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Techniques of Water-Resources Investigations of the United States Geological Survey

Chapter B7

ANALYTICAL SOLUTIONS FOR ONE-, TWO-, AND THREE-DIMENSIONAL SOLUTE TRANSPORT IN GROUND-WATER SYSTEMS WITH UNIFORM FLOW

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Book 3 APPLICATIONS OF HYDRAULICS

Attachment 1.—Derivation of Selected Analytical Solutions

Aquifer of infinite width and height with finite-width and finite-height solute source Aquifer of finite width and height with finite-width and finite-height solute source Aquifer of infinite width and height with continuous point source

AQUIFER OF INFINITE WIDTH AND HEIGHT WITH FINITE-WIDTH AND FINITE-HEIGHT SOLUTE SOURCE

The following is a step-by-step derivation of the analytical solution for solute transport in an aquifer of infinite length, width, and height containing a solute source of finite width and finite height (patch source) in a steady flow field (eq. 121 in the text).

The governing three-dimensional solute-transport equation is

$$\frac{\partial c}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - V \frac{\partial C}{\partial x} - \lambda C.$$
(A1.1)

Boundary and initial conditions are

$$\begin{array}{l} C = C_{o}, \; x = 0 \; \text{and} \; Y_{1} < \; y < Y_{2} \\ \text{and} \; Z_{1} < z < Z_{2} \end{array} \tag{A1.2a}$$

$$C (\infty, y, z, t) = 0$$
 (A1.3)

$$C(x, \pm \infty, z, t) = 0$$
 (A1.4)

C (x, y,
$$\pm \infty$$
, t)=0 (A1.5)

$$C(x, y, z, 0)=0$$
 (A1.6)

where

V is the velocity in x-direction,

Y₁, is the y-coordinate of the lower limit of solute source,

 Y_2 is the y-coordinate of the upper limit of solute source,

 Z_1 , is the z-coordinate of the lower limit of solute source, and

 Z_2 is the z-coordinate of the upper limit of solute source.

STEP 1:

To solve equation A1.1 for the patch source, first solve the partial differential equation for solute transport in an aquifer with an instantaneous point source at the inflow end (at x=0). The governing equations are identical, but the boundary condition at x=0 (eq. A1.2) is rewritten as

C (0, y, z, t)=C_o
$$\delta(y-y') \delta(z-z') \delta(t-t')$$
 at x=0,

where

 δ () is the dirac delta function,

y' and z' are the coordinates of the point source, and

t' is time at which the instantaneous point source starts and ends.

STEP 2:

A variable transformation is applied to remove the advective and solute-decay terms, where

$$c = C \exp\left[-\frac{Vx}{2D_x} + \frac{V^2 t}{4D_x} + \lambda t\right].$$
 (A1.7)

The resulting transformed solute-transport equation and boundary and initial conditions are

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

c (o, y, z, t)=C_o exp $\left[\frac{V^2 t}{4D_x} + \lambda t\right] \delta(y-y') \delta(z-z') \delta(t-t')$ (A1.8)

$$c (\infty, y, z, t) = 0$$
 (A1.9)

$$c (x, \pm \infty, z, t) = 0$$
 (A1.10)

$$c (x, y, \pm \infty, t) = 0$$
 (A1.11)

$$c (x, y, z, 0) = 0$$
 (A1.12)

STEP 3:

The x-derivative term is removed by applying the Fourier sine transform, defined by Churchill (1972, p. 401–402) as

S [F(x)]=
$$\overline{F}(\alpha) = \int_{\alpha}^{\infty} F(x) \sin(\alpha x) dx$$
 (A1.13)

with inverse

$$S^{-1}[\overline{F}(\alpha)] = F(x) = \frac{2}{\pi} \int_{0}^{\infty} \overline{F}(\alpha) \sin(\alpha x) d\alpha$$
 (A1.14)

and with an operational property

$$S\left[\frac{d^{2}F(x)}{dx^{2}}\right] = -\alpha^{2}\overline{F} + \alpha F(0), \qquad (A1.15)$$

where F(0) is the function evaluated at x=0. The transformed equation and boundary and initial conditions are

$$\frac{\partial \bar{c}}{\partial t} + \alpha^2 D_x \bar{c} - D_y \frac{\partial^2 \bar{c}}{\partial y^2} - D_z \frac{\partial^2 \bar{c}}{\partial z^2} - \alpha D_x C_o \exp\left[\frac{V^2 t}{4D_x} + \lambda t\right] \delta(y - y') \,\,\delta(z - z') \,\,\delta(t - t') = 0 \quad (A1.16)$$

$$\bar{c} (\alpha, \pm \infty, z, t) = 0$$
(A1.17)

$$\bar{c} (\alpha, y, \pm \infty, t) = 0$$
 (A1.18)

$$\bar{c} (\alpha, y, z, 0) = 0.$$
 (A1.19)

STEP 4:

The y-derivative is removed by applying the exponential Fourier transform, defined by Churchill (1972, p. 384–385) as

$$E [G(y)] = \overline{G}(\beta) = \int_{-\infty}^{+\infty} G(y) \exp [-i\beta y] dy$$
 (A1.20)

with inverse

$$\mathbf{E}^{-1}\left[\bar{\mathbf{G}}(\boldsymbol{\beta})\right] = \mathbf{G}(\mathbf{y}) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \bar{\mathbf{G}}(\boldsymbol{\beta}) \exp\left[-\mathrm{i}\boldsymbol{\beta}\mathbf{y}\right] d\boldsymbol{\beta}$$
(A1.21)

and with an operational property

$$\mathbf{E}\left[\frac{\mathrm{d}^{2}\mathbf{G}(\mathbf{y})}{\mathrm{d}\mathbf{y}^{2}}\right] = -\beta^{2} \ \bar{\mathbf{G}}(\beta), \tag{A1.22}$$

where $i=\sqrt{-1}$. The transformed equation and boundary and initial conditions are

$$\frac{\partial \overline{\overline{c}}}{\partial t} + \alpha^2 D_x \overline{\overline{c}} + \beta^2 D_y \overline{\overline{c}} - D_z \frac{\partial^2 \overline{\overline{c}}}{\partial z^2} - \alpha D_x C_o \exp\left[\frac{V^2 t}{4D_x} + \lambda t\right]$$
$$\cdot \int_{-\infty}^{+\infty} e^{-i\beta y} \,\delta(y - y') \,\delta(z - z') \,\delta(t - t') \,dy = 0$$
(A1.23)

$$\overline{\overline{c}} (\alpha, \beta, \pm \infty, t) = 0$$
 (A1.24)

$$\overline{\overline{c}} (\alpha, \beta, z, o) = 0.$$
(A1.25)

STEP 5:

The exponential Fourier transform is applied again to remove the z-derivative. Also, by definition, the integral of a function multiplied by the dirac delta function (last term in eq. A1.23) is equal to the function evaluated at the coordinate of the point source; that is

$$\int F(x)\delta(x-x')dx = F(x').$$
 (A1.26)

Thus, the transformed equation and initial condition are given by

$$\frac{d\overline{\overline{c}}}{dt} + \left(\alpha^2 D_x + \beta^2 D_y + \gamma^2 D_z\right)\overline{\overline{c}} - \alpha D_x C_o \exp\left[\frac{V^2 t}{4D_x} + \lambda t - i\beta y' - i\gamma z'\right] \cdot \delta(t - t') = 0$$
(A1.27)

$$\overline{\overline{c}} (\alpha, \beta, \gamma, 0) = 0.$$
(A1.28)

STEP 6:

