Lecture 15:
The Mathematics of Water

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Water is of key importance in the living world.

Continuous description versus motion of individual H_20 molecules

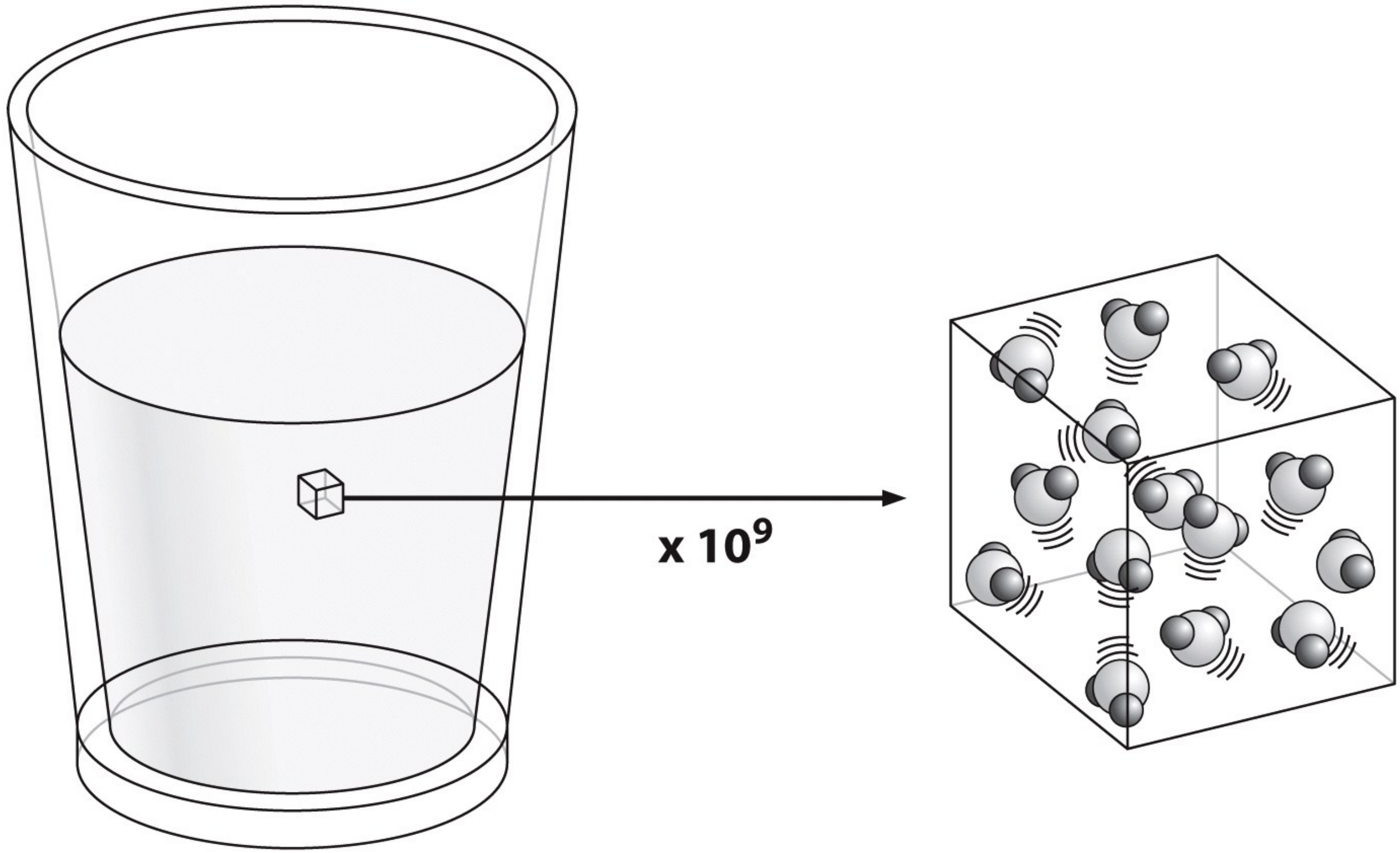


Figure 12.1 Physical Biology of the Cell (© Garland Science 2009)

Continuous description of water uses the velocity field, which in general can change with a spacial position (x,y,z) of a small volume of water and time:

$$\mathbf{v}(\mathbf{r}, t)$$

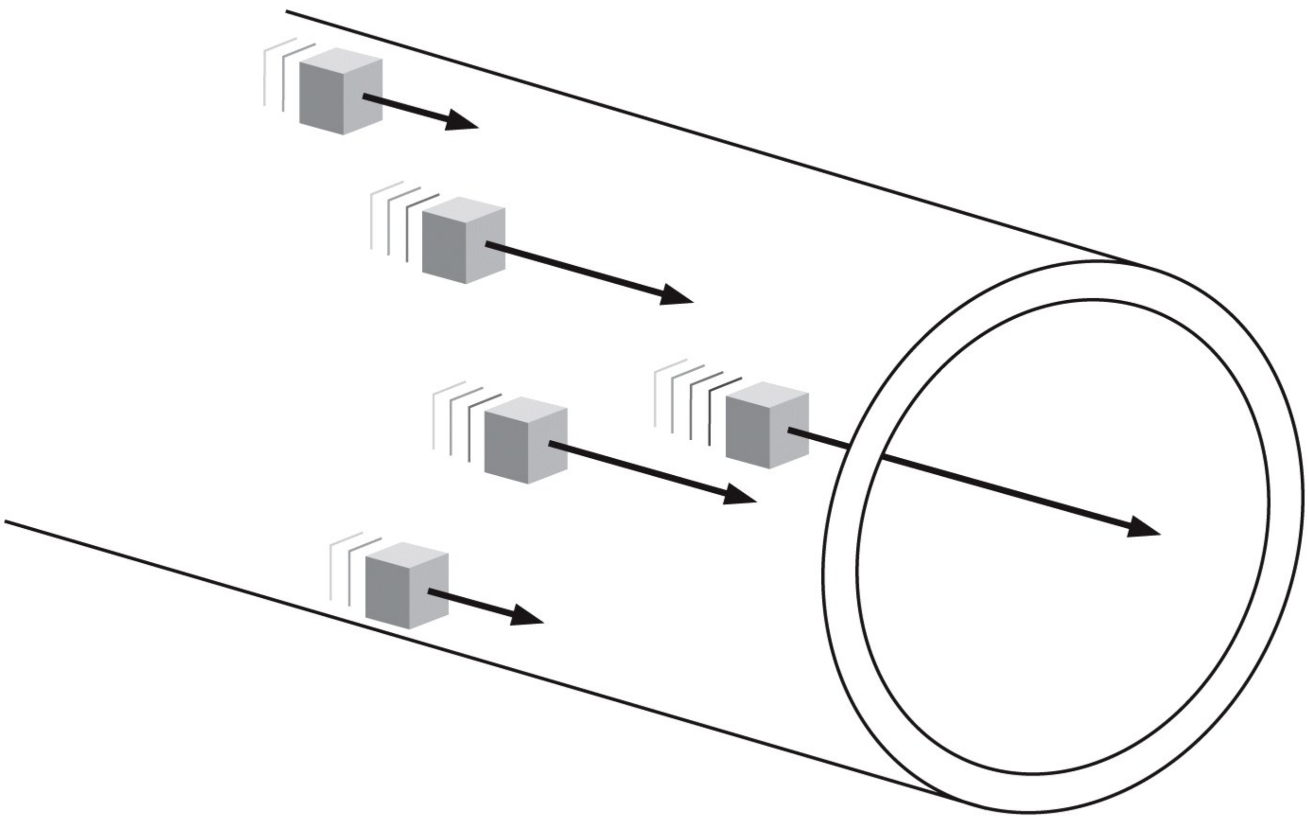


Figure 12.2 Physical Biology of the Cell (© Garland Science 2009)

Q: What distinguishes liquids from solids?

A: Solids and liquids respond to applied forces differently: Solids undergo deformation, liquids flow.

Mechanical properties of liquids are described by *viscosity* (in analogy to Young modulus E that describes solids).

For simple, Newtonian fluids: pulling force Results in a constant velocity fluid motion:

$$\frac{F}{A} = \eta \frac{v}{d}$$

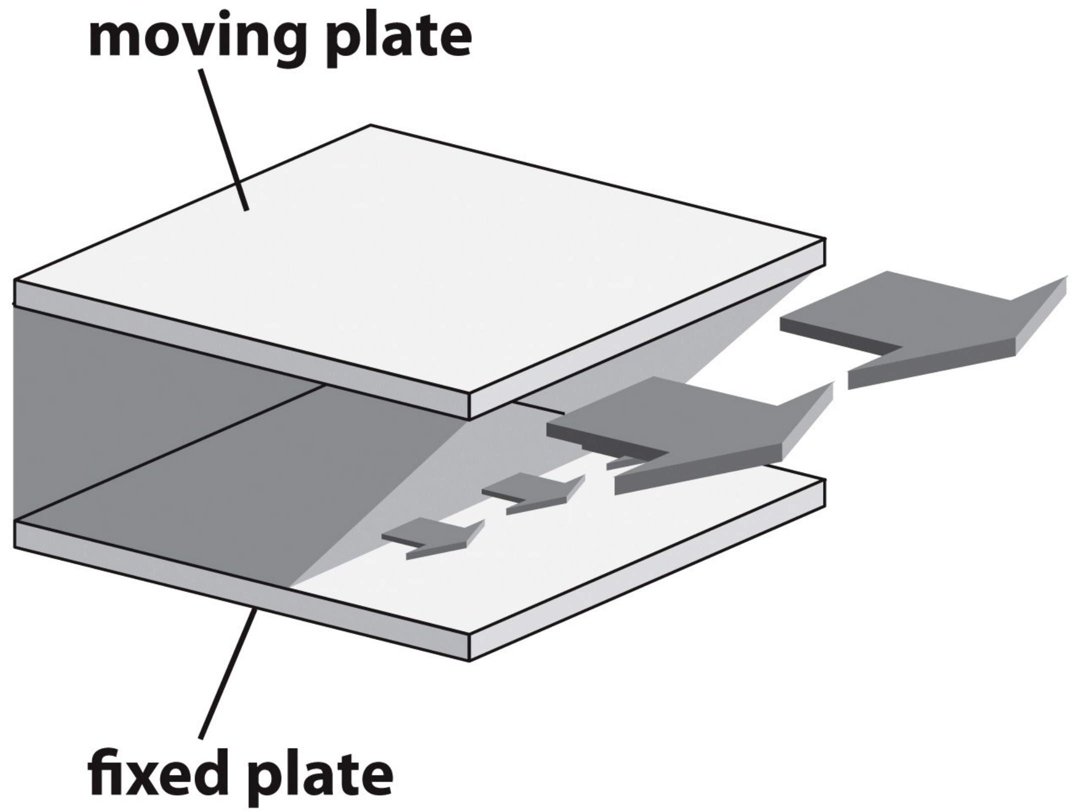


Figure 12.3 Physical Biology of the Cell (© Garland Science 2009)

