HST.410J/6.021J **Lecture 6**

February 27, 2007

Last time: Quantitative models of diffusion.

Diffusion: transport of solute due to gradient in solute concentration.

Fick's law: $$\phi(x,t) = -D\frac{\partial c(x,t)}{\partial x}$$

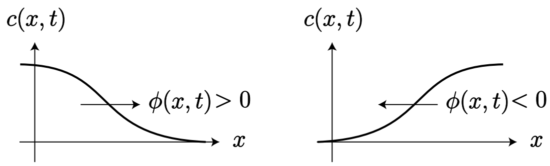
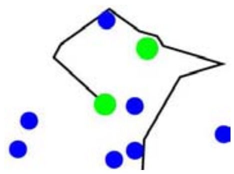


Figure from Weiss, T. F. *Cellular Biophysics, Vol. I.* Cambridge, MA: MIT Press, 1996. Courtesy of MIT Press. Used with permission.

Microscopic basis: Random walk model.



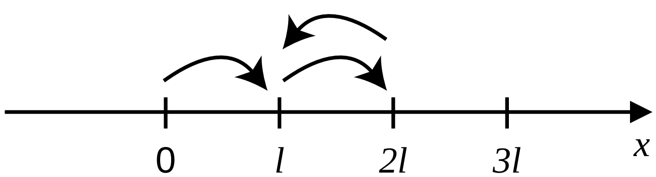
Random Walk Model

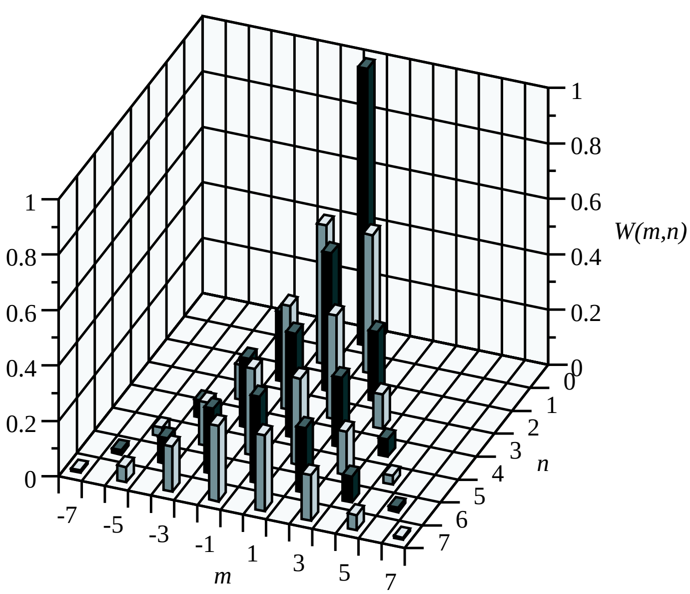
- number of solute particles << number of solvent particles
- motion of solute determined by collisions with solvent (ignore solute-solute interactions)
- focus on 1 solute particle, assume motions of others are statistically identical

Every τ seconds, solute particle gets hit by solvent particle.

In response, solute particle is equally likely to move $+l$ or $-l$.

