Friction in Fluids

• We learned that diffusion is a dissipative process. It tends to erase ordered arrangements of molecules.
• Friction is dissipative, too. It tends to erase ordered motion.
• In biology, dynamics of small molecules can be envisioned as a marble dropped into a jar of honey.
• We will learn that water acts like a highly viscous fluid for small molecules.
• Viscous friction dominates mechanics in the nanoworld.
• We learned that $v = \frac{F}{\zeta}$ small particles fall under gravity because the nominator ($F$) increases by the mass ($m$) of particle which is proportional to $R^3$, whereas the drag coefficient ($\zeta$) increases by $R$. Therefore $v_{drift}$ is proportional to $R^2$.

How about small particles?
Biased Diffusion

- A force $F$ exerted on a particle results in a drift velocity:

$$F = \zeta v_{drift}$$

- The movement of particles under the same net $v_{drift}$ would generate a net flux:

$$j_F = \frac{1}{A \Delta t} \Delta N$$

where $\Delta N$ is the number of particles moving under the drift velocity to right.

$$\Delta N = cA \Delta t \cdot v_{drift}$$

$$j_F = cv_{drift} = c \frac{F}{\zeta}$$

- We can write the total flux due to random diffusion and net movement under the drift velocity:

$$j(x) = -D \frac{dc}{dx} + \frac{F}{\zeta} c$$
\[ j(x) = -D \frac{dc}{dx} + \frac{F}{\zeta} \]

In equilibrium, the net flux vanishes, \( J(x) = 0 \)

\[ D \frac{dc}{dx} = \frac{F}{\zeta} \]

Nonuniform concentration gradient can be set up by force.

\[ \text{using separation of variables, } \zeta D \frac{dc}{c} = F dx \]

\( \zeta D = kT \) and \( F = -dU/dx \)

\[ \frac{c(x)}{c(0)} = \frac{e^{-U(x)/kT}}{e^{-U(0)/kT}} \]
\[ j(x) = -D \frac{dc}{dx} + \frac{F}{\zeta} \]

Out of equilibrium,

\[ \frac{\partial c}{\partial t} = -\frac{\partial j}{\partial x} \]

\[ \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - \frac{F}{\zeta} \frac{\partial c}{\partial x} \quad (Nernst – Planck Equation) \]

- Nernst – Planck Equation describes process that involve both external forcing and diffusion.
Pulse Equation under Bias

You release 1 billion molecules at position $x = 0$ in the middle of a narrow tube. The molecules, diffusion constant is $100 \, \mu\text{m}^2\text{s}^{-1}$. An electric field pulls the molecules to the right with drift velocity of $1 \, \mu\text{m/s}$. After 80s, what percentage of molecules will be on the left?

We learned that without bias, $c(x,t) = \frac{1}{\sqrt{4\pi Dt}} e^{-x^2/4Dt}$ in one dimension.

In the presence of bias, the whole distribution of molecules shift to right

$$\Delta x = v_{\text{drift}} t$$

so, if we replace $x \to x - v_{\text{drift}} t$ on the right hand side of the equation

$$c(x,t) = \frac{1}{\sqrt{4\pi Dt}} e^{-(x-v_{\text{drift}} t)^2/4Dt}$$
the number of molecules on the left, \( N \):

\[
N = 10^9 \int_{-\infty}^{0} c(x, t) \, dx = 10^9 \int_{-\infty}^{0} \frac{1}{\sqrt{4\pi Dt}} e^{-\left(x - v_{\text{drift}} t\right)^2 / 4Dt} \, dx
\]

\[
u = (x - v_{\text{drift}} t) / \sqrt{4Dt}
\]

\[
d\nu = dx / \sqrt{4Dt}
\]

\[
x = 0 \Rightarrow \nu = -v_{\text{drift}} t / \sqrt{4Dt} = -z
\]

