Chapter 7

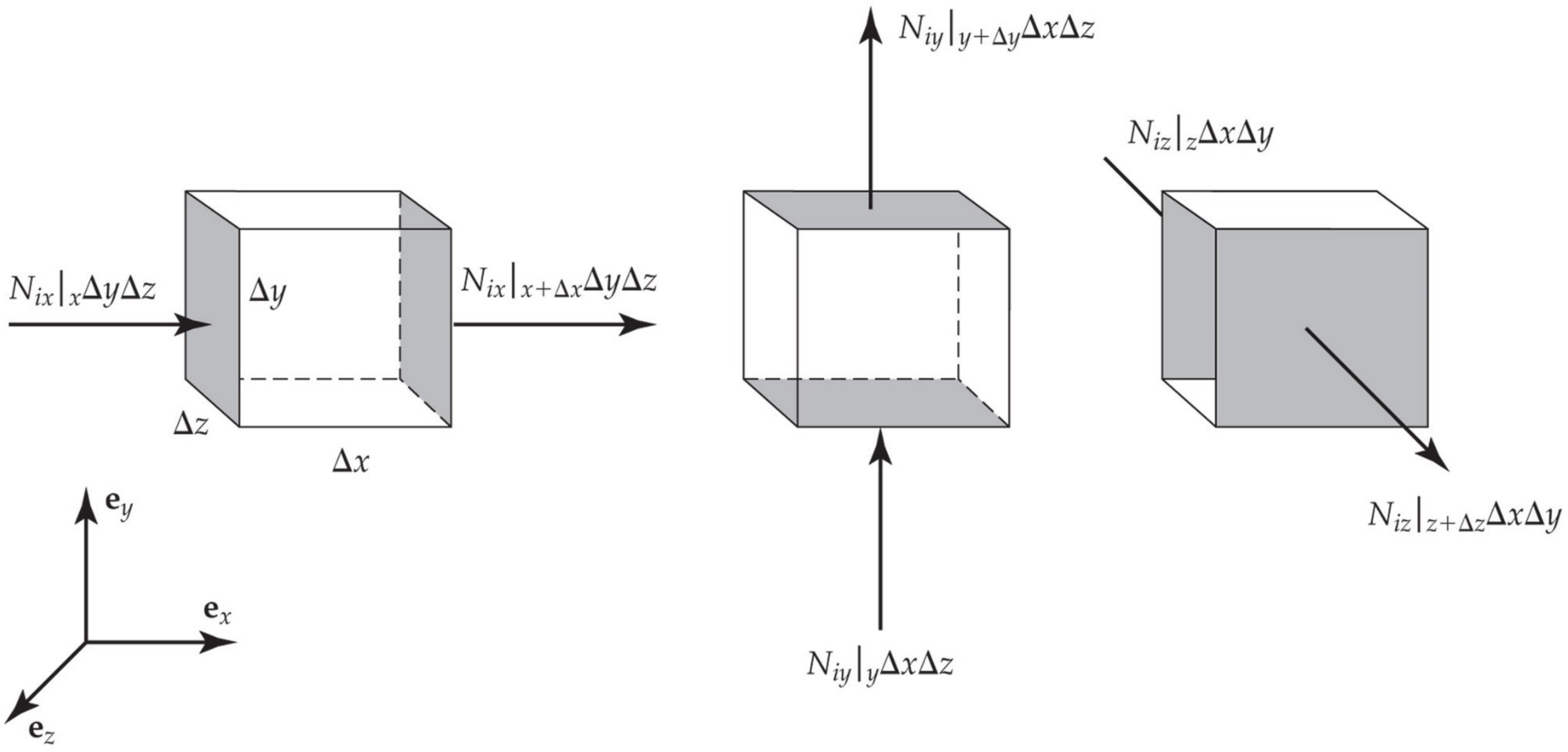
7.2

Dilute systems with convection…

$$N_i = -D_{ij}^{o}\nabla C_i + C_i v_i$$

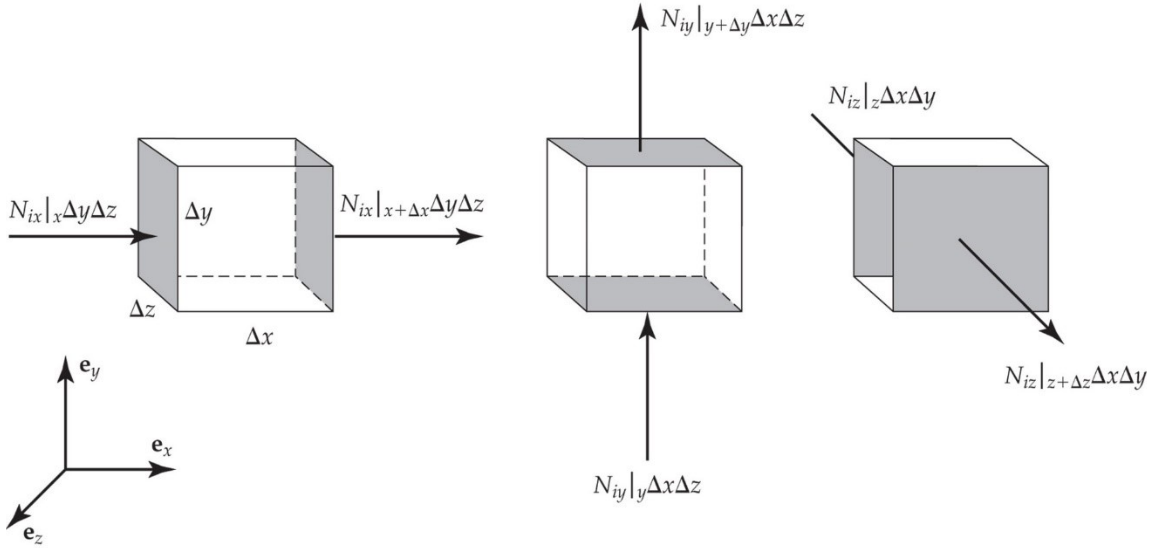
7.3

Figure 7.1 Schematic of components of solute flux.



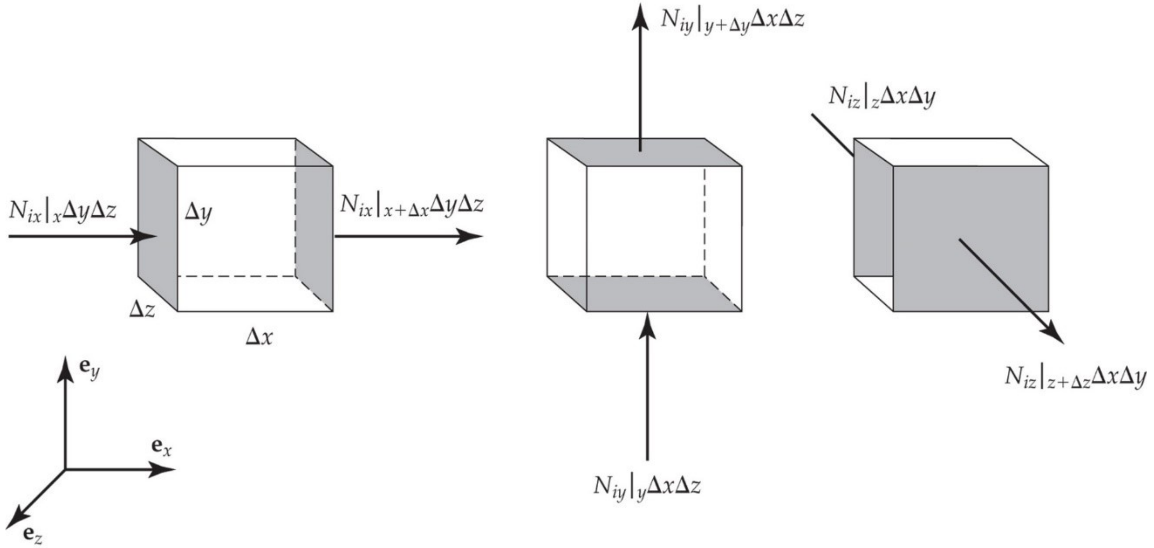
What does this mean?

Conservation of mass...



$$\Delta x\Delta y\Delta z\frac{\partial \rho_i}{\partial t} = [N_{i@x} - N_{i@x+\Delta x}]\Delta y\Delta z + [N_{i@y} - N_{i@y+\Delta y}]\Delta x\Delta z + [N_{i@z} - N_{i@z+\Delta z}]\Delta x\Delta y + r_i\Delta x\Delta y\Delta z$$

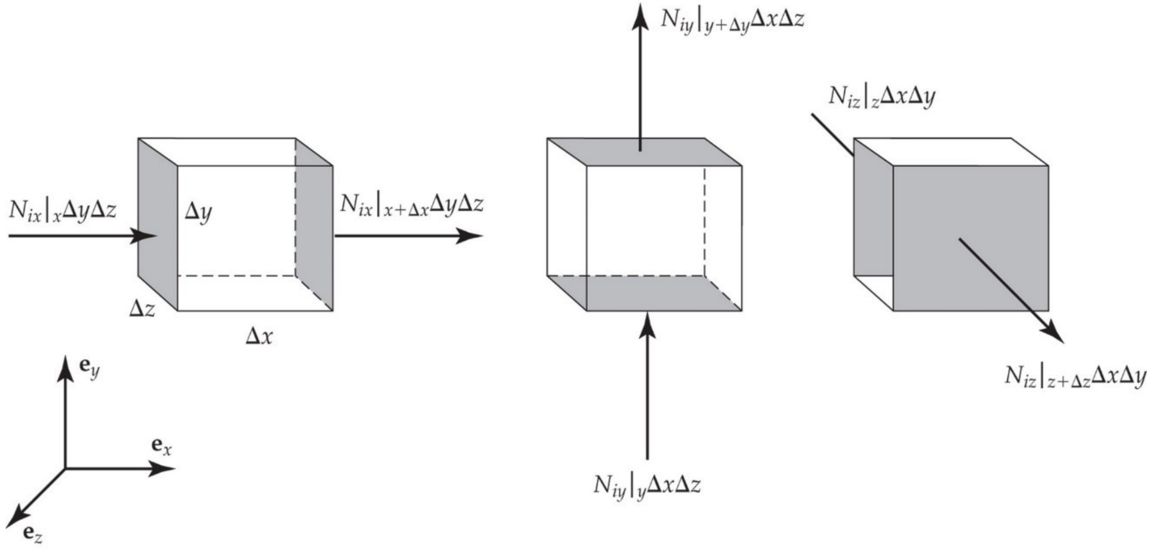
Conservation of mass…



$$
\begin{aligned}
\Delta x \Delta y \Delta z \frac{\partial \rho_i}{\partial t}
&= [N_{i@x} - N_{i@x+\Delta x}]\Delta y \Delta z \\
&+ [N_{i@y} - N_{i@y+\Delta y}]\Delta x \Delta z \\
&+ [N_{i@z} - N_{i@z+\Delta z}]\Delta x \Delta y \\
&+ r_i \Delta x \Delta y \Delta z
\end{aligned}
$$

What if we divided everything by volume?…

Conservation of mass…

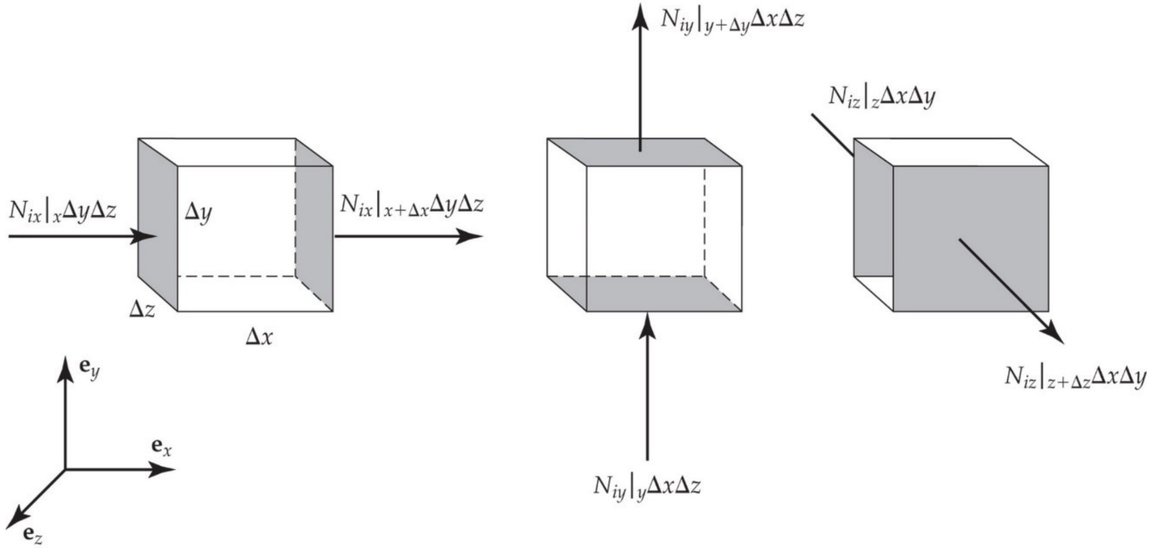


$$\Delta x\Delta y\Delta z\frac{\partial\rho_i}{\partial t} = [N_{i@x} - N_{i@x+\Delta x}]\Delta y\Delta z + [N_{i@y} - N_{i@y+\Delta y}]\Delta x\Delta z + [N_{i@z} - N_{i@z+\Delta z}]\Delta x\Delta y + r_i\Delta x\Delta y\Delta z$$

What if we divided everything by volume?…

$$\frac{\left[\Delta x\Delta y\Delta z\frac{\partial\rho_i}{\partial t} = [N_{i@x} - N_{i@x+\Delta x}]\Delta y\Delta z + [N_{i@y} - N_{i@y+\Delta y}]\Delta x\Delta z + [N_{i@z} - N_{i@z+\Delta z}]\Delta x\Delta y + r_i\Delta x\Delta y\Delta z\right]}{[\Delta x\Delta y\Delta z]}$$

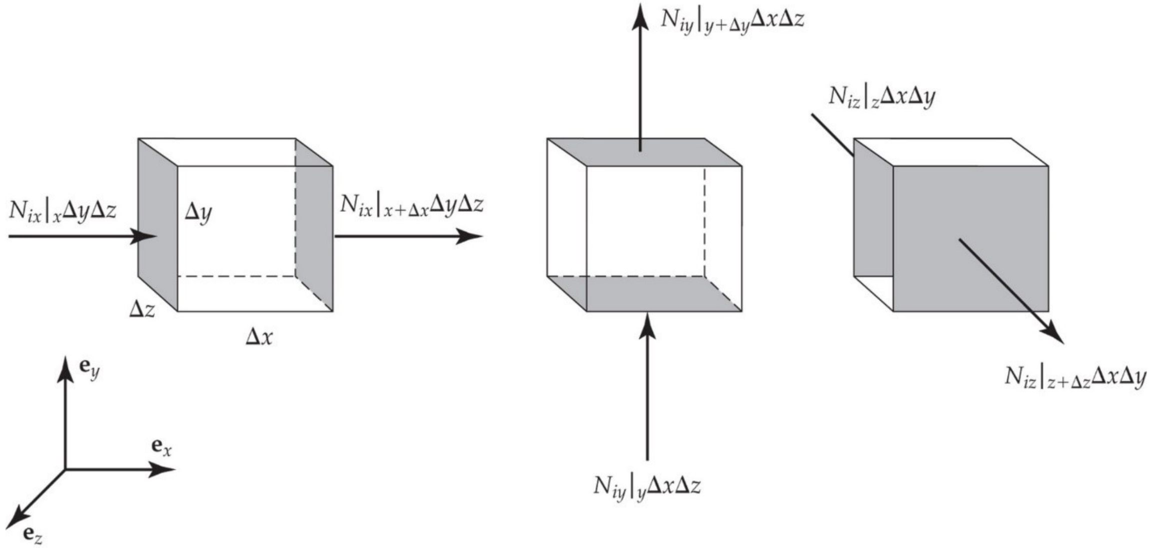
Conservation of mass...



$$\frac{\left[\Delta x \Delta y \Delta z \frac{\partial \rho_i}{\partial t} = [N_{i@x} - N_{i@x+\Delta x}]\Delta y \Delta z + [N_{i@y} - N_{i@y+\Delta y}]\Delta x \Delta z + [N_{i@z} - N_{i@z+\Delta z}]\Delta x \Delta y + r_i \Delta x \Delta y \Delta z\right]}{[\Delta x \Delta y \Delta z]}$$

What is this?

Conservation of mass…

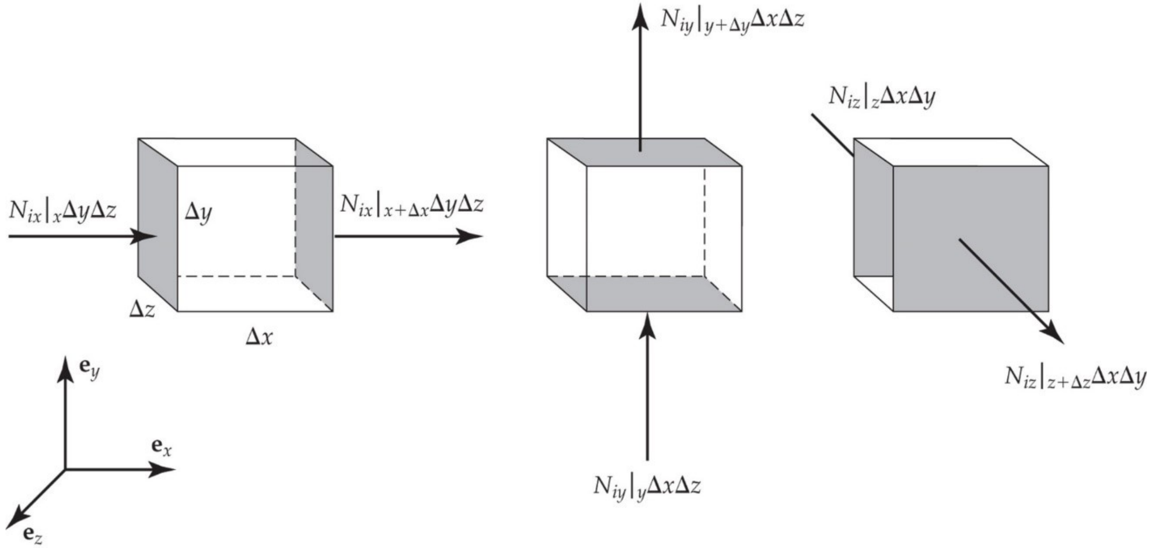


$$\frac{\left[\Delta x \Delta y \Delta z \frac{\partial \rho_i}{\partial t} = [N_{i@x} - N_{i@x+\Delta x}]\Delta y \Delta z + [N_{i@y} - N_{i@y+\Delta y}]\Delta x \Delta z + [N_{i@z} - N_{i@z+\Delta z}]\Delta x \Delta y + r_i \Delta x \Delta y \Delta z\right]}{[\Delta x \Delta y \Delta z]}$$

What is this?

$$\left[\frac{\partial \rho_i}{\partial t} = \frac{[N_{i@x} - N_{i@x+\Delta x}]}{\Delta x} + \frac{[N_{i@y} - N_{i@y+\Delta y}]}{\Delta y} + \frac{[N_{i@z} - N_{i@z+\Delta z}]}{\Delta z} + r_i\right]$$

Conservation of mass...