τ = mean free time; l = mean free path





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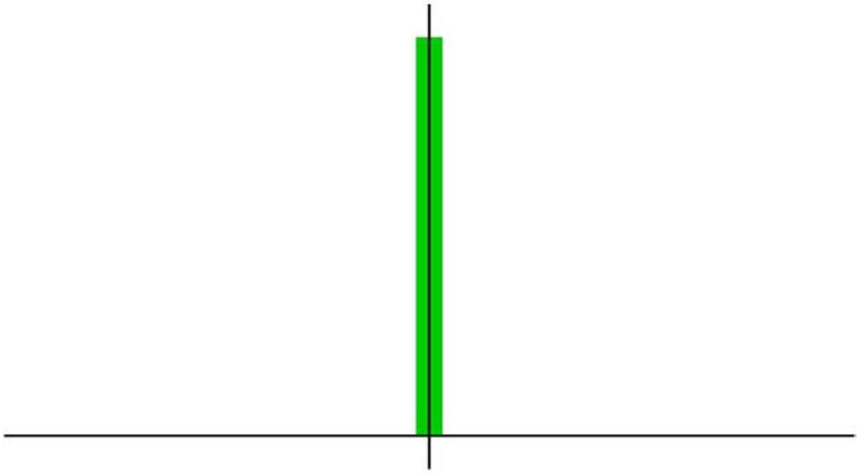
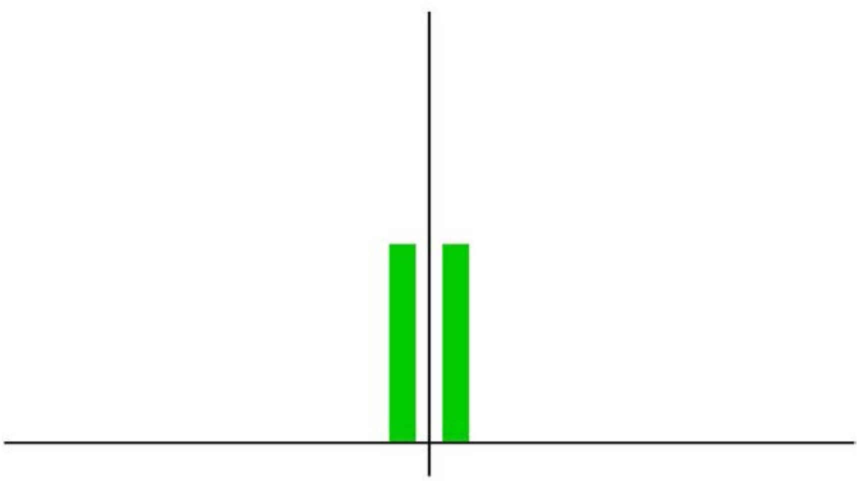
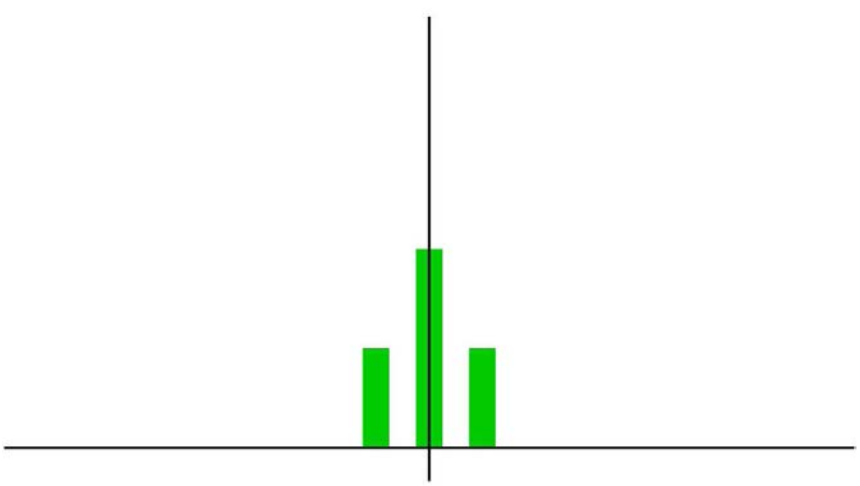
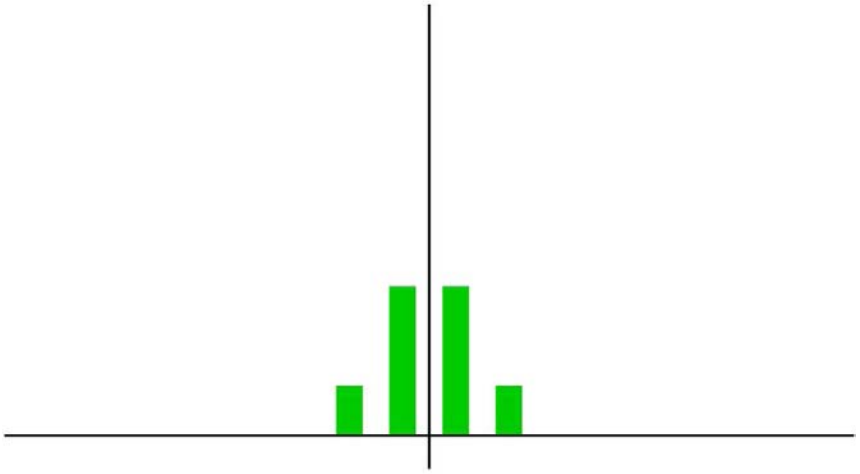








$$
\begin{array}{ccccccccc}
 & & & & 1 & & & & \\
 & & & \frac{1}{2} & & \frac{1}{2} & & & \\
 & & \frac{1}{4} & & \frac{2}{4} & & \frac{1}{4} & & \\
 & \frac{1}{8} & & \frac{3}{8} & & \frac{3}{8} & & \frac{1}{8} & \\
\frac{1}{16} & & \frac{4}{16} & & \frac{6}{16} & & \frac{4}{16} & & \frac{1}{16}
\end{array}
$$