\[
z = \frac{1 \, \mu m s^{-1} \times 180 s}{\sqrt{4.100 \, \mu m^2 s^{-1} \times 1.80 s}} \approx \frac{80 \, \mu m}{125 \, \mu m} = 0.6
\]

\[
x = -\infty \Rightarrow \nu = -\infty
\]

\[
N = \frac{10^9 \sqrt{4Dt}}{\sqrt{4\pi Dt}} \int_{-\infty}^{-z} e^{-\nu^2} \, d\nu
\]
\[ N = \frac{10^9 \sqrt{4Dt}}{\sqrt{4\pi Dt}} \int_{-\infty}^{-z} e^{-u^2} du \]

This integral is equivalent to the complementary error function:

\[ \text{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_{z}^{\infty} e^{-u^2} du \approx 1 - \frac{2}{\sqrt{\pi}} \left( z - \frac{z^3}{3!} + \frac{z^5}{5!} + \frac{z^7}{7!} \ldots \right) \] for small values of \( z \)

since the function is symmetric, \( \int_{z}^{\infty} e^{-u^2} du = \int_{-\infty}^{-z} e^{-u^2} du \)

\[ N = \frac{10^9}{\sqrt{\pi}} \int_{-\infty}^{-z} e^{-u^2} du \approx \frac{10^9}{\sqrt{\pi}} \left[ \frac{\sqrt{\pi}}{2} - \left( z - \frac{z^3}{3!} + \frac{z^5}{5!} + \frac{z^7}{7!} \ldots \right) \right] \]

\[ N = \frac{10^9}{\sqrt{\pi}} \left[ \frac{\sqrt{\pi}}{2} - 0.53 \right] = 1.9 \times 10^8 \text{ molecules on the left} \]

only 19% of molecules stay on the left.
Stokes Drag at a Single Molecule Level

• ATP synthase is a rotary motor which turns 120° counterclockwise per ATP produced.
• To demonstrate the rotation of the enzyme, fluorescently tagged actin filament was attached to the F1 subunit. [http://www.youtube.com/watch?v=QeHCAFKaWM8](http://www.youtube.com/watch?v=QeHCAFKaWM8)
• Myosin V motor carries a micron-sized bead in optical trap experiments, demonstrating its ability to carry large vesicles and organelles.
• Viscous drag produced in these experiments is:
  \[ \zeta = 6\pi \eta R = 6\pi \times 10^{-3} \text{ Pa.s x 0.5 x 10}^{-6} \text{ m} \]
  \[ F_s = \zeta \cdot v_{\text{motor}} = 6\pi \times 10^{-3} \text{ Pa.s x 0.5 x 10}^{-6} \text{ m x 10}^{-6} \frac{m}{s} = 0.01 \text{ pN} \]

Drag force is small compared to force production of a single motor (2-6 pN)
Small Particles Remain in Suspension in Water

• Most proteins have slightly higher densities than water.
• Gravity pulls the object downward.
• Buoyant force reduces the effect of gravity.

\[ \nu_{\text{drift}} = \frac{F_{\text{net}}}{\zeta} \quad \text{where} \quad F_{\text{net}} = F_{\text{buoyant}} + F_{\text{gravity}} \]

\[ F_{\text{buoyant}} = (V_{\text{molecule}} \, \rho_{\text{water}})g \quad F_{\text{gravity}} = -(V_{\text{molecule}} \, \rho_{\text{molecule}})g \]

\[ F_{\text{net}} = -V_{\text{molecule}} \, (\rho_{\text{molecule}} - \rho_{\text{water}})g = -m_{\text{net}} \, g \]

\[ U(z) = -m_{\text{net}} \, gz \]

Thermal agitation will create a distribution of molecules at equilibrium.

\[ c(z) = c \, e^{-m_{\text{net}} \, gz/kT} \quad \text{(Boltzmann Distribution)} \]

For example: Myoglobin has \( m = 17000 \, \frac{g}{mole} \) and \( m_{\text{net}} = 0.25m \)

define scale height \( z_* = \frac{kT}{m_{\text{net}} \, g} \approx 59 \text{ meters} \)

\[ c(z) = c \, e^{-z/z_*} \] concentration at the top of a 4 cm test tube is equal to that of bottom.