The transformed ordinary differential equation is solved for $\overline{\overline{c}}$ using an integrating factor; that is, given a differential equation of the form

$$\frac{\mathrm{d}w}{\mathrm{d}t} + gw = h(t), \tag{A1.29}$$

the solution is given by

$$w = \frac{1}{p(t)} \int_{t_o}^{t} p(\tau) h(\tau) d\tau + w_o \frac{p(t)}{p(t_o)},$$
 (A1.30)

where the integrating factor p(t) is given by

$$p(t) = \exp[\int g(\tau) d\tau]. \tag{A1.31}$$

Applied to equation A1.27, this yields

$$\overline{\overline{c}} = \frac{\alpha D_x C_o \exp[-i\beta y' - i\gamma z']}{\exp[\alpha^2 D_x t + \beta^2 D_y t + \gamma^2 D_z t]} \int_0^t \exp\left[\alpha^2 D_x + \beta^2 D_y + \gamma^2 D_z + \frac{V^2}{4D_x} + \lambda\right] \cdot \tau \,\,\delta(\tau - t') \,\,d\tau. \,(A1.32)$$

Integrating equation A1.32 and grouping like terms gives

$$\overline{\overline{c}} = \alpha D_x C_o \exp\left[\frac{V^2 t'}{4D_x} + \lambda t' - \alpha^2 D_x (t - t') - i\beta y' - \beta^2 D_y (t - t') - i\gamma z' - \gamma^2 D_z (t - t')\right].$$
(A1.33)

STEP 7:

The inverse Fourier sine transform (eq. A1.14) is applied to remove the α term; that is

$$\overline{\overline{c}} = D_{x}C_{o} \exp\left[\frac{V^{2}t'}{4D_{x}} + \lambda t' - i\beta y' - \beta^{2}D_{y}(t-t') - i\gamma z' - \gamma^{2}D_{z}(t-t')\right]$$

$$\cdot S^{-1}\left\{\alpha \exp\left[-\alpha^{2}D_{x}(t-t')\right]\right\}.$$
(A1.34)

From a table of inverse Fourier sine transforms given in Churchill (1972, p. 424, eq. D.1.26)

$$S^{-1}\left[\alpha \exp\left(-a\alpha^{2}\right)\right] = \frac{x}{2a\sqrt{\pi a}} \exp\left(\frac{-x^{2}}{4a}\right).$$
(A1.35)

Applied to equation A1.35, this yields

$$\overline{\overline{c}} = C_{o} \exp\left[\frac{V^{2}t'}{4D_{x}} + \lambda t' - i\beta y' - \beta^{2}D_{y}(t-t') - i\gamma z' - \gamma^{2}D_{z}(t-t')\right]$$

$$\cdot \frac{x}{2(t-t')\sqrt{\pi D_{x}(t-t')}} \exp\left[\frac{-x^{2}}{4D_{x}(t-t')}\right].$$
(A1.36)

STEP 8:

The inverse exponential Fourier transform (eq. A1.21) is applied to remove the β terms; that is

$$\bar{c} = \frac{C_{o}x}{2(t-t')\sqrt{\pi D_{x}(t-t')}} \exp\left[\frac{V^{2}t'}{4D_{x}} + \lambda t' - \frac{x^{2}}{4D_{x}(t-t')} - i\gamma z' - \gamma^{2}D_{z}(t-t')\right]$$

$$\cdot E^{-1}\left\{\exp\left[-i\beta y' - \beta^{2} D_{y}(t-t')\right]\right\}.$$
(A1.37)

Multiplying through by $\frac{2\sqrt{\pi D_y(t-t')}}{2\sqrt{\pi D_y(t-t')}}$

and using the shift theorem (Churchill, 1972, p. 471, eq. C.1.5) given by

$$\mathbf{E}^{-1} \{ \exp[i\alpha\beta] \overline{\mathbf{G}}(\beta) \} = \mathbf{G}(\mathbf{y} + \mathbf{a})$$
(A1.38)

and equation C.1.20 from the table of inverse exponential Fourier transforms (Churchill, 1972, p. 472) given by

$$\mathbf{E}^{-1}[2\sqrt{\pi a}\exp[-a\beta^2]] = \exp\left[-\frac{y^2}{4a}\right],\tag{A1.39}$$

yields

$$\bar{c} = \frac{C_{o}x}{4\pi(t-t')^{2}\sqrt{D_{x}D_{y}}} exp\left[\frac{V^{2}t'}{4D_{x}} + \lambda t' - \frac{x^{2}}{4D_{x}(t-t')} - i\gamma z' - \gamma^{2}D_{z}(t-t')\right] \cdot exp\left[-\frac{(y-y')^{2}}{4D_{y}(t-t')}\right].$$
(A1.40)

STEP 9:

Next multiply through by $\frac{2\sqrt{\pi D_z(t-t')}}{2\sqrt{\pi D_z(t-t')}}$ and apply the inverse exponential Fourier transform (eq. A1.21) to remover the γ terms; that is

$$c = \frac{C_{o}x}{8\pi^{-3/2}(t-t')^{-5/2}\sqrt{D_{x}D_{y}D_{z}}} exp\left[\frac{V^{2}t'}{4D_{x}} + \lambda t' - \frac{x^{2}}{4D_{x}(t-t')} - \frac{(y-y')^{2}}{4D_{y}(t-t')}\right]$$

• $E^{-1}\left\{2\sqrt{\pi D_{z}(t-t')}exp\left[-i\gamma z' - \gamma^{2}D_{z}(t-t')\right]\right\}.$ (A1.41)

Applying the shift theorem and inverse transform (eqs. A1.38 and A1.39) yields

$$c = \frac{C_o x}{8\pi^{3/2} (t-t')^{5/2} \sqrt{D_x D_y D_z}} exp \left[\frac{V^2 t'}{4D_x} + \lambda t' - \frac{x^2}{4D_x (t-t')} - \frac{(y-y')^2}{4D_y (t-t')} - \frac{(z-z')^2}{4D_z (t-t')} \right].$$
(A1.42)

STEP 10:

The transformed variable is converted back from c to C by multiplying both sides of equation A1.42 by

$$exp \left[\frac{Vx}{2D_x} - \frac{V^2t}{4D_x} - \lambda t \right]$$

(see eq. A1.7) to yield the analytical solution to the solute-transport equation for an *instantaneous point* source

$$C = \frac{C_{0}x}{8\pi^{3/2}(t-t')^{5/2}\sqrt{D_{x}D_{y}D_{z}}} exp\left[-\frac{V^{2}(t-t')}{4D_{x}} - \lambda(t-t') + \frac{Vx}{2D_{x}} - \frac{x^{2}}{4D_{x}(t-t')} - \frac{(y-y')^{2}}{4D_{y}(t-t')} - \frac{(z-z')^{2}}{4D_{z}(t-t')}\right].$$
(A1.43)

STEP 11:

The equation for an instantaneous line source of finite length along the y-axis is derived by integrating equation A1.43 from $y'=Y_1$ to $y'=Y_2$; that is

$$C = \frac{C_{0}x}{8\pi^{3/2} (t-t')^{5/2} \sqrt{D_{x}D_{y}D_{z}}} exp\left[-\frac{V^{2}(t-t')}{4D_{x}} - \lambda(t-t') + \frac{Vx}{2D_{x}} - \frac{x^{2}}{4D_{x}(t-t')} - \frac{(z-z')^{2}}{4D_{z}(t-t')}\right]$$

$$\bullet \int_{Y_{1}}^{Y_{2}} exp\left[-\frac{(y-y')^{2}}{4D_{y}(t-t')}\right] dy'.$$
(A1.44)