Viscosity: $\eta[\text{Pa}\cdot\text{s}]$, where $1\,\text{Pa} = 10^{-5}\,\text{N/m}^2 = 10^{-5}\,\text{atm}$

Viscosity of water: $\eta = 1\,\text{mPa}\cdot\text{s} = 10^{-8}\,\text{N/m}^2\cdot\text{s} = 10^{-8}\,\text{atm}\cdot\text{s}$

Equation of motion for a Newtonian fluid: $\mathbf{F} = m\mathbf{a}$

Consider a small fluid element and apply Newton's second law to its motion:

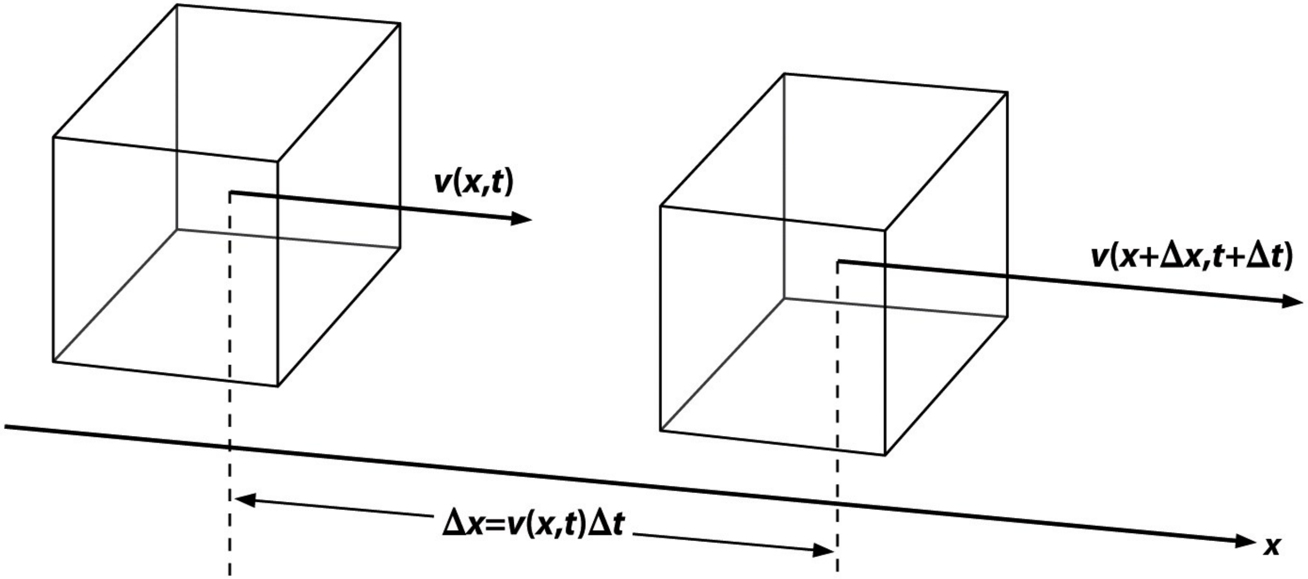


Figure 12.4 Physical Biology of the Cell (© Garland Science 2009)

In general, we need to consider: $\mathbf{r}=(x, v, z)$ $\quad \mathbf{v}=(v_x, v_y, v_z)$

To derive the equation of motion, we will assume a one-dimensional Problem:

$$\mathbf{v}(x,t)=v(x,t)\,\mathbf{e}_x \qquad \mathbf{e}_x \text{...unit vector along } x-\text{direction}$$

$$v(x+\Delta x, t+\Delta t) = v(x,t) + \frac{\partial v}{\partial x}\Delta x + \frac{\partial v}{\partial t}\Delta t$$

The element moves along the x-direction by Δx in time Δt:

$$v(x,t) = \frac{\Delta x}{\Delta t} \quad \rightarrow \quad \frac{\partial v}{\partial x}\Delta x = \frac{\partial v}{\partial x}\cdot\frac{\Delta x}{\Delta t}\cdot\Delta t = \frac{\partial v}{\partial x}\cdot v\cdot\Delta t$$

Thus we can calculate the change of velocity and thus acceleration along the x-direction:

$$\Delta v(x,t) = \left[\frac{\partial v}{\partial t} + v(x,t)\frac{\partial v}{\partial x}\right]\Delta t \quad \rightarrow$$

$$a(x,t) = \frac{\Delta v(x,t)}{\Delta t} = \frac{\partial v(x,t)}{\partial t} + v(x,t)\frac{\partial v(x,t)}{\partial x}$$

We can express the acceleration of a fluid element at position x and at time t as a *material derivative*:

$$\mathbf{a} = \frac{D\mathbf{v}}{Dt}$$

which is defined as: $$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla$$

Material derivative consists of two parts:

(1) conventional explicit time dependence reflecting the field variable v that is changing with time

(2) convective term: a material particle can be dragged into a region of space, where the field is different

Example of a temperature field T(x, t):

(1) fluid is resting but T is changing with time (e.g. heating): $$\frac{D}{Dt} = \frac{\partial}{\partial t}$$

(2) fluid is moving, steady state T gradient: $$\frac{D}{Dt} = \mathbf{v}_x\cdot\nabla$$

Two different kinds of forces are acting on a fluid volume element

$$\Delta x \times \Delta y \times \Delta z$$

pressure force **viscous stress force**

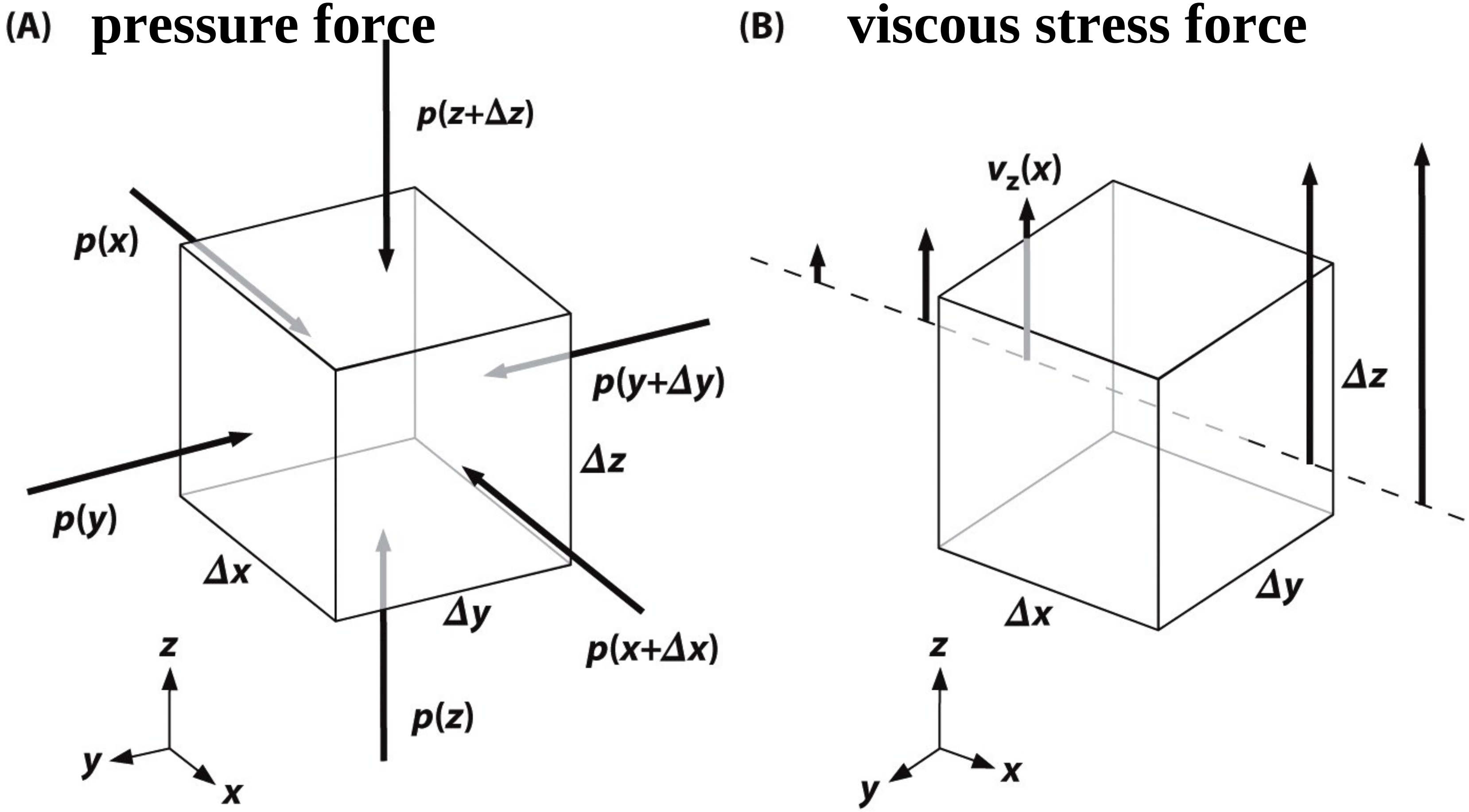


Figure 12.5 Physical Biology of the Cell (© Garland Science 2009)