The solution never settles out, makes a colloidal suspension.
Centrifugation

• While the molecules stay homogenously distributed under Earth’s gravity, they can be forced to sediment under centrifugal acceleration with many orders of magnitude of $g$.

The particle wants to move in a straight line (no acceleration).

The centripetal acceleration points toward the axis of rotation.

This force can only come from frictional drag force of the surrounding fluid.

Therefore, particle remains in solution, while slowly drifting towards the bottom of the tube.

Centrifugation artificially increases the gravity.

\[
F_C = -m\omega^2 r
\]

\[
F_{fr} = \zeta v_{drift} \quad \text{where} \quad \zeta = kT/D
\]

since \( F_{fr} = -F_C \), \quad \( v_{drift} = m\omega^2 rD/kT \)

\[
\text{drift flux:} \quad j_{drift} = -cv_{drift} = -cm\omega^2 rD/kT
\]
Sedimentation

Centrifugation can be used to separate particles with different sizes from each other.

At equilibrium, the flux \( j = 0 \).

\[
j = j_{\text{drift}} + j_{\text{diffusion}} = -D \left( \frac{cm \omega^2 r}{kT} + \frac{dc}{dr} \right) = 0
\]

\[
c(r) = \text{constant. } e^{-\frac{m \omega^2 r^2}{2kT}} \quad \text{(Sedimentation Equilibrium)}
\]

**Sedimentation Coefficient**

\[
s = \frac{v_{\text{drift}}}{g} = \frac{m_{\text{net}}}{\zeta} \quad \text{defines time required for a particle to reach terminal velocity}
\]

It is expressed in units of svedbergs, equals to \(10^{-13}\) seconds.

Small particles reach terminal velocity almost immediately, and slowly moves toward the bottom of the tube.
Separation of Molecules by Ultracentrifugation

- Under centrifugation, molecules both undergo diffusional motion and drifted motion.
- Each species of particles will have different $v_{drift}$ and $D$, depending its density and size.
- Width of the band of molecules will increase by diffusive law
  \[ \Delta x = \sqrt{2Dt} \]
- The center position of the band will be given by
  \[ x_c = v_{drift}t \]
- Since particle moves linearly with time, by dissipate by the square root of time, the method allows separation of molecules.
Separation of Molecules by Sucrose Gradient

- Solutions containing sucrose at different densities are layered on top of each other.
- High sucrose density at the bottom, low density is at the top of the tube.
- Ultracentrifugation allows molecules to drift towards the bottom of the tube.
- Once molecules reach to a layer whose density is equal to theirs, $v_{drift} = 0$
- Macromolecules with different mass densities separate into bands.
Viscosity of Fluids, revisited

- The response of a fluid to applied force is flow.
- If you rapidly pull a spoon from a jar of honey, the whole jar will come along.
- If you pull slowly, there will be little force resisting it.
- Viscosity is a mechanical property of a fluid, resisting motion.
- (Right) When you move one plate with force $F$, it shears the hypothetical layers of water.
- The force will create a linear velocity gradient from the top to the bottom plate.
- Velocity is equal to zero at the bottom plate surface.

http://www.youtube.com/watch?v=X4zd4Qpsbs8
http://www.youtube.com/watch?v=f2XQ97XHjVw
Shearing of Water

Shear Modulus of Solids

\[ \frac{F}{A} = G \frac{\Delta x}{l} \]  where \( G \) is the shear modulus.

Viscosity of Fluids

\[ \frac{F}{A} = \eta \frac{v}{d} \]  where \( \eta \) is the viscosity of a fluid.

