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Information Flow to Dissipate an Ionic Fluctuation through a Membrane Channel

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The flux of information that a hypothetical system on a cell membrane would have to process in order to dissipate an ionic fluctuation in the solution through a membrane channel is calculated on the basis of nonequilibrium thermodynamics. The developed formula contemplates the relative size and initial relaxation time of the fluctuation, the concentration of the solution, and the size of the ionic channel. It is found that for a wide range of biological concentrations this flux is on the order of 1 Mbit/s for a 10% fluctuation. © 1996 Academic Press, Inc.

Key Words: **information flow; ionic fluctuation; channel transport.**

INTRODUCTION

When a fluctuation occurs, a local order is established and a knowledge (for example number of particles) of this local molecular system can be attained by a device able to process information faster than the relaxation time of the fluctuation.

The objective of this paper is to estimate, without entering into the mechanisms of the process (see Refs. (1) and (2) for possible mechanisms), the ‘‘minimum’’ flow of information (bit/s) a device would have to process in order to dissipate an ionic fluctuation in a solution through a channel of the size of a biological channel, and to compare this result with some of the already existent man-made devices.

In doing so we make use of the relation between entropy production and information lost (bit/s) when a fluctuation is dissipating in a volume of the size of a biological channel. Of course, the device would have to process information in a faster way in order to decide whether this fluctuation could be utilized by a cell or not. Procopio and Fornés (3) analyzed the possibility that naturally occurring ionic fluctuations could be utilized by a cell membrane system to create a transient ionic flow, and eventually to produce ion concentration gradients across the membrane. It was found that there is a broad range of concentrations for which significant fluctuations take place in enclosing volumes having diameters comparable to the membrane thickness. In these cases, the dissipation of a fluctuation close to the membrane could result in a transient net flow of the corresponding ionic species through the channel. In order for a channel to correlate its state of aperture to the phase of a nearby ion density fluctuation, a flow of information is required by the second law of thermodynamics (Brillouin (4) and Bennett (1)). Molecular entities such as biological channels, ‘‘carriers,’’ and eventually ATPases may be important molecular devices for an efficient processing of information in the form of fast conformational changes. Such structures are in principle capable of performing the coupling of fluctuating parameters such as concentration or density to fast molecular conformational changes. Studies employing various techniques have shown (5) that channel proteins experience important conformational changes in response to binding or proximity of ions, and also (5) that computer simulations of internal motions of proteins can be carried out for time periods of the order of a few hundred ps. Our calculation is a first step in the quantification of the process, showing the possibility of its existence.

THEORY

We consider here an ionic channel placed along the x axis at a distance d from the origin (see Fig. 1). The entropy production (J/K·m^3·s) while an ionic species a is being dissipated in the solution at the neighborhood of the channel mouth was given by Fornés (6) as

$$\sigma_a = Q[(x-d)^2 + y^2 + z^2] \times \exp\left[-\frac{(x-d)^2 + y^2 + z^2}{2D_a(t+\tau_0)}\right], \quad [1]$$

where Q is given by

$$Q = \frac{RK_a c_a \nu_a \tau_0^3 \epsilon^2}{4M_a D_a (t+\tau_0)^5}, \quad [2]$$

with K_a given by

$$K_a = 1 - \frac{e^3}{2\epsilon_{\mathrm{m}}^{3/2}}\left[\frac{N_{\mathrm{A}}\pi}{(kT)^3}\right]^{1/2} z_a^4 \left(\sum_a c_a z_a^2\right)^{-1/2}, \quad [3]$$

where c_a is the concentration in moles/m^3, N_A is the Avogadro number, ν_a is the number of ions of type a in one molecule of the electrolyte, z_a is its corresponding valence, ϵ_m is the dielectric constant of the medium, e is the elementary charge (esu), T the absolute temperature, k is the Boltzmann constant, R is the gas constant, M_a is the atomic weight of the ion a, τ_0 is the initial relaxation time of the fluctuation, D_a is the diffusion coefficient, and $\epsilon = \delta c_a / c_a$ is the relative amplitude of the fluctuation. For a symmetrical monovalent electrolyte of concentration c, Eq. [3] transforms to

$$K_a = 1 - \frac{e^3 (N_A \pi)^{1/2}}{(2\epsilon_m kT)^{3/2}} c^{-1/2}. \qquad [4]$$