***Pressure Force*: due to variations in the pressure along x, y, z**
***Viscous Stress Force*: friction on the volume element due to a velocity gradient along x, y, z**

The total pressure force along the x-direction:

$$\delta F_x^p = p(x,y,z,t)\,\Delta y\,\Delta z - p(x+\Delta x,y,z,t)\,\Delta y\,\Delta z$$

$$p(x+\Delta x,y,z,t) \approx p(x,y,z,t) + \frac{\partial p}{\partial x}\Delta x \quad \rightarrow$$

$$\delta \mathbf{F}^p = -\nabla p\,\Delta x\,\Delta y\,\Delta z \quad \text{where} \quad \nabla p = \left(\frac{\partial p}{\partial x},\frac{\partial p}{\partial y},\frac{\partial p}{\partial z}\right)$$

The viscous force on the face at position x is:

$$-\eta\frac{\partial v_z(x)}{\partial x}\Delta y\,\Delta z\;\mathbf{e}_z$$

whereas on the face at position x + Δx is:

$$+\eta\frac{\partial v_z(x+\Delta x)}{\partial x}\Delta y\,\Delta z\;\mathbf{e}_z$$

The total viscous stress force is then a sum of the two:

$$\delta F_z^v = -\eta \frac{\partial v_z(x)}{\partial x} \Delta y \Delta z \mathbf{e}_z + \eta \frac{\partial v_z(x+\Delta x)}{\partial x} \Delta y \Delta z \mathbf{e}_z$$

$$\frac{\partial v_z(x+\Delta x)}{\partial x} \approx \frac{\partial v_z(x)}{\partial x} + \frac{\partial^2 v_z(x)}{\partial x^2} \Delta x$$

$$\delta F_z^v = \eta \frac{\partial^2 v_z(x)}{\partial x^2} \Delta x \Delta y \Delta z$$

In general, the total viscous stress force can be written as:

$$\delta \mathbf{F}^v = (\eta \nabla^2 \mathbf{v} + \eta' \nabla (\nabla \cdot \mathbf{v})) \Delta x \Delta y \Delta z$$

If we only consider incompressible fluids, then $\nabla \cdot \mathbf{v} = 0$ **and:**

$$\delta \mathbf{F}^v = \eta \nabla^2 \mathbf{v} \; \Delta x \Delta y \Delta z$$

Incompressible fluids: the flow can distort and stretch the fluid element but preserves its volume.
Consider a volume element at a time t:

$$\Delta x \times \Delta y \times \Delta z$$

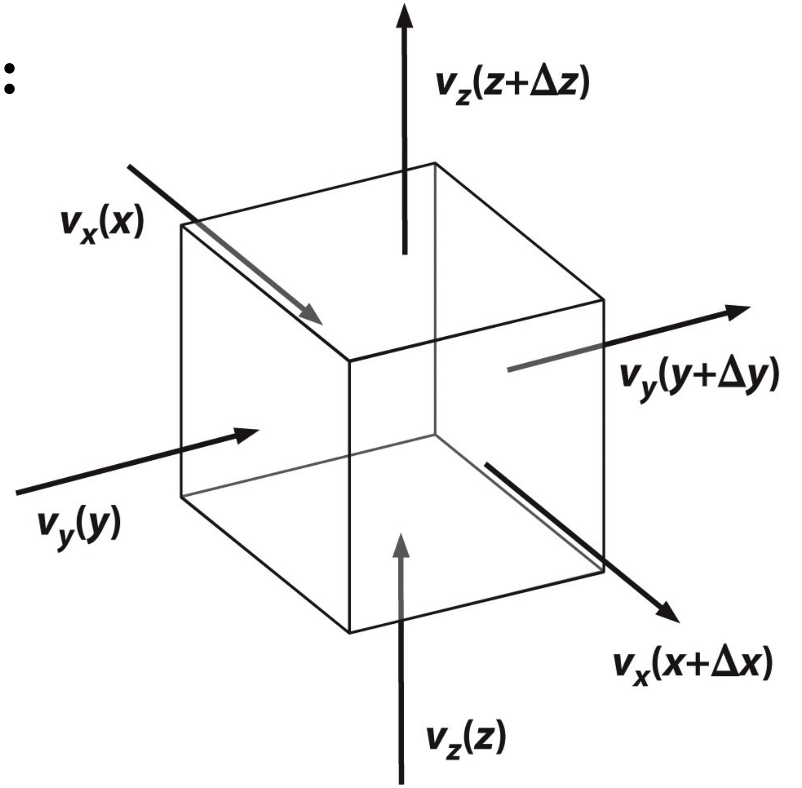


Figure 12.6 Physical Biology of the Cell (© Garland Science 2009)

A moment later, at t + Δt:

$$\Delta x' = \Delta x\left(1 + \frac{\partial v_x}{\partial x}\Delta t\right)$$

$$\Delta y' = \Delta y\left(1 + \frac{\partial v_y}{\partial y}\Delta t\right)$$

$$\Delta z' = \Delta z\left(1 + \frac{\partial v_z}{\partial z}\Delta t\right)$$

Thus the volume change is:

$$\Delta x'\,\Delta y'\,\Delta z' = \Delta x\,\Delta y\,\Delta z\left[1 + \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}\right)\right]$$

$$\Delta x'\,\Delta y'\,\Delta z' = \Delta x\,\Delta y\,\Delta z\left(1 + \nabla \cdot \mathbf{v}\right)$$

The Newtonian Fluid and the Navier-Stokes Equation

$$\Delta m \mathbf{a} = \delta \mathbf{F}_p + \delta \mathbf{F}_v \quad \text{where} \quad \Delta m = \rho \Delta x \Delta y \Delta z$$

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{v} \quad \text{where} \quad \nu = \frac{\eta}{\rho}$$

kinematic viscosity

The Navier-Stokes equation is a second-order partial differential equation: need to specify the boundary conditions:

no-slip condition = at a solid boundary the fluid is at rest with respect to the solid

Fluid Dynamics of Blood

- **a process of blood circulation**
- **blood vessels ranging in size from 2 μm to 1 cm**
- **use cylindrical symmetry to describe the blood flow**

$$\mathbf{v} = v(r)\,\mathbf{e}_z$$

- **consider only steady state:** $\dfrac{\partial \mathbf{v}}{\partial t} = 0$

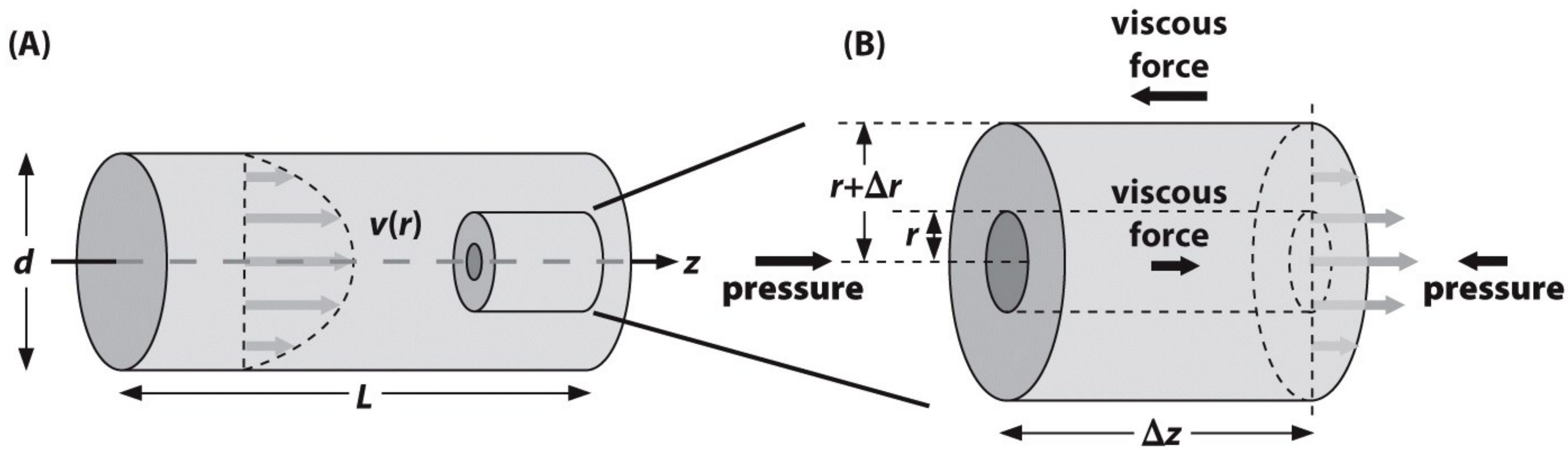


Figure 12.7 Physical Biology of the Cell (© Garland Science 2009)

Consider a small volume element in the shape of a hollow cylinder and calculate the opposing pressure forces:

$$\delta F_z^p = [p(z) - p(z+\Delta z)] 2\pi r \Delta r = -\frac{dp}{dz} 2\pi r \Delta r \Delta z$$

and the opposing viscous stress forces:

$$\delta F_z^v = \eta v'(r+\Delta r) 2\pi (r+\Delta r) \Delta z - \eta v'(r) 2\pi r \Delta z \quad \text{where} \quad v' = \frac{dv}{dr}$$