- Solids shear under force and come to an equilibrium.
- Fluids flow under force.
- The unit of viscosity is \( \text{Pa.s} \)
- Velocity is inversely proportional to viscosity.
Laminar and Turbulent Flow

When a fluid encounters an obstacle, it flows the way around it.

If the viscosity of the fluid is high, and velocity is low, it will display a laminar flow.

In contrast, fluid with low viscosity forms turbulent flow at high velocity.

http://www.youtube.com/watch?v=pmnOgk2McvU
Reynolds Number

- Assume that motion of a small fluid element, a cube with a side length of \( l \), encounters an obstacle with a diameter of \( R \).
- To sidestep the sphere, fluid must undergo radial acceleration

\[
\alpha_R = \omega^2 R = \frac{v^2}{R}
\]

- Newton’s Law of motion says that

\[
F_{\text{net}} = F_{\text{friction}} + F_{\text{external}}
\]

\[
F_{\text{net}} = ma \quad \text{(inertial term)}
\]

\[
m = V\rho = l^3\rho
\]

\[
inertial \ term = l^3\rho v^2/R
\]
Reynolds Number

• To estimate the frictional force, we need to generalize Newtonian Fluid relation where the velocity of fluid is not uniform.

\[
\frac{F}{A} = \eta \frac{v}{d} \Rightarrow \frac{F}{A} = -\eta \frac{dv}{dx}
\]

\[A = l^2\]

• The net frictional force on a fluid is the force exerted above it, minus the force exerted below it.

\[f_{friction} = F(x) - F(x + l)\]

when \(l \to 0\), \(f_{friction} = -l \frac{dF}{dx} = \eta l^3 \frac{d^2v}{dx^2}\) (Taylor Series Expansion)

we estimate \(\frac{dv}{dx} = \frac{v}{R}\) and \(\frac{d^2v}{dx^2} = \frac{v}{R^2}\) (Uniform Circular Motion)

Therefore, friction term = \(\eta l^3 \frac{v}{R^2}\)
Reynolds Number

- The Reynolds number is the ratio of inertial and friction terms

\[ Re = \frac{\text{inertial term}}{\text{friction term}} = \frac{l^3 \rho v^2 / R}{\eta l^3 \frac{v}{R^2}} = \frac{\rho v R}{\eta} \]

Note that \( R \sim l \), length scale is similar to the size of the molecule.

- In other words, kinetic energy of a particle travelling with a velocity \( v \):

\[ KE \approx l^3 \rho v^2 \]

- Energy dissipated by viscous friction:

\[ W = \frac{\eta}{l} v l^2 \times l = \eta v l^2 \]

Viscous stress  Area  Distance traveled

- Ratio of these terms again give the Reynolds number.
The Life at Low Reynolds Number

• When $Re$ is small, friction term dominates.
• When $Re$ is large, inertial term dominates.
• In the low $Re$ world, momentum (or kinetic energy) is rapidly dissipated by friction.

• In other words, when a ship stops its engines, it still moves a long distance (due to its inertia) before it stops. 
• When a fish swims in water, friction has some effect on its motion. Fish can move a distance similar to its size without swimming before it stops completely. 
• When a bacteria stops its engines, it stops moving in 0.1 Å. Water acts like an intensely viscous environment.
Dissipative Time Scales and the Reynolds Number

• We can estimate the time to dissipate kinetic energy of the molecule in a fluid.

\[ \tau_{\text{viscous}} \approx \frac{K.E.}{\text{the power of friction}} = \frac{K.E.}{v \cdot F_{\text{friction}}} = \frac{l^3 \rho v^2}{\eta l^3 \frac{v^2}{R^2}} = \frac{\rho R^2}{\eta} \]

• Time it takes a molecule to move comparable to its size:

\[ \tau_{\text{inertia}} \approx \frac{l}{v} \]

• The ratio of these two terms again yields the Reynolds number \((R \sim l)\)

\[ Re = \frac{\rho vl}{\eta} \]
Dissipative Time Scales and the Reynolds Number

• Dissipation of kinetic energy by viscous drag:

\[ P = \frac{dE}{dt} \rightarrow F_s \cdot v \approx \frac{mv^2}{\tau_{viscous}} \rightarrow \tau_{viscous} = \frac{mv^2}{\zeta v \cdot v} = \frac{m}{\zeta} \]

• At times greater than \( \tau_{viscous} \), the inertial term can be dropped in above equation.