$E[m|n=0]=0 \qquad E[m^2|n=0]=0$

$E[m|n=1]=0 \qquad E[m^2|n=1]=1$

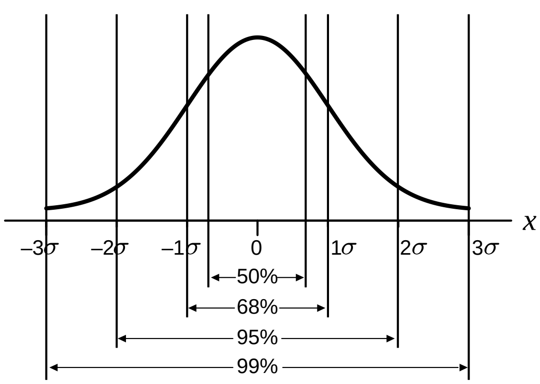
$E[m|n=2]=0 \qquad E[m^2|n=2]=2$

$E[m|n=3]=0 \qquad E[m^2|n=3]=3$

$E[m|n=4]=0 \qquad E[m^2|n=4]=4$

$E[m|n=n_0]=0 \qquad E[m^2|n=n_0]=n_0$

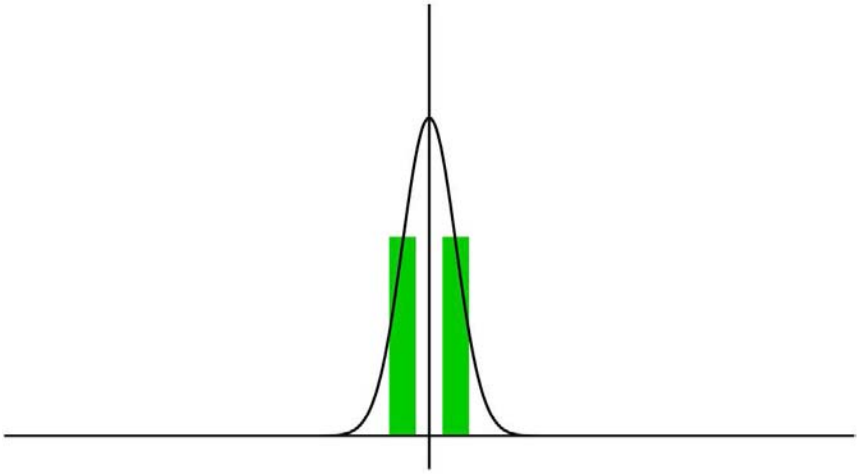
$x >> l \quad t >> \tau$ binomial $\rightarrow$ gaussian