Use the Taylor expansion:

$$v'(r+\Delta r) \approx v'(r) + \frac{dv'}{dr} \Delta r$$

To derive the expression for the viscous stress force:

$$\delta F_z^v = \eta v' 2\pi \Delta r \Delta z + \eta \frac{dv'}{dr} 2\pi r \Delta r \Delta z$$

In a steady state, a force balance on the hollow fluid cylinder is:

$$\delta F_z^p + \delta F_z^v = 0$$

This results in a differential equation relating the pressure and velocity fields:

$$\frac{1}{\eta}\frac{dp}{dz} = \frac{1}{r}\frac{dv}{dr} + \frac{d^2 v}{dr^2} = \frac{1}{r}\frac{d}{dr}\left(r\frac{dv}{dr}\right)$$

Laplacian of the velocity field in cylindrical coordinates

How do we solve this equation?
Integrate both sides along the z direction along the length L:

$$\frac{-1}{\eta}\Delta p = \frac{1}{r}\frac{d}{dr}\left(r\frac{dv}{dr}\right)L \quad \text{where} \quad \Delta p = p(0) - p(L)$$

pressure drop along the length of the pipe

Now integrate twice along r to get a solution:

$$v(r) = -\frac{\Delta p}{\eta L}\left(\frac{r^2}{4} - \frac{C_1}{r^2} + C_2\right)$$

Take into account the boundary conditions:

$$v(r=0)<\infty \quad \rightarrow \quad C_1=0$$

$$v\left(r=\frac{d}{2}\right)=0 \quad \text{no}-\text{slip} \quad \rightarrow \quad C_2=\frac{-d^2}{16}$$

We derive the final expression for the fluid velocity in the pipe:

$$v(r) = \frac{\Delta p}{4\eta L}\left(\frac{d^2}{4} - r^2\right)$$

The fluid moves the fastest in the center of the pipe and not at all at the boundaries. We need an average velocity $\langle v \rangle$ which can be related to the flow rate Q:

$$Q = \frac{\langle v \rangle \pi d^2}{4}$$

The average velocity and the resulting flow rate are:

$$\langle v \rangle = \frac{\int_0^{d/2} v(r) 2\pi r\, dr}{\frac{\pi d^2}{4}} = \frac{\Delta p\, d^4}{128\eta L} \quad \rightarrow \quad Q = \frac{\pi \Delta p\, d^4}{128\eta L}$$

Estimated blood flow through capillaries:

$$d \approx 5\,\mu m \quad \text{for most animals}$$

A measured pressure difference across a capillary and its length:

$$\Delta p \approx 20 \text{ mmHg} \approx 3000\,\text{Pa}$$

$$L \approx 1 \text{ cm}$$

The average flow velocity through a capillary:

$$v = \frac{\Delta p\, d^2}{32\,\eta L} \approx 0.02\,\text{cm/s} \qquad (\eta \approx \eta_{water} = 10^{-3}\,\text{Pa})$$

But the viscosity of blood is higher than that of water:

$$\eta \approx 3\,\eta_{water} \quad \rightarrow \quad v \approx 0.007 \text{ cm/s} \qquad \text{too small!}$$

$$v_{measured} \approx 0.05 \text{ cm/s}$$

Can blood be well represented as a Newtonian liquid? Not really.

Blood carries red blood cells and white blood cells (leukocytes)

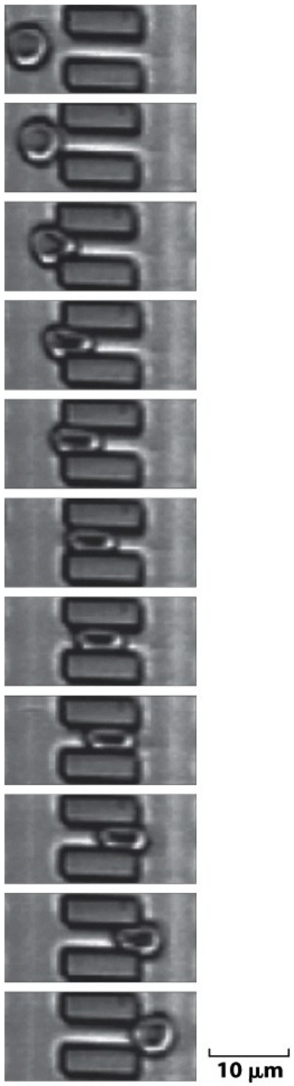


Figure 2.11 Physical Biology of the Cell (© Garland Sci

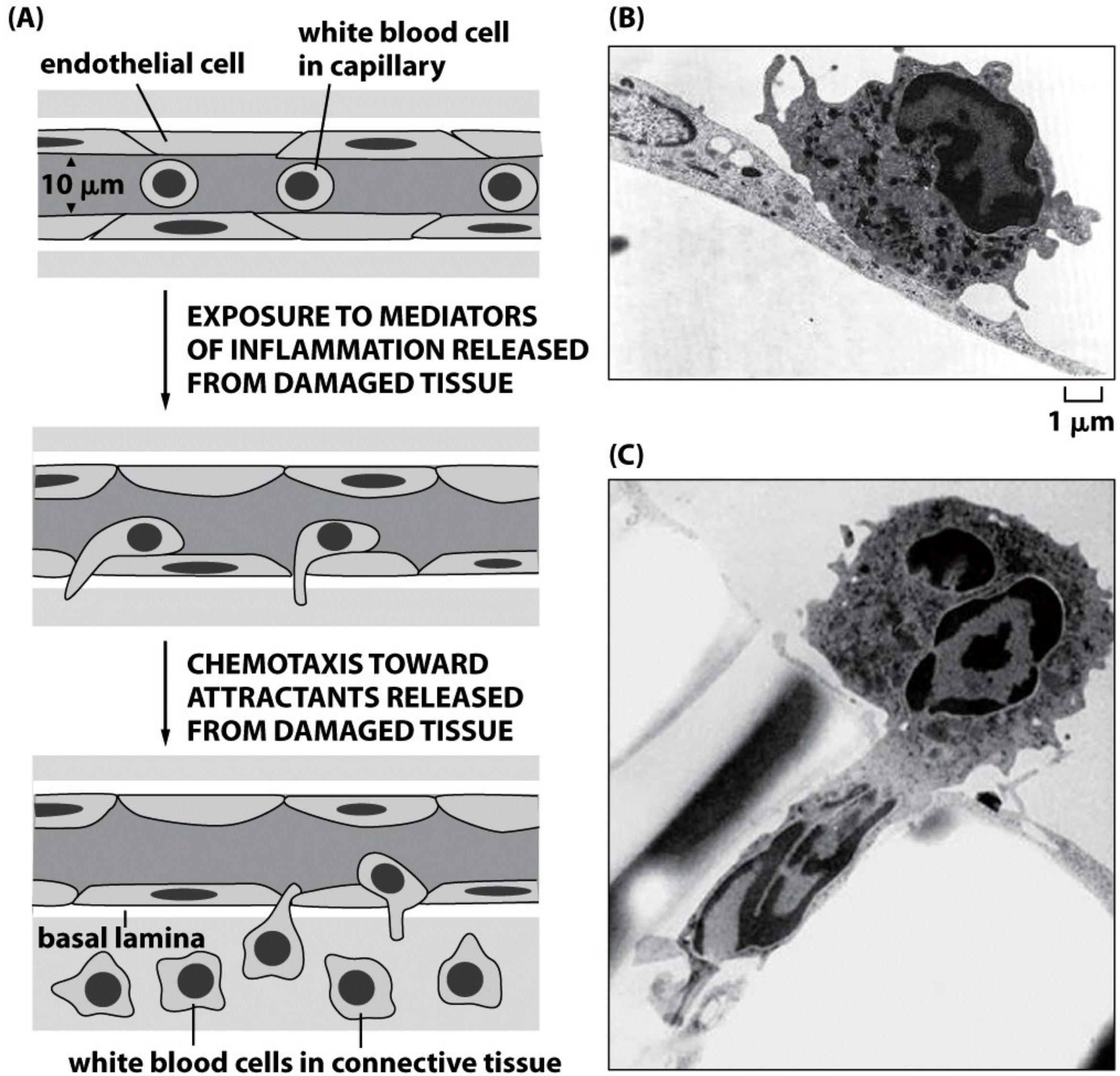


Figure 12.8 Physical Biology of the Cell (© Garland Science 2009)

The Low Reynolds number World

The 100 years experiment with a very viscous fluid: 1 drop every 10 years!

Figure 12.9 Physical Biology of the Cell (© Garland Science 2009)

This system has the same viscous properties as water to the *E. coli* bacterium.

What is a Reynolds number Re?
Re = intertial term of N.-S. Eq. /
visocus term of N.-S. Eq.