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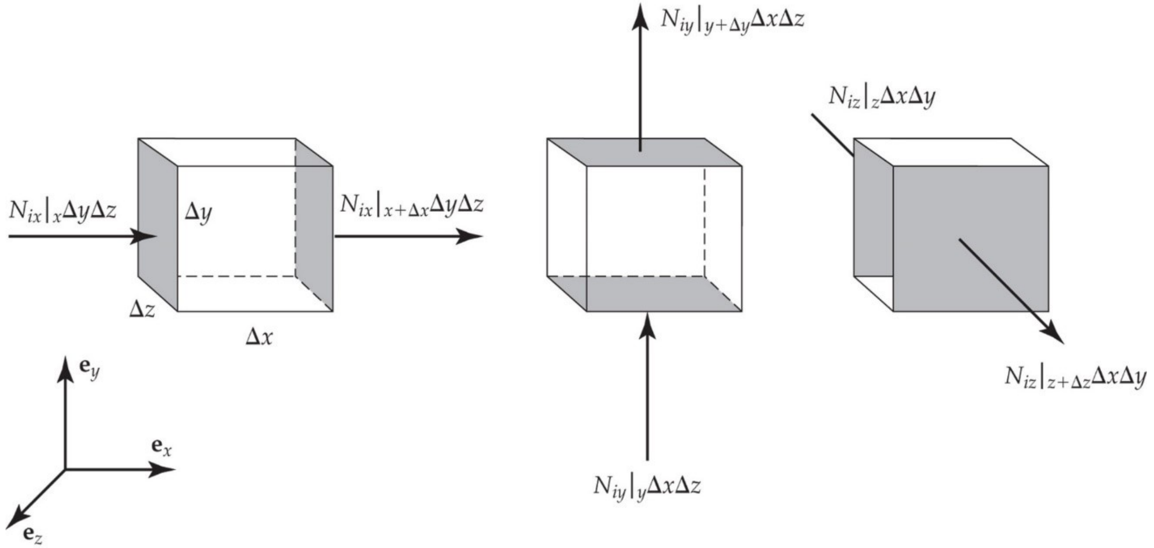
What is this?

$$\left[\frac{\partial \rho_i}{\partial t} = \frac{[N_{i@x} - N_{i@x+\Delta x}]}{\Delta x} + \frac{[N_{i@y} - N_{i@y+\Delta y}]}{\Delta y} + \frac{[N_{i@z} - N_{i@z+\Delta z}]}{\Delta z} + r_i\right]$$

What is this?

Conservation of mass…



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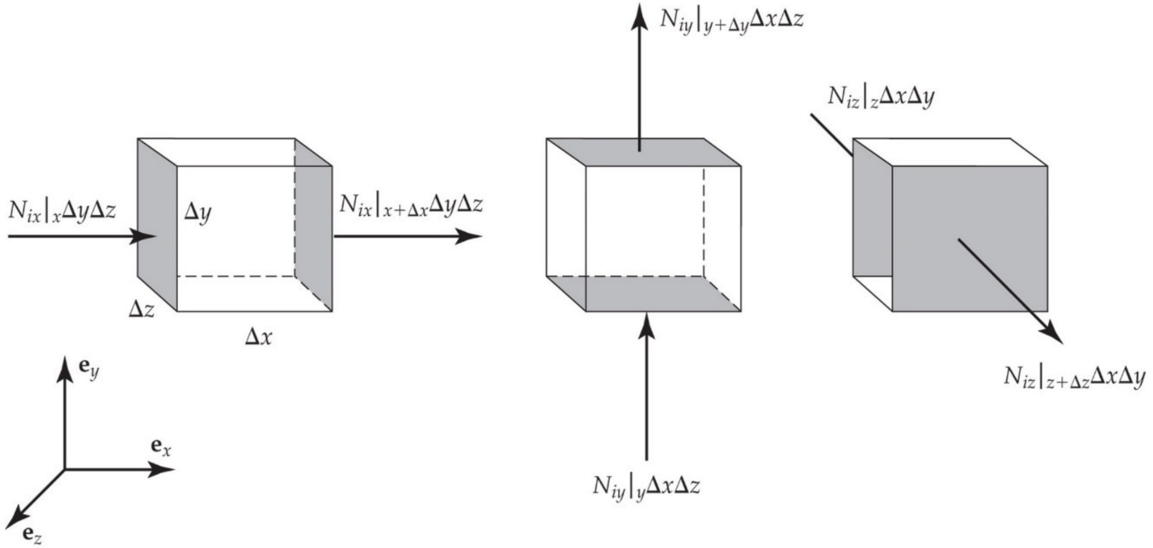
What is this?

$$\left[\frac{\partial \rho_i}{\partial t} = \frac{[N_{i@x} - N_{i@x+\Delta x}]}{\Delta x} + \frac{[N_{i@y} - N_{i@y+\Delta y}]}{\Delta y} + \frac{[N_{i@z} - N_{i@z+\Delta z}]}{\Delta z} + r_i\right]$$

What is this?

Conservation of mass…



$$\frac{\left[\Delta x \Delta y \Delta z \frac{\partial \rho_i}{\partial t} = [N_{i@x} - N_{i@x+\Delta x}]\Delta y \Delta z + [N_{i@y} - N_{i@y+\Delta y}]\Delta x \Delta z + [N_{i@z} - N_{i@z+\Delta z}]\Delta x \Delta y + r_i \Delta x \Delta y \Delta z\right]}{[\Delta x \Delta y \Delta z]}$$

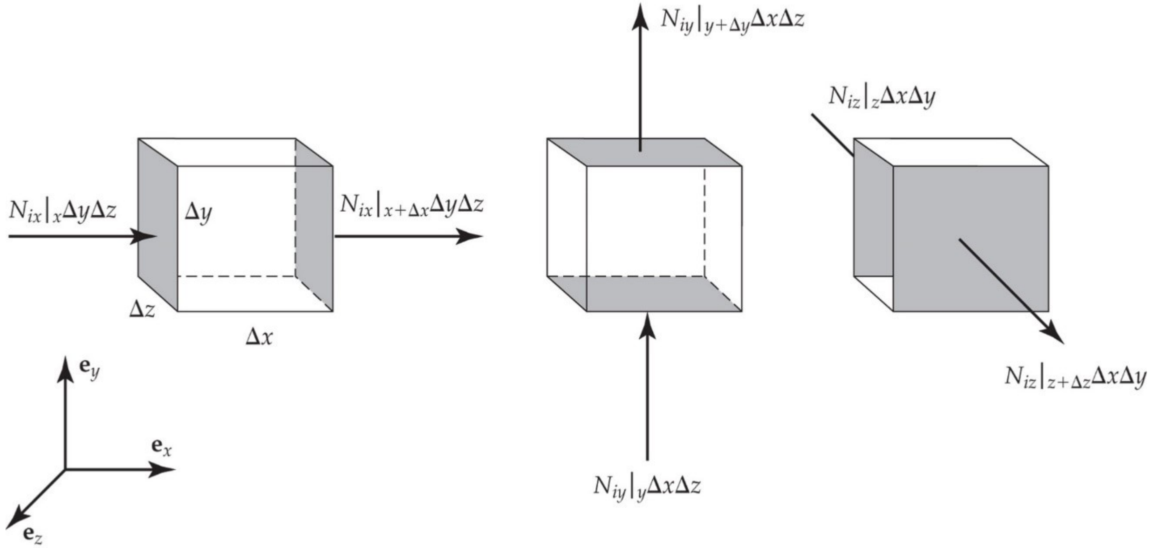
What is this?

$$\left[\frac{\partial \rho_i}{\partial t} = \frac{[N_{i@x} - N_{i@x+\Delta x}]}{\Delta x} + \frac{[N_{i@y} - N_{i@y+\Delta y}]}{\Delta y} + \frac{[N_{i@z} - N_{i@z+\Delta z}]}{\Delta z} + r_i\right]$$

What is this?

$$\frac{\partial \rho_i}{\partial t} = -\left(\frac{\partial N_i}{\partial x} + \frac{\partial N_i}{\partial y} + \frac{\partial N_i}{\partial z}\right) + r_i$$

Conservation of mass…



$$\frac{\left[\Delta x\Delta y\Delta z\frac{\partial\rho_i}{\partial t} = [N_{i@x} - N_{i@x+\Delta x}]\Delta y\Delta z + [N_{i@y} - N_{i@y+\Delta y}]\Delta x\Delta z + [N_{i@z} - N_{i@z+\Delta z}]\Delta x\Delta y + r_i\Delta x\Delta y\Delta z\right]}{[\Delta x\Delta y\Delta z]}$$

What is this?

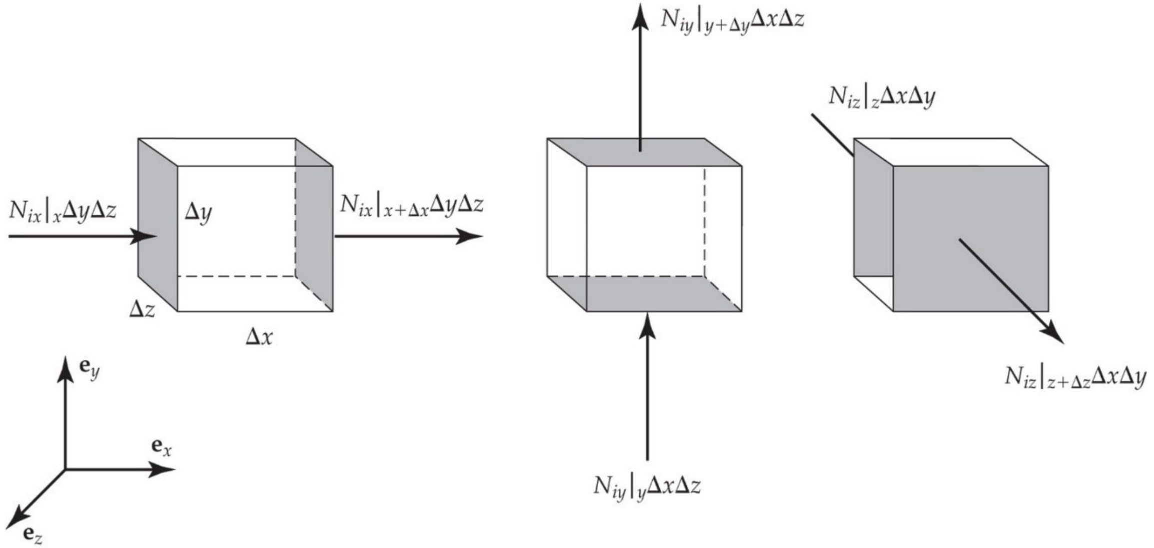
$$\left[\frac{\partial\rho_i}{\partial t} = \frac{[N_{i@x} - N_{i@x+\Delta x}]}{\Delta x} + \frac{[N_{i@y} - N_{i@y+\Delta y}]}{\Delta y} + \frac{[N_{i@z} - N_{i@z+\Delta z}]}{\Delta z} + r_i\right]$$

What is this?

$$\frac{\partial\rho_i}{\partial t} = -\left(\frac{\partial N_i}{\partial x} + \frac{\partial N_i}{\partial y} + \frac{\partial N_i}{\partial z}\right) + r_i$$

What is this?

Conservation of mass…



$$\frac{\left[\Delta x \Delta y \Delta z \frac{\partial \rho_i}{\partial t} = [N_{i@x} - N_{i@x+\Delta x}]\Delta y \Delta z + [N_{i@y} - N_{i@y+\Delta y}]\Delta x \Delta z + [N_{i@z} - N_{i@z+\Delta z}]\Delta x \Delta y + r_i \Delta x \Delta y \Delta z\right]}{[\Delta x \Delta y \Delta z]}$$

What is this?

$$\left[\frac{\partial \rho_i}{\partial t} = \frac{[N_{i@x} - N_{i@x+\Delta x}]}{\Delta x} + \frac{[N_{i@y} - N_{i@y+\Delta y}]}{\Delta y} + \frac{[N_{i@z} - N_{i@z+\Delta z}]}{\Delta z} + r_i\right]$$

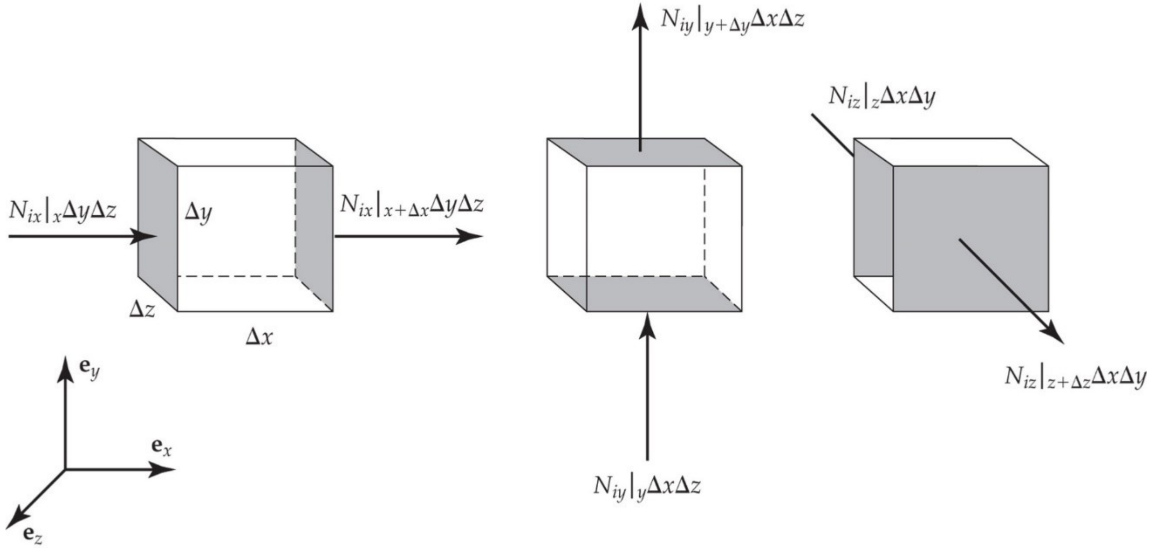
What is this?

$$\frac{\partial \rho_i}{\partial t} = -\left(\frac{\partial N_i}{\partial x} + \frac{\partial N_i}{\partial y} + \frac{\partial N_i}{\partial z}\right) + r_i$$

What is this?

$$\frac{\partial \rho_i}{\partial t} = -\nabla N_i + r_i$$

Conservation of mass…



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What is this?

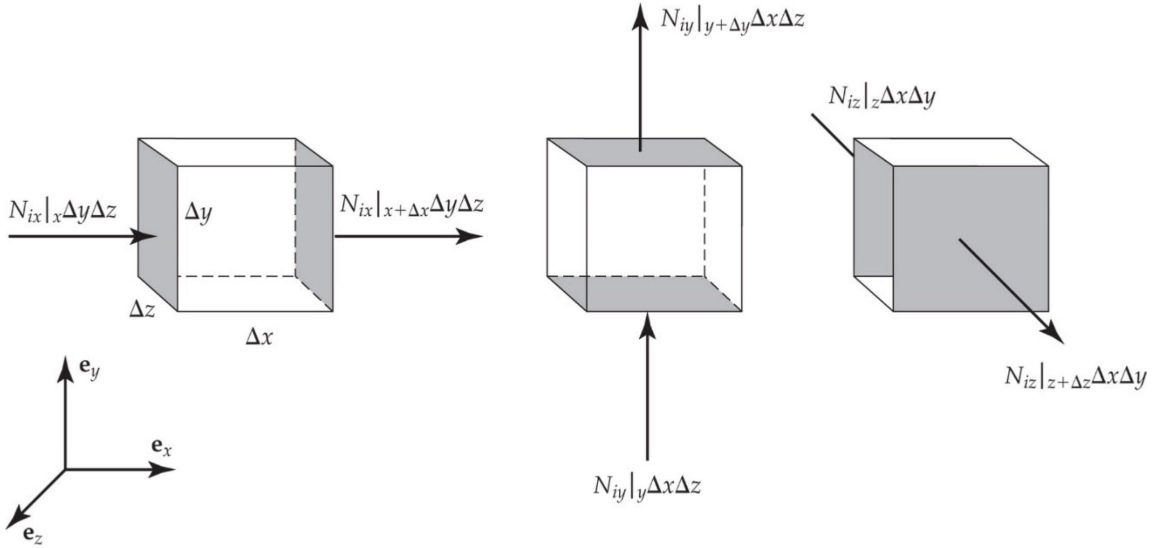
$$\frac{\partial\rho_i}{\partial t} = -\left(\frac{\partial N_i}{\partial x} + \frac{\partial N_i}{\partial y} + \frac{\partial N_i}{\partial z}\right) + r_i$$

What is this?

$$\frac{\partial\rho_i}{\partial t} = -\nabla N_i + r_i$$

What about everything?

Conservation of mass…



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What is this?

$$\left[\frac{\partial \rho_i}{\partial t} = \frac{[N_{i@x} - N_{i@x+\Delta x}]}{\Delta x} + \frac{[N_{i@y} - N_{i@y+\Delta y}]}{\Delta y} + \frac{[N_{i@z} - N_{i@z+\Delta z}]}{\Delta z} + r_i\right]$$

What is this?

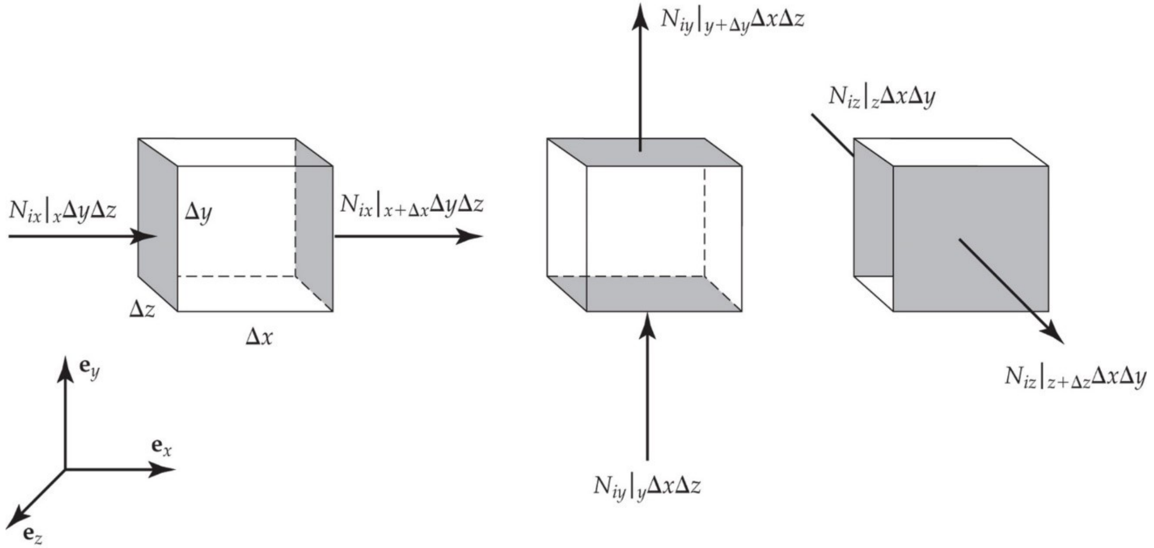
$$\frac{\partial \rho_i}{\partial t} = -\left(\frac{\partial N_i}{\partial x} + \frac{\partial N_i}{\partial y} + \frac{\partial N_i}{\partial z}\right) + r_i$$

What is this?

$$\frac{\partial \rho_i}{\partial t} = -\nabla N_i + r_i$$

What about everything? $\frac{\partial \rho}{\partial t} = -\nabla \sum_i^n N_i + \sum_i^n r_i$

Conservation of mass…



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$$\left[\frac{\partial \rho_i}{\partial t} = \frac{[N_{i@x} - N_{i@x+\Delta x}]}{\Delta x} + \frac{[N_{i@y} - N_{i@y+\Delta y}]}{\Delta y} + \frac{[N_{i@z} - N_{i@z+\Delta z}]}{\Delta z} + r_i\right]$$

What is this?

$$\frac{\partial \rho_i}{\partial t} = -\left(\frac{\partial N_i}{\partial x} + \frac{\partial N_i}{\partial y} + \frac{\partial N_i}{\partial z}\right) + r_i$$

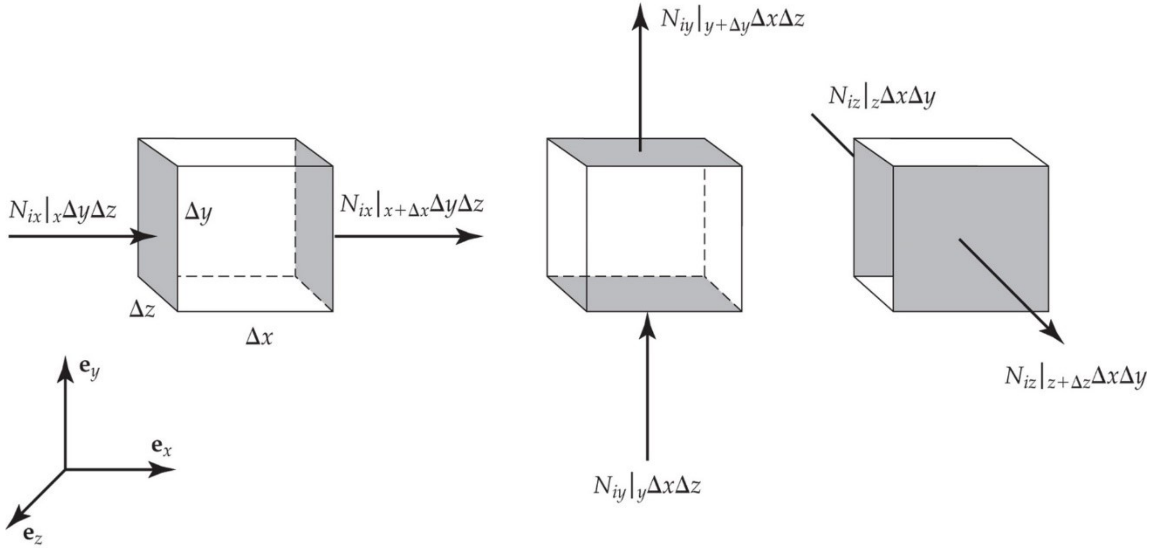
What is this?

$$\frac{\partial \rho_i}{\partial t} = -\nabla N_i + r_i$$

?