The integral in equation A1.44 can be found in a table of integrals by Abramowitz and Stegun (1964, p. 303, eq. 7.4.32) given as

$$\int \exp\left[-(ax^2+2bx+c)\right] dx = \frac{1}{2}\sqrt{\frac{\pi}{a}} \exp\left[\frac{b^2-ac}{a}\right] \cdot \exp\left(\sqrt{a}x + \frac{b}{\sqrt{a}}\right) + C, \quad (A1.45)$$

where erf(x) is the error function, and C is an arbitrary constant. Letting

$$x=y', \eta=4D_y(t-t'), a=\frac{1}{\eta}, b=\frac{-y}{\eta}, and c=\frac{y^2}{\eta},$$

the integral in equation A1.44 can be simplified to

$$I = \frac{\sqrt{\pi\eta}}{2} \left\{ \frac{\operatorname{erf}(Y_2 - y)}{\sqrt{\eta}} - \frac{\operatorname{erf}(Y_1 - y)}{\sqrt{\eta}} \right\}$$
(A1.46)

 \mathbf{or}

$$I = \sqrt{\pi D_{y}(t-t')} \left\{ erfc \left[\frac{Y_{1} - y}{2\sqrt{D_{y}(t-t')}} \right] - erfc \left[\frac{Y_{2} - y}{2\sqrt{D_{y}(t-t')}} \right] \right\},$$
(A1.47)

where erfc is the complementary error function, 1 - erf(x); thus, the analytical solution for an *instantaneous line* source is given by

$$C = \frac{C_{o}x}{8\pi(t-t')^{2}\sqrt{D_{x}D_{z}}} \exp\left[-\frac{V^{2}(t-t')}{4D_{x}} - \lambda(t-t') + \frac{Vx}{2D_{x}} - \frac{x^{2}}{4D_{x}(t-t')} - \frac{(z-z')^{2}}{4D_{z}(t-t')}\right] \\ \cdot \left\{ \operatorname{erfc}\left[\frac{Y_{1}-y}{2\sqrt{D_{y}(t-t')}}\right] - \operatorname{erfc}\left[\frac{Y_{2}-y}{2\sqrt{D_{y}(t-t')}}\right] \right\}.$$
(A1.48)

STEP 12:

The z' terms in equation A1.44 are integrated similarly from $z'=Z_1$ to $z'=Z_2$ to obtain the solution for an *instantaneous patch* source using equation A1.47; that is

$$C = \frac{C_{o}x}{8\sqrt{\pi D_{x}(t-t')}} \exp\left[-\frac{V^{2}(t-t')}{4D_{x}} - \lambda(t-t') + \frac{Vx}{2D_{x}} - \frac{x^{2}}{4D_{x}(t-t')}\right] \cdot \left\{ \operatorname{erfc}\left[\frac{Y_{1}-y}{2\sqrt{D_{y}(t-t')}}\right] - \operatorname{erfc}\left[\frac{Y_{2}-y}{2\sqrt{D_{y}(t-t')}}\right] \right\} \cdot \left\{ \operatorname{erfc}\left[\frac{Z_{1}-z}{2\sqrt{D_{z}(t-t')}}\right] - \operatorname{erfc}\left[\frac{Z_{2}-z}{2\sqrt{D_{z}(t-t')}}\right] \right\}.$$
(A1.49)

STEP 13:

To derive a solution for a continuous patch source, integrate equation A1.49 from t'=0 to t'=t. To simplify the integration, let $\tau=(t-t')$ and $d\tau=-dt'$; that is

$$C = \frac{C_{o}x \exp\left[\frac{Vx}{2D_{x}}\right]}{8\sqrt{\pi D_{x}}} \int_{0}^{t} \tau^{-3/2} \exp\left[-\frac{V^{2}\tau}{4D_{x}} - \lambda\tau - \frac{x^{2}}{4D_{x}\tau}\right] \cdot \left\{ \operatorname{erfc}\left[\frac{(Y_{1}-y)}{2\sqrt{D_{y}\tau}}\right] - \operatorname{erfc}\left[\frac{(Y_{2}-y)}{2\sqrt{D_{y}\tau}}\right] \right\}$$
$$\cdot \left\{ \operatorname{erfc}\left[\frac{(Z_{1}-z)}{2\sqrt{D_{z}\tau}}\right] - \operatorname{erfc}\left[\frac{(Z_{2}-z)}{2\sqrt{D_{z}\tau}}\right] \right\} d\tau.$$
(A1.50)

Equation A1.50 is identical to equation 121a in the text. The integral in the solution could not easily be simplified further and must be evaluated numerically.

AQUIFER OF FINITE WIDTH AND HEIGHT WITH FINITE-WIDTH AND FINITE-HEIGHT SOLUTE SOURCE

The following is a step-by-step derivation of the analytical solution for solute transport in an aquifer of infinite length and finite width and height containing a solute source of finite width and finite height (patch source) in a steady flow field (eq. 114 in the text).

The governing three-dimensional solute-transport equation is

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - V \frac{\partial C}{\partial x} - \lambda C.$$
(A1.51)

Boundary and initial conditions are

C (o, y, z, t)=C_o, for
$$Y_1 < y < Y_2$$

 $Z_1 < z < Z_2$ (A1.52)

C (o, y, z, t)=0, for
$$y < Y_1$$
 or $y > Y_2$
 $z < Z_1$ or $z > Z_2$

C,
$$\frac{\partial C}{\partial y} = 0$$
, $y = 0$, $y = W$ (A1.53)

C,
$$\frac{\partial C}{\partial z} = 0$$
, $z=0$, $z=H$ (A1.54)

C,
$$\frac{\partial C}{\partial x} = 0$$
, $x = \infty$ (A1.55)

C
$$(x, y, z, 0)=0,$$
 (A1.56)

where

V is the velocity in x-direction,

Y₁ is the y-coordinate of the lower limit of solute source,

 Y_2 is the y-coordinate of the upper limit of solute source,

 Z_1 is the z-coordinate of the lower limit of solute source,

 Z_2 is the z-coordinate of the upper limit of solute source,

W is the aquifer width, and

H is the aquifer height.

STEP 1:

To solve equation A1.51 for the patch source, a variable transformation is applied to remove the advective and solute-decay terms, where

$$c = C \exp\left[-\frac{Vx}{2D_x} + \frac{V^2 t}{4D_x} + \lambda t\right].$$
(A1.57)

The resulting transformed solute-transport equation and boundary and initial conditions are

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

c (o, y, z, t)=C_o exp
$$\left[\frac{V^2 t}{4D_x} + \lambda t\right]$$
, for Y₁2
Z₁2 (A1.58)

c,
$$\frac{\partial c}{\partial y} = 0$$
, $y = 0$, $y = W$ (A1.59)

c,
$$\frac{\partial c}{\partial z} = 0$$
, $z = 0$, $z = H$ (A1.60)

c,
$$\frac{\partial c}{\partial x} = 0$$
, $x = \infty$ (A1.61)

$$c (x, y, z, 0) = 0.$$
 (A1.62)

STEP 2:

The x-derivative term is removed by applying the Fourier sine transform as defined by Churchill (1972, p. 401–402); that is

$$S[F(x)] = \overline{F}(\alpha) = \int_{0}^{\infty} F(x) \sin(\alpha x) dx \qquad (A1.63)$$

with inverse

$$S^{-1}[\overline{F}(\alpha)] = F(x) = \frac{2}{\pi} \int_{0}^{\infty} \overline{F}(\alpha) \sin(\alpha x) d\alpha$$
 (A1.64)

and with an operational property

$$S\left[\frac{d^2F(x)}{dx^2}\right] = -\alpha^2 \overline{F} + \alpha F(0), \qquad (A1.65)$$

where F(0) is the function evaluated at x=0. The transformed equation and boundary and initial conditions are

$$\frac{\partial \bar{c}}{\partial t} + \alpha^2 D_x \bar{c} - D_y \frac{\partial^2 \bar{c}}{\partial y^2} - D_z \frac{\partial^2 \bar{c}}{\partial z^2} - \alpha D_x c (0, y, z, t) = 0$$
(A1.66)

$$\mathbf{c}, \frac{\partial \mathbf{\bar{c}}}{\partial \mathbf{y}} = 0 \qquad \mathbf{y} = 0, \ \mathbf{y} = \mathbf{W}$$
 (A1.67)

c,
$$\frac{\partial \bar{c}}{\partial z} = 0$$
 z=0, z=H (A1.68)

$$\bar{c} (\alpha, y, z, 0) = 0,$$
 (A1.69)

where c (0, y, z, t) is the patch source boundary condition specified in equation A1.58.