For a rigid body of length L moving with a speed U:

$$\text{Re.N.} = \frac{\rho U^2/L}{\eta U/L^2} = \frac{\rho L U}{\eta} = \frac{L U}{\nu}$$

For small Reynolds numbers, the Navier-Stokes equation simplifies into the Stokes equation:

$$\nabla p = \eta \nabla^2 \mathbf{v} \qquad \text{incompressibility:} \quad \nabla \cdot \mathbf{v} = 0$$

The meaning of Reynolds number can be found by comparing the kinetic energy to the work done by the viscous stress dissipation of an object of linear dimension a and speed u (where u/a is the rate of change of the fluid velocity):

$$KE \approx \rho a^3 u^2 \qquad W \approx \eta \frac{u}{a} \times a^2 \times a \quad \rightarrow \quad \text{Re.N.} = \frac{KE}{W} = \frac{a u}{\nu}$$

Another way: compare the time needed to dissipate KE of the fluid element to the time needed to move a distance comparable to its size:

$$\tau_{\text{viscous}} = \frac{\rho a^2}{\eta} \quad \ll \quad \tau_{\text{inertial}} = \frac{a}{u} \quad \rightarrow \quad \text{Re.N.} = \frac{\tau_{\text{viscous}}}{\tau_{\text{inertial}}}$$

Flow around a sphere at different Reynolds numbers

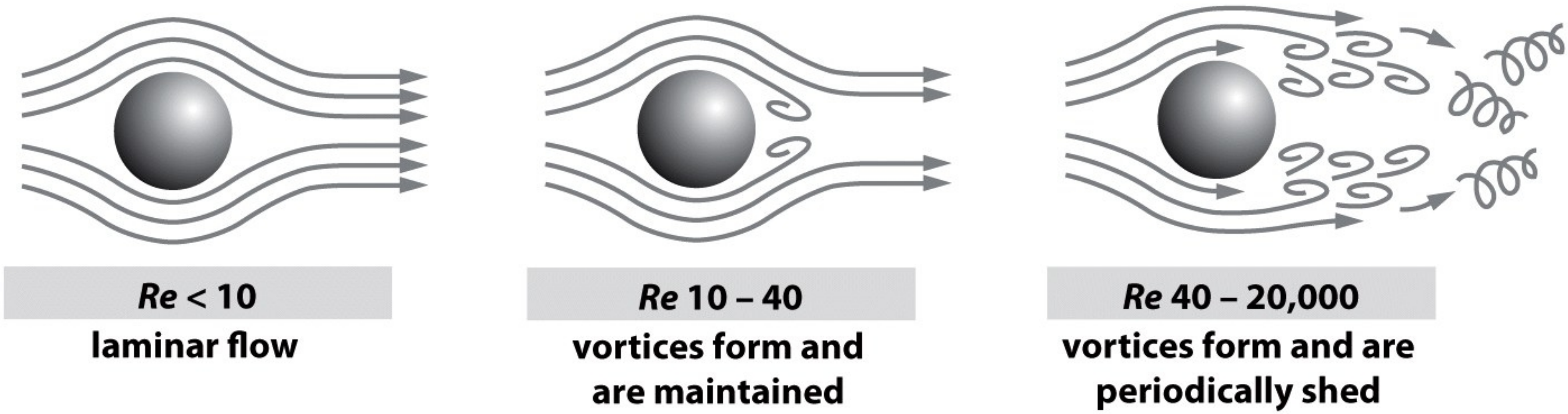


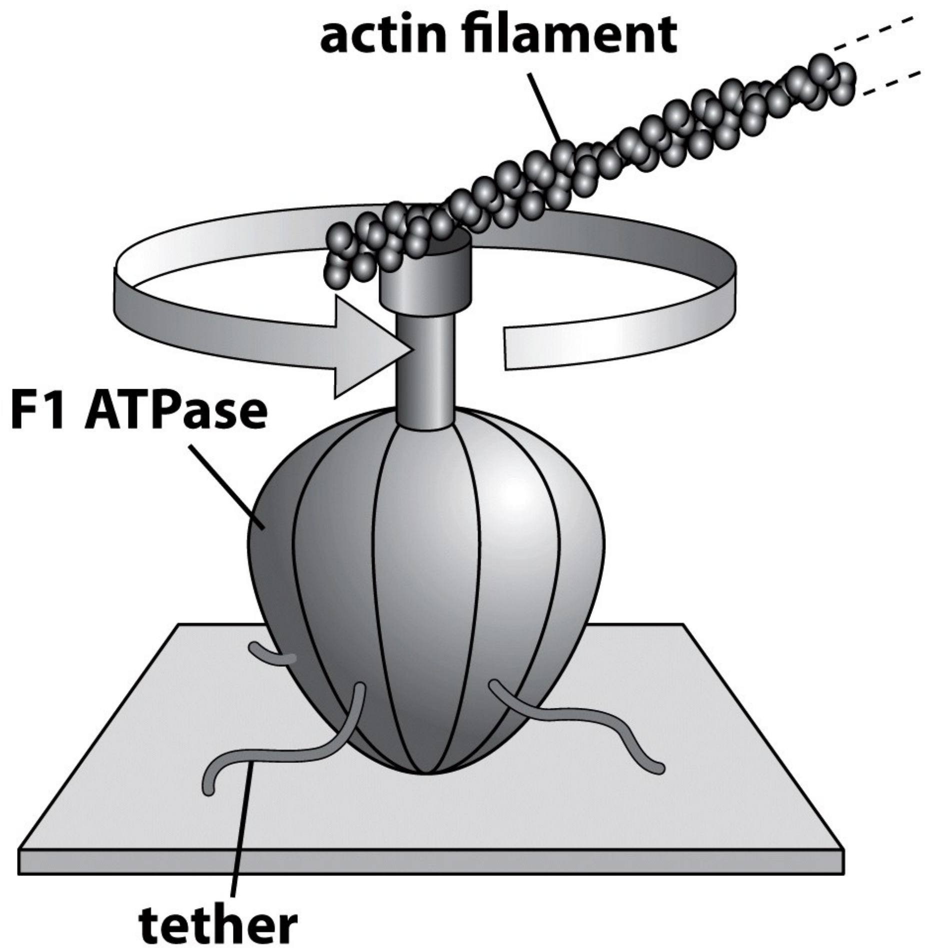
Figure 12.10 Physical Biology of the Cell (© Garland Science 2009)

The Stokes formula for a drag force on a sphere

- need to integrate the viscous stress and the pressure over the surface of a sphere
- viscous stress proportional to the spatial derivative of the speed $\frac{v}{R}$
- the area of the surface of the sphere: $4\pi R^2$
- the Stokes force/drag is then: $F_S = C\eta \frac{v}{R} \times 4\pi R^2 = 6\pi\eta R\nu$

Stokes Drag in Single-Molecule Experiments

- ATP synthase is a rotary motor
- actin filament attached to this motor is tagged by a fluorescent molecule
- when the motor rotates, the filament spins around and the fluorescent tag allows us to measure the rotation
- existence of pauses in molecular motors



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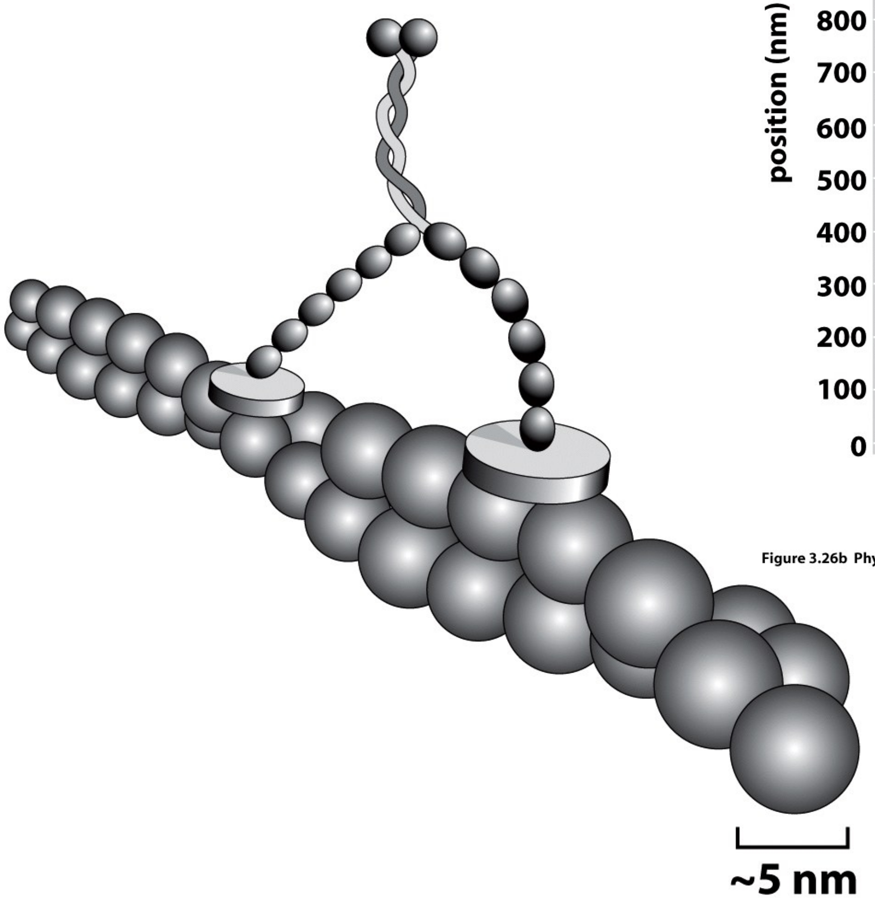
Molecular motor: Motion of myosin on an actin filament