What about everything? $\frac{\partial \rho}{\partial t} = -\nabla \sum_i^n N_i + \sum_i^n r_i$

Conservation of mass…



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What is this?

$$\left[\frac{\partial \rho_i}{\partial t} = \frac{[N_{i@x} - N_{i@x+\Delta x}]}{\Delta x} + \frac{[N_{i@y} - N_{i@y+\Delta y}]}{\Delta y} + \frac{[N_{i@z} - N_{i@z+\Delta z}]}{\Delta z} + r_i\right]$$

What is this?

0

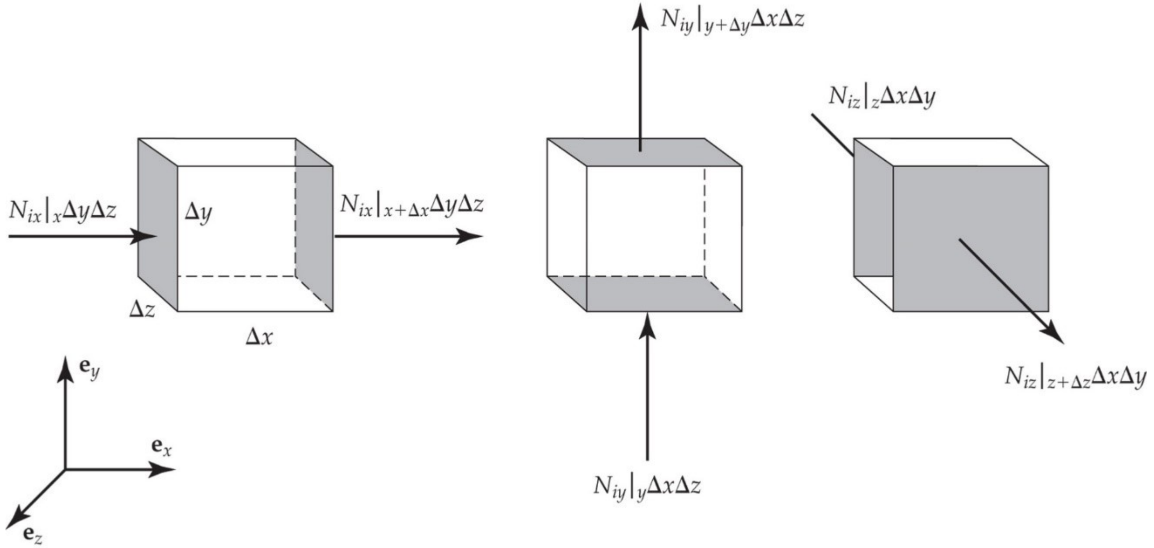
$$\frac{\partial \rho_i}{\partial t} = -\left(\frac{\partial N_i}{\partial x} + \frac{\partial N_i}{\partial y} + \frac{\partial N_i}{\partial z}\right) + r_i$$

What is this?

$$\frac{\partial \rho_i}{\partial t} = -\nabla N_i + r_i$$

What about everything? $\frac{\partial \rho}{\partial t} = -\nabla \sum_i^n N_i + \sum_i^n r_i$

Conservation of mass…



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What is this?

$$\left[\frac{\partial \rho_i}{\partial t} = \frac{[N_{i@x} - N_{i@x+\Delta x}]}{\Delta x} + \frac{[N_{i@y} - N_{i@y+\Delta y}]}{\Delta y} + \frac{[N_{i@z} - N_{i@z+\Delta z}]}{\Delta z} + r_i\right]$$

What is this?

$$\frac{\partial \rho_i}{\partial t} = -\left(\frac{\partial N_i}{\partial x} + \frac{\partial N_i}{\partial y} + \frac{\partial N_i}{\partial z}\right) + r_i$$

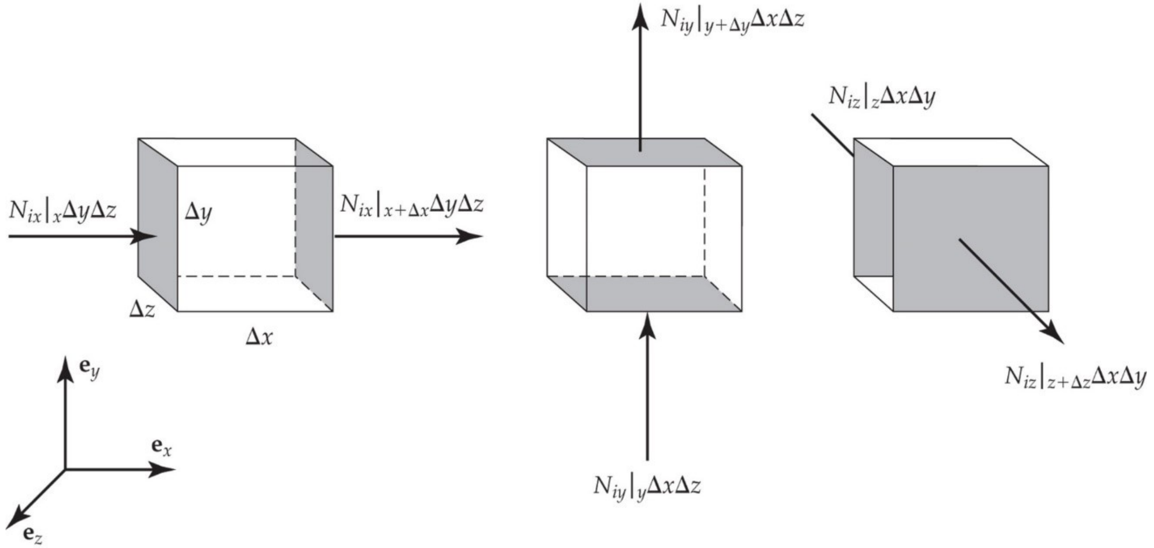
What is this?

$$\frac{\partial \rho_i}{\partial t} = -\nabla N_i + r_i$$

? **0**

What about everything? $\frac{\partial \rho}{\partial t} = -\nabla \sum_i^n N_i + \sum_i^n r_i$

Conservation of mass…



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What is this?

$$\left[\frac{\partial \rho_i}{\partial t} = \frac{[N_{i@x} - N_{i@x+\Delta x}]}{\Delta x} + \frac{[N_{i@y} - N_{i@y+\Delta y}]}{\Delta y} + \frac{[N_{i@z} - N_{i@z+\Delta z}]}{\Delta z} + r_i\right]$$

What is this?

ρVel **0**

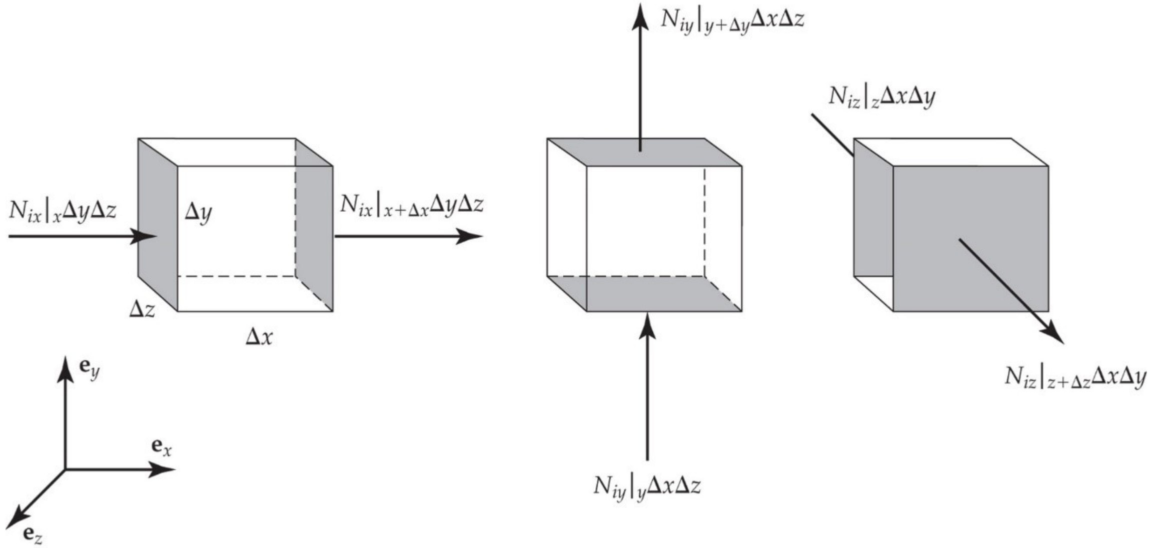
$$\frac{\partial \rho_i}{\partial t} = -\left(\frac{\partial N_i}{\partial x} + \frac{\partial N_i}{\partial y} + \frac{\partial N_i}{\partial z}\right) + r_i$$

What is this?

$$\frac{\partial \rho_i}{\partial t} = -\nabla N_i + r_i$$

What about everything? $\frac{\partial \rho}{\partial t} = -\nabla \sum_i^n N_i + \sum_i^n r_i$

Conservation of mass…



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What is this?

$$\left[\frac{\partial \rho_i}{\partial t} = \frac{[N_{i@x} - N_{i@x+\Delta x}]}{\Delta x} + \frac{[N_{i@y} - N_{i@y+\Delta y}]}{\Delta y} + \frac{[N_{i@z} - N_{i@z+\Delta z}]}{\Delta z} + r_i\right]$$

What is this?

ρVel **0**

$$\frac{\partial \rho_i}{\partial t} = -\left(\frac{\partial N_i}{\partial x} + \frac{\partial N_i}{\partial y} + \frac{\partial N_i}{\partial z}\right) + r_i$$

What is this?

Also…

$$\frac{\partial C_i}{\partial t} = \frac{\partial \rho_i}{\partial t} = -\nabla N_i + r_i$$

What about everything? $\frac{\partial \rho}{\partial t} = -\nabla \sum_i^n N_i + \sum_i^n r_i$

So…

$$N_i = -D_{ij}^{o}\nabla C_i + C_i v_i$$

TABLE 7.1

Conservation of Mass Using Molar Fluxes Based on Fixed Coordinates

Rectangular	$\frac{\partial C_i}{\partial t} = -\left(\frac{\partial N_{i_x}}{\partial x} + \frac{\partial N_{i_y}}{\partial y} + \frac{\partial N_{i_z}}{\partial z}\right) + R_i$	(7.3.9a)
Cylindrical	$\frac{\partial C_i}{\partial t} = -\left(\frac{1}{r}\frac{\partial (rN_{i_r})}{\partial r} + \frac{1}{r}\frac{\partial N_{i_\theta}}{\partial \theta} + \frac{\partial N_{i_z}}{\partial z}\right) + R_i$	(7.3.9b)
Spherical	$\frac{\partial C_i}{\partial t} = -\left(\frac{1}{r^2}\frac{\partial (r^2 N_{i_r})}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial (N_{i\theta}\sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial N_{i_\phi}}{\partial \phi}\right) + R_i$	(7.3.9c)

Conservation of Mass Using Molar Fluxes Based on Fixed Coordinates

Rectangular
$$\frac{\partial C_i}{\partial t} = -\left(\frac{\partial N_{i_x}}{\partial x} + \frac{\partial N_{i_y}}{\partial y} + \frac{\partial N_{i_z}}{\partial z}\right) + R_i \qquad (7.3.9a)$$

Cylindrical
$$\frac{\partial C_i}{\partial t} = -\left(\frac{1}{r}\frac{\partial (rN_{i_r})}{\partial r} + \frac{1}{r}\frac{\partial N_{i_\theta}}{\partial \theta} + \frac{\partial N_{i_z}}{\partial z}\right) + R_i \qquad (7.3.9b)$$

Spherical
$$\frac{\partial C_i}{\partial t} = -\left(\frac{1}{r^2}\frac{\partial (r^2 N_{i_r})}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial (N_{i\theta}\sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial N_{i_\phi}}{\partial \phi}\right) + R_i \qquad (7.3.9c)$$

$$N_i = -D_{ij}^{o}\nabla C_i + C_i v_i$$

TABLE 7.2

TABLE 7.2

Conservation Relatic

Rectangular
$$\frac{\partial C_i}{\partial t} + v_x\frac{\partial C_i}{\partial x} + v_y\frac{\partial C_i}{\partial y} + v_z\frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i \qquad (7.3.13a)$$

Cylindrical
$$\frac{\partial C_i}{\partial t} + v_r\frac{\partial C_i}{\partial r} + \frac{v_\theta}{r}\frac{\partial C_i}{\partial \theta} + v_z\frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_i}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 C_i}{\partial \theta^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i \qquad (7.3.13b)$$

Spherical
$$\frac{\partial C_i}{\partial t} + v_r\frac{\partial C_i}{\partial r} + \frac{v_\theta}{r}\frac{\partial C_i}{\partial \theta} + \frac{v_\phi}{r\sin\theta}\frac{\partial C_i}{\partial \phi}$$
$$= D_{ij}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_i}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial C_i}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 C_i}{\partial \phi^2}\right) + R_i \qquad (7.3.13c)$$

Conservation of Mass Using Molar Fluxes Based on Fixed Coordinates

Rectangular
$$\frac{\partial C_i}{\partial t} = -\left(\frac{\partial N_{i_x}}{\partial x} + \frac{\partial N_{i_y}}{\partial y} + \frac{\partial N_{i_z}}{\partial z}\right) + R_i \qquad (7.3.9a)$$

Cylindrical
$$\frac{\partial C_i}{\partial t} = -\left(\frac{1}{r}\frac{\partial (rN_{i_r})}{\partial r} + \frac{1}{r}\frac{\partial N_{i_\theta}}{\partial \theta} + \frac{\partial N_{i_z}}{\partial z}\right) + R_i \qquad (7.3.9b)$$

Spherical
$$\frac{\partial C_i}{\partial t} = -\left(\frac{1}{r^2}\frac{\partial (r^2 N_{i_r})}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial (N_{i\theta}\sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial N_{i_\phi}}{\partial \phi}\right) + R_i \qquad (7.3.9c)$$

$$N_i = -D_{ij}^{o}\nabla C_i + C_i v_i$$

TABLE 7.2

Conservation Relation

? Rectangular
$$\frac{\partial C_i}{\partial t} + v_x\frac{\partial C_i}{\partial x} + v_y\frac{\partial C_i}{\partial y} + v_z\frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i \qquad (7.3.13a)$$

Cylindrical
$$\frac{\partial C_i}{\partial t} + v_r\frac{\partial C_i}{\partial r} + \frac{v_\theta}{r}\frac{\partial C_i}{\partial \theta} + v_z\frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_i}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 C_i}{\partial \theta^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i \qquad (7.3.13b)$$

Spherical
$$\frac{\partial C_i}{\partial t} + v_r\frac{\partial C_i}{\partial r} + \frac{v_\theta}{r}\frac{\partial C_i}{\partial \theta} + \frac{v_\phi}{r\sin\theta}\frac{\partial C_i}{\partial \phi}$$
$$= D_{ij}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_i}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial C_i}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 C_i}{\partial \phi^2}\right) + R_i \qquad (7.3.13c)$$

Conservation of Mass Using Molar Fluxes Based on Fixed Coordinates

Rectangular
$$\frac{\partial C_i}{\partial t} = -\left(\frac{\partial N_{i_x}}{\partial x} + \frac{\partial N_{i_y}}{\partial y} + \frac{\partial N_{i_z}}{\partial z}\right) + R_i \qquad (7.3.9a)$$

Cylindrical
$$\frac{\partial C_i}{\partial t} = -\left(\frac{1}{r}\frac{\partial (rN_{i_r})}{\partial r} + \frac{1}{r}\frac{\partial N_{i_\theta}}{\partial \theta} + \frac{\partial N_{i_z}}{\partial z}\right) + R_i \qquad (7.3.9b)$$

Spherical
$$\frac{\partial C_i}{\partial t} = -\left(\frac{1}{r^2}\frac{\partial (r^2 N_{i_r})}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial (N_{i\theta}\sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial N_{i_\phi}}{\partial \phi}\right) + R_i \qquad (7.3.9c)$$

$$N_i = -D_{ij}^{o}\nabla C_i + C_i v_i$$

TABLE 7.2

Conservation Relation

Fick's 2nd + ?

Rectangular
$$\frac{\partial C_i}{\partial t} + v_x\frac{\partial C_i}{\partial x} + v_y\frac{\partial C_i}{\partial y} + v_z\frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i \qquad (7.3.13a)$$

Cylindrical
$$\frac{\partial C_i}{\partial t} + v_r\frac{\partial C_i}{\partial r} + \frac{v_\theta}{r}\frac{\partial C_i}{\partial \theta} + v_z\frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_i}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 C_i}{\partial \theta^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i \qquad (7.3.13b)$$

Spherical
$$\frac{\partial C_i}{\partial t} + v_r\frac{\partial C_i}{\partial r} + \frac{v_\theta}{r}\frac{\partial C_i}{\partial \theta} + \frac{v_\phi}{r\sin\theta}\frac{\partial C_i}{\partial \phi}$$
$$= D_{ij}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_i}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial C_i}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 C_i}{\partial \phi^2}\right) + R_i \qquad (7.3.13c)$$

Conservation of Mass Using Molar Fluxes Based on Fixed Coordinates

Rectangular
$$\frac{\partial C_i}{\partial t} = -\left(\frac{\partial N_{i_x}}{\partial x} + \frac{\partial N_{i_y}}{\partial y} + \frac{\partial N_{i_z}}{\partial z}\right) + R_i \qquad (7.3.9a)$$

Cylindrical
$$\frac{\partial C_i}{\partial t} = -\left(\frac{1}{r}\frac{\partial (rN_{i_r})}{\partial r} + \frac{1}{r}\frac{\partial N_{i_\theta}}{\partial \theta} + \frac{\partial N_{i_z}}{\partial z}\right) + R_i \qquad (7.3.9b)$$

Spherical
$$\frac{\partial C_i}{\partial t} = -\left(\frac{1}{r^2}\frac{\partial (r^2 N_{i_r})}{\partial r} + \frac{1}{r\sin\theta}\frac{\partial (N_{i\theta}\sin\theta)}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial N_{i_\phi}}{\partial \phi}\right) + R_i \qquad (7.3.9c)$$

$$N_i = -D_{ij}^o \nabla C_i + C_i v_i$$

TABLE 7.2

Conservation Relation

Fick's 2nd + convection

Rectangular
$$\frac{\partial C_i}{\partial t} + v_x\frac{\partial C_i}{\partial x} + v_y\frac{\partial C_i}{\partial y} + v_z\frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i \qquad (7.3.13a)$$

Cylindrical
$$\frac{\partial C_i}{\partial t} + v_r\frac{\partial C_i}{\partial r} + \frac{v_\theta}{r}\frac{\partial C_i}{\partial \theta} + v_z\frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_i}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 C_i}{\partial \theta^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i \qquad (7.3.13b)$$

Spherical
$$\frac{\partial C_i}{\partial t} + v_r\frac{\partial C_i}{\partial r} + \frac{v_\theta}{r}\frac{\partial C_i}{\partial \theta} + \frac{v_\phi}{r\sin\theta}\frac{\partial C_i}{\partial \phi} = D_{ij}\left(\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial C_i}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial C_i}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 C_i}{\partial \phi^2}\right) + R_i \qquad (7.3.13c)$$

Example 7.1

Figure 7.2 Schematic of transport across a membrane with convection.