STEP 3:

The y-derivative is removed by applying the finite Fourier cosine transform as defined by Churchill (1972, p. 354-356); that is

$$F_{c}[G(y)] = \overline{G}(n) = \int_{0}^{W} G(y) \cos\left(\frac{n\pi y}{W}\right) dy$$
(A1.70)

with inverse

$$F_{c}^{-1}[\bar{G}(n)] = G(y) = \frac{\bar{G}(0)}{w} + \frac{2}{W} \sum_{n=1}^{\infty} \bar{G}(n) \cos\left(\frac{n\pi y}{W}\right)$$
(A1.71)

and with an operational property

$$F_{c} \left[\frac{d^{2}G(y)}{dy^{2}} \right] = (-1)^{n} \frac{dG}{dy} \left| \right|_{y=W} - \frac{dG}{dy} \left| \right|_{y=0} - \frac{n^{2} \pi^{2}}{W^{2}} \overline{G}.$$
(A1.72)

The transformed equation and boundary and initial conditions are

$$\frac{\partial \overline{\overline{c}}}{\partial t} + \alpha^2 D_x \overline{\overline{c}} + \eta^2 D_y \overline{\overline{c}} - D_z \frac{\partial^2 \overline{\overline{c}}}{\partial z^2} - \alpha D_x \int_0^{\infty} c (0, y, z, t) \cos(\eta y) \, dy = 0$$
(A1.73)

$$\overline{c}, \frac{\partial \overline{c}}{\partial z} = 0, \quad z = 0, \ z = H$$
 (A1.74)

$$\overline{c}$$
 (a, n, z, 0)=0. (A1.75)

where $\eta = \frac{n\pi}{W}$.

STEP 4:

The finite Fourier cosine transform is applied again to remove the z-derivative. Note that when equation A1.58 is used to define the patch source boundary term, the integral in equation A1.73 has a nonzero value only over the interval from Y_1 to Y_2 and from Z_1 to Z_2 . Thus, the transformed equation and initial condition are given by

$$\frac{d\overline{\overline{c}}}{dt} + \left(\alpha^2 D_x + \eta^2 D_y + \zeta^2 D_z\right) \overline{\overline{c}} - \alpha D_x C_o \exp\left[\frac{V^2 t}{4D_x} + \lambda t\right] \cdot \int_{Z_1}^{Z_2} \int_{Y_1}^{Y_2} \cos(\eta y) \cos(\zeta z) dy dz = 0 \text{ (A1.76)}$$
$$\overline{\overline{c}} (\alpha, n, m, 0) = 0, \qquad (A1.77)$$

where $\zeta = \frac{m\pi}{H}$.

STEP 5:

The transformed ordinary differential equation is solved for $\overline{\overline{c}}$ using an integrating factor (see eqs. A1.29 to A1.31); that is

$$\overline{\overline{c}} = \frac{\alpha D_x C_o I_{zy}}{\exp[\alpha^2 D_x t + \eta^2 D_y t + \zeta^2 D_z t]} \int_0^t \exp\left[\alpha^2 D_x + \eta^2 D_y + \zeta^2 D_z + \frac{V^2}{4D_x} + \lambda\right] \cdot \tau \, d\tau, \qquad (A1.78)$$

where

$$I_{zy} = \int_{Z_1}^{Z_2} \int_{Y_1}^{Y_2} \cos(\eta y) \, \cos(\zeta z) \, dy \, dz.$$

Integrating equation A1.78 over time gives

$$\overline{\overline{c}} = \frac{\alpha D_x C_o I_{zy}}{\left(\alpha^2 D_x + \eta^2 D_y + \zeta^2 D_z + \frac{V^2}{4D_x} + \lambda\right)} \left\{ \exp\left[\frac{V^2 t}{4D_x} + \lambda t\right] - \exp\left[-\alpha^2 D_x t - \eta^2 D_y t - \zeta^2 D_z t\right] \right\}.$$
(A1.79)

STEP 6:

The inverse Fourier sine transform (eq. A1.64) is applied to remove the α term; that is

$$\begin{split} \bar{c} &= C_{o} I_{zy} \Biggl\{ exp \Biggl[\frac{V^{2}t}{4D_{x}} + \lambda t \Biggr] S^{-1} \Biggl[\frac{\alpha}{\alpha^{2} + \frac{\eta^{2}D_{y}}{D_{x}} + \frac{\zeta^{2}D_{z}}{D_{x}} + \frac{V^{2}}{4D_{x}^{-2}} + \frac{\lambda}{D_{x}}} \Biggr] \\ &- exp [-\eta^{2}D_{y}t - \zeta^{2}D_{z}t] S^{-1} \Biggl[\frac{\alpha exp [-\alpha^{2}D_{x}t]}{\alpha^{2} + \frac{\eta^{2}D_{y}}{D_{x}} + \frac{\zeta^{2}D_{z}}{D_{x}} + \frac{V^{2}}{4D_{x}^{-2}} + \frac{\lambda}{D_{x}}} \Biggr] \Biggr\}.$$
(A1.80)

The first inverse transform can be evaluated using equation D.1.16 in the table of inverse Fourier sine transforms in Churchill (1972, p. 474), where

$$S^{-1}\left[\frac{\alpha}{\alpha^2 + b^2}\right] = \exp(-bx). \tag{A1.81}$$

Unfortunately, the second inverse transform cannot be found in the tables. Instead, it can be determined by performing the integration as defined in equation A1.64, where

$$S^{-1}\left[\frac{[\alpha \exp[-a\alpha^2]}{\alpha^2 + b^2}\right] = \frac{2}{\pi} \int_0^\infty \frac{\alpha \exp[-a\alpha^2]}{\alpha^2 + b^2} \sin \alpha x d\alpha.$$
(A1.82)

The integral in equation A1.82 is given in Gradshteyn and Ryzhik (1980, p. 497, eq. 3.954); that is

$$I = -\frac{\pi}{4} \exp[ab^2] \left\{ 2\sinh(xb) + \exp[-xb] \operatorname{erf}\left[b\sqrt{a} - \frac{x}{2\sqrt{a}}\right] - \exp[xb] \operatorname{erf}\left[b\sqrt{a} + \frac{x}{2\sqrt{a}}\right] \right\}, \quad (A1.83)$$

where $\sinh(xb)$ is the hyperbolic sine. When written in terms of the complementary error function, erfc, the inverse Fourier sine transform can be written as

$$S^{-1}\left[\frac{\alpha \exp[-a\alpha^{2}]}{\alpha^{2}+b^{2}}\right] = \frac{1}{2} \exp[ab^{2}] \left\{ \exp[-xb] \operatorname{erfc}\left[b\sqrt{a}-\frac{x}{2\sqrt{a}}\right] -\exp[xb] \operatorname{erfc}\left[b\sqrt{a}+\frac{x}{2\sqrt{a}}\right] \right\}.$$
(A1.84)