• Dependence of the velocity of the object on its initial velocity also drops out if viscous time scale is shorter than time it takes to travel a distance of \( x(0) \). Without bias, swimming objects lose their momentum within the dissipative timescale.

\[ \tau_{viscous} = \frac{mv^2}{\zeta v \cdot v} = \frac{m}{\zeta} \ll \frac{x_0}{v_0} \]
A block of mass $m$ slides along a horizontal surface lubricated with a thick oil which provides a drag force proportional to its velocity: $F_D = -\varsigma v$

a. If $v = v_0$ at $t = 0$, determine $v$ as a function of time.
b. Determine $x$ as function of time. Assume that $x = 0$ at $t = 0$.
c. Determine the maximum distance the block can travel.

\begin{align*}
\int \frac{-\varsigma}{m} dt &= \int \frac{dv}{v} \\
-\frac{\varsigma t}{m} &= \ln v + c \\
v(t) &= v_0 e^{-\frac{\varsigma t}{m}}
\end{align*}

\begin{align*}
\int dx &= \int v dt = \int v_0 e^{-\frac{\varsigma t}{m}} dt \\
x(t) &= c - \frac{m}{\varsigma} v_0 e^{-\frac{\varsigma t}{m}} \\
&\quad \text{and } x = 0 \text{ at } t = 0
\end{align*}

\begin{align*}
\Delta x_{max} &= \int_0^\infty v_0 e^{-\frac{\varsigma t}{m}} dt = \frac{m}{\varsigma} v_0
\end{align*}
Example: Swimming of Fish

\[ \rho_{fish} \approx 1 \frac{kg}{lt} \quad (similar \, to \, water) \]

\[ v_{fish} \approx 1 \, m/s \]

\[ l_{fish} \approx 10 \, cm \]

\[ \eta_{water} \approx 10^{-3} \, Pa. \, s \]

\[ \tau_{viscous} \approx \frac{\rho l^2}{\eta} = \frac{\left( \frac{1 \, kg}{10^{-3} \, m^3} \right) (10^{-1} \, m)^2}{10^{-3} \, kg \, \frac{m}{s^2} \frac{1}{m^2} \, s} = 10^4 \, s \]

\[ Re_{fish} = \frac{\rho vl}{\eta} = 10^5 \]

- Fish will stop moving on the order of 10000 seconds.
- Fish has a high Reynolds number.
Example: Swimming of *E. Coli*

\[ \rho_{Ecoli} \approx 1 \frac{kg}{lt} \text{ (similar to water)} \]

\[ \nu_{Ecoli} \approx 10 \ \mu m/s \]

\[ l_{Ecoli} \approx 1 \ \mu m \]

\[ \eta_{water} \approx 10^{-3} Pa.s \]

\[ \tau_{viscous} \approx \frac{\rho l^2}{\eta} = \left( \frac{1 \ kg}{10^{-3} \ m^3} \right) \left( 10^{-6} \ m \right)^2 = 10^{-6} s \]

\[ Re_{Ecoli} = \frac{\rho vl}{\eta} = 10^{-5} \]

- Bacteria will stop moving on the order of 1 microseconds.
- It will stop moving in 0.01 nm.
- Bacteria has a low Reynolds number.
- Viscosity of medium should be ten orders of magnitude higher than water, in order for fish to experience similar kinematic viscosity to *E.coli.*
How Do Small Organisms Swim?