Example 7.1 Consider steady-state one-dimensional diffusion and convection across a membrane of thickness L (Figure 7.2). Such a membrane may be a synthetic membrane or a cellular layer. No chemical reactions are occurring. At $z = 0$, $C = \Phi C_0$ and at $z = L$, $C = \Phi C_L$, where Φ is the partition coefficient of the solute in the membrane. Determine the concentration profile and flux across the membrane, and compare it with results for diffusion only.

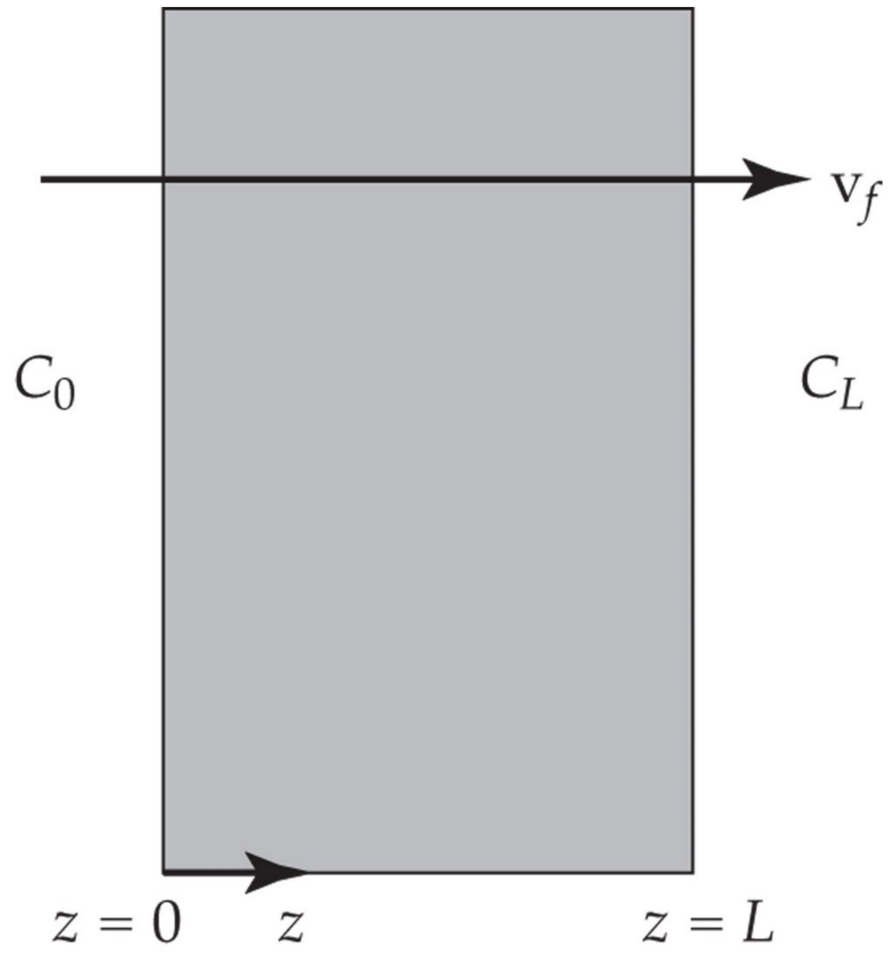


Figure 7.2 Schematic of transport across a membrane with convection.

Example 7.1 Consider steady-state one-dimensional diffusion and convection across a membrane of thickness L (Figure 7.2). Such a membrane may be a synthetic membrane or a cellular layer. No chemical reactions are occurring. At $z = 0$, $C = \Phi C_0$ and at $z = L$, $C = \Phi C_L$, where Φ is the partition coefficient of the solute in the membrane. Determine the concentration profile and flux across the membrane, and compare it with results for diffusion only.

Where to start?
What coordinates are we using?

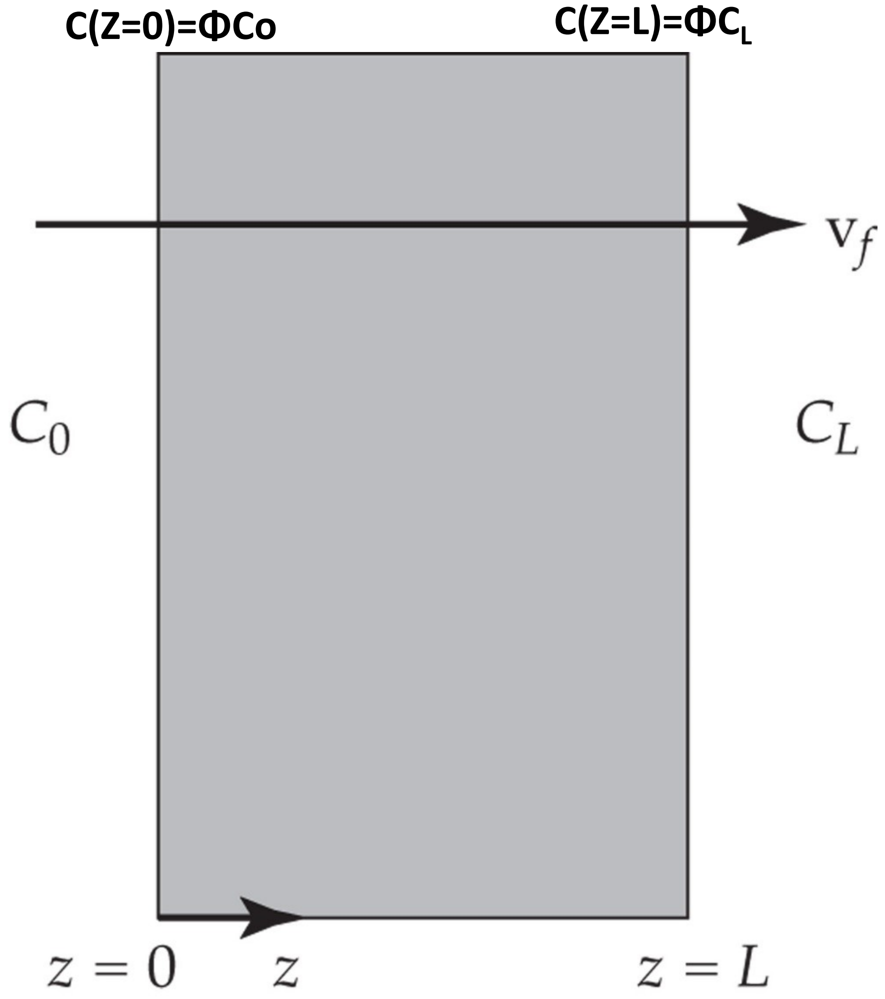
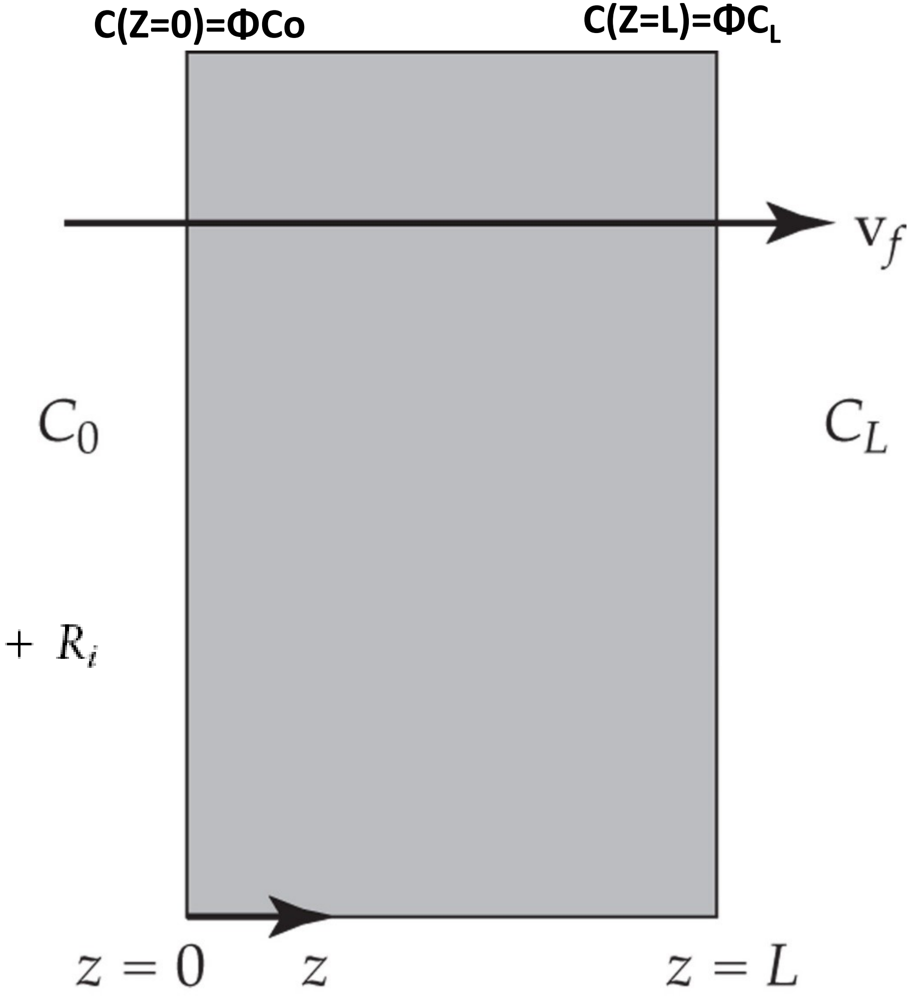


Figure 7.2 Schematic of transport across a membrane with convection.

Example 7.1 Consider steady-state one-dimensional diffusion and convection across a membrane of thickness L (Figure 7.2). Such a membrane may be a synthetic membrane or a cellular layer. No chemical reactions are occurring. At $z = 0$, $C = \Phi C_0$ and at $z = L$, $C = \Phi C_L$, where Φ is the partition coefficient of the solute in the membrane. Determine the concentration profile and flux across the membrane, and compare it with results for diffusion only.



Where to start?

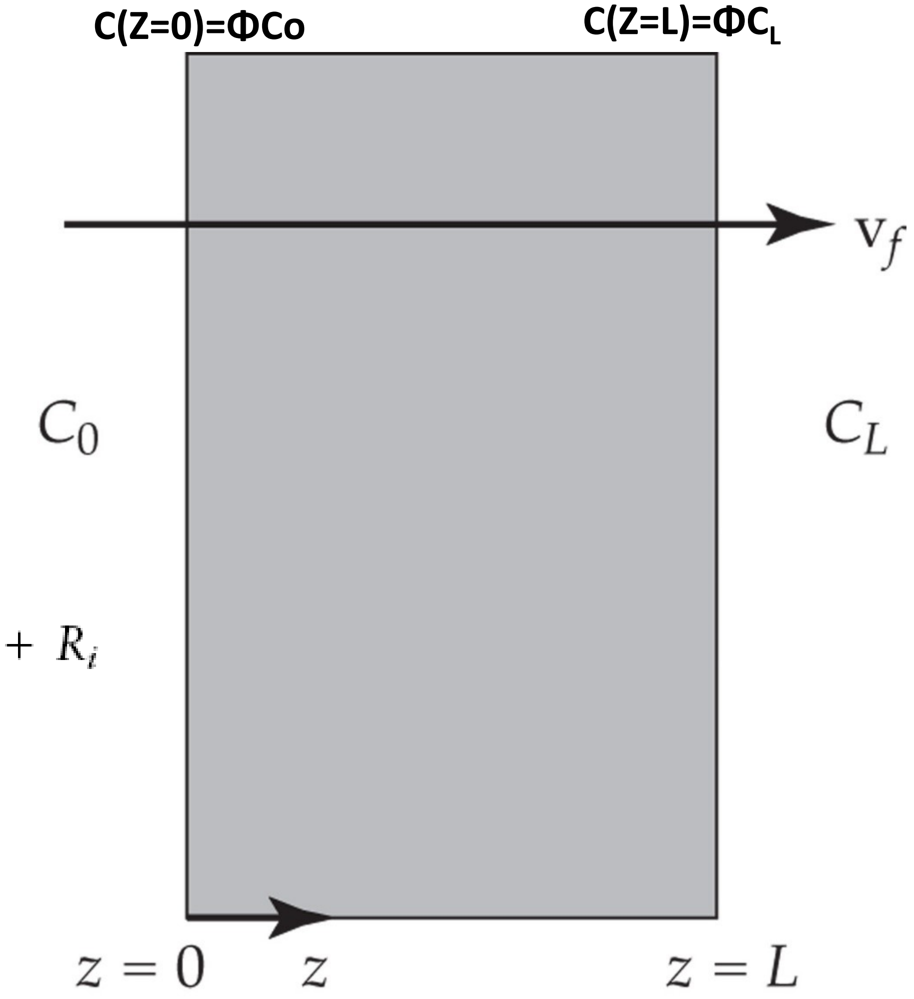
What coordinates are we using?

Rectangular
$$\frac{\partial C_i}{\partial t} + v_x\frac{\partial C_i}{\partial x} + v_y\frac{\partial C_i}{\partial y} + v_z\frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

Fick's 2nd + Convection… Yay!

Figure 7.2 Schematic of transport across a membrane with convection.

Example 7.1 Consider steady-state one-dimensional diffusion and convection across a membrane of thickness L (Figure 7.2). Such a membrane may be a synthetic membrane or a cellular layer. No chemical reactions are occurring. At $z = 0$, $C = \Phi C_0$ and at $z = L$, $C = \Phi C_L$, where Φ is the partition coefficient of the solute in the membrane. Determine the concentration profile and flux across the membrane, and compare it with results for diffusion only.



Where to start?

What coordinates are we using?

Rectangular $$\frac{\partial C_i}{\partial t} + v_x \frac{\partial C_i}{\partial x} + v_y \frac{\partial C_i}{\partial y} + v_z \frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

Fick's 2nd + Convection… Yay!

Figure 7.2 Schematic of transport across a membrane with convection.

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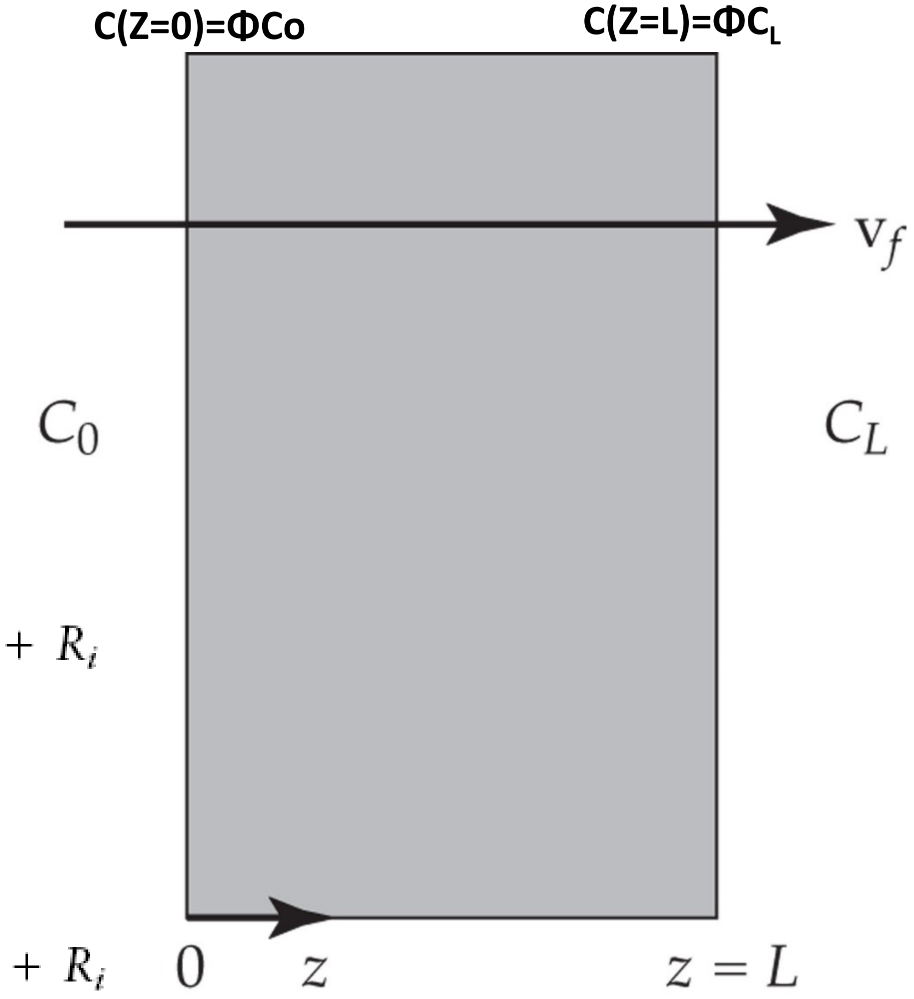


Where to start?
What coordinates are we using?

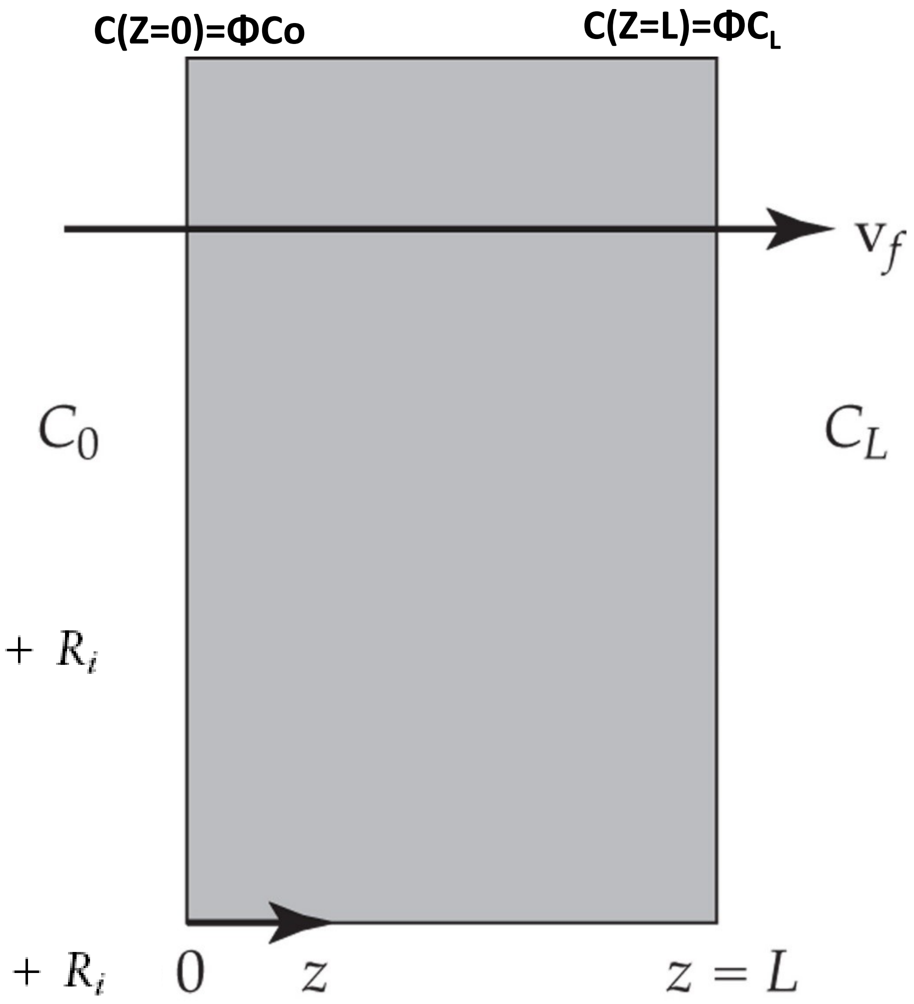
Rectangular $$\frac{\partial C_i}{\partial t} + v_x \frac{\partial C_i}{\partial x} + v_y \frac{\partial C_i}{\partial y} + v_z \frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

Fick's 2nd + Convection… Yay!