Letting a=D_xt and b= $\left(\frac{\eta^2 D_y}{D_x} + \frac{\zeta^2 D_z}{D_x} + \frac{V^2}{4D_x^2} + \frac{\lambda}{D_x}\right)^{1/2}$, equation A1.80 can be evaluated as

$$\begin{split} \overline{\overline{c}} &= C_{o} I_{zy} \bigg\{ exp \bigg[\frac{V^{2} t}{4 D_{x}} + \lambda t - \frac{\beta x}{2 D_{x}} \bigg] - \frac{1}{2} exp \bigg[\frac{V^{2} t}{4 D_{x}} + \lambda t - \frac{\beta x}{2 D_{x}} \bigg] erfc \bigg[\frac{\beta t - x}{2 \sqrt{D_{x} t}} \bigg] \\ &+ \frac{1}{2} exp \bigg[\frac{V^{2} t}{4 D_{x}} + \lambda t + \frac{\beta x}{2 D_{x}} \bigg] erfc \bigg[\frac{\beta t + x}{2 \sqrt{D_{x} t}} \bigg] \bigg\}, \end{split}$$
(A1.85)

where $\beta = [V^2 + 4D_x(\lambda + \eta^2 D_y + \zeta^2 D_z)]^{1/2}$. The second term in equation A1.85 can be rewritten using the identity erfc (-x)=2-erfc(x) to cancel the first term, yielding

$$\overline{\overline{c}} = C_o \frac{I_{zy}}{2} \exp\left[\frac{V^2 t}{4D_x} + \lambda t\right] \left\{ \exp\left[\frac{-\beta x}{2D_x}\right] \exp\left[\frac{x - \beta t}{2\sqrt{D_x t}}\right] + \exp\left[\frac{\beta x}{2D_x}\right] \exp\left[\frac{x + \beta t}{2\sqrt{D_x t}}\right] \right\}.$$
 (A1.86)

STEP 7:

The inverse finite Fourier cosine transform (eq. A1.71) is applied to remove the n terms; that is

$$\overline{c} = \frac{\overline{\overline{c}}}{W} \bigg|_{n=0} + \frac{2}{W} \sum_{n=1}^{\infty} \overline{\overline{c}}(n) \cos(\eta y).$$
(A1.87)

Integrals involving n in the term $I_{\rm zy}$ are also evaluated at this point to give

$$\bar{c} = C_{o} \frac{(Y_{2} - Y_{1})}{2W} \int_{Z_{1}}^{Z_{2}} \cos(\zeta z) dz \cdot \exp\left[\frac{V^{2}t}{4D_{x}} + \lambda t\right] \left\{ \exp\left[\frac{-\gamma x}{2D_{x}}\right] \operatorname{erfc}\left[\frac{x - \gamma t}{2\sqrt{D_{x}t}}\right] \right\} \\ + \exp\left[\frac{\gamma x}{2D_{x}}\right] \operatorname{erfc}\left[\frac{x + \gamma t}{2\sqrt{D_{x}t}}\right] \right\} + \frac{C_{o}}{W} \int_{Z_{1}}^{Z_{2}} \cos(\zeta z) dz \cdot \sum_{n=1}^{\infty} \left[\frac{\sin(\eta Y_{2}) - \sin(\eta Y_{1})}{\eta}\right] \\ \cdot \cos(\eta y) \exp\left[\frac{V^{2}t}{4D_{x}} + \lambda t\right] \left\{ \exp\left[\frac{-\beta x}{2D_{x}}\right] \operatorname{erfc}\left[\frac{x - \beta t}{2\sqrt{D_{x}t}}\right] + \exp\left[\frac{\beta x}{2D_{x}}\right] \operatorname{erfc}\left[\frac{x + \beta t}{2\sqrt{D_{x}t}}\right] \right\}, \quad (A1.88)$$

where

$$\gamma = [V^2 + 4D_x(\lambda + \zeta^2 D_z)]^{1/2}.$$

STEP 8:

Apply the inverse finite Fourier cosine transform to remove the m terms; that is

$$\begin{split} \mathbf{c} &= \frac{\mathbf{C}_{o}}{2} \left[\frac{(\mathbf{Y}_{2} - \mathbf{Y}_{1})}{\mathbf{W}} \right] \left[\frac{(\mathbf{Z}_{2} - \mathbf{Z}_{1})}{\mathbf{H}} \right] \exp\left[\frac{\mathbf{V}^{2} \mathbf{t}}{4\mathbf{D}_{x}} + \lambda \mathbf{t} \right] \left\{ \exp\left[\frac{-\omega \mathbf{x}}{2\mathbf{D}_{x}} \right] \operatorname{erfc}\left[\frac{\mathbf{x} - \omega \mathbf{t}}{2\sqrt{\mathbf{D}_{x}} \mathbf{t}} \right] \right\} \\ &+ \exp\left[\frac{\omega \mathbf{x}}{2\mathbf{D}_{x}} \right] \operatorname{erfc}\left[\frac{\mathbf{x} + \omega \mathbf{t}}{2\sqrt{\mathbf{D}_{x}} \mathbf{t}} \right] \right\} + \mathbf{C}_{o} \left(\frac{\mathbf{Z}_{2} - \mathbf{Z}_{1}}{\mathbf{H}} \right) \sum_{n=1}^{\infty} \left[\frac{\sin(\eta \mathbf{Y}_{2}) - \sin(\eta \mathbf{Y}_{1})}{n\pi} \right] \operatorname{cos} \eta \mathbf{y} \\ &\cdot \exp\left[\frac{\mathbf{V}^{2} \mathbf{t}}{4\mathbf{D}_{x}} + \lambda \mathbf{t} \right] \left\{ \exp\left[\frac{-\epsilon \mathbf{x}}{2\mathbf{D}_{x}} \right] \operatorname{erfc}\left[\frac{\mathbf{x} - \epsilon \mathbf{t}}{2\sqrt{\mathbf{D}_{x}} \mathbf{t}} \right] + \exp\left[\frac{\epsilon \mathbf{x}}{2\mathbf{D}_{x}} \right] \operatorname{erfc}\left[\frac{\mathbf{x} + \epsilon \mathbf{t}}{2\sqrt{\mathbf{D}_{x}} \mathbf{t}} \right] \right\} \\ &+ \mathbf{C}_{o} \left(\frac{\mathbf{Y}_{2} - \mathbf{Y}_{1}}{\mathbf{W}} \right) \sum_{m=1}^{\infty} \left[\frac{\sin((\zeta \mathbf{Z}_{2}) - \sin(\zeta \mathbf{Z}_{1})}{m\pi} \right] \operatorname{cos}(\zeta z) \\ &\cdot \exp\left[\frac{\mathbf{V}^{2} \mathbf{t}}{4\mathbf{D}_{x}} + \lambda \mathbf{t} \right] \left\{ \exp\left[\frac{-\gamma \mathbf{x}}{2\mathbf{D}_{x}} \right] \operatorname{erfc}\left[\frac{\mathbf{x} - \gamma \mathbf{t}}{2\sqrt{\mathbf{D}_{x}} \mathbf{t}} \right] + \exp\left[\frac{\gamma \mathbf{x}}{2\mathbf{D}_{x}} \right] \operatorname{erfc}\left[\frac{\mathbf{x} + \gamma \mathbf{t}}{2\sqrt{\mathbf{D}_{x}} \mathbf{t}} \right] \right\} \\ &+ 2\mathbf{C}_{o} \sum_{m=1}^{\infty} \left[\frac{\sin(\zeta \mathbf{Z}_{2}) - \sin(\zeta \mathbf{Z}_{1})}{m\pi} \right] \operatorname{cos}(\mathbf{z} \mathbf{z}) \sum_{n=1}^{\infty} \left[\frac{\sin(\eta \mathbf{Y}_{2}) - \sin(\eta \mathbf{Y}_{1})}{n\pi} \right] \operatorname{cos}(\eta \mathbf{y}) \\ &\cdot \exp\left[\frac{\mathbf{V}^{2} \mathbf{t}}{4\mathbf{D}_{x}} + \lambda \mathbf{t} \right] \left\{ \exp\left[\frac{-\beta \mathbf{x}}{2\mathbf{D}_{x}} \right] \operatorname{erfc}\left[\frac{\mathbf{x} - \beta \mathbf{t}}{2\sqrt{\mathbf{D}_{x}} \mathbf{t}} \right] + \exp\left[\frac{\beta \mathbf{x}}{2\mathbf{D}_{x}} \right] \operatorname{erfc}\left[\frac{\mathbf{x} + \beta \mathbf{t}}{2\sqrt{\mathbf{D}_{x}} \mathbf{t}} \right] \right\}, \quad (A1.89) \\ \text{where} \qquad \omega = (\mathbf{V}^{2} + 4\lambda \mathbf{D}_{x})^{1/2} \\ \mathrm{and} \qquad \qquad \varepsilon = [\mathbf{V}^{2} + 4\mathbf{D}_{x}(\lambda + \eta^{2}\mathbf{D}_{y})]^{1/2}. \end{aligned}$$

