APPENDIX A

The advective mass transport occurs due to the groundwater movement and its real velocity is calculated from Darcy velocity and effective porosity as

$$V_i = \frac{u_i}{n_e} \qquad \text{(A.1)}$$

where V_i is the real velocity, u_i is the Darcy velocity and n_e is the effective porosity.

The advective mass transport in a small cube is considered (Figure A.1). If the change of volumetric concentration ΔC_{adv} occurs in the small cube during an increment of time Δt, the stored mass inside of the small cube during the increment of time Δt is expressed as $(\rho\theta\Delta C_{\mathrm{adv}})\Delta x\Delta y\Delta z$,

$$(\rho\theta\Delta C_{\mathrm{adv}})\Delta x\Delta y\Delta z = \Delta t\left\{\frac{\partial(\rho\theta V_x c)}{\partial x} + \frac{\partial(\rho\theta V_y c)}{\partial y} + \frac{\partial(\rho\theta V_z c)}{\partial z}\right\}\Delta x\Delta y\Delta z \qquad \text{(A.2)}$$

where ρ is the fluid density, θ is the volume water content and c is the volumetric concentration.

Dividing both side of Eq. (A.1) by $\Delta x\Delta y\Delta z$ and considering $\Delta t \rightarrow 0$ and $\Delta x, \Delta y, \Delta z \rightarrow 0$, the following equation is obtained.

$$\frac{\partial(\rho\theta C_{\mathrm{adv}})}{\partial \mathrm{t}} = \frac{\partial}{\partial x_i}(\rho\theta V_i c) \quad (i=1, 2, 3) \qquad \text{(A.3)}$$

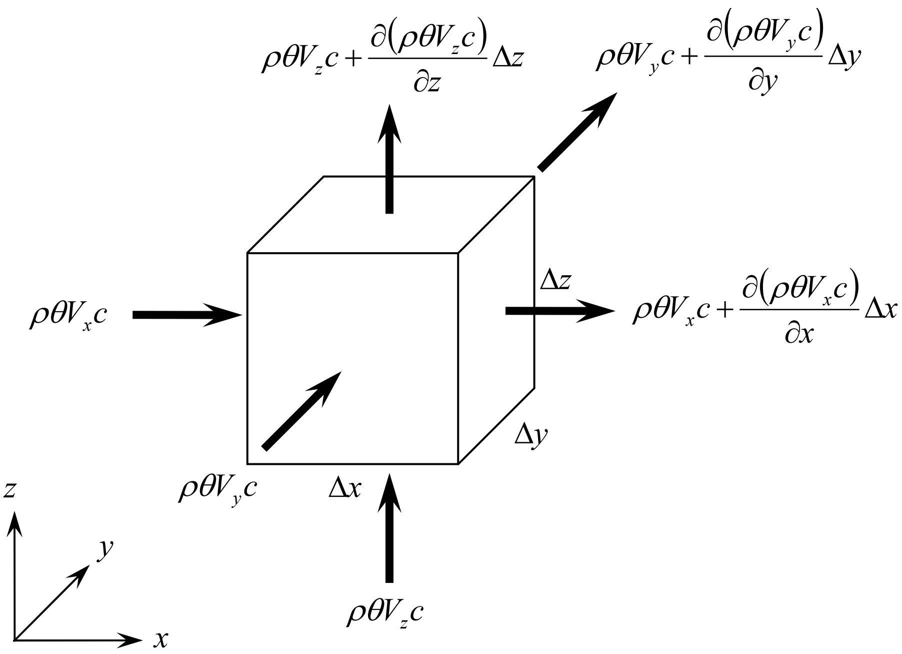

Figure A.1. The mass balance in a small cube due to advective mass transport.

The dispersive mass transport in the small cubic volume is also considered in the same way (Figure A.2).

$$
\begin{aligned}
&(\rho\theta\Delta C_{\mathrm{dis}})\Delta x\Delta y\Delta z \\
&= \Delta t\left\{\frac{\partial}{\partial x}\left(\rho\theta D_x\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial y}\left(\rho\theta D_y\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial z}\left(\rho\theta D_z\frac{\partial c}{\partial z}\right)\right\}\Delta x\Delta y\Delta z \qquad \text{(A.4)}
\end{aligned}
$$

where D is the dispersivity tensor.