Rectangular $$\frac{\partial C_i}{\partial t} + v_x \frac{\partial C_i}{\partial x} + v_y \frac{\partial C_i}{\partial y} + v_z \frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

Figure 7.2 Schematic of transport across a membrane with convection.

Example 7.1 Consider steady-state one-dimensional diffusion and convection across a membrane of thickness L (Figure 7.2). Such a membrane may be a synthetic membrane or a cellular layer. No chemical reactions are occurring. At $z = 0$, $C = \Phi C_0$ and at $z = L$, $C = \Phi C_L$, where Φ is the partition coefficient of the solute in the membrane. Determine the concentration profile and flux across the membrane, and compare it with results for diffusion only.



Where to start?

What coordinates are we using?

Rectangular $$\frac{\partial C_i}{\partial t} + v_x \frac{\partial C_i}{\partial x} + v_y \frac{\partial C_i}{\partial y} + v_z \frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

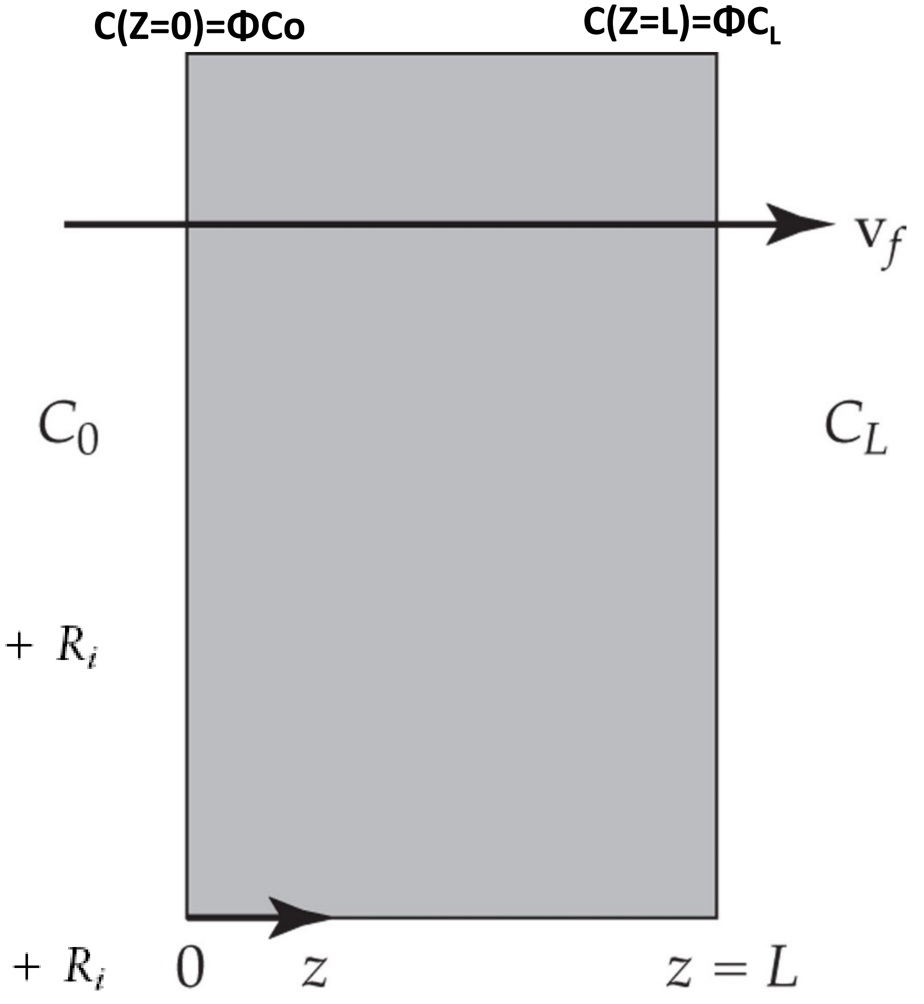
Fick's 2nd + Convection… Yay!

Rectangular $$\frac{\partial C_i}{\partial t} + v_x \frac{\partial C_i}{\partial x} + v_y \frac{\partial C_i}{\partial y} + v_z \frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

?

Figure 7.2 Schematic of transport across a membrane with convection.

Example 7.1 Consider steady-state one-dimensional diffusion and convection across a membrane of thickness L (Figure 7.2). Such a membrane may be a synthetic membrane or a cellular layer. No chemical reactions are occurring. At $z = 0$, $C = \Phi C_0$ and at $z = L$, $C = \Phi C_L$, where Φ is the partition coefficient of the solute in the membrane. Determine the concentration profile and flux across the membrane, and compare it with results for diffusion only.



Where to start?
What coordinates are we using?

Rectangular $$\frac{\partial C_i}{\partial t} + v_x\frac{\partial C_i}{\partial x} + v_y\frac{\partial C_i}{\partial y} + v_z\frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

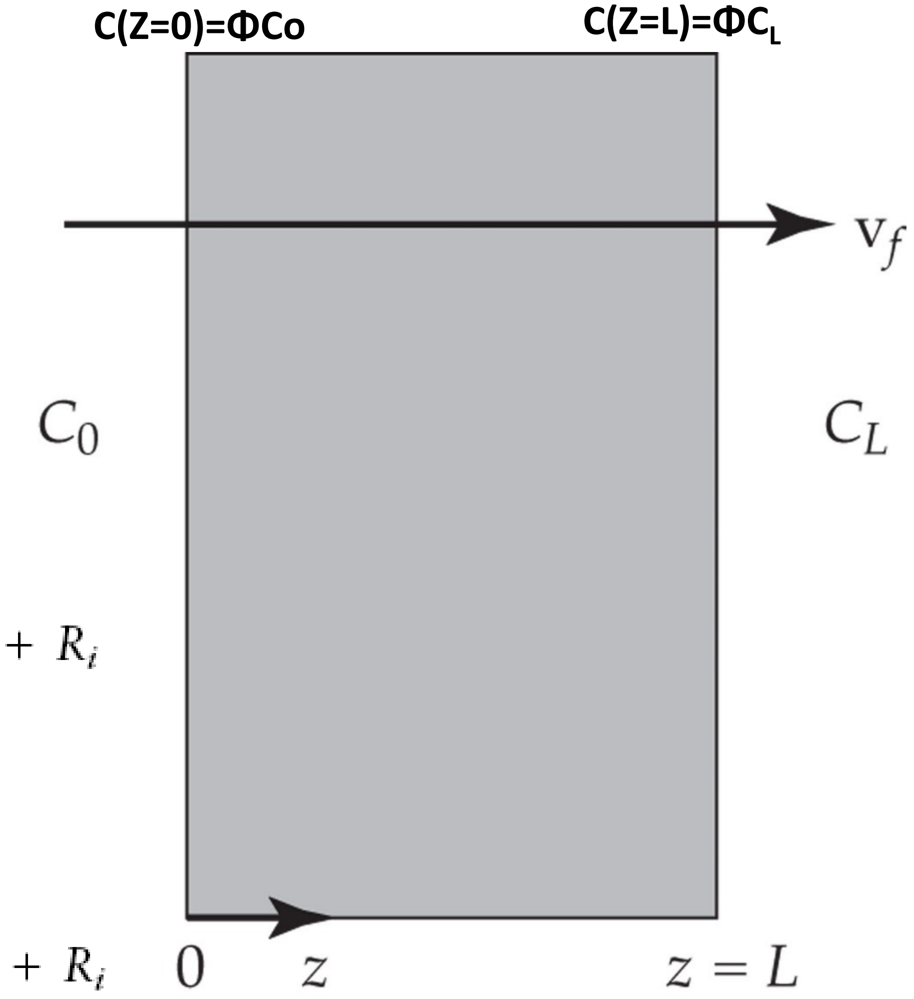
Fick's 2nd + Convection… Yay!

Rectangular $$\frac{\partial C_i}{\partial t} + v_x\frac{\partial C_i}{\partial x} + v_y\frac{\partial C_i}{\partial y} + v_z\frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

S.S ?

Figure 7.2 Schematic of transport across a membrane with convection.

Example 7.1 Consider steady-state one-dimensional diffusion and convection across a membrane of thickness L (Figure 7.2). Such a membrane may be a synthetic membrane or a cellular layer. No chemical reactions are occurring. At $z = 0$, $C = \Phi C_0$ and at $z = L$, $C = \Phi C_L$, where Φ is the partition coefficient of the solute in the membrane. Determine the concentration profile and flux across the membrane, and compare it with results for diffusion only.



Where to start?
What coordinates are we using?

Rectangular $$\frac{\partial C_i}{\partial t} + v_x \frac{\partial C_i}{\partial x} + v_y \frac{\partial C_i}{\partial y} + v_z \frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

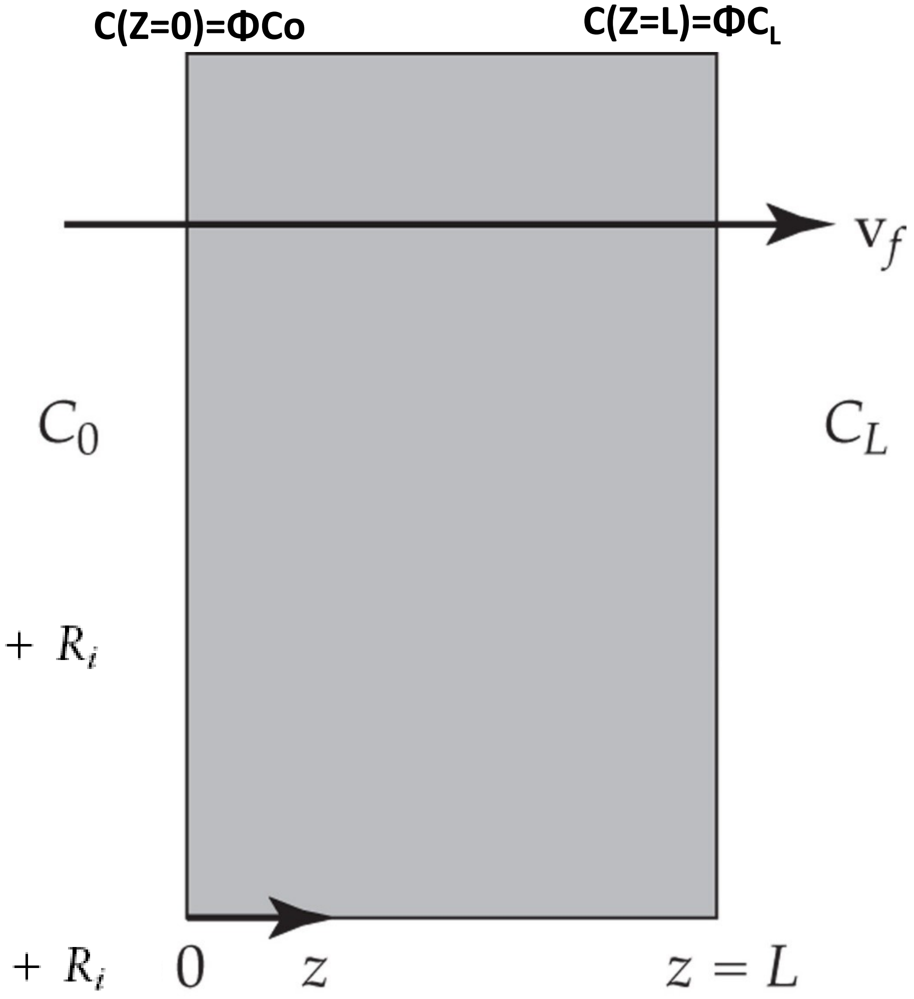
Fick's 2nd + Convection… Yay!

Rectangular $$\frac{\partial C_i}{\partial t} + v_x \frac{\partial C_i}{\partial x} + v_y \frac{\partial C_i}{\partial y} + v_z \frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

S.S N/A ?

Figure 7.2 Schematic of transport across a membrane with convection.

Example 7.1 Consider steady-state one-dimensional diffusion and convection across a membrane of thickness L (Figure 7.2). Such a membrane may be a synthetic membrane or a cellular layer. No chemical reactions are occurring. At $z = 0$, $C = \Phi C_0$ and at $z = L$, $C = \Phi C_L$, where Φ is the partition coefficient of the solute in the membrane. Determine the concentration profile and flux across the membrane, and compare it with results for diffusion only.



Where to start?
What coordinates are we using?

Rectangular $$\frac{\partial C_i}{\partial t} + v_x \frac{\partial C_i}{\partial x} + v_y \frac{\partial C_i}{\partial y} + v_z \frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

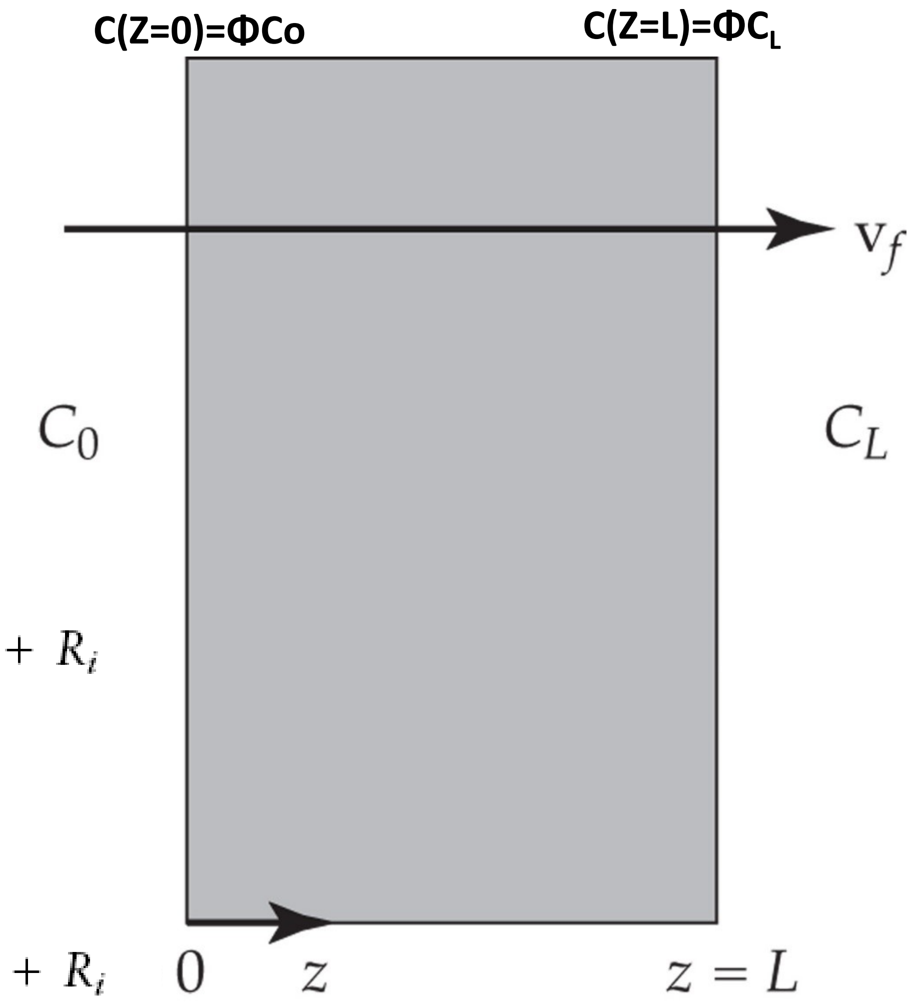
Fick's 2nd + Convection… Yay!

Rectangular $$\frac{\partial C_i}{\partial t} + v_x \frac{\partial C_i}{\partial x} + v_y \frac{\partial C_i}{\partial y} + v_z \frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

S.S N/A N/A ?

Figure 7.2 Schematic of transport across a membrane with convection.

Example 7.1 Consider steady-state one-dimensional diffusion and convection across a membrane of thickness L (Figure 7.2). Such a membrane may be a synthetic membrane or a cellular layer. No chemical reactions are occurring. At $z = 0$, $C = \Phi C_0$ and at $z = L$, $C = \Phi C_L$, where Φ is the partition coefficient of the solute in the membrane. Determine the concentration profile and flux across the membrane, and compare it with results for diffusion only.



Where to start?
What coordinates are we using?

Rectangular $$\frac{\partial C_i}{\partial t} + v_x\frac{\partial C_i}{\partial x} + v_y\frac{\partial C_i}{\partial y} + v_z\frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

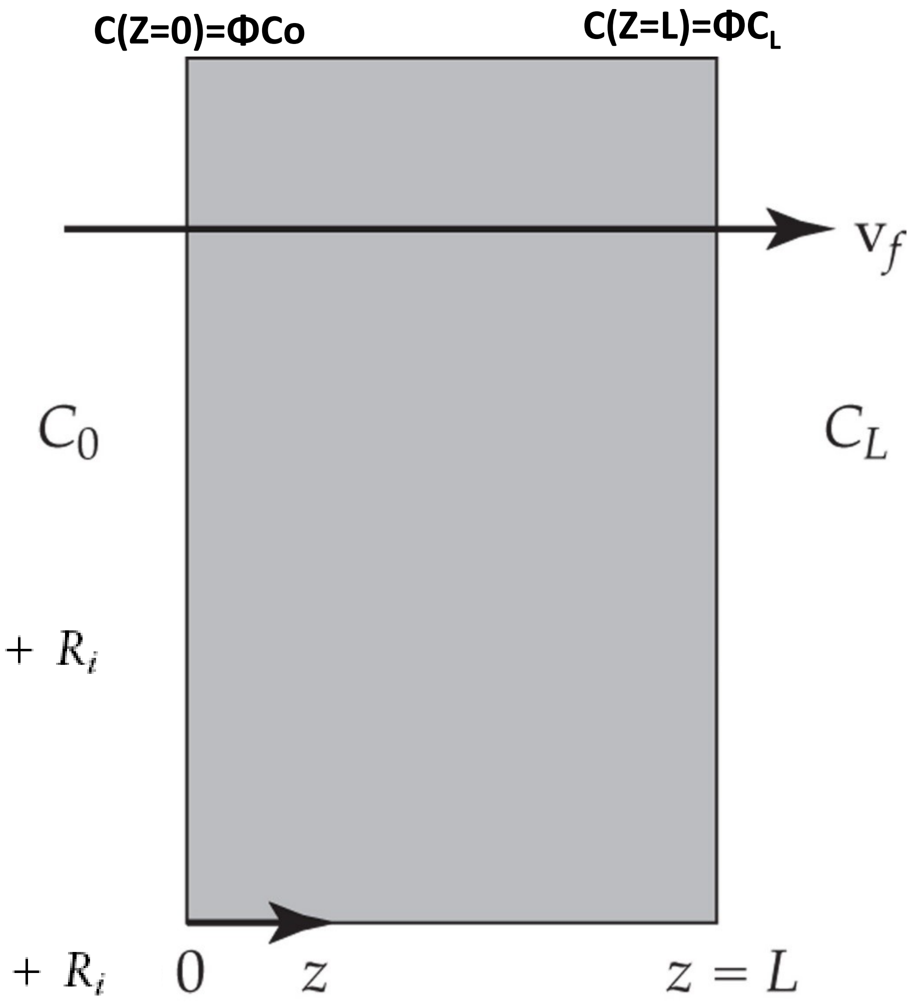
Fick's 2nd + Convection… Yay!

