ENTROPY IN BIOLOGY

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Lecture 6: Rotary Motors Driven by Transmembrane Ionic Currents

Rotary motors driven by transmembrane ionic currents

There are two rotary motors in biology: ATP synthase, and the bacterial flagellar motor. Both span membranes and are driven by transmembrane ionic currents. The ions flow through multiple channels that are arranged in a symmetrical array around the part of the motor that rotates, which is called the rotor. The ion channels run parallel to the axis of rotation.

For this arrangement to produce rotation, it is necessary that the rotor carry fixed charges with something like helical symmetry, so that the ions as they flow across the membrane can interact with these charges in much the same way as fluid interacts with the blades of a turbine to produce rotation.

Here, we consider an idealized model of such a motor.

The rotor is an infinitely long cylinder of radius r. It carries a fixed, negative surface charge density with helical symmetry.

The ions that drive the motor each have charge $+q$. Instead of being confined to discrete channels, they flow on the surface of a cylinder that is co-axial with the rotor and only slightly larger than the rotor, so that the two surfaces may be regarded as coincident.

The existence of the channels in the real motor is modeled here by constraining the ions to move in the z-direction only.

The ions move according to the drift-diffusion equation, but they are also constrained by electroneutrality to balance the charge distribution on the rotor. These conditions together determine the form of the electrostatic potential.

The governing equations are (1-4), see next page.

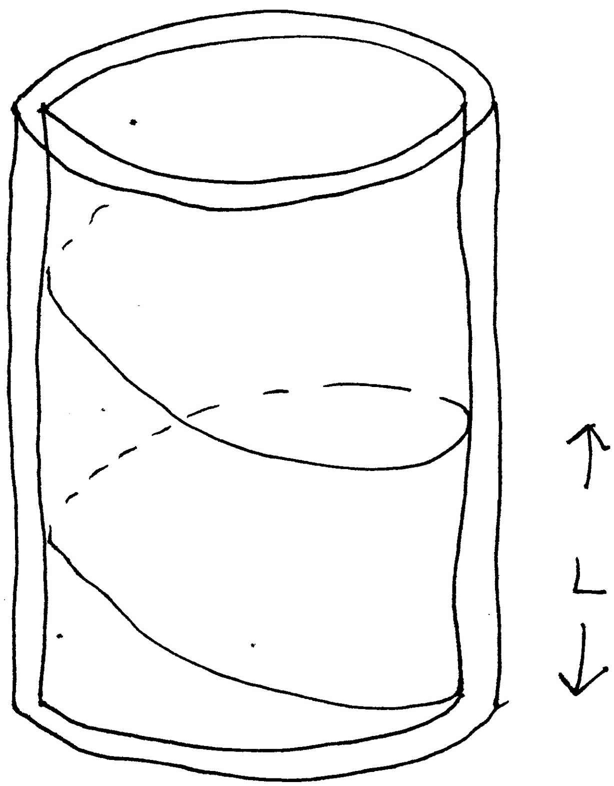
Equation (1) describes the charge distribution on the rotor, with its helical symmetry.

ω is the angular velocity of rotation, positive clockwise. Here and throughout, the words "clockwise" and "counterclockwise" refer to the view from above, looking down the z axis.

Equation (2) is the condition of electroneutrality, with σ as the charge density of the ions

Equation (3) is continuity equation for the ions, with J as the current density in the z direction. (Note the units:
$\sigma \sim$ charge/area, $J \sim$ current/length)

Equation (4) is the drift-diffusion equation for ions of charge $+q$ (expressed here ~~as~~ in terms of current density and charge density instead of flux and concentration.)



(1) $$\sigma_0 = -f\left(\theta + \omega t + 2\pi \frac{z}{L}\right)$$

where $f(\theta + 2\pi) = f(\theta) > 0$

(2) $$\sigma = -\sigma_0 = f\left(\theta + \omega t + 2\pi \frac{z}{L}\right)$$

(3) $$\frac{\partial \sigma}{\partial t} + \frac{\partial J}{\partial z} = 0$$

(4) $$J = -D\left(\frac{\partial \sigma}{\partial z} + \frac{q}{b}\frac{\sigma}{kT}\frac{\partial \phi}{\partial z}\right)$$

let

(5) $$\frac{\partial\phi}{\partial z} = E\left(\theta + \omega t + \frac{2\pi z}{L}\right)$$

with $E(\theta + 2\pi) = E(\theta)$. Then E is the z component of the electric field, positive downward

(6) $$J = -D\left(\frac{2\pi}{L} f' + \frac{q}{kT} f E\right)$$

(7) $$\frac{\partial J}{\partial z} = -\left(\frac{2\pi}{L}\right) D \left(\frac{2\pi}{L} f'' + \frac{q}{kT}(fE)'\right)$$