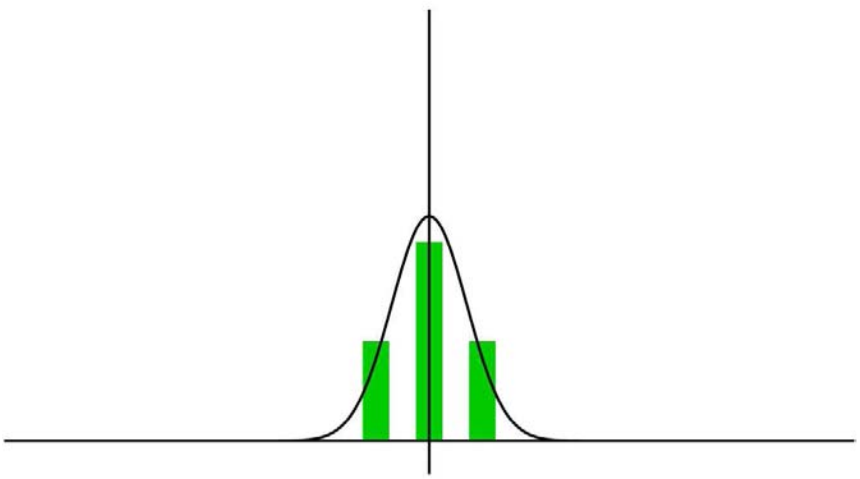


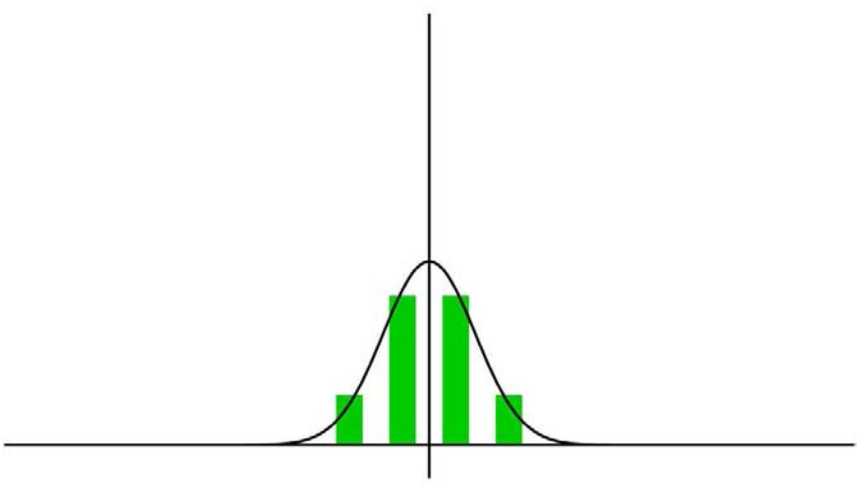
$$\frac{1}{\sqrt{2\pi}\,\sigma} e^{-\frac{x^2}{2\sigma^2}}$$

$$\sigma^2 \propto t$$

$$\sigma^2 = 2Dt$$







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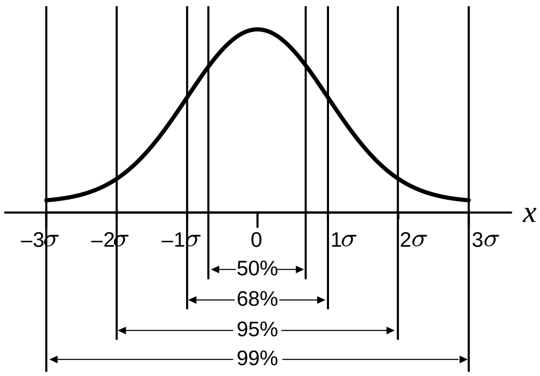