If the change of volumetric concentration ΔC_{dis} occurs in the small cube during the increment of time Δt, the stored mass inside of the small cube during the time Δt is expressed as $(\rho\theta\Delta C_{\mathrm{dis}})\Delta x\Delta y\Delta z$.

Dividing both side of Eq. (A.4) by $\Delta x\Delta y\Delta z$ and considering $\Delta t \rightarrow 0$ and $\Delta x, \Delta y, \Delta z \rightarrow 0$, the following equation is obtained.

$$
\frac{\partial(\rho\theta\Delta C_{\mathrm{dis}})}{\partial t} = \frac{\partial}{\partial x_i}\left(\rho\theta D_i\frac{\partial c}{\partial x_i}\right) \quad (i=1, 2, 3) \qquad \text{(A.5)}
$$

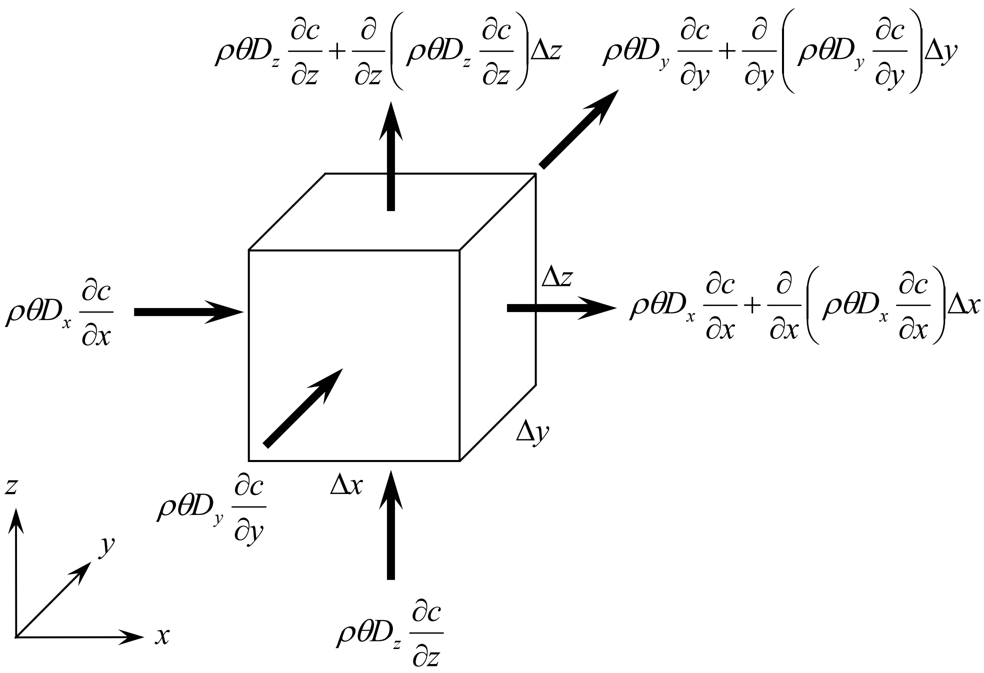

Figure A.2. The mass valance in a small cube due to dispersive mass transport.

Combining Eqs. (A.3) and (A.5), the general form of the advection-dispersion equation can be obtained as follows,

$$\frac{\partial(\rho\theta c)}{\partial t} = \frac{\partial}{\partial x_i}\left(\rho\theta D_{ij} \frac{\partial c}{\partial x_i}\right) - \frac{\partial}{\partial x_i}(\rho\theta V_i c) + Q_c \tag{A.6}$$

where θ is volume water content, ρ is fluid density, D_{ij} is dispersivity tensor, c is volumetric concentration, V_i is real velocity and Q_c is source/sink term.

Here the left hand side of Eq. (A.6) is

$$\frac{\partial(\rho\theta c)}{\partial t} = c\frac{\partial(\rho\theta)}{\partial t} + \rho\theta\frac{\partial c}{\partial t} \tag{A.7}$$

and the second term of right hand side of Eq. (A.6) becomes

$$-\frac{\partial}{\partial x_i}(\rho\theta V_i c) = -\left(c\frac{\partial}{\partial x_i}(\rho\theta V_i) + \rho\theta V\frac{\partial c}{\partial x_i}\right) \tag{A.8}$$