(8) $$0 = \frac{\partial \sigma}{\partial t} + \frac{\partial J}{\partial z}$$

$$= \omega f' - \left(\frac{2\pi}{L}\right) D \left(\frac{2\pi}{L} f'' + \frac{q}{kT}(fE)'\right)$$

Integration of the above equation gives

(9) $$C = \omega f - \frac{2\pi}{L} D\left(\frac{2\pi}{L} f' + \frac{q}{kT} f E\right)$$

and this can be divided by f (recall $f > 0$):

(10) $$C f^{-1} = \omega - \left(\frac{2\pi}{L}\right) D\left(\frac{2\pi}{L}\left(\frac{f'}{f}\right) + \frac{qE}{kT}\right)$$

Let

(11) $$\overline{E} = \frac{1}{2\pi}\int_0^{2\pi} E(\theta)\, d\theta$$

$$= \frac{1}{2\pi}\int_0^{L} E\left(\frac{2\pi z}{L}\right) \frac{2\pi}{L} dz$$

$$= \frac{1}{L}\int_0^{L} E\left(\frac{2\pi z}{L}\right) dz$$

$$= \frac{1}{L}\int_0^{L} E\left(\theta + \omega t + \frac{2\pi z}{L}\right) dz$$

We can express G in terms of $\overline{E}$ by integrating both sides of (10) over $(0, 2\pi)$:

(12) $$G \int_0^{2\pi} f^{-1}(\theta)\,d\theta = 2\pi\omega - \frac{2\pi}{L} D \frac{q}{kT} 2\pi \overline{E}$$

Let

(13) $$f_H = \frac{2\pi}{\int_0^{2\pi} f^{-1}(\theta)\,d\theta} = \frac{1}{\frac{1}{2\pi}\int_0^{2\pi} f^{-1}(\theta)\,d\theta}$$

so that f_H is the harmonic mean of f.
Then

(14) $$G = \left(\omega - \frac{2\pi}{L} D \frac{q\overline{E}}{kT}\right) f_H$$

In the following, we regard $\overline{E}$ as a given parameter, and this equation determines G in terms of $\overline{E}$ and ω.

Next, we evaluate the current I, positive <u>downwards</u>.

(15) $$I = -\int_0^{2\pi} J \, r \, d\theta$$

$$= r\int_0^{2\pi} D\left(\frac{2\pi}{L} f' + \frac{q}{kT} f E\right) d\theta$$

$$= r \int_0^{2\pi} D \frac{q}{kT}(fE) \, d\theta$$

Integrating both sides of (9) over $(0, 2\pi)$, we get

(16) $$2\pi C = 2\pi w \bar{f} - \frac{2\pi}{L} \int_0^{2\pi} D \frac{q}{kT}(fE) \, d\theta$$

where

(17) $$\bar{f} = \frac{1}{2\pi} \int_0^{2\pi} f \, d\theta$$

Therefore

(18) $$I = rL\left(\omega \bar{f} - C\right)$$

$$= rL\,\omega\left(\bar{f} - f_H\right) + 2\pi r \frac{D}{kT} q \bar{E} f_H$$

The units are correct here, since

(19) $$I \sim \frac{\text{charge}}{\text{time}}$$

(20) $$\bar{f},\ f_H \sim \frac{\text{charge}}{\text{area}}$$

(21) $$r,\ L \sim \text{length}$$

(22) $$\frac{D}{kT} q \tilde{E} \sim \text{velocity}$$

(23) $$\omega \sim \frac{1}{\text{time}}$$

We claim that

(24) $$f_H \leq \overline{f}$$

with equality only if f is constant.

To prove this, we use the Schwarz inequality, as follows:

(25) $$2\pi = \int_0^{2\pi} f^{1/2} f^{-1/2}\, d\theta$$

$$\leq \left(\int_0^{2\pi} f\, d\theta\right)^{1/2} \left(\int_0^{2\pi} f^{-1}\, d\theta\right)^{1/2}$$

Squaring both sides and then dividing by $(2\pi)^2$ gives

(26) $$1 \leq \frac{1}{2\pi}\int_0^{2\pi} f\, d\theta \quad \frac{1}{2\pi}\int_0^{2\pi} f^{-1}\, d\theta$$

$$= \overline{f} / f_H$$

which is equivalent to (24)

We have equality in the foregoing only if

$$f^{1/2}(\theta) = c\, f^{-1/2}(\theta) \tag{27}$$

for some constant c, and this is equivalent to

$$f(\theta) = c \tag{28}$$

It makes sense that the coupling coefficient between I and ω in (18) always has the same sign (and that this sign is positive with the various choices of sign that we have made), and of course it also makes sense that this coefficient vanishes when the charge density on the rotor is uniform.