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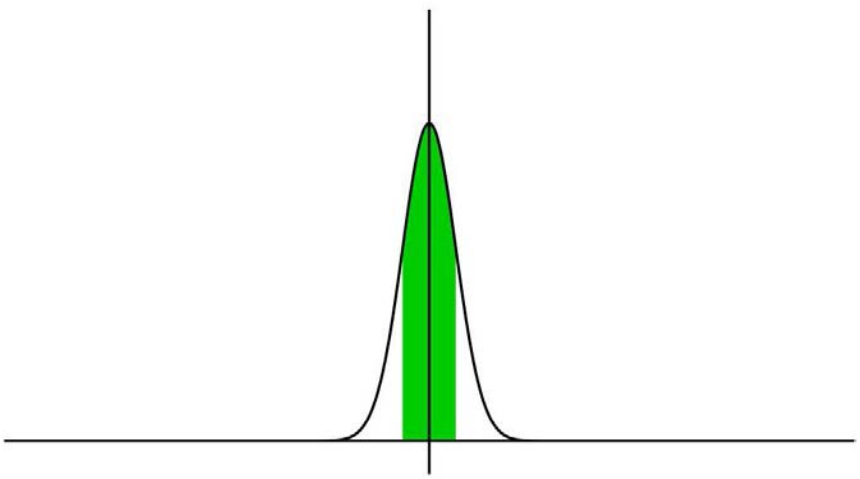
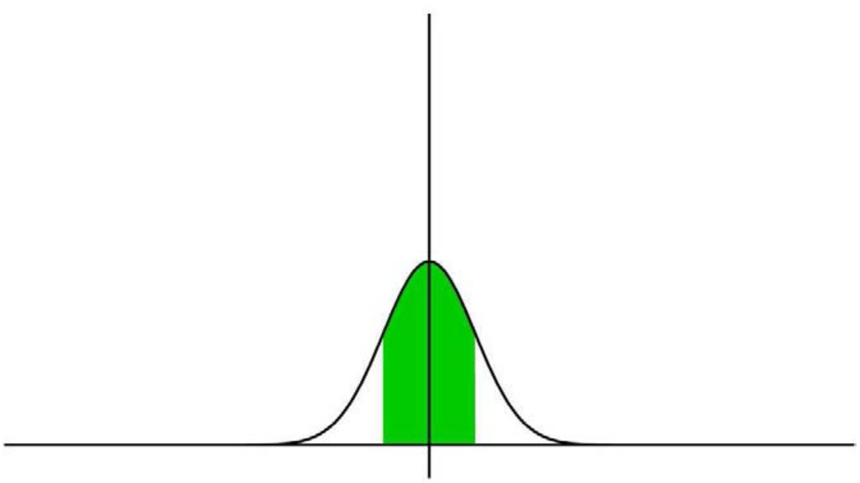
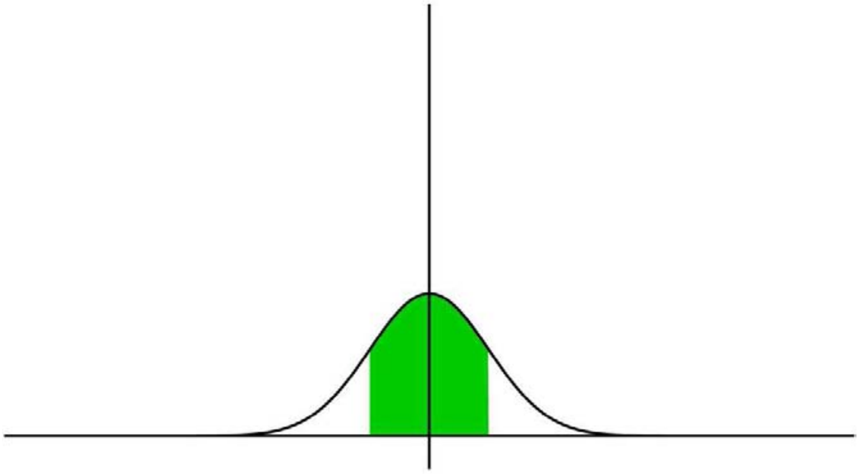


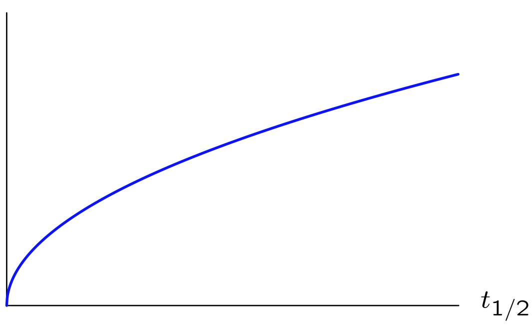




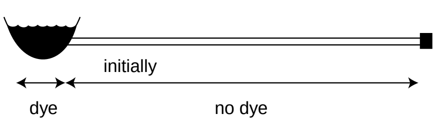
Speed of diffusion

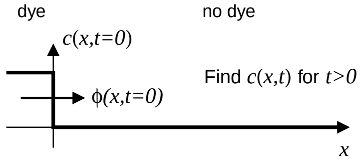
$$D = \frac{\left(x_{1/2}\right)^2}{t_{1/2}}$$

$$x_{1/2} = \sqrt{D\, t_{1/2}}$$



Apply Fick's law to dye demonstration



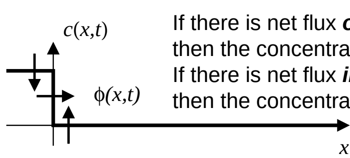


Find $c(x,t)$ for $t>0$

Fick's law:

$$\phi(x,t) = -D\frac{\partial c(x,t)}{\partial x}$$

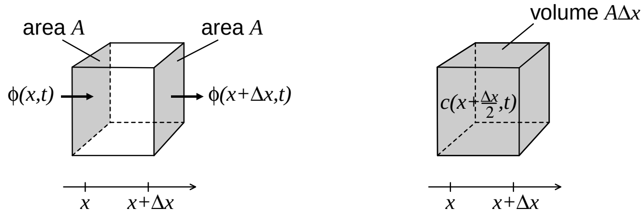
- provides information about time "t" only
- need new information to get from time "t" to time "$t+\Delta t$"



If there is net flux ***out*** of a region,
then the concentration in that region must ***fall***.
If there is net flux ***into*** a region,
then the concentration in that region must ***rise***.