STEP 9:

Multiply both sides of equation A1.90 by

$$exp \left[\frac{Vx}{2D_x} - \frac{V^2 t}{4D_x} - \lambda t \right]$$

to convert the transformed variable c back to C (see eq. A1.57) which yields

$$\begin{split} \mathbf{c} &= \frac{\mathbf{C}_{0}}{2} \left[\frac{(\mathbf{Y}_{2} - \mathbf{Y}_{1})}{\mathbf{W}} \right] \left[\frac{(\mathbf{Z}_{2} - \mathbf{Z}_{1})}{\mathbf{H}} \right] \left\{ \exp\left[\frac{\mathbf{x}(\mathbf{v} - \boldsymbol{\omega})}{2\mathbf{D}_{x}} \right] \exp\left[\mathbf{c}\left[\frac{\mathbf{x} - \boldsymbol{\omega}t}{2\sqrt{\mathbf{D}_{x}t}} \right] + \exp\left[\frac{\mathbf{x}(\mathbf{v} + \boldsymbol{\omega})}{2\mathbf{D}_{x}} \right] \exp\left[\frac{\mathbf{x} + \boldsymbol{\omega}t}{2\sqrt{\mathbf{D}_{x}t}} \right] \right] \right\} \\ &+ \mathbf{C}_{0} \frac{(\mathbf{Z}_{2} - \mathbf{Z}_{1})}{\mathbf{H}} \sum_{n=1}^{\infty} \left[\frac{\sin(\eta \mathbf{Y}_{2}) - \sin(\eta \mathbf{Y}_{1})}{n\pi} \right] \cos(\eta \mathbf{y}) \\ &\cdot \left\{ \exp\left[\frac{\mathbf{x}(\mathbf{v} - \boldsymbol{\epsilon})}{2\mathbf{D}_{x}} \right] \exp\left[\frac{\mathbf{x} - \boldsymbol{\epsilon}t}{2\sqrt{\mathbf{D}_{x}t}} \right] + \exp\left[\frac{\mathbf{x}(\mathbf{v} + \boldsymbol{\epsilon})}{2\mathbf{D}_{x}} \right] \exp\left[\frac{\mathbf{x} + \boldsymbol{\epsilon}t}{2\sqrt{\mathbf{D}_{x}t}} \right] \right\} \\ &+ \mathbf{C}_{0} \frac{(\mathbf{Y}_{2} - \mathbf{Y}_{1})}{\mathbf{W}} \sum_{m=1}^{\infty} \left[\frac{\sin(\zeta \mathbf{Z}_{2}) - \sin(\zeta \mathbf{Z}_{1})}{m\pi} \right] \cos(\zeta \mathbf{z}) \\ &\cdot \left\{ \exp\left[\frac{\mathbf{x}(\mathbf{v} - \boldsymbol{\gamma})}{\mathbf{W}} \right] \exp\left[\frac{\mathbf{x} - \mathbf{\gamma}t}{2\sqrt{\mathbf{D}_{x}t}} \right] + \exp\left[\frac{\mathbf{x}(\mathbf{v} + \boldsymbol{\gamma})}{2\mathbf{D}_{x}} \right] \exp\left[\frac{\mathbf{x} + \mathbf{\gamma}t}{2\sqrt{\mathbf{D}_{x}t}} \right] \right\} \\ &+ 2\mathbf{C}_{0} \sum_{m=1}^{\infty} \left[\frac{\sin(\zeta \mathbf{Z}_{2}) - \sin(\zeta \mathbf{Z}_{1})}{m\pi} \right] \cos(\zeta \mathbf{z}) \cdot \sum_{n=1}^{\infty} \left[\frac{\sin(\eta \mathbf{Y}_{2}) - \sin(\eta \mathbf{Y}_{1})}{n\pi} \right] \cos(\eta \mathbf{y}) \\ &\cdot \left\{ \exp\left[\frac{\mathbf{x}(\mathbf{v} - \boldsymbol{\beta})}{2\mathbf{D}_{x}} \right] \exp\left[\frac{\mathbf{x} - \mathbf{\beta}t}{2\sqrt{\mathbf{D}_{x}t}} \right] + \exp\left[\frac{\mathbf{x}(\mathbf{v} + \boldsymbol{\beta})}{2\mathbf{D}_{x}} \right] \exp\left[\frac{\mathbf{x} + \mathbf{\beta}t}{2\sqrt{\mathbf{D}_{x}t}} \right] \right\}, \tag{A1.90}$$

Equation A1.90 represents a final form of the analytical soltuion for the patch source. It can also be written in a form similar to that of Cleary and Ungs (1978, p. 24-25) and equation 114 in the text; that is

$$C = C_{o} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} L_{mn} O_{m} P_{n} \cos(\zeta z) \cos(\eta y)$$

$$\cdot \left\{ exp \left[\frac{x(v-\beta)}{2D_{x}} \right] erfc \left[\frac{x-\beta t}{2\sqrt{D_{x}t}} \right] + exp \left[\frac{x(v+\beta)}{2D_{x}} \right] erfc \left[\frac{x+\beta t}{2\sqrt{D_{x}t}} \right] \right\},$$
(A1.91)

m=0, and n=0

where

$$\begin{split} \mathbf{L}_{mn} = \begin{cases} \frac{1}{2} & \text{m=0, and } n=0 \\ 1 & \text{m=0, and } n>0 \\ 1 & \text{m>0, and } n=0 \\ 2 & \text{m>0, and } n>0 \\ \end{bmatrix} \\ O_{m} = \begin{cases} \frac{\mathbf{Z}_{2} - \mathbf{Z}_{1}}{\mathbf{H}} & \text{m=0} \\ \frac{\mathbf{Z}_{2} - \mathbf{Z}_{1}}{\mathbf{H}} & \text{m=0} \\ \frac{\left[\frac{\left[\sin\left(\zeta \mathbf{Z}_{2}\right) - \sin\left(\zeta \mathbf{Z}_{1}\right)\right]}{\mathbf{m}\pi}\right]}{\mathbf{m}\pi} & \text{m>0} \end{cases} \end{split}$$

$$P_{n} = \begin{cases} \frac{Y_{2} - Y_{1}}{W} & n = 0\\ \left[\frac{\sin(\eta Y_{2}) - \sin(\eta Y_{1})}{n\pi}\right] & n > 0 \end{cases}$$

AQUIFER OF INFINITE WIDTH AND HEIGHT WITH CONTINUOUS POINT SOURCE

The following is a step-by-step derivation of the analytical solution for solute transport in an aquifer of infinite length, width, and height containing a continuous point solute source injecting solute with a concentration C_o at a rate Q in a steady flow field (eq. 105 in the text).