• Suppose you flap a paddle, then bring it back to its original position by the same path.
  • *No net progress!*
• Reciprocal motion won’t work for swimming.
  • *It must be periodic so that it can be repeated.*
• Swimming cycle can be divided into two strokes that are time reversals of one another.
• Scallop model (three plates and two hinges) has been proposed to explain swimming motility of Spiroplasma.

http://www.youtube.com/watch?v=9b-NYvQTWYc

http://www.youtube.com/watch?v=hHSbdbQHk9M&list=PLF550BB0E03777E11
• *E. coli* possesses a 20 nm thick 10 μm long flagella.

• Flagellum is too thin to generate any reasonable amount of force to push it against the friction of water.

• *Instead, E. coli* rotates its flagellum at its base by a bacterial flagellar motor (utilizing proton motive force), to use its flagella as a propeller.

http://www.youtube.com/watch?v=hLTFiEKwFy8

http://www.youtube.com/watch?v=6bEacq-ow50
Bacterial Flagella Generates Net Force in Direction of Motion

- Tangential velocity per small section of flagellum experiences a drag force that resists its motion.
- Viscous drag coefficient for motion parallel to the axis is SMALLER than the one in perpendicular axis of motion.
- Therefore, force vector is not parallel to the velocity vector, and is closer to the perpendicular direction.
- $x$ and $y$ components of force cancel out (symmetry), but the one in $z$ does not.
$L = 10 \mu m$

$f = 100 \text{ Hz}$

$Pitch = 2 \mu m$

$D = 0.5 \mu m$

take a small segment of length $l$, which has angle $\theta$ with respect to the z axis

$v = \omega R = \pi D f$

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

$S_{\text{parallel}} = 2\pi \eta l$

$S_{\text{perpendicular}} = 4\pi \eta l$

$F_{\text{parallel}} = -S_{\text{parallel}} \, v \sin \theta$

$F_{\text{perpendicular}} = S_{\text{perpendicular}} \, v \cos \theta$

$z$ components of each forces are:

$F_{\text{parallel}} -z = F_{\text{parallel}} \cos \theta = -2\pi \eta lv \cos \theta \sin \theta$

$F_{\text{perpendicular}} -z = F_{\text{perpendicular}} \sin \theta = 4\pi \eta lv \cos \theta \sin \theta$

$F_z = F_{\text{parallel}} -z + F_{\text{perpendicular}} -z = 2\pi \eta lv \cos \theta \sin \theta$
each segment \( \left( N = \frac{L}{l} \right) \) has the same angle with respect to the z axis

\[
F_{\text{flagella}} = \frac{L}{l} F_z = 2\pi \eta L v \cos \theta \sin \theta
\]

if the bacteria is travelling with a velocity of \( V \), it will experience \( F_D = -2\pi \eta L V \)

To cruise at constant speed, \( F_{\text{net}} = F_{\text{flagella}} + F_D = 0 \)

\[
2\pi \eta L v \cos \theta \sin \theta = 2\pi \eta L V
\]

\[
V = \pi D f \cos \theta \sin \theta
\]

- velocity of bacteria is 30 \( \mu \)m/sec.
- Why does bacteria swim? If the food is plenty, diffusion is sufficient to feed the bacteria.
- It is only relevant, when diffusion takes much longer, or food is rare.
- Bacteria moves in a straight line, pauses, and takes off in a new random direction.
- While swimming, cell continuously sample the environment for rich nutrients.
- Biased random walk. http://www.youtube.com/watch?v=N2M_82mArXk
Ciliary Beating

• 5-10 μm long, 200 nm thick.
• Has sufficient thickness to generate significant amount of force.
• Powerstroke is in perpendicular axis to cell surface
• Recovery stroke is in parallel axis.

http://www.youtube.com/watch?v=BbI47I2nbDQ
Eukaryotic Flagella

http://www.youtube.com/watch?v=C_N-_v2cYjY

http://www.youtube.com/watch?v=0xo77Q09Brc