Rectangular $$\frac{\partial C_i}{\partial t} + v_x\frac{\partial C_i}{\partial x} + v_y\frac{\partial C_i}{\partial y} + v_z\frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

S.S N/A N/A f ?

Figure 7.2 Schematic of transport across a membrane with convection.

Example 7.1 Consider steady-state one-dimensional diffusion and convection across a membrane of thickness L (Figure 7.2). Such a membrane may be a synthetic membrane or a cellular layer. No chemical reactions are occurring. At $z = 0$, $C = \Phi C_0$ and at $z = L$, $C = \Phi C_L$, where Φ is the partition coefficient of the solute in the membrane. Determine the concentration profile and flux across the membrane, and compare it with results for diffusion only.



Where to start?
What coordinates are we using?

Rectangular $$\frac{\partial C_i}{\partial t} + v_x\frac{\partial C_i}{\partial x} + v_y\frac{\partial C_i}{\partial y} + v_z\frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

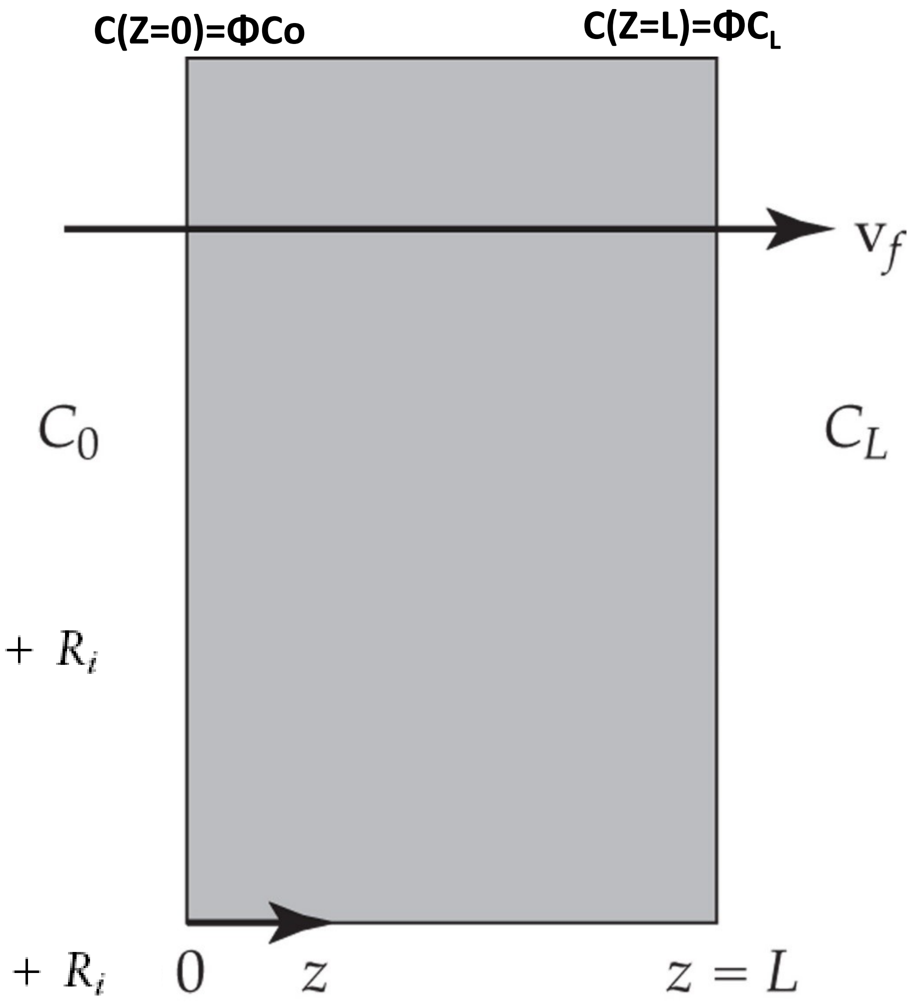
Fick's 2nd + Convection… Yay!

Rectangular $$\frac{\partial C_i}{\partial t} + v_x\frac{\partial C_i}{\partial x} + v_y\frac{\partial C_i}{\partial y} + v_z\frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

S.S N/A N/A f Deff ?

Figure 7.2 Schematic of transport across a membrane with convection.

Example 7.1 Consider steady-state one-dimensional diffusion and convection across a membrane of thickness L (Figure 7.2). Such a membrane may be a synthetic membrane or a cellular layer. No chemical reactions are occurring. At $z = 0$, $C = \Phi C_0$ and at $z = L$, $C = \Phi C_L$, where Φ is the partition coefficient of the solute in the membrane. Determine the concentration profile and flux across the membrane, and compare it with results for diffusion only.



Where to start?
What coordinates are we using?

Rectangular $$\frac{\partial C_i}{\partial t} + v_x \frac{\partial C_i}{\partial x} + v_y \frac{\partial C_i}{\partial y} + v_z \frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

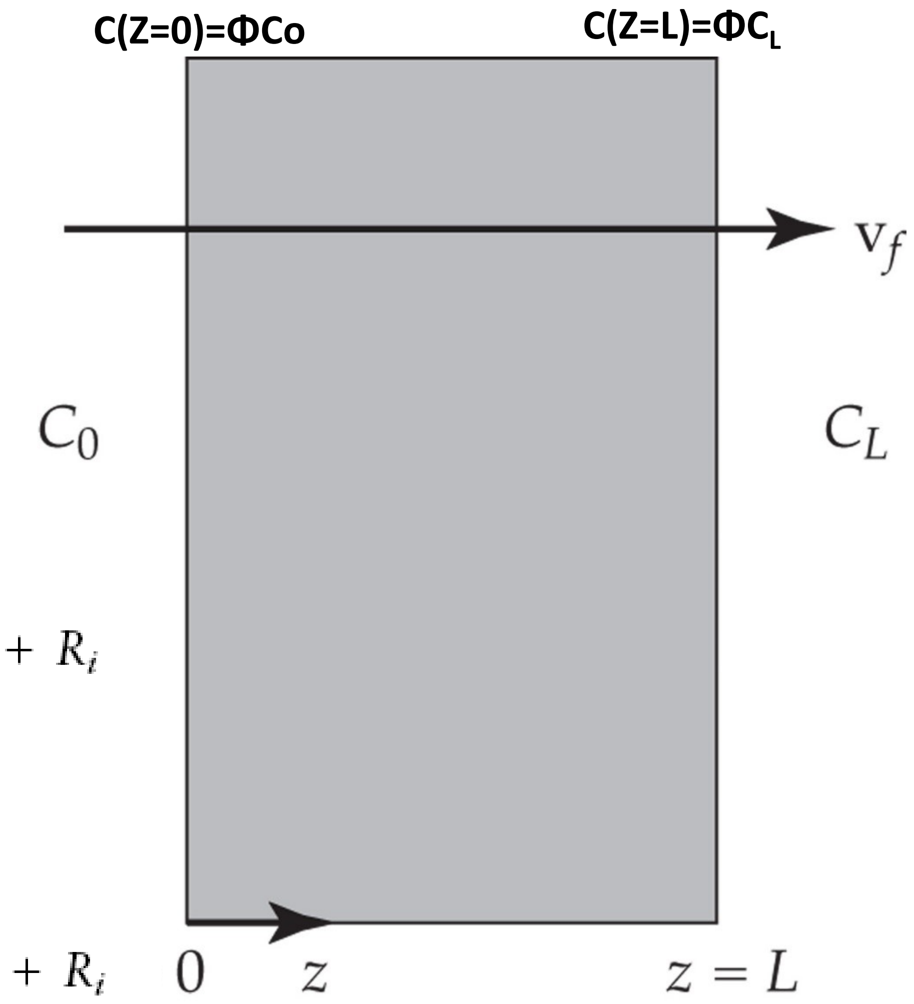
Fick's 2nd + Convection… Yay!

Rectangular $$\frac{\partial C_i}{\partial t} + v_x \frac{\partial C_i}{\partial x} + v_y \frac{\partial C_i}{\partial y} + v_z \frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

S.S N/A N/A f Deff N/A ?

Figure 7.2 Schematic of transport across a membrane with convection.

Example 7.1 Consider steady-state one-dimensional diffusion and convection across a membrane of thickness L (Figure 7.2). Such a membrane may be a synthetic membrane or a cellular layer. No chemical reactions are occurring. At $z = 0$, $C = \Phi C_0$ and at $z = L$, $C = \Phi C_L$, where Φ is the partition coefficient of the solute in the membrane. Determine the concentration profile and flux across the membrane, and compare it with results for diffusion only.



Where to start?
What coordinates are we using?

Rectangular $$\frac{\partial C_i}{\partial t} + v_x \frac{\partial C_i}{\partial x} + v_y \frac{\partial C_i}{\partial y} + v_z \frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$$

Fick's 2nd + Convection… Yay!

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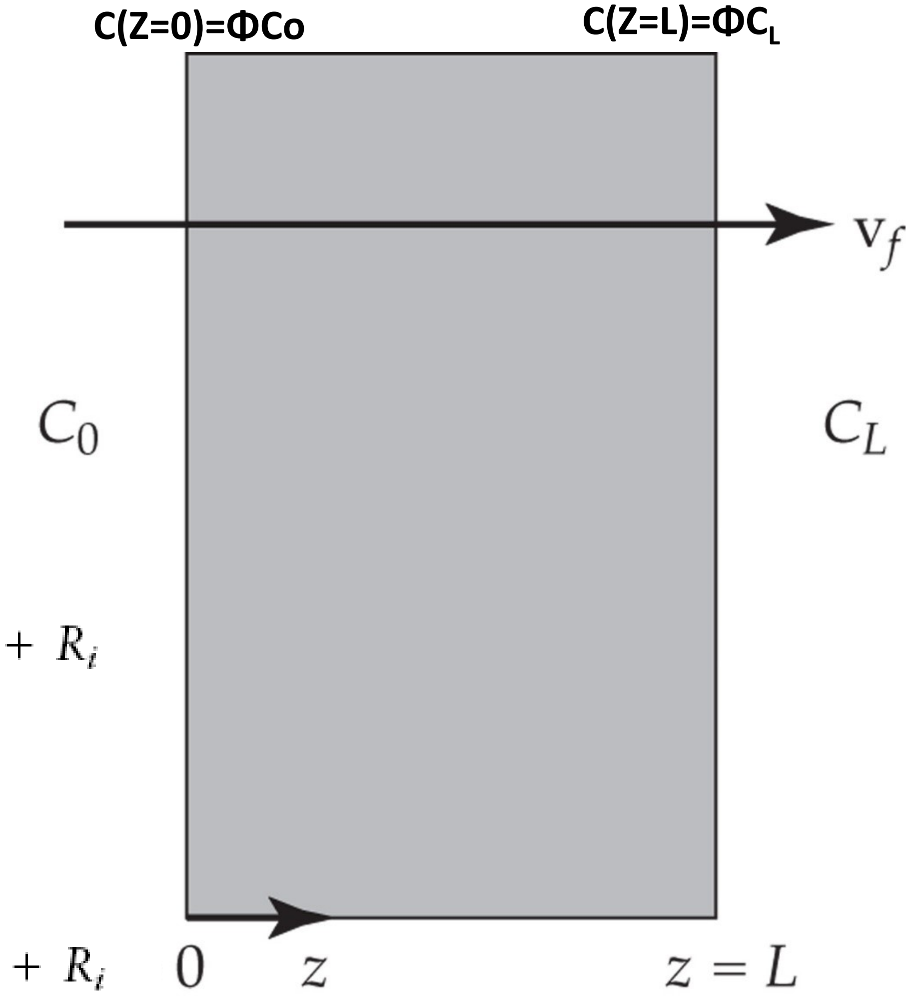
S.S N/A N/A f Deff N/A N/A ?

Figure 7.2 Schematic of transport across a membrane with convection.

Example 7.1 Consider steady-state one-dimensional diffusion and convection across a membrane of thickness L (Figure 7.2). Such a membrane may be a synthetic membrane or a cellular layer. No chemical reactions are occurring. At $z = 0$, $C = \Phi C_0$ and at $z = L$, $C = \Phi C_L$, where Φ is the partition coefficient of the solute in the membrane. Determine the concentration profile and flux across the membrane, and compare it with results for diffusion only.



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S.S N/A N/A f Deff N/A N/A Need ?

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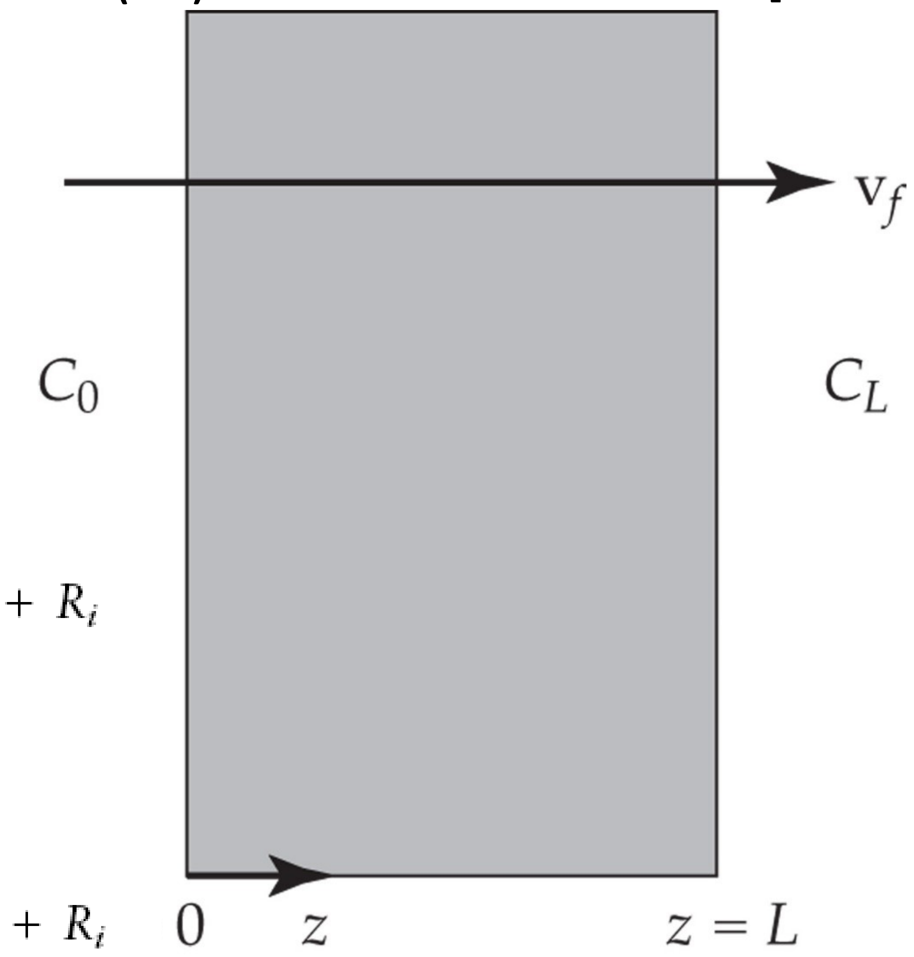
C(Z=0)=ΦCo **C(Z=L)=ΦC$_L$**



Where to start?
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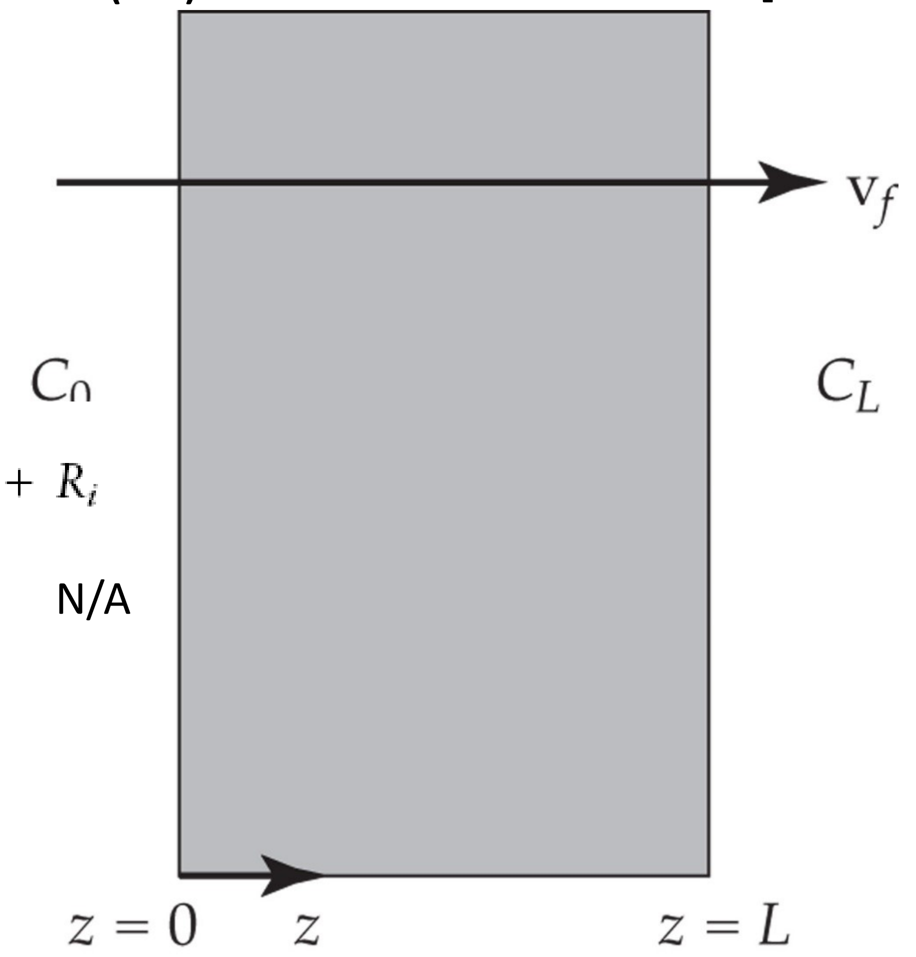

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S.S N/A N/A f Deff N/A N/A Need N/A

$$V_f\frac{dC_i}{dz} = D_{eff}\frac{d^2C_i}{dz^2}$$

Figure 7.2 Schematic of transport across a membrane with convection.