The governing three-dimensional solute-transport equation is

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - V \frac{\partial C}{\partial x} - \lambda C + \frac{Qdt}{n} C_o \delta(x - X_c) \delta(y - Y_c) \delta(z - Z_c).$$
(A1.92)

Boundary and initial conditions are

C,
$$\frac{\partial C}{\partial x} = 0$$
, $x = \pm \infty$ (A1.93)

C,
$$\frac{\partial C}{\partial y} = 0$$
, $y = \pm \infty$ (A1.94)

C,
$$\frac{\partial C}{\partial z} = 0$$
, $z = \pm \infty$ (A1.95)

C (x, y, z, 0)=0
$$(A1.96)$$

where

V is the velocity in x-direction,

Qdt C_o is the mass of solute injected into aquifer over the time period dt,

n is the aquifer porosity,

 X_c, Y_c, Z_c are the coordinates of the point source, and

 $\delta(\)$ is the dirac delta function.

STEP 1:

To solve equation A1.91 for the continuous point source, first solve the partial differential equation for solute transport in an aquifer with an *instantaneous point* source. The governing equation is rewritten as

$$\frac{\partial C}{\partial t} = D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - V \frac{\partial C}{\partial x} - \lambda c + \frac{Qdt}{n} C_o \delta(x - X_c) \delta(y - Y_c) \delta(z - Z_c) \delta(t - t'), \quad (A1.97)$$

where t' is time at which the instantaneous point source starts and ends. Boundary conditions remain the same.

STEP 2:

A variable transformation is applied to remove the advective and solute-decay terms, where

$$\int_{A} \mathbf{c} = \mathbf{C} \, \exp\left[-\frac{\mathbf{V}\mathbf{x}}{2\mathbf{D}_{\mathbf{x}}} + \frac{\mathbf{V}^{2}\mathbf{t}}{4\mathbf{D}_{\mathbf{x}}} + \lambda\mathbf{t}\right]. \tag{A1.98}$$

The resulting transformed solute-transport equation and boundary and initial conditions are

$$\frac{\partial \mathbf{c}}{\partial t} = \mathbf{D}_{\mathbf{x}} \frac{\partial^2 \mathbf{c}}{\partial \mathbf{x}^2} + \mathbf{D}_{\mathbf{y}} \frac{\partial^2 \mathbf{c}}{\partial \mathbf{y}^2} + \mathbf{D}_{\mathbf{z}} \frac{\partial^2 \mathbf{c}}{\partial \mathbf{z}^2} + \frac{\mathbf{Q}dt}{\mathbf{n}} \mathbf{C}_{\mathbf{o}} \exp\left[-\frac{\mathbf{V}\mathbf{x}}{2\mathbf{D}_{\mathbf{x}}} + \frac{\mathbf{V}^2 \mathbf{t}}{4\mathbf{D}_{\mathbf{x}}} + \lambda \mathbf{t}\right]$$

• $\delta(\mathbf{x} - \mathbf{X}_c)\delta(\mathbf{y} - \mathbf{Y}_c)\delta(\mathbf{z} - \mathbf{Z}_c)\delta(\mathbf{t} - \mathbf{t}')$ (A1.99)

c,
$$\frac{\partial c}{\partial x} = 0$$
, $x = \pm \infty$ (A1.100)

c,
$$\frac{\partial c}{\partial y} = 0$$
, $y = \pm \infty$ (A1.101)

c,
$$\frac{\partial c}{\partial z} = 0$$
, $z = \pm \infty$ (A1.102)

$$c (x, y, z, 0) = 0$$
 (A1.103)

STEP 3:

The x-derivative term is removed by applying the exponential Fourier transform as defined by Churchill (1972, p. 384-385); that is

$$\mathbf{E}[\mathbf{F}(\mathbf{x})] = \overline{\mathbf{F}}(\alpha) = \int_{-\infty}^{+\infty} \mathbf{F}(\mathbf{x}) \exp[-i\alpha \mathbf{x}] d\mathbf{x}$$
(A1.104)

with inverse

$$\mathbf{E}^{-1}[\overline{\mathbf{F}}(\alpha)] = \mathbf{F}(\mathbf{x}) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \overline{\mathbf{F}}(\alpha) \exp[i\alpha \mathbf{x}] d\alpha$$
(A1.105)

and with an operational property

$$\mathbf{E}\left[\frac{\mathrm{d}^{2}\mathbf{F}(\mathbf{x})}{\mathrm{d}\mathbf{x}^{2}}\right] = -\alpha^{2}\overline{\mathbf{F}}(\alpha), \qquad (A1.106)$$

where $i=\sqrt{-1}$. The y- and z-derivatives can be removed similarly yielding the transformed equation and initial condition

$$\frac{\partial \overline{\overline{c}}}{\partial t} + \left[\alpha^2 D_x + \beta^2 D_y + \gamma^2 D_z \right] \overline{\overline{c}} - \frac{Qdt}{n} C_o \exp\left[\frac{V^2 t}{4 D_x} + \lambda t \right] \cdot \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \exp\left[-i\alpha x - \frac{Vx}{2 D_x} - i\beta y - i\gamma z \right]$$

$$\delta(x - X_c) \delta(y - Y_c) \delta(z - Z_c) \delta(t - t') dx dy dz = 0$$
(A1.107)

$$\delta(\mathbf{x} - \mathbf{X}_{c})\delta(\mathbf{y} - \mathbf{Y}_{c})\delta(\mathbf{z} - \mathbf{Z}_{c})\delta(\mathbf{t} - \mathbf{t}')d\mathbf{x} d\mathbf{y} d\mathbf{z} = 0$$
(A1.107)

$$\overline{\overline{c}} (\alpha, \beta, \gamma, 0) = 0.$$
 (A1.108)

By definition, the integral of a function multiplied by the dirac delta function (last term in eq. A1.107) is equal to the function evaluated at the coordinate of the point source. Thus, the transformed equation is given by

$$\frac{d\overline{\overline{c}}}{dt} + (\alpha^2 D_x + \beta^2 D_y + \gamma^2 D_z)\overline{\overline{c}} - \frac{Qdt}{n}C_o exp\left[\frac{V^2 t}{4D_x} + \lambda t - i\alpha X_c - \frac{VX_c}{2D_x} - i\beta Y_c - i\gamma Z_c\right]\delta(t - t') = 0$$
(A1.109)

STEP 4:

The transformed ordinary differential equation is solved for c using an integrating factor (see eqs. A1.29 to A1.31); that is

$$\begin{split} & = \frac{Qdt}{c} C_{o} exp \left[-i\alpha X_{c} - \frac{VX_{c}}{2D_{x}} - i\beta Y_{c} - i\gamma Z_{c} \right]}{exp(\alpha^{2}D_{x}t + \beta^{2}D_{y}t + \gamma^{2}D_{z}t]} \int_{0}^{t} exp \left[\alpha^{2}D_{x} + \beta^{2}D_{y} + \gamma^{2}D_{z}t + \gamma^{2}D_{z}t \right] \\ & + \gamma^{2}D_{z} + \frac{V^{2}}{4D_{x}} + \lambda \right] \cdot \tau \delta(\tau - t') d\tau. \end{split}$$
(A1.110)