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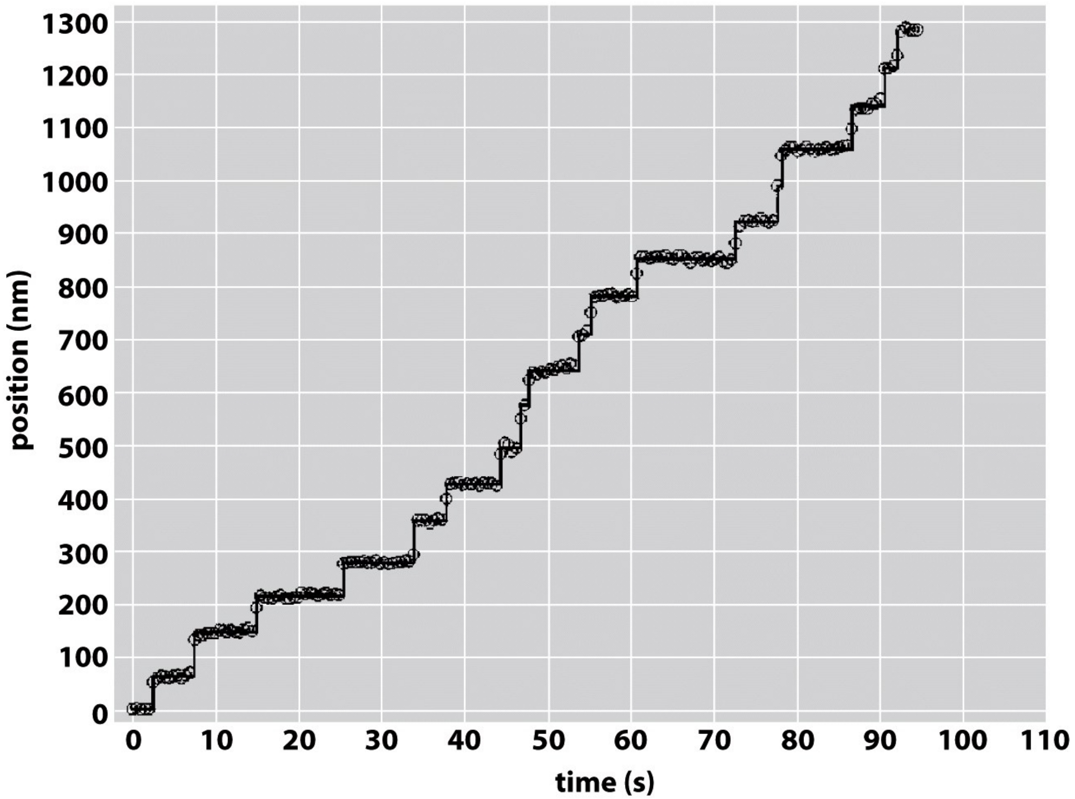

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Position as a function of time

Stokes Drag can be Neglected in Optical Tweezers Experiments

- can measure the speed of the motor as a function of the applied load
- How large is a drag force due to a bead tethered to the motor?
- the bead: 1 μm diameter

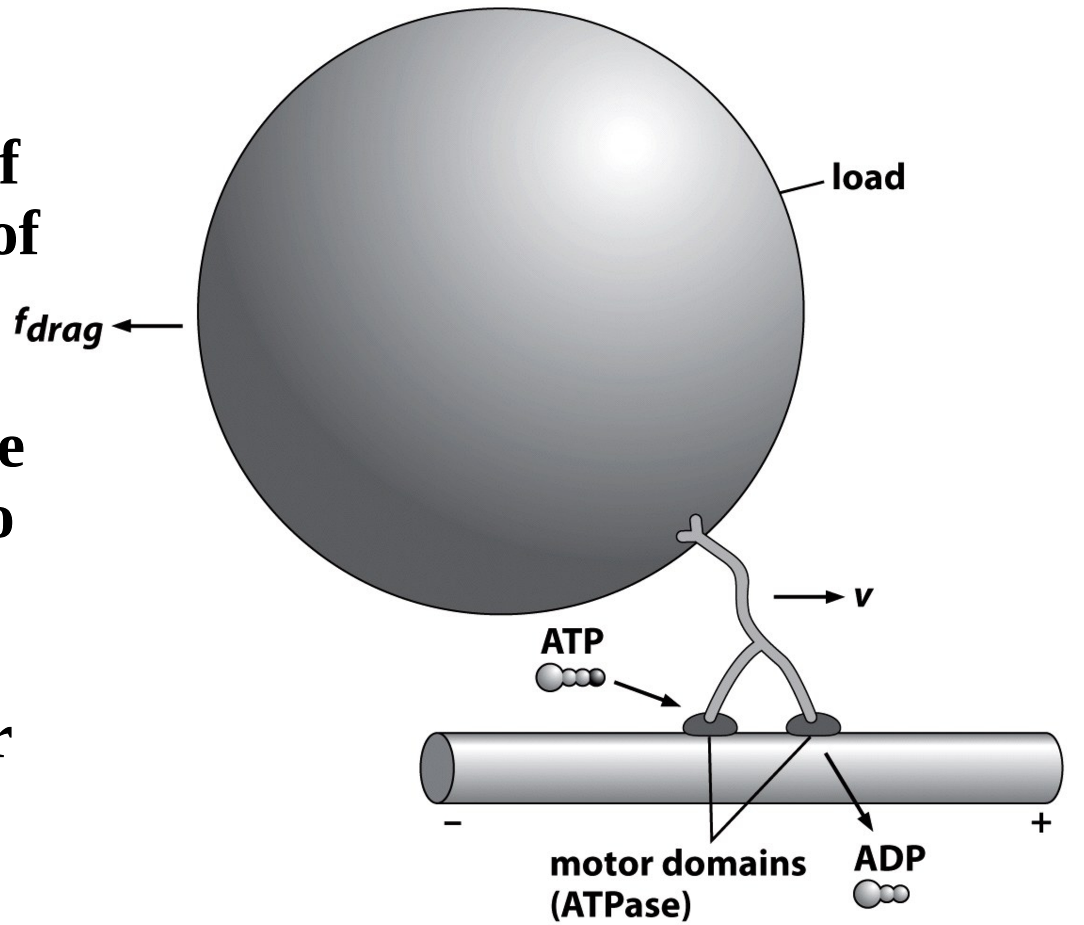


Figure 12.12 Physical Biology of the Cell (© Garland Science 2009)

$$F_S \approx 6\pi \times 10^{-3} \mathrm{Ns/m^2} \times 5 \times 10^{-7} \mathrm{m} \times 10^{-6} \mathrm{m/s} \approx 10^{-2} \mathrm{pN} \ll 5 \mathrm{pN}$$

Dissipative Time Scales and the Reynolds Number

Consider a damped harmonic oscillator and analyze its behavior at low Reynolds numbers:

$$m\frac{d^2x}{dt^2} + \gamma\frac{dx}{dt} + kx = 0$$

A low Reynolds number means that the time scale over which the kinetic energy dissipates is small:

$$\frac{m(dx/dt)^2}{\tau_{viscous}} \approx \gamma(dx/dt)^2$$

(rate of dissipation on the right is a viscous force times velocity)

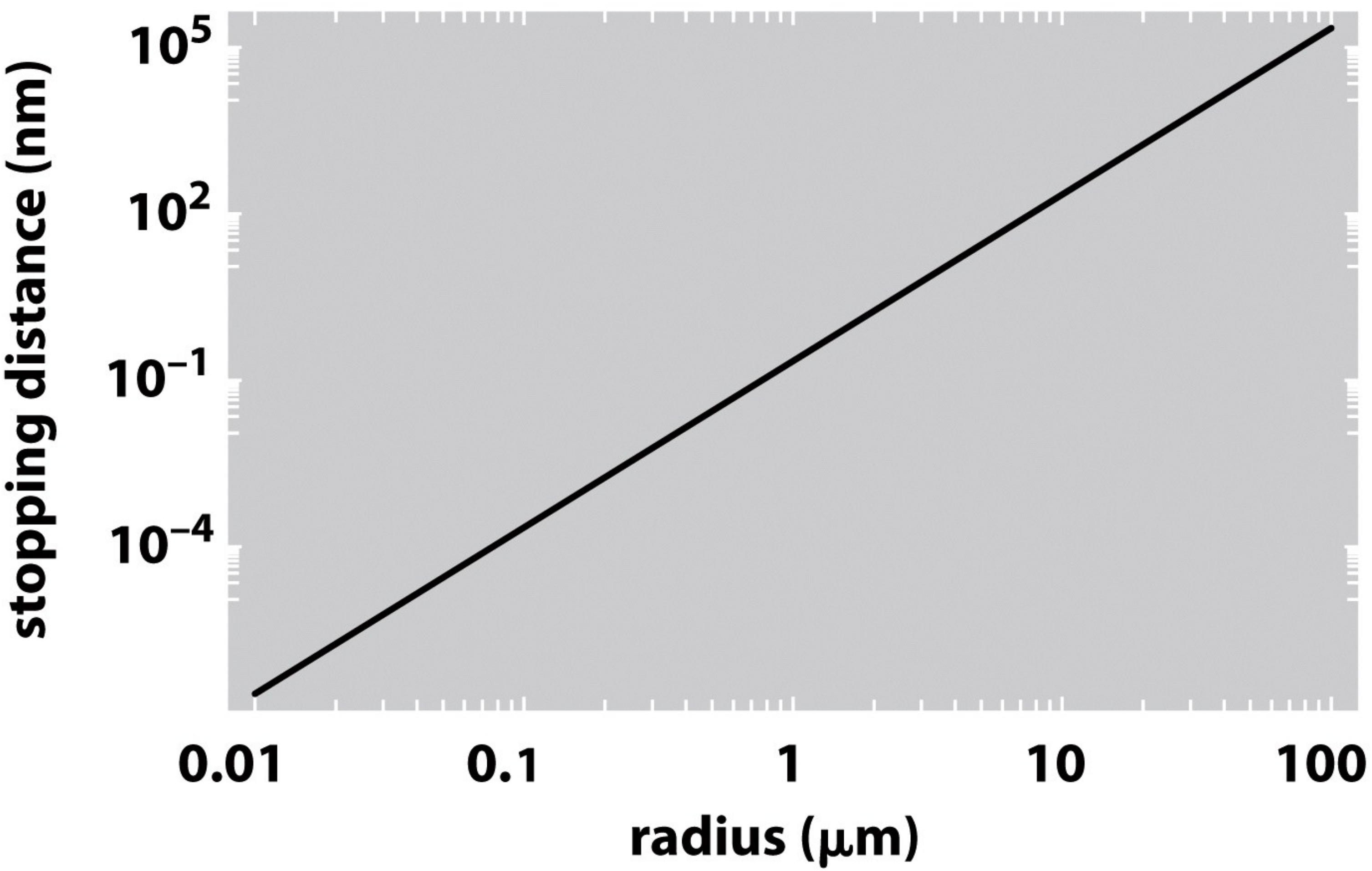
Thus we get a simple expression:

$$\tau_{viscous} = \frac{m}{\gamma}$$

which means that we can neglect the inertial term in the equation and get

$$\gamma\frac{dx}{dt} + kx = 0 \quad \text{with a solution:} \quad x(t) = x_0 e^{-(k/\gamma)t}$$

