\frac{1}{2}} \right\} erfc\left\{ \frac{x}{2\sqrt{D_x^{'}t}} - \left(\frac{v'^2}{4D_x^{'}} + \lambda \right)^{\frac{1}{2}} \sqrt{t} \right\} \right.$$

$$\left. + \exp\left\{ \frac{x}{\sqrt{D_x^{'}}} \left(\frac{v'^2}{4D_x^{'}} + \lambda \right)^{\frac{1}{2}} \right\} erfc\left\{ \frac{x}{2\sqrt{D_x^{'}t}} + \left(\frac{v'^2}{4D_x^{'}} + \lambda \right)^{\frac{1}{2}} \sqrt{t} \right\} \right)$$

$$+ \frac{2}{\pi} \exp\left\{ \frac{xv'}{2D_x^{'}} \right\} \sum_{n=1}^{\infty} \frac{1}{n} \left[\sin\left(\frac{n\pi z_2}{B} \right) - \sin\left(\frac{n\pi z_1}{B} \right) \right] \cos\left(\frac{n\pi z}{B} \right) \frac{\sqrt{\pi D_x^{'}}}{x}$$

$$\cdot \left(\exp\left\{ -\frac{x}{\sqrt{D_x^{'}}} \mu_n \right\} erfc\left\{ \frac{x}{2\sqrt{D_x^{'}t}} - \mu_n \sqrt{t} \right\} \right.$$

$$\left.\left.\left. + \exp\left\{ \frac{x}{\sqrt{D_x^{'}}} \mu_n \right\} erfc\left\{ \frac{x}{2\sqrt{D_x^{'}t}} + \mu_n \sqrt{t} \right\} \right) \right]\!\!\right]$$

Simplifying yields the final form of the solution:

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

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.,

$$\boxed{\begin{aligned} z_1 &= 0 \\ z_2 &= B \\ y_0 &\to \infty \end{aligned}}$$

For this case the general solution reduces to:

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

a. <u>Constant Inflow Concentration</u>

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

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

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

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

Expanding the exponential term in the integrand:

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

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:

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

Substituting for *a* and *b*:

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

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

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

$$\therefore \quad I = \frac{\sqrt{\pi D_x^{'}}}{x}\left(\exp\left\{-\frac{x}{\sqrt{D_x^{'}}}\left(\frac{v'^2}{4D_x^{'}} + \lambda\right)^{\frac{1}{2}}\right\} erfc\left\{\frac{1}{\sqrt{t}}\left[\left(\frac{x^2}{4D_x^{'}}\right)^{\frac{1}{2}} - \left(\frac{v'^2}{4D_x^{'}} + \lambda\right)^{\frac{1}{2}} t\right]\right\}\right.$$

$$\left. + \exp\left\{\frac{x}{\sqrt{D_x^{'}}}\left(\frac{v'^2}{4D_x^{'}} + \lambda\right)^{\frac{1}{2}}\right\} erfc\left\{\frac{1}{\sqrt{t}}\left[\left(\frac{x^2}{4D_x^{'}}\right)^{\frac{1}{2}} + \left(\frac{v'^2}{4D_x^{'}} + \lambda\right)^{\frac{1}{2}} t\right]\right\}\right)$$

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

$$
\begin{aligned}
c &= c_0 \frac{x}{2\sqrt{\pi D_x'}} \exp\left\{ -\frac{xv'}{4D_x'} \right\} \frac{\sqrt{\pi D_x'}}{x} \\
&\cdot \left(\exp\left\{ -\frac{x\mu}{\sqrt{D_x'}} \right\} erfc\left\{ \frac{x}{2\sqrt{D_x' t}} - \mu\sqrt{t} \right\} + \exp\left\{ \frac{x\mu}{\sqrt{D_x'}} \right\} erfc\left\{ \frac{x}{2\sqrt{D_x' t}} + \mu\sqrt{t} \right\} \right)
\end{aligned}
$$

Simplifying:

$$
\boxed{
\begin{aligned}
c &= c_0 \frac{1}{2} \exp\left\{ -\frac{xv'}{4D_x'} \right\} \\
&\cdot \left(\exp\left\{ -\frac{x\mu}{\sqrt{D_x'}} \right\} erfc\left\{ \frac{x}{2\sqrt{D_x' t}} - \mu\sqrt{t} \right\} + \exp\left\{ \frac{x\mu}{\sqrt{D_x'}} \right\} erfc\left\{ \frac{x}{2\sqrt{D_x' t}} + \mu\sqrt{t} \right\} \right)
\end{aligned}
}
$$

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:

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

the solution becomes:

$$\boxed{\begin{aligned}c = \frac{1}{2}\exp\left\{\frac{xv'}{4D_x^{'}}\right\}\sum_{i=1}^{NP}\Delta c_i\Bigg(&\exp\left\{-\frac{x\mu}{\sqrt{D_x^{'}}}\right\}erfc\left\{\frac{x}{2\sqrt{D_x^{'}\left(t-t_i\right)}}-\mu\sqrt{t-t_i}\right\}\\ &+\exp\left\{\frac{x\mu}{\sqrt{D_x^{'}}}\right\}erfc\left\{\frac{x}{2\sqrt{D_x^{'}\left(t-t_i\right)}}+\mu\sqrt{t-t_i}\right\}\Bigg)\end{aligned}}$$

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

c. <u>Exponentially-decaying Inflow Concentration</u>

- General solution:

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

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

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

Substituting into the solution yields:

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

Alternative solution:

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

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

and the alternate solution can be written as:

$$\boxed{\begin{aligned} c = \frac{c_0}{2}\exp\left\{-\gamma t + \frac{xv'}{2D_x'}\right\}\Bigg(&\exp\left\{-\frac{x\mu}{\sqrt{D_x'}}\right\} erfc\left\{\frac{x}{2\sqrt{D_x' t}} - \mu\sqrt{t}\right\} \\ &+ \exp\left\{\frac{x\mu}{\sqrt{D_x'}}\right\} erfc\left\{\frac{x}{2\sqrt{D_x' t}} + \mu\sqrt{t}\right\}\Bigg) \end{aligned}}$$

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