Integrating equation A1.110 and grouping like terms gives

$$\begin{split} &= \frac{Qdt}{n} C_{o} exp \left[\frac{V^{2}t'}{4D_{x}} + \lambda t' - i\alpha X_{c} - \frac{VX_{c}}{2D_{x}} - \alpha^{2} D_{x}(t-t') - i\beta Y_{c} - \beta^{2} D_{y}(t-t') - i\gamma Z_{c} \right. \\ &\left. - \gamma^{2} D_{z}(t-t') \right]. \end{split}$$

$$(A1.111)$$

STEP 5:

The inverse exponential Fourier transform (eq. A1.105) is applied three times to remove the α , β , and γ terms; that is

$$\mathbf{c} = \frac{\mathrm{Qdt}}{\mathrm{n}} \mathrm{C}_{\mathrm{o}} \mathrm{exp} \left[\frac{\mathrm{V}^{2} \mathrm{t}'}{4\mathrm{D}_{\mathrm{x}}} + \lambda \mathrm{t}' - \frac{\mathrm{VX}_{\mathrm{c}}}{2\mathrm{D}_{\mathrm{x}}} \right] \bullet \mathrm{E}^{-1} \left\{ \mathrm{exp} \left[-\mathrm{i}\alpha \mathrm{X}_{\mathrm{c}} - \alpha^{2} \mathrm{D}_{\mathrm{x}} (\mathrm{t} - \mathrm{t}') \right] \right\}$$
$$\bullet \mathrm{E}^{-1} \left\{ \mathrm{exp} \left[-\mathrm{i}\beta \mathrm{Y}_{\mathrm{c}} - \beta^{2} \mathrm{D}_{\mathrm{y}} (\mathrm{t} - \mathrm{t}') \right] \right\} \bullet \mathrm{E}^{-1} \left\{ \mathrm{exp} \left[-\mathrm{i}\gamma \mathrm{Z}_{\mathrm{c}} - \gamma^{2} \mathrm{D}_{\mathrm{z}} (\mathrm{t} - \mathrm{t}') \right] \right\}.$$
(A1.112)

Multiplying through by

$$\frac{2\sqrt{\pi D_x(t-t')}\bullet 2\sqrt{\pi D_y(t-t')}\bullet 2\sqrt{\pi D_z(t-t')}}{8\pi^{3/2}\ (t-t')^{3/2}\sqrt{D_xD_yD_z}}$$

and using the shift theorem (Churchill, 1972, p. 471, eq. C.1.5) given by

$$\mathbf{E}^{-1}[\exp[\mathbf{i}\alpha\alpha]\mathbf{F}(\alpha)] = \mathbf{F}(\mathbf{x}+\mathbf{a})$$
(A1.113)

and equation C.1.20 from the table of inverse exponential Fourier transforms (Churchill, 1972, p. 472) given by

$$\mathbf{E}^{-1}\left\{2\sqrt{\pi a}\exp\left[-\mathbf{a}(\alpha)^{2}\right]\right\} = \exp\left[-\frac{\mathbf{x}^{2}}{4a}\right],\tag{A1.114}$$

yields

$$c = \frac{Qdt C_{o}}{8n\pi^{3/2}(t-t')^{3/2}\sqrt{D_{x}D_{y}D_{z}}} exp \left[\frac{V^{2}t'}{4D_{x}} + \lambda t' - \frac{VX_{c}}{2D_{x}} - \frac{(x-X_{c})^{2}}{4D_{x}(t-t')} - \frac{(y-Y_{c})^{2}}{4D_{z}(t-t')} - \frac{(z-Z_{c})^{2}}{4D_{z}(t-t')}\right] (A1.115)$$

STEP 6:

The transformed variable is converted back from c to C by multiplying both sides of equation A1.115 by

$$\exp\!\left[\frac{Vx}{2D_x}\!-\!\frac{V^2t}{4D_x}\!-\lambda t\right]$$

(see eq. A1.98) to yield the analytical solution to the solute-transport equation for an *instantaneous point* source (similar to eq. 104 in the text); that is

$$c = \frac{Qdt C_{o}}{8n\pi^{3/2}(t-t')^{3/2}\sqrt{D_{x}D_{y}D_{z}}} exp\left[-\frac{V^{2}(t-t')}{4D_{x}} - \lambda(t-t') + \frac{V(x-X_{c})}{2D_{x}} - \frac{(x-X_{c})^{2}}{4D_{x}(t-t')} - \frac{(y-Y_{c})^{2}}{4D_{y}(t-t')} - \frac{(z-Z_{c})^{2}}{4D_{z}(t-t')}\right].$$
(A1.116)

STEP 7:

To derive a solution for a continuous point source, integrate equation A1.116 from t'=0 to t'=t. To simplify the integration, let $\tau = (t-t')$ and $d\tau = -dt'$:

$$C = \frac{C_{o} Q \exp\left[\frac{V(x-X_{c})}{2D_{x}}\right]}{8n\pi^{3/2}\sqrt{D_{x}D_{y}D_{z}}} \cdot \int_{t}^{o} -\tau^{-3/2} \exp\left[-\frac{(x-X_{c})^{2}}{4D_{x}\tau} \frac{(y-Y_{c})^{2}}{4D_{y}\tau} \frac{(z-Z_{c})^{2}}{4D_{z}\tau} -\left(\frac{V^{2}}{4D_{x}} + \lambda\right)\tau\right] d\tau.$$
(A1.117)

The integral in equation A1.117 can be evaluated by first reversing the limits of integration and then using an indefinite integral given in a table by Cho (1971, eq. 2.9.5), where

$$\int_{0}^{t} \tau^{-3/2} \exp\left[-\frac{a^{2}}{\tau} - b^{2}\tau\right] d\tau = \frac{\sqrt{\pi}}{2a} \left\{ \exp\left[-2ab\right] \operatorname{erfc}\left[\frac{a}{\sqrt{t}} - b\sqrt{t}\right] + \exp\left[2ab\right] \operatorname{erfc}\left[\frac{a}{\sqrt{t}} + b\sqrt{t}\right] \right\}.$$
(A1.118)
Letting $\gamma = \left[(x - X_{c})^{2} + \frac{D_{x}}{D_{y}} (y - Y_{c})^{2} + \frac{D_{x}}{D_{z}} (z - Z_{c})^{2} \right]^{1/2}$

 $\beta = (\mathrm{V}^2 + 4\mathrm{D}_{\mathrm{x}}\lambda)^{1/2},$ and

the integral can be rewritten as

$$I = \frac{\sqrt{\pi D_{x}}}{\gamma} \left\{ exp\left[-\frac{\gamma\beta}{2D_{x}} \right] erfc\left[\frac{\gamma - \beta t}{2\sqrt{D_{x}t}} \right] + exp\left[\frac{\gamma\beta}{2D_{x}} \right] erfc\left[\frac{\gamma + \beta t}{2\sqrt{D_{x}t}} \right] \right\}.$$
 (A1.119)

Substituting in equation A1.117 yields the final closed form of the analytical solution for a continuous point source (similar to eq. 105 in the text); that is

$$C = \frac{C_{o} Q \exp\left[\frac{V(x - X_{c})}{2D_{x}}\right]}{8n\pi\gamma\sqrt{D_{y}D_{z}}} \left\{ \exp\left[-\frac{\gamma\beta}{2D_{x}}\right] \operatorname{erfc}\left[\frac{\gamma - \beta t}{2\sqrt{D_{x}t}}\right] + \exp\left[\frac{\gamma\beta}{2D_{x}}\right] \operatorname{erfc}\left[\frac{\gamma + \beta t}{2\sqrt{D_{x}t}}\right] \right\}.$$
(A1.120)

At steady state, the solution is given by

$$C = \frac{C_o Q}{4n\pi\gamma\sqrt{D_y D_z}} exp\left[\frac{V(x-X_c)-\gamma\beta}{2D_x}\right].$$
 (A1.121)