$\rightarrow$ conservation of solute

Continuity Equation



Amount of solute entering through edges during $(t, t+\Delta t)$

Change in amount of solute in volume from t to $t+\Delta t$

—— left —— —— right —— —— time 2 —— —— time 1 ——

$$\phi(x,t+\tfrac{\Delta t}{2})\, A\, \Delta t - \phi(x+\Delta x,t+\tfrac{\Delta t}{2})\, A\, \Delta t = c(x+\tfrac{\Delta x}{2},t+\Delta t)\, A\, \Delta x - c(x+\tfrac{\Delta x}{2},t)\, A\, \Delta x$$

equal if solute is neither created nor destroyed

$$\frac{\phi(x,t+\frac{\Delta t}{2}) - \phi(x+\Delta x,t+\frac{\Delta t}{2})}{\Delta x} = \frac{c(x+\frac{\Delta x}{2},t+\Delta t) - c(x+\frac{\Delta x}{2},t)}{\Delta t}$$

Take limit as $\Delta x \to 0$ and $\Delta t \to 0$

$$-\frac{\partial \phi(x,t)}{\partial x} = \frac{\partial c(x,t)}{\partial t}$$

Fick's First Law:
$$\phi(x,t) = -D\frac{\partial c(x,t)}{\partial x}$$

Continuity Equation:
$$\frac{\partial \phi(x,t)}{\partial x} = -\frac{\partial c(x,t)}{\partial t}$$

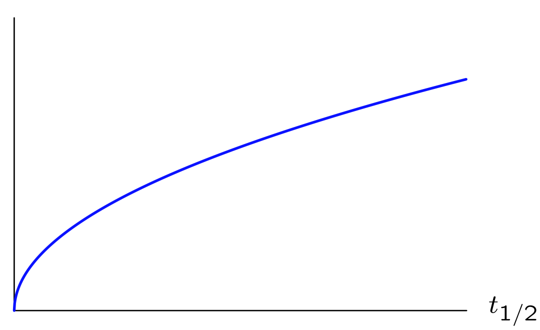
Diffusion Equation:
$$\frac{\partial c(x,t)}{\partial t} = D\frac{\partial^2 c(x,t)}{\partial x^2}$$

Solution:
$$c(x,t) = \frac{n_0}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}}$$

Speed of diffusion

$$D = \frac{\left(x_{1/2}\right)^2}{t_{1/2}}$$

$$x_{1/2} = \sqrt{D\, t_{1/2}}$$



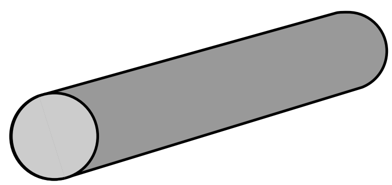
Importance of Scale

$$t_{1/2} = \frac{x_{1/2}^2}{D} \quad ; \quad D = 10^{-5}\,\frac{\text{cm}^2}{\text{s}} \quad \text{for small solutes (e.g., Na}^+\text{)}$$

	$x_{1/2}$	$t_{1/2}$
membrane sized	10 nm	$\frac{1}{10}$ µsec
cell sized	10 µm	$\frac{1}{10}$ sec
dime sized	10 mm	10^5 sec ≈ 1 day

Fluid Dynamics: Flows through Channels

tube flow



1D tube ($L \times \infty \times \infty$)

Fluid Properties

- density ρ
- viscosity
  - dynamic viscosity μ
  - kinematic viscosity $\nu = \mu/\rho$ (diffusivity of momentum)

Which is more important?
Let V = convection speed.
Let v = speed of momentum diffusion.
Then Reynold's number $R = \frac{V}{v}$.
Diffusivity $\nu = \frac{L^2}{\tau}$ where τ = time to diffuse distance L.
Thus $v = \frac{L}{\tau} = \frac{\nu}{L}$
and $R = \frac{VL}{\nu}$.