Substituting Eqs. (A.7) and (A.8) into Eq. (A.6), the following equation is obtained

$$c\frac{\partial(\rho\theta)}{\partial t}+\rho\theta\frac{\partial c}{\partial t}=\frac{\partial}{\partial x_i}\left(\rho\theta D_{ij}\frac{\partial c}{\partial x_i}\right)-\left(c\frac{\partial}{\partial x_i}(\rho\theta V_i)+\rho\theta V\frac{\partial c}{\partial x_i}\right)+Q_c \quad \text{(A.9)}$$

On the other hand, the continuity equation is expressed as

$$\frac{\partial(\rho\theta)}{\partial t}=-\frac{\partial(\rho\theta V_i)}{\partial x_i} \quad \text{(A.10)}$$

Introducing Eq. (A.10) in Eq. (A.9), the latter becomes

$$\rho\theta\frac{\partial c}{\partial t}=\frac{\partial}{\partial x_i}\left(\rho\theta D_{ij}\frac{\partial c}{\partial x_i}\right)-\rho\theta V\frac{\partial c}{\partial x_i}+Q_c \quad \text{(A.11)}$$

If retardation effect and decay are considered, Eq. (A.11) becomes as follows using retardation coefficient R and decay rate λ,

$$R\rho\theta\frac{\partial c}{\partial t}=\frac{\partial}{\partial x_i}\left(\rho\theta D_{ij}\frac{\partial c}{\partial x_i}\right)-\rho\theta V\frac{\partial c}{\partial x_i}-R\rho\theta\lambda c+Q_c \quad \text{(A.12)}$$

Introducing the following Lagrangian description in Eq. (A.12),

$$\frac{d}{dt}=\frac{\partial}{\partial t}+\frac{V_i}{R}\frac{\partial}{\partial x_i} \quad \text{(A.13)}$$

it becomes,

$$R\rho\theta\left(\frac{dc}{dt}-\frac{V_i}{R}\frac{\partial c}{\partial x_i}\right)=\frac{\partial}{\partial x_i}\left(\rho\theta D_{ij}\frac{\partial c}{\partial x_i}\right)-\rho\theta V\frac{\partial c}{\partial x_i}-R\rho\theta\lambda c+Q_c \quad \text{(A.14)}$$

Since the second terms in both sides are the same, Eq. (A.14) becomes

$$R\rho\theta\frac{dc}{dt}=\frac{\partial}{\partial x_i}\left(\rho\theta D_{ij}\frac{\partial c}{\partial x_i}\right)-R\rho\theta\lambda c+Q_c \quad \text{(A.15)}$$

Now it is assumed that the volumetric concentration c can be divided into two parts related to advection $\bar{c}$ and dispersion $\tilde{c}$ as follows.

$$c(x_i,t)=\bar{c}(x_i,t)+\tilde{c}(x_i,t) \tag{A.16}$$

Substituting Eq. (A.16) into Eq. (A.17), the following equation is obtained,

$$R\rho\theta\frac{d(\bar{c}+\tilde{c})}{dt}=\frac{\partial}{\partial x_i}\left(\rho\theta D_{ij}\frac{\partial c}{\partial x_i}\right)-R\rho\theta\lambda(\bar{c}+\tilde{c})+Q_c \tag{A.17}$$

or

$$R\rho\theta\frac{d\bar{c}}{dt}+R\rho\theta\frac{d\tilde{c}}{dt}=\frac{\partial}{\partial x_i}\left(\rho\theta D_{ij}\frac{\partial c}{\partial x_i}\right)-R\rho\theta\lambda\bar{c}-R\rho\theta\lambda\tilde{c}+Q_c \tag{A.18}$$

If the advective transport is focused on, the following governing equation can be obtained,

$$\frac{d\bar{c}}{dt}=-\lambda\bar{c} \tag{A.19}$$

On the other hand, the governing equation for dispersive transport can be obtained by subtracting advection part from Eq. (A.18)

$$R\rho\theta\left(\frac{dc}{dt}-\frac{d\bar{c}}{dt}\right)=\frac{\partial}{\partial x_i}\left(\rho\theta D_{ij}\frac{\partial c}{\partial x_i}\right)-R\rho\theta\lambda(c-\bar{c})+Q_c \tag{A.20}$$

or

$$R\rho\theta\frac{d\tilde{c}}{dt}=\frac{\partial}{\partial x_i}\left(\rho\theta D_{ij}\frac{\partial(\bar{c}+\tilde{c})}{\partial x_i}\right)-R\rho\theta\lambda\tilde{c}+Q_c \tag{A.21}$$

Eqs. (A.19) and (A.20) are two independent problems that can be solved separately.