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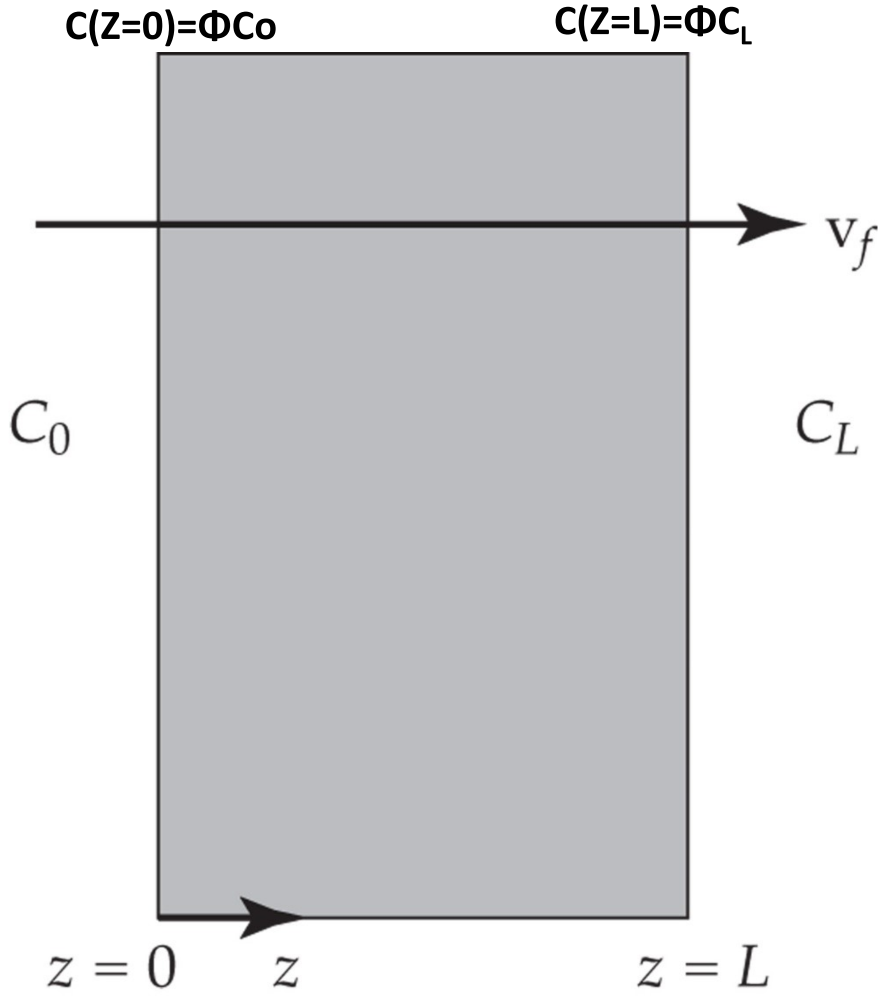
$$V_f \frac{dC_i}{dz} = D_{eff} \frac{d^2 C_i}{dz^2}$$

How do we solve this for C_i?



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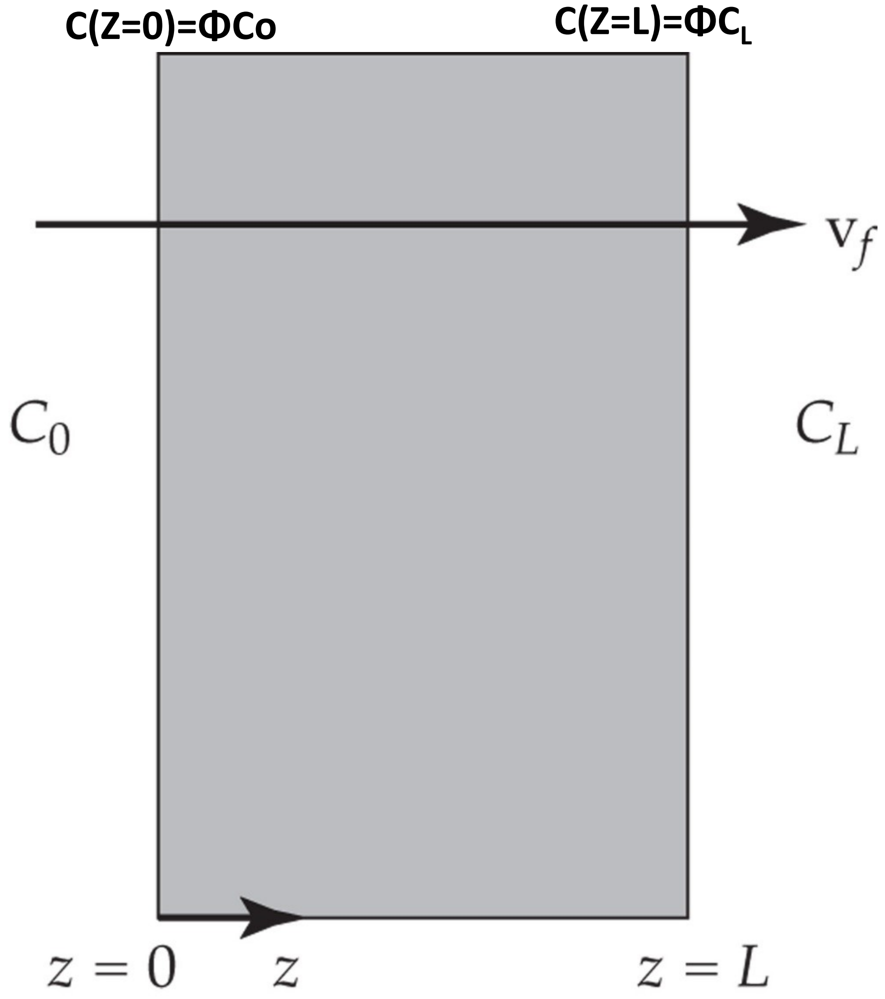

$$V_f \frac{dC_i}{dz} = D_{eff} \frac{d^2 C_i}{dz^2} \qquad u = \frac{dC_i}{dz}$$

$$V_f u = D_{eff} \frac{du}{dz}$$

$$\int \frac{V_f}{D_{eff}} dz = \int \frac{1}{u} du$$

$$\frac{V_f z}{D_{eff}} + C_1 = \ln u + C_2 \qquad C_1 - C_2 = C_3$$

$$e^{\left(\frac{V_f z}{D_{eff}} + C_3\right)} = e^{\ln u} = u = \frac{dC_i}{dz}$$

$$\int dz \frac{dC_i}{dz} = \int e^{\left(\frac{V_f z}{D_{eff}} + C_3\right)} dz \qquad \text{call } C_3 = -C_5$$

$$C_4 + C_i = \int e^{\left(\frac{V_f z}{D_{eff}} - C_5\right)} dz = \int \frac{e^{\left(\frac{V_f z}{D_{eff}}\right)}}{e^{C_5}} dz \quad \& \ \frac{1}{e^{C_5}} = C_6$$

$$C_4 + C_i = C_6 \int e^{\frac{V_f z}{D_{eff}}} dz \qquad \frac{V_f}{D_{eff}} = m$$

$$C_4 + C_i = C_6 \cdot \left(\frac{1}{m} e^{mz} + C_7\right) = \frac{C_6 D_{eff}}{V_f} e^{\frac{V_f z}{D_{eff}}} + C_6 C_7 \qquad C_6 C_7 = C_8$$

$$\& \ \frac{C_6 D_{eff}}{V_f} = C_9$$

$$C_i = C_9 e^{\frac{V_f z}{D_{eff}}} + C_8 - C_4 \qquad C_8 - C_4 = C_{10}$$

$$C_i = C_9 e^{\frac{V_f z}{D_{eff}}} + C_{10}$$

B.C.

@ $z = 0$, $C = C_0 \Phi$

@ $z = L$, $C = C_L \Phi$

$$C_0 \Phi = C_9 e^{\frac{V_f (z=0)}{D_{eff}}} + C_{10} = C_9 + C_{10} \quad \text{so} \quad C_9 = -C_{10} + C_0 \Phi$$

$$C_L \Phi = C_9 e^{\frac{V_f L}{D_{eff}}} + C_{10} \quad \text{so} \quad C_{10} = C_L \Phi - C_9 e^{\frac{V_f L}{D_{eff}}}$$

& solve for C_{10}

& Done

what is $\frac{V_f L}{D_{eff}} = ?$

peclet #!

& simplify

7.4

Table 7

TABLE 7.3

Dimensionless Groups Arising in Mass Transfer and Chemical Reactions

Group	Definition	Physical interpretation	Applications
Schmidt number	$\mathrm{Sc} = \frac{\nu}{D_{ij}}$	$\frac{\text{Momentum transport}}{\text{Diffusive transport}}$	Convective-diffusion problems
Fourier number	$t^* = \frac{tD_{ij}}{L^2}$	$\frac{\text{Time}}{\text{Diffusion time}}$	Unsteady diffusion
Dimensionless residence time	$\tau = \frac{t\langle \mathrm{v} \rangle}{\mathrm{L}}$	$\frac{\text{Time}}{\text{Residence time}}$	Flow problems
Peclet number	$\mathrm{Pe} = \frac{\langle \mathrm{v} \rangle L}{D_{ij}} = \mathrm{ReSc}$	$\frac{\text{Diffusion time}}{\text{Convection time}}$	Convective-diffusion problems
Sherwood number	$\mathrm{Sh} = \frac{k_f L}{D_{ij}}$	$\frac{\text{Mass transfer}}{\text{Diffusion}}$	Convective-diffusion problems
Biot number	$\mathrm{Bi} = \frac{k_f L}{D_{\mathrm{eff}}}$	$\frac{\text{Mass transfer}}{\text{Internal diffusion}}$	Interphase mass transfer
Damkohler number	$\mathrm{Da} = \frac{kL}{k_f}$	$\frac{\text{Chemical reaction}}{\text{Mass transfer}}$	Mass transfer and surface reaction
Thiele modulus	$\phi = \sqrt{\frac{k_n L^2 C^{n-1}}{D_{ij}}}$	$\frac{\text{Diffusion time}}{\text{Reaction time}}$	Chemical reactions and diffusion
Reaction rate modulus	$R_i^* = \frac{R_i L^2}{C_0 D_{ij}}$	$\frac{\text{Diffusion time}}{\text{Reaction time}}$	Chemical reactions and diffusion

k_f is the mass transfer coefficient (length time^{-1}).
k is the rate coefficient for the first-order reaction (time^{-1}).
D_{eff} is the effective diffusion coefficient in the solid phase (length^2 time^{-1}).
k_n is the reaction rate coefficient for a reaction of order n ((volume/moles)$^{n-1}$ time^{-1}).

Laplace Equation

TABLE 7.2

Conservation Relations for Dilute Solutions		
Rectangular	$\frac{\partial C_i}{\partial t} + v_x \frac{\partial C_i}{\partial x} + v_y \frac{\partial C_i}{\partial y} + v_z \frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$	(7.3.13a)

- What if it is at steady state and without a reaction?

- If the Pe# is approximately zero then what does that mean about the velocity?

Laplace equation (has nothing to do with Laplace Transformations which we will do later in the semester):
If you take Fick's second law and pass 5 tau units the concentration is no longer changing (much) in time. Thus dC/dt = 0 = D gradient^2(C), thus 0 = gradient^2(C). This is known as the Laplace equation.

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Rectangular	$\frac{\partial C_i}{\partial t} + v_x \frac{\partial C_i}{\partial x} + v_y \frac{\partial C_i}{\partial y} + v_z \frac{\partial C_i}{\partial z} = D_{ij}\left(\frac{\partial^2 C_i}{\partial x^2} + \frac{\partial^2 C_i}{\partial y^2} + \frac{\partial^2 C_i}{\partial z^2}\right) + R_i$	(7.3.13a)

- What if it is at steady state and without a reaction?

- If the Pe# is approximately zero then what does that mean about the velocity?
- Close to zero…

$$\frac{\partial C_i}{\partial t} = D_{ij}\nabla^2 C_i \qquad 0 = \nabla^2 C_i$$

Laplace equation…

Laplace equation (has nothing to do with Laplace Transformations which we will do later in the semester):
If you take Fick's second law and pass 5 tau units the concentration is no longer changing (much) in time. Thus dC/dt = 0 = D gradient^2(C), thus 0 = gradient^2(C). This is known as the Laplace equation.

Nernst Plank Equation

TANGENT

Nernst Plank Equation…

$$N_i = -D_{ij}\nabla C_i - \frac{D_{ij} C_i z_i F}{RT} \nabla\psi + C_i v$$

- F = Faraday's Constant = 1.602e-19 Coloumbs*Avogadro's # (C/mol of ion)
- R = J/(mol*Kelvin)
- RT = J/mol
- z = charge of ion
- Note: current density i = NF

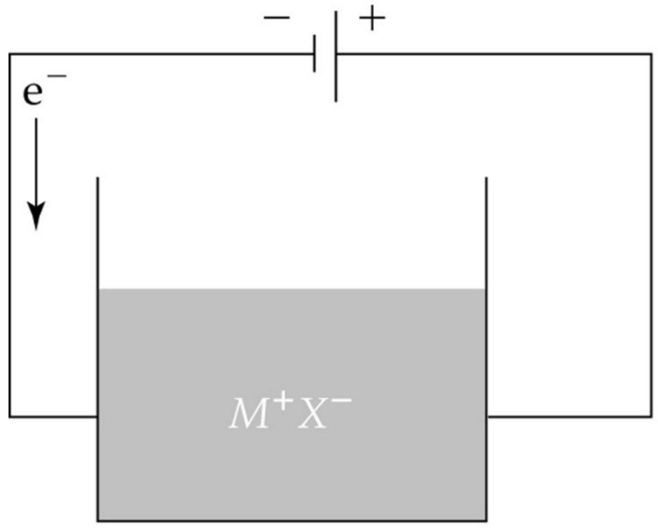
TABLE 7.4

Diffusion Coefficients of Anions and Cations at 25°C

Cation	Charge, z_+	$D_+ \times 10$ cm^2 s^{-1}	Anion	Charge, z_-	$D_- \times 10$ cm^2 s^{-1}
H^+	+1	9.312	OH^-	−1	5.260
Na^+	+1	1.334	Cl^-	−1	2.032
K^+	+1	1.957	NO_3^-	−1	1.902
NH_4^+	+1	1.954	HCO_3^-	−1	1.105
Mg^{++}	+2	0.7063	HCO_2^-	−1	1.454
Ca^{++}	+2	0.7920	$SO_4^=$	−2	1.065
Cu^{++}	+2	0.72	HSO_4^-	−1	1.33

Source: Adapted from Ref. [5]. Used with permission.

Figure 7.4 (a) Schematic of electrical potential difference $\Delta\psi$ applied to a solution of the 1:1 electrolyte M^+X^-.



z=0 cathode z z=L anode

(a)

Note that electrons react with M+ only and not X- so
Current density = F*N of + or current density = F for cation
And N = 0 for anion

$$N_i = -D_{ij}\nabla C_i - \frac{D_{ij}C_i z_i F}{RT}\nabla\psi + C_i v$$

$$N^+ = \frac{i}{F} = -D^+\frac{dC}{dz} - \frac{D^+CF}{RT}\frac{d\psi}{dz}$$

B.C.: C = C0 at z=0 and C=CL at z=L; Δψ= ?; i = ?

$$N^- = 0 = -D^-\frac{dC}{dz} + \frac{D^-CF}{RT}\frac{d\psi}{dz}$$

B.C.: C = C0 at z=0 and C=CL at z=L; Δψ= ?

$$\sum_{i=1}^{n} C_i z_i = 0 \; and \; F\sum_{i=1}^{n} N_i z_i = i$$

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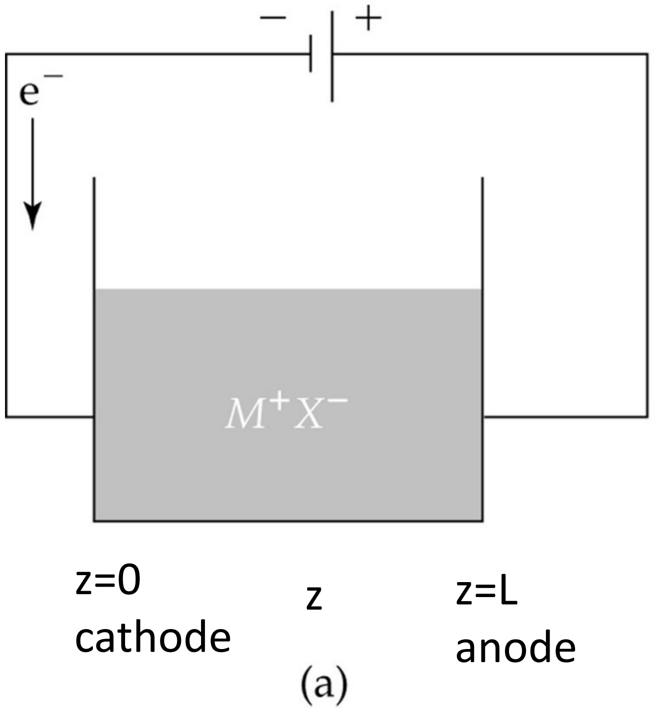

Counter-current assumption;
Analogous to mass-countering...

$$\sum_{i=1}^{n} C_i z_i = 0 \ and \ F\sum_{i=1}^{n} N_i z_i = i$$

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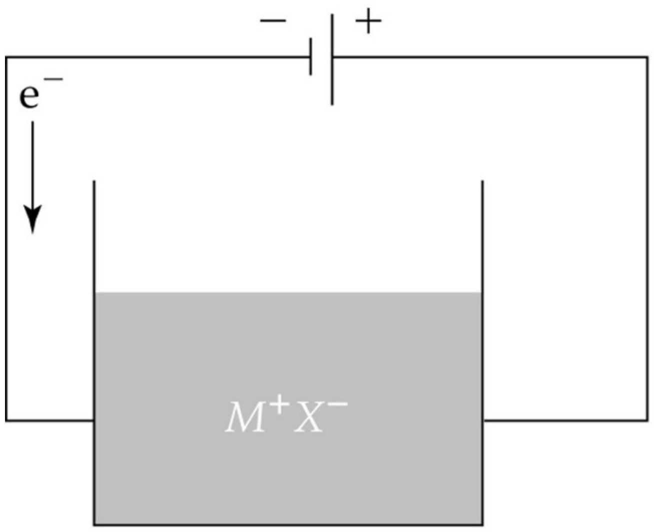


z=0
cathode

z

z=L
anode

(a)

$$N^+ = \frac{i}{F} = -D^+\frac{dC}{dz} - \frac{D^+CF}{RT}\frac{d\psi}{dz}$$

B.C.: C = C0 at z=0 and C=CL at z=L; Δψ= ?; i = ?

$$N^- = 0 = -D^-\frac{dC}{dz} + \frac{D^-CF}{RT}\frac{d\psi}{dz}$$

B.C.: C = C0 at z=0 and C=CL at z=L; Δψ= ?

Hint: solve for the differential of potential with respect to z in the N^- equation and plug in to the N^+ flux and solve for i.