Our next task is to evaluate the torque per unit length acting on the rotor, and for this we need the θ component of the electric field, which is evaluated from $\partial\phi/\partial\theta$. We have to be careful here because ϕ by itself is not merely a function of $\theta + \omega t + \frac{2\pi}{L}z$. Instead, we assume that

(29) $$\phi(\theta, t, z) = \Phi\left(\theta + \omega t + \frac{2\pi}{L}z\right) + \bar{E}z$$

Differentiating both sides of this equation with respect to z, and making use of equation (5), we get

(30) $$E\left(\theta + \omega t + \frac{2\pi}{L}z\right) = \frac{2\pi}{L}\Phi'\left(\theta + \omega t + \frac{2\pi}{L}z\right) + \bar{E}$$

Now we can replace $\theta + \omega t + \frac{2\pi}{L}z$ by θ and rearrange (30) to read

(31) $$\frac{2\pi}{L}\Phi'(\theta) = E(\theta) - \bar{E}$$

Since $E(\theta)$ and $\bar{E}$ are known, see equations (10) & (14), and recall that we are regarding $\bar{E}$ as known, equation (31) determines Φ and therefore ϕ up to an arbitrary constant. By integration on both sides of (31) over an interval of the form $(\theta, \theta+2\pi)$, we see that

(32) $$\Phi(\theta+2\pi) = \Phi(\theta)$$

From (29) & (31), we immediately get a formula for the θ component of the electric field, as follows

(33) $$-\frac{1}{r}\frac{\partial \phi}{\partial \theta}(\theta,t,z) = -\frac{1}{r}\Phi'\left(\theta+\omega t+\frac{2\pi}{L}z\right)$$

$$= -\left(\frac{L}{2\pi r}\right)\left(E\left(\theta+\omega t+\frac{2\pi}{L}z\right)-\bar{E}\right)$$

Let τ be the torque per unit length*, counterclockwise positive, applied by the electric field to the rotor. This is the same as the torque per unit length, clockwise positive that must be applied by an external agent to maintain the steady state.

*the units of torque/length are those of force.

Then τ is given by

(34) $$\tau = r\int_0^{2\pi}\left(-\frac{1}{r}\frac{\partial\phi}{\partial\theta}(\theta,t,z)\right)\left(-f\left(\theta+\omega t+\frac{2\pi}{L}z\right)\right) r\,d\theta$$

$$= \frac{rL}{2\pi}\int_0^{2\pi}\left(E(\theta)-\bar{E}\right) f(\theta)\,d\theta$$

$$= \frac{rL}{2\pi}\int_0^{2\pi} E(\theta)f(\theta)\,d\theta - rL\bar{E}\bar{f}$$

$$= \frac{L}{2\pi}\,\frac{I}{D\left(\frac{g}{kT}\right)} - rL\bar{E}\bar{f}$$

See equation (15). Thus, we can express I in terms of τ and $\bar{E}$ as follows:

(35) $$I = g\left(\frac{D}{kT}\right)\frac{2\pi}{L}\left(\tau + rL\bar{f}\bar{E}\right)$$

$$= g\left(\frac{D}{kT}\right)\left(\frac{2\pi}{L}\tau + 2\pi r\bar{f}\bar{E}\right)$$

We can similarly express ω in terms of τ and $\bar{E}$ by solving (18) for ω and then using (35) to eliminate I:

(36) $$\omega = \frac{I - 2\pi r g \frac{D}{kT} f_H \bar{E}}{rL(\bar{f} - f_H)}$$

$$= \frac{g\left(\frac{D}{kT}\right)\left(\frac{2\pi}{L}\tau + 2\pi r(\bar{f} - f_H)\bar{E}\right)}{rL(\bar{f} - f_H)}$$

$$= \frac{g\left(\frac{D}{kT}\right) 2\pi}{rL^2(\bar{f} - f_H)}\tau + g\left(\frac{D}{kT}\right)\frac{2\pi}{L}\bar{E}$$

Equations (35-36) can be summarized in matrix form:

(37) $$\begin{pmatrix} \omega \\ I \end{pmatrix} = g\left(\frac{D}{kT}\right)\left(\frac{2\pi}{L}\right)\begin{pmatrix} \frac{1}{rL(\bar{f} - f_H)} & 1 \\ 1 & rL\bar{f} \end{pmatrix}\begin{pmatrix} \tau \\ \bar{E} \end{pmatrix}$$

The symmetry of this matrix is an Onsager relation.