Observation of stopping distances for objects of different sizes: Consider a spherical object with initial velocity equal to a diameter of a sphere per second



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E. coli moves by rotating its flagella

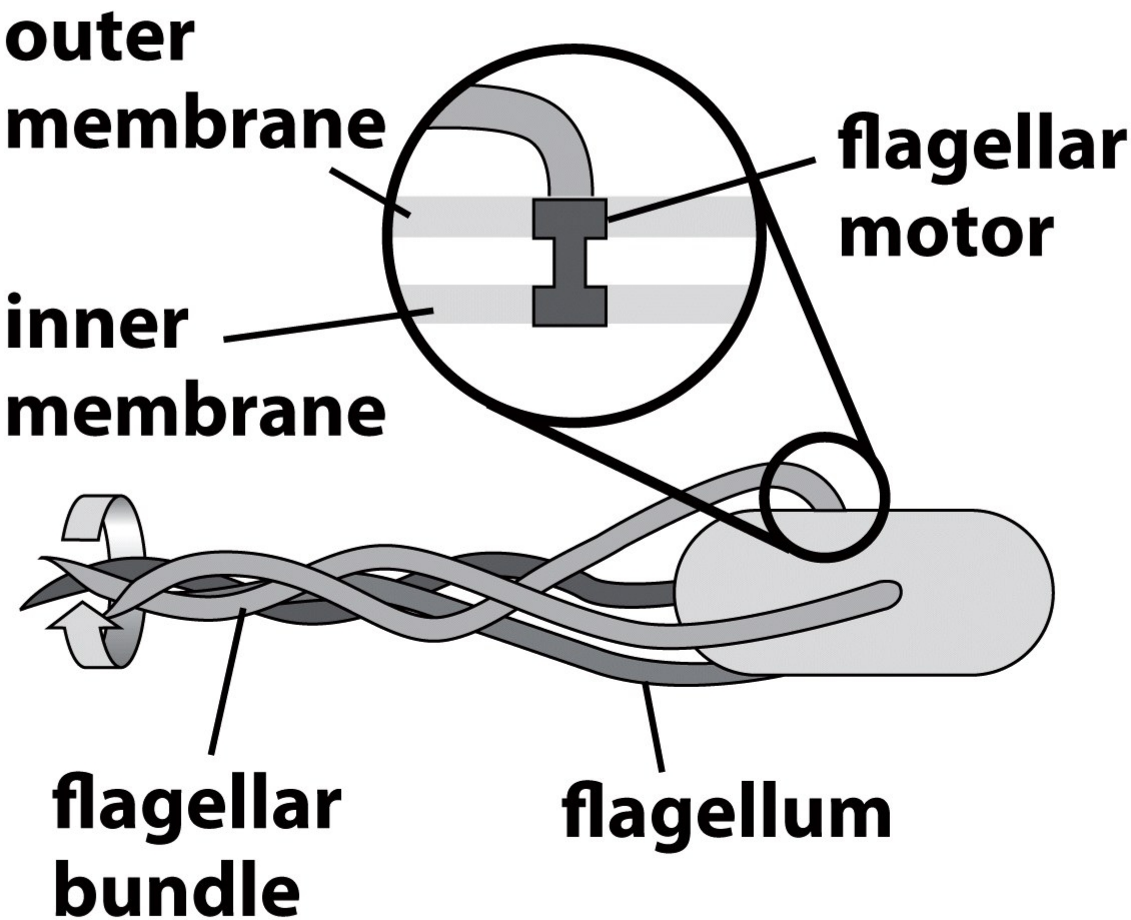


Figure 4.16a Physical Biology of the Cell (© Garland Science 2009)

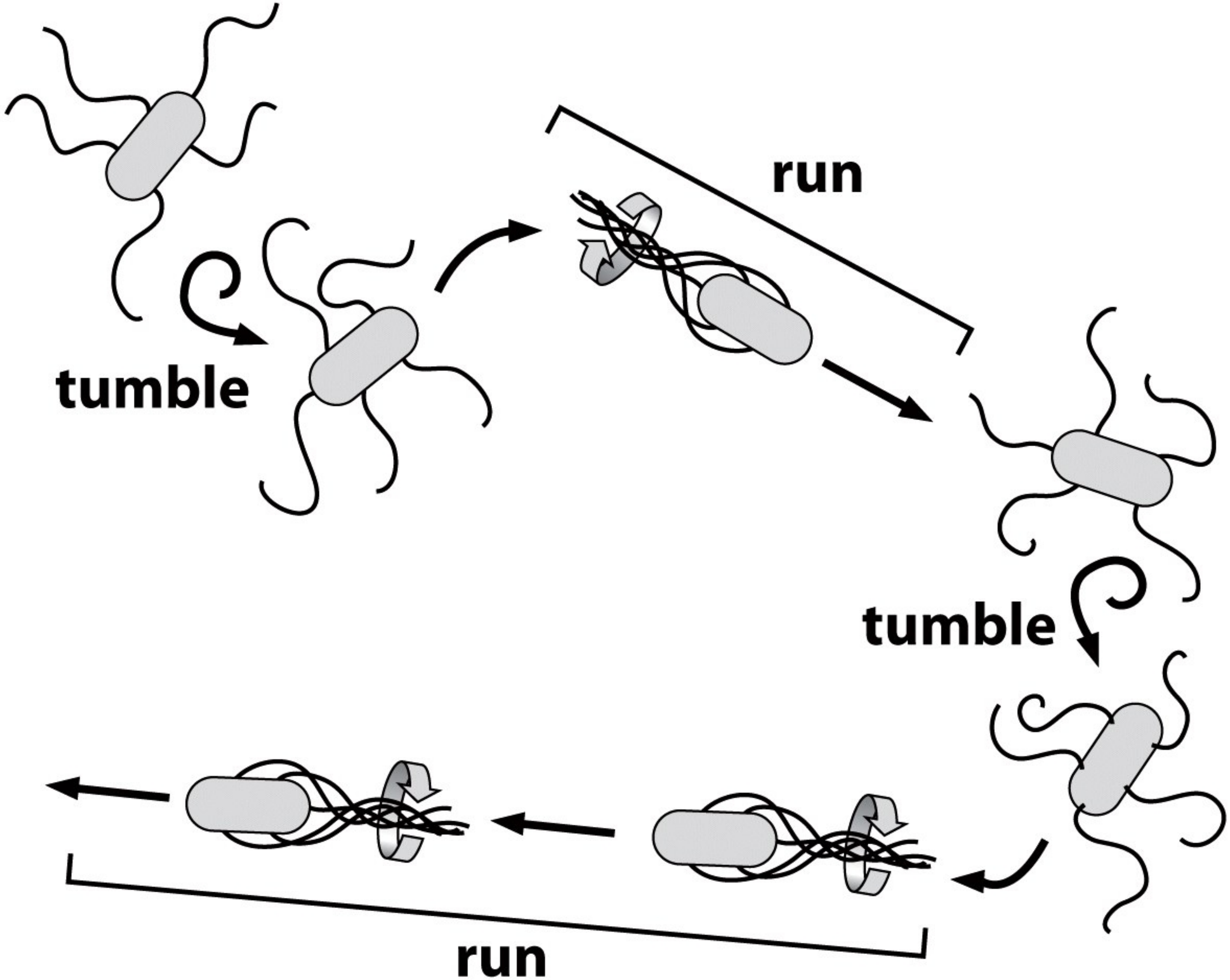


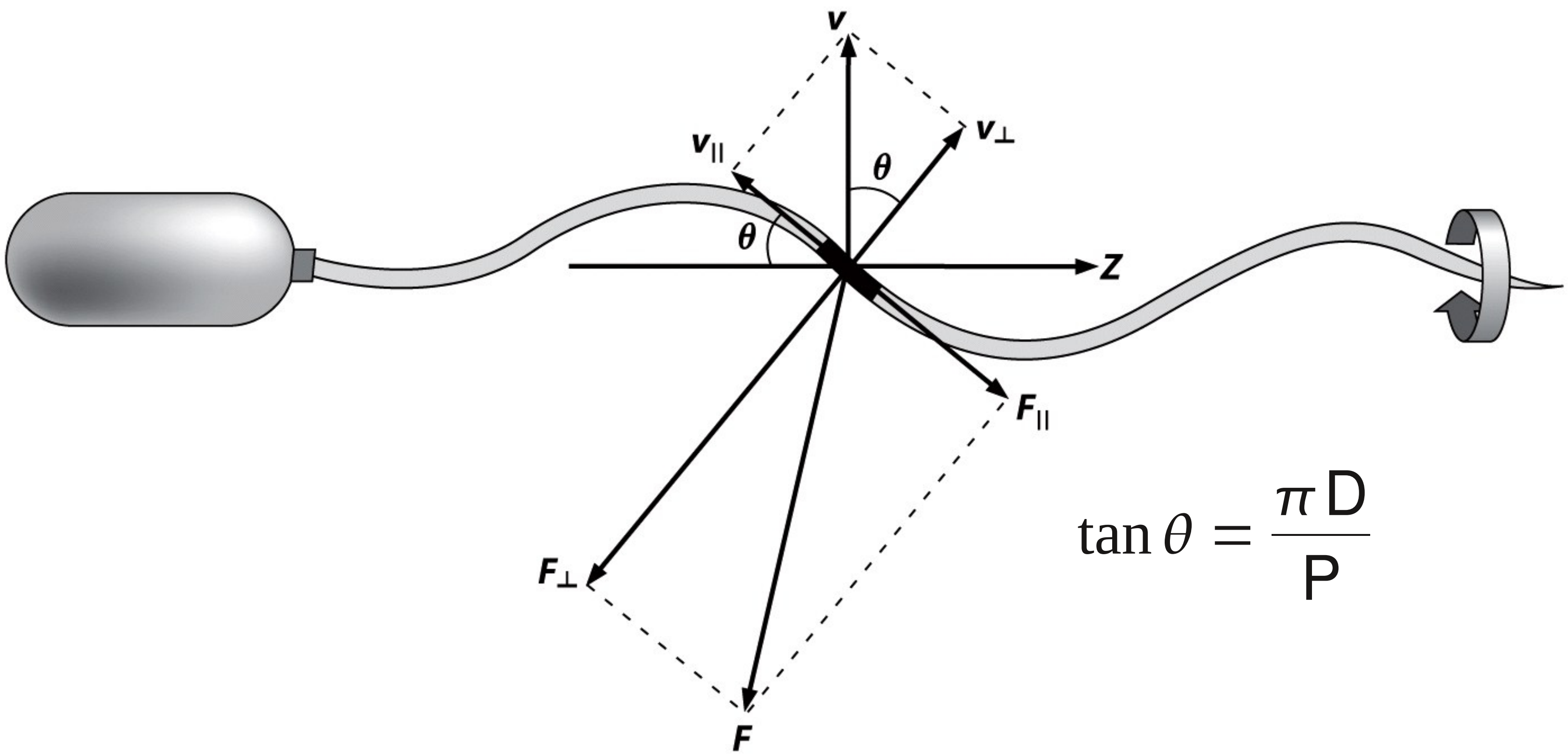
Figure 4.16b Physical Biology of the Cell (© Garland Science 2009)