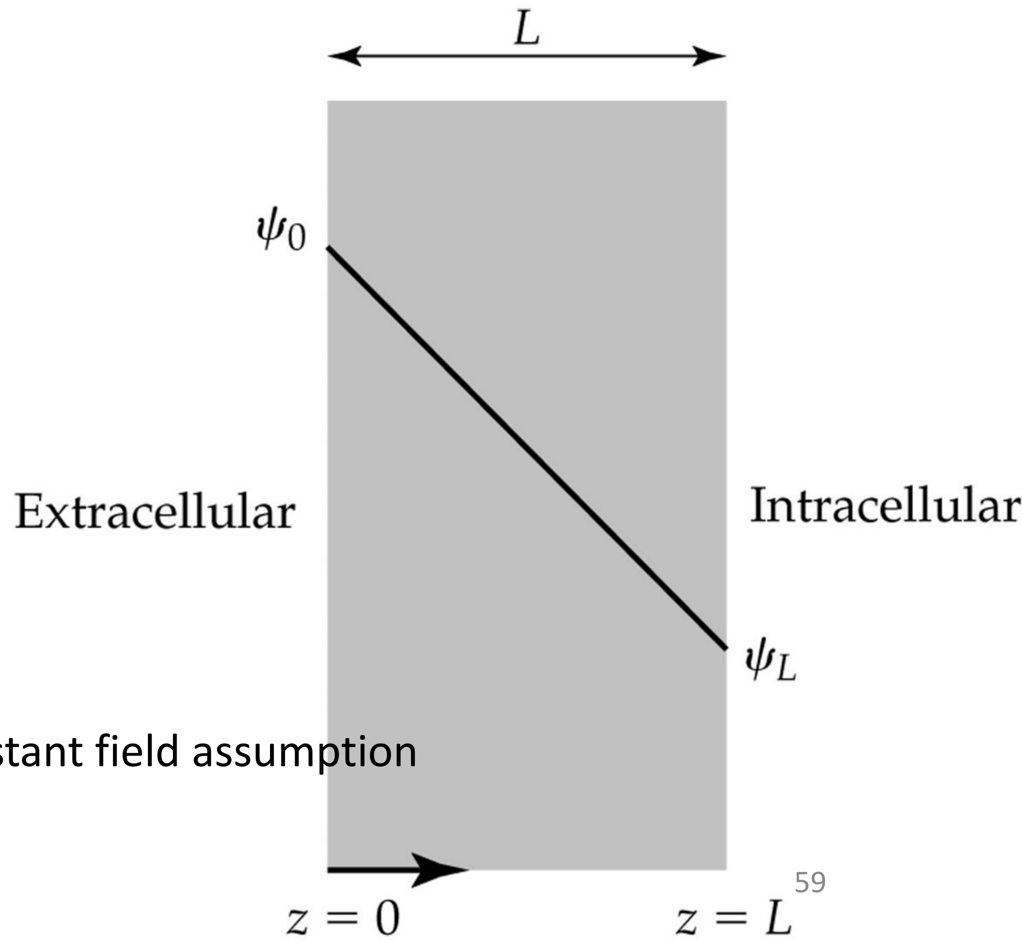
Figure 7.5

Figure 7.5 Potential difference across a charged cellular membrane. The transmembrane potential V_m equals the potential inside the cell minus the potential outside the cell, Ψ_i - Ψ_0 or **Vm**

Because ion transport across membranes is important in biological and biotechnological applications, it is worth examining in some detail. Ion transport is affected by the charge of the membrane and the manner in which ions are transported across the membrane. Transport across uncharged membranes is a straightforward extension of previous concepts, and an example is provided next. For charged membranes, both the concentration gradient and potential gradient must be determined.

$$N_i = -D_{ij}\nabla C_i - \frac{D_{ij} C_i z_i F}{RT}\nabla\psi + C_i v$$

$$\frac{d\psi}{dz} = \frac{V_m}{L}$$



3 Assumptions:

1) The electric potential varies linearly across the membrane = constant field assumption
2) Each ion because independently
3) Membrane properties are uniform across

$$\frac{\partial C_i}{\partial t} = -\nabla N_i + r_i$$

$$N_i = -D_{ij}\nabla C_i - \frac{D_{ij} C_i z_i F}{RT}\nabla\psi + C_i v$$

$$\frac{\partial C_i}{\partial t} + v\nabla C = D\nabla^2 C + \frac{DzF}{RT}\nabla(C\nabla\psi)$$

7.5.20a (pg. 362)

$$\frac{\partial C_i}{\partial t} + v\nabla C = D^-\nabla^2 C + \frac{D^- z^- F}{RT}\nabla(C\nabla\psi)$$

—

7.5.20b

$$\frac{\partial C_i}{\partial t} + v\nabla C = D^+\nabla^2 C + \frac{D^+ z^+ F}{RT}\nabla(C\nabla\psi)$$

$$\nabla(C\nabla\psi) = \frac{RT}{F}\left(\frac{[D^- - D^+]}{z^- D^- - z^+ D^+}\right)\nabla^2 C$$

$$\frac{\partial C_i}{\partial t} + v\nabla C = D_{eff}\nabla^2 C$$

$$D_{eff} = \left(\frac{(z^+ - z^-)[D^+ D^-]}{z^+ D^+ - z^- D^-}\right)$$

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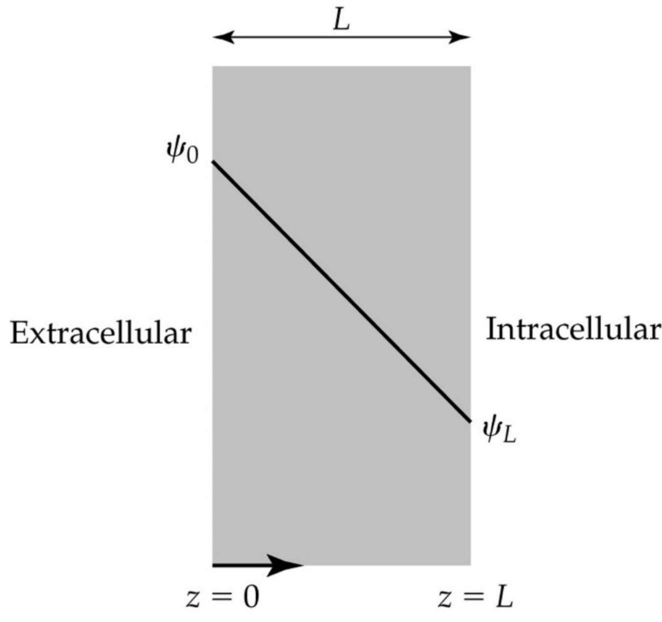


$$N_i = -D_{ij}\nabla C_i - \frac{D_{ij}C_i z_i F}{RT}\nabla\psi + C_i v$$

$$\frac{d\psi}{dz} = \frac{V_m}{L}$$

Counter –current assumption...

Net current across = 0 so… $z^+N^+ = z^-N^-$ and solve for the differential of potential (respect to space)

B.C.: C = C0 at z=0 and C=CL at z=L; Δψ= ?

$$\nabla\psi = -\frac{RT}{F}\left(\frac{[D^+ - D^-]}{z^+D^+ - z^-D^-}\right)\frac{1}{C^+}\nabla C$$

Δψ= ?

What does this mean About different Ds of Ions and the voltage?
= diffusion potential

Nernst-Planck Equation + Conserv. Relation

$$\frac{\partial C_i}{\partial t} = -\nabla N_i + r_i$$

$$N_i = -D_{ij}\nabla C_i - \frac{D_{ij} C_i z_i F}{RT}\nabla\psi + C_i v$$

$$\frac{\partial C_i}{\partial t} + v\nabla C = D\nabla^2 C + \frac{DzF}{RT}\nabla(C\nabla\psi)$$

$$0 + 0 = D\nabla^2 C + \frac{DzF}{RT}\nabla\left(\frac{CV_m}{L}\right)$$

$$0 = D\nabla^2 C + \frac{DzF}{RT}\frac{Vm}{L}\nabla C$$

Algebra will be “prettier” if multiply both Sides by a negative…

Solve for Ci (equation 7.5.30a) and remember fick’s first law to get N=-Dgrad(C) 7.5.30b)

Assume counter current or sum of the fluxes = 0 (do this for potassium, sodium, and chloride) and calculate Vm

B.C.

(Make prettier with permeabilities (= ΦD/L))

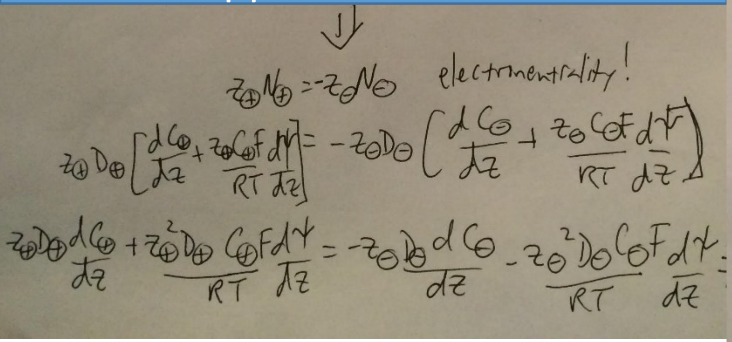
At z=0, Ci = ΦiCo

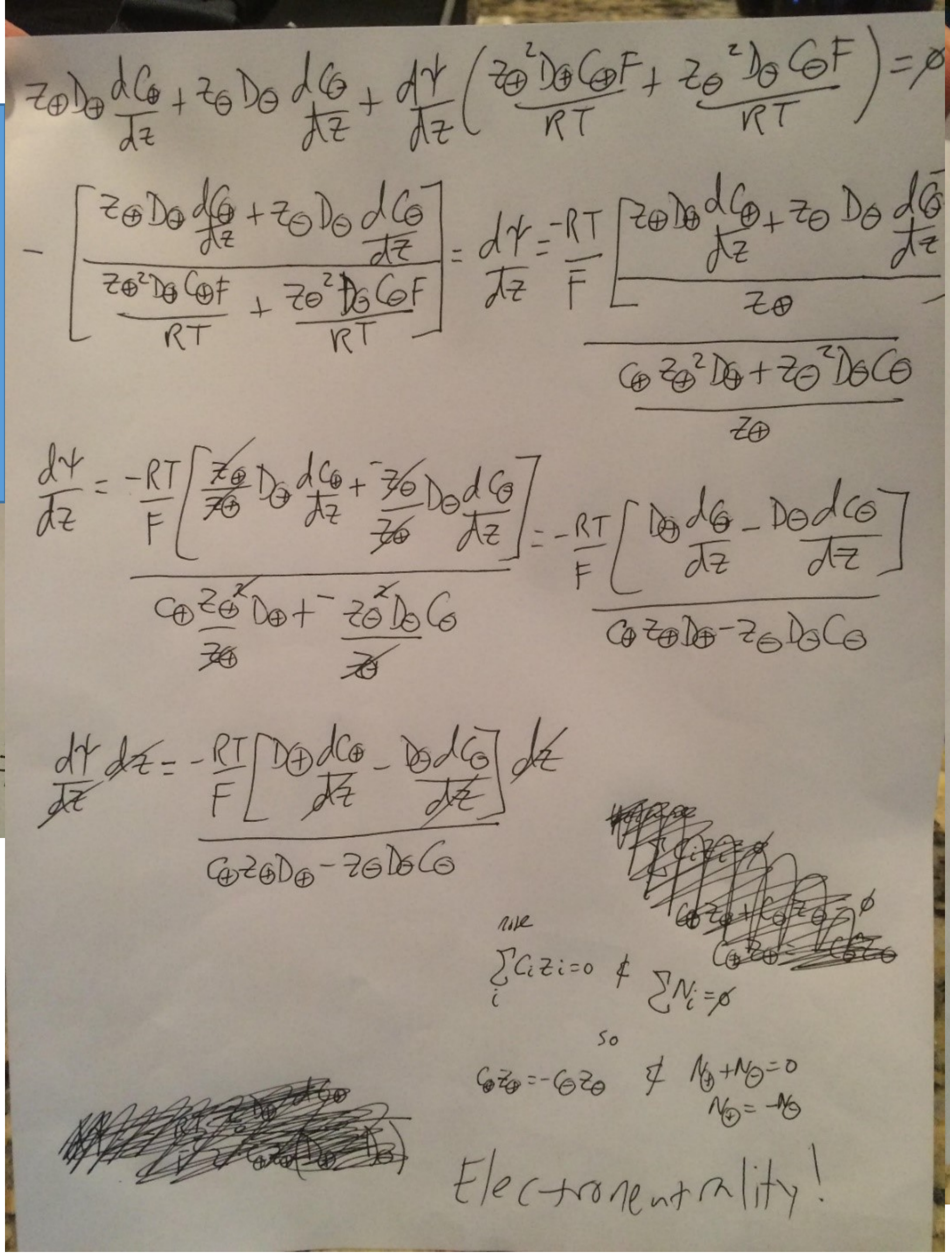
At z=L, Ci= ΦiCL

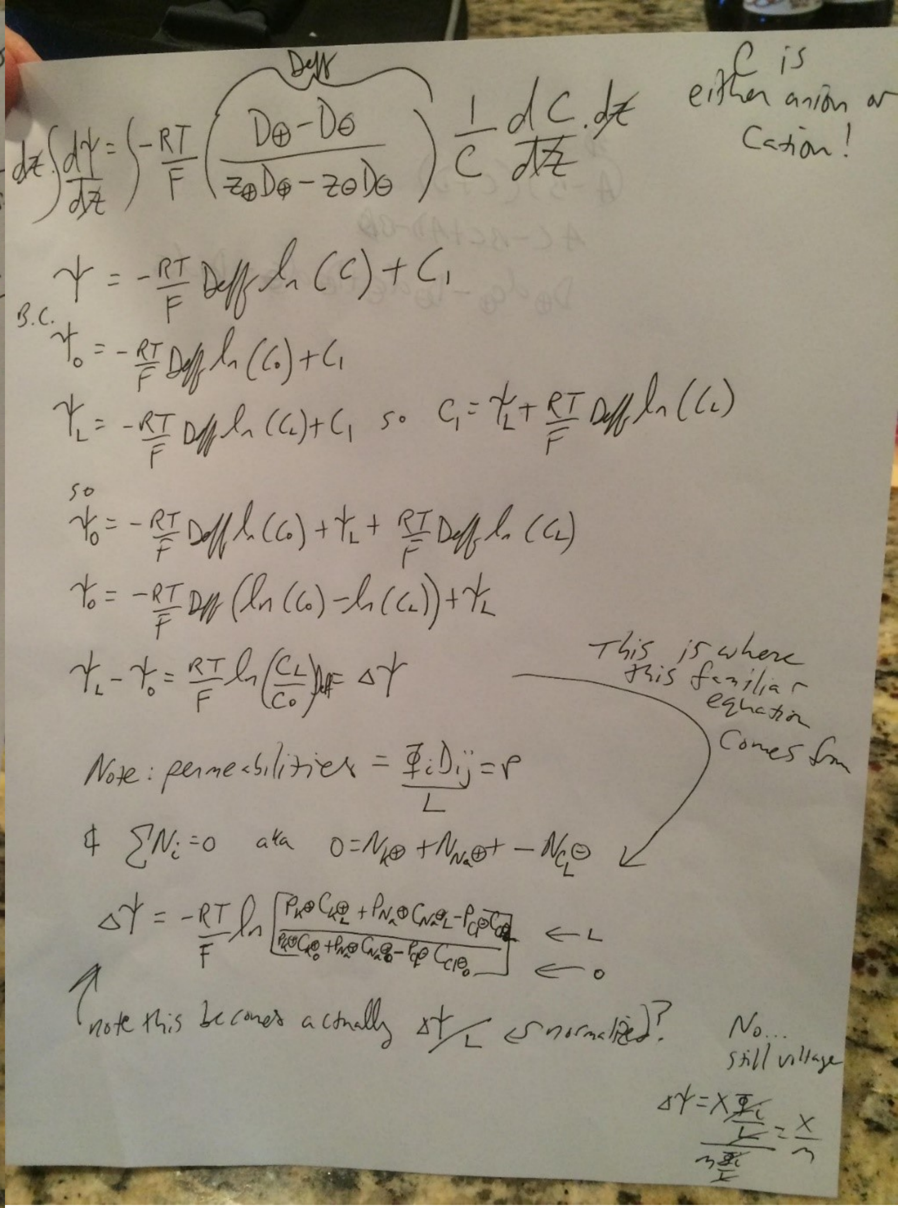
1-D (use z)

Example 7.4

The book references 7.3.9a
dC/dt = gradient(N)+Ri
No reaction and it is at steady state so 0=dN/dz.
We assume 7.5.6 (sum of zN=0) applies here so…







$$z_\oplus D_\oplus \frac{dC_\oplus}{dz} + z_\ominus D_\ominus \frac{dC_\ominus}{dz} + \frac{d\psi}{dz}\left(\frac{z_\oplus^2 D_\oplus C_\oplus F}{RT} + \frac{z_\ominus^2 D_\ominus C_\ominus F}{RT}\right) = \emptyset$$

$$-\left[\frac{z_\oplus D_\oplus \frac{dC_\oplus}{dz} + z_\ominus D_\ominus \frac{dC_\ominus}{dz}}{\frac{z_\oplus^2 D_\oplus C_\oplus F}{RT} + \frac{z_\ominus^2 D_\ominus C_\ominus F}{RT}}\right] = \frac{d\psi}{dz} = \frac{-RT}{F}\left[\frac{\frac{z_\oplus D_\oplus \frac{dC_\oplus}{dz} + z_\ominus D_\ominus \frac{dC_\ominus}{dz}}{z_\oplus}}{\frac{C_\oplus z_\oplus^2 D_\oplus + z_\ominus^2 D_\ominus C_\ominus}{z_\oplus}}\right]$$

$$\frac{d\psi}{dz} = \frac{-RT}{F}\frac{\left[\frac{z_\oplus}{z_\oplus} D_\oplus \frac{dC_\oplus}{dz} + \frac{z_\ominus}{z_\ominus} D_\ominus \frac{dC_\ominus}{dz}\right]}{C_\oplus \frac{z_\oplus^2}{z_\oplus} D_\oplus + \frac{z_\ominus^2 D_\ominus C_\ominus}{z_\ominus}} = -\frac{RT}{F}\frac{\left[D_\oplus \frac{dC_\oplus}{dz} - D_\ominus \frac{dC_\ominus}{dz}\right]}{C_\oplus z_\oplus D_\oplus - z_\ominus D_\ominus C_\ominus}$$

$$\frac{d\psi}{dz}dz = -\frac{RT}{F}\frac{\left[D_\oplus \frac{dC_\oplus}{dz} - D_\ominus \frac{dC_\ominus}{dz}\right]}{C_\oplus z_\oplus D_\oplus - z_\ominus D_\ominus C_\ominus}dz$$

use $\sum_i C_i z_i = 0$ & $\sum N_i = \emptyset$

so $C_\oplus z_\oplus = -C_\ominus z_\ominus$ & $N_\oplus + N_\ominus = 0$, $N_\oplus = -N_\ominus$

Electroneutrality!

$$\int dz \frac{d\psi}{dz} = \int -\frac{RT}{F}\overbrace{\left(\frac{D_\oplus - D_\ominus}{z_\oplus D_\oplus - z_\ominus D_\ominus}\right)}^{D_{eff}}\frac{1}{C}\frac{dC}{dz}dz$$

C is either anion or Cation!

$$\psi = -\frac{RT}{F}D_{eff}\ln(C) + C_1$$

B.C.

$$\psi_0 = -\frac{RT}{F}D_{eff}\ln(C_0) + C_1$$

$$\psi_L = -\frac{RT}{F}D_{eff}\ln(C_L) + C_1 \quad \text{so} \quad C_1 = \psi_L + \frac{RT}{F}D_{eff}\ln(C_L)$$

so

$$\psi_0 = -\frac{RT}{F}D_{eff}\ln(C_0) + \psi_L + \frac{RT}{F}D_{eff}\ln(C_L)$$

$$\psi_0 = -\frac{RT}{F}D_{eff}\left(\ln(C_0) - \ln(C_L)\right) + \psi_L$$

$$\psi_L - \psi_0 = \frac{RT}{F}\ln\left(\frac{C_L}{C_0}\right)D_{eff} = \Delta\psi$$

This is where this familiar equation comes from

Note: permeabilities $= \frac{\Phi_i D_{ij}}{L} = P$

& $\sum N_i = 0$ aka $0 = N_{K^\oplus} + N_{Na^\oplus} - N_{Cl^\ominus}$

$$\Delta\psi = -\frac{RT}{F}\ln\left[\frac{P_{K^\oplus}C_{K^\oplus_L} + P_{Na^\oplus}C_{Na^\oplus_L} - P_{Cl^\ominus}C_{Cl^\ominus_L}}{P_{K^\oplus}C_{K^\oplus_0} + P_{Na^\oplus}C_{Na^\oplus_0} - P_{Cl^\ominus}C_{Cl^\ominus_0}}\right] \begin{array}{l}\leftarrow L \\ \leftarrow 0\end{array}$$

note this becomes actually $\Delta\psi/L$ ← normalized?

No... still voltage

$$\Delta\psi = X\frac{\Phi_i}{L} \Big/ \frac{n\Phi_i}{L} = \frac{X}{n}$$

Poisson Equation:

$$\nabla^2\psi = -\frac{F}{\varepsilon}\sum z_i C_i$$

Charge distribution

Debye length and what is the relationship with Zeta Potential? Distance the voltage drops by 1/e…

- Represents the characteristic distance over which counterion concentration is elevated around the central ion…
- ε= permittivity (units are Farads/m)
- What's a Farad
- Permittivity = # of coulombs to cause 1 volt in 1 m
- F = Faraday's constant = coloumbs/m
- How units cancel to be distance

$$\lambda = \sqrt{\frac{\varepsilon RT}{F^2\sum z_i^2 C_i}}$$

A special thank you to Wikipedia.