Helically shaped flagella with a diameter D and pitch P:

$\mathrm{D} \approx 0.5\,\mu\mathrm{m}$...diameter of the helically shaped flagellum

$\mathrm{P} \approx 2\,\mu\mathrm{m}$...pitch of the helix (length of one helical turn)

f...propulsion frequency $\quad$ $v = \pi \mathrm{D} f$...linear velocity



$$\tan\theta = \frac{\pi \mathrm{D}}{\mathrm{P}}$$

Figure 12.14 Physical Biology of the Cell (© Garland Science 2009)

The propulsive force relies on the difference in the drag coefficients between parallel and perpendicular motion of a rod:

- **force parallel to the rod is:**

$$F_{\parallel} = \gamma_{\parallel} v \sin\theta \quad , \quad \text{where } \gamma_{\parallel} = 2\pi\nu L$$

- **force perpendicular to the rod is:**

$$F_{\perp} = \gamma_{\perp} v \sin\theta \quad , \quad \text{where } \gamma_{\perp} = 4\pi\nu L$$

- **the total force projected onto the negative z-direction (direction of motion) is then:** $F_p = -F_{\parallel}\cos\theta + F_{\perp}\sin\theta$

$$F_p = -2\pi\eta L v \sin\theta\cos\theta + 4\pi\eta L v \cos\theta\sin\theta = 2\pi\eta L v \sin\theta\cos\theta$$

- **the propulsion force is balanced by the drag force:**

$$F_D = 2\pi\eta L V$$

- **which results in the final speed of:**

$$V = \pi D f \sin\theta\cos\theta \approx 70\,\mu m/s \quad (30\,\mu m/s \ \text{exp.}) \quad (v = \pi D f)$$

Centrifugation and Sedimentation

- **biochemical purification: to separate macromolecules or their complexes from the solution**

- ***centrifugation*: a simple example of diffusion in the presence of drift using the Stokes formula**

- **What is centrifugation? Spinning at up to 100,000 rpm ~ 10^6 g**

- **the centrifugal force that all molecules in the solution experience:**

$$m\omega^2 r$$

- **assume: the size of the sample much smaller than the distance from the rotation axis**

- **The mass of the molecule in the solvent needs to be corrected by the mass of displaced solvent:** $m \rightarrow (\rho_P - \rho) V$

The centrifugal force imparts a drift velocity to the biomolecules (low Reynolds numbers): centrifugal force equal to the frictional Force:

$$v_{drift} = \frac{m g_c}{\gamma} \quad \text{for a sphereical molecule:} \quad \gamma = 6\pi\eta R$$

The quantity m/γ **is quoted for different biomolecules in units of Svedberg:**

$$1\,\text{svedberg} = 10^{-13}\,\text{s}$$

which corresponds to a globular protein with a radius of 1 nm in water. Typical density of proteins: $1.35\,\text{g/cm}^3$

***The drift velocity is then a quadratic function of the size of the Biomolecule*:**

$$v_{drift} = \frac{(\rho_P - \rho) 4/3\pi R^3}{6\pi\eta R} = \frac{2(\rho_P - \rho)}{9\eta} R^2 g_c$$

which allows for an effective separation of particles based on their respective sizes.

Rate Zonal Versus Isopycnic Centrifugation

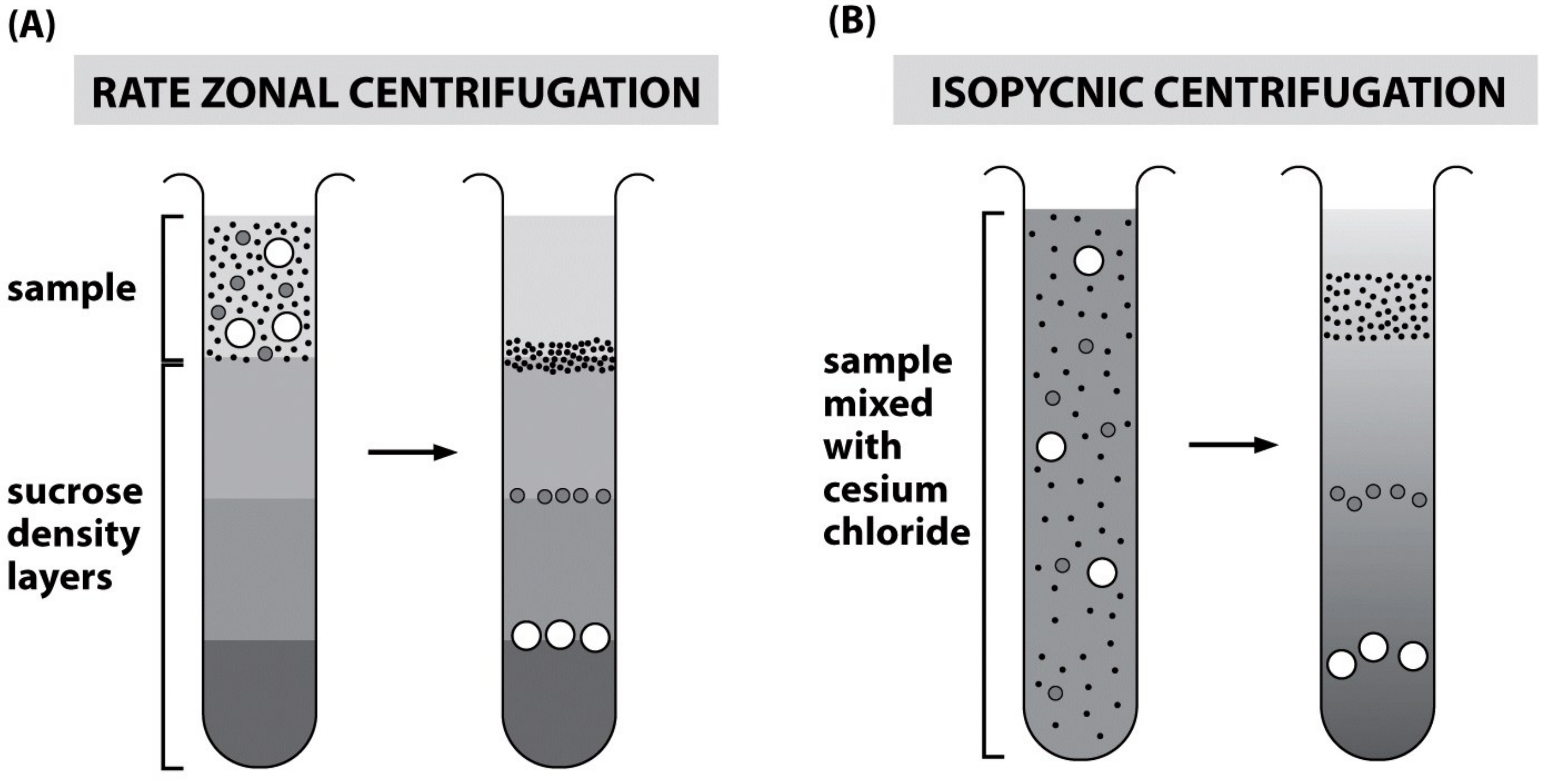


Figure 12.16 Physical Biology of the Cell (© Garland Science 2009)

$$x_c = v_{drift}\, t$$

$$\Delta x = \sqrt{2Dt}$$

Diffusion of biomolecules due to thermal fluctuations: a negative effect on the separation. A condition for separation:

$$\left|v_{drift1} - v_{drift2}\right| t > (\sqrt{2D_1} + \sqrt{2D_2})\sqrt{t}$$

which shows that we just need to wait long enough for two types of molecules to separate:

$$t_{sep} = \left(\frac{\sqrt{2D_1} + \sqrt{2D_2}}{\left|v_{drift1} - v_{drift2}\right|} \right)^2$$

However, a test tube has a finite length, so the separation needs to occur before the molecules reach the bottom of the tube, that is, the speed of spinning needs to be large enough:

$$v_{drift} t_{sep} < L \quad \rightarrow \quad g_c > \frac{1}{L} \frac{m_1}{\gamma_1} \left(\frac{\sqrt{2D_1} + \sqrt{2D_2}}{m_1/\gamma_1 - m_2/\gamma_2} \right)^2$$

The other separation method: isopycnic centrifugation relies on a density gradient of the solvent and different densities of the various macromolecules that needs to be separated.