Then the rate at which entropy is being created inside the channel (J/K·s) will be given by

$$\sigma'_{a,\mathrm{ch}} = Q \int_d^{l+d} \int_0^r [(x-d)^2 + \rho^2] \times \exp\left[- \frac{(x-d)^2 + \rho^2}{2D_a(t+\tau_0)} \right] 2\pi\rho d\rho dx, \qquad [5]$$

where l is the channel length and r the channel radius. After performing the integrations in Eq. [5] we obtain

$$\sigma'_{a,\mathrm{ch}} = \frac{c_a \nu_a f_a^5 D_a^4 K_a}{M_a} 2^2 \pi \tau_0^3 \epsilon^2 R [\sqrt{\pi} \mathrm{erf}(f_a l) \times \left[\exp(-(rf_a)^2) \left[\frac{1}{2} + (rf_a)^2 \right] + \frac{3}{2} \right] - (lf_a) \exp(-(lf_a)^2)[1 - \exp(-(rf_a)^2)]], \qquad [6]$$

where $f_a = [2D_a(t + \tau_0)]^{-1/2}$ and erf is the error function defined as $\mathrm{erf}(u) = (2/\sqrt{\pi}) \int_0^u \exp(-x^2) dx$. In order to ensure the fluctuation will dissipate inside the channel we chose $\tau_0 = l^2/(2D_a)$ in Eq. [6]. The mean rate of which entropy is produced inside the channel by the ionic species a will be

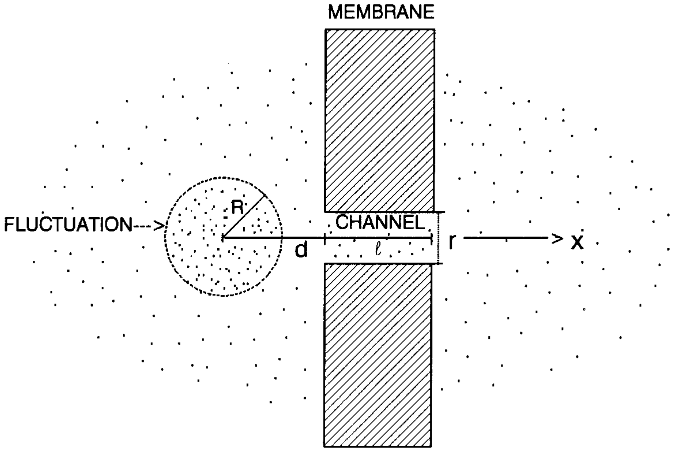

FIG. 1. Ionic fluctuation close to a membrane channel.

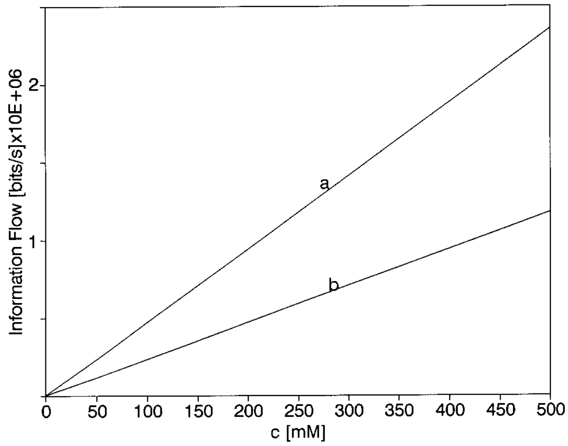

FIG. 2. Information flow to dissipate an ionic fluctuation ($\epsilon = 0.1$) through a membrane channel. Na$^+$ ion from a symmetrical monovalent electrolyte ($D_{Na^+} = 1.33 \times 10^{-9}$ m^2/s) at room temperature (298 K). (a) $\tau_0 = 9.38 \times 10^{-9}$ s (channel size: r = 5 Å, l = 50 Å); (b) $\tau_0 = 2.34 \times 10^{-9}$ s (channel size: r = 5 Å, l = 25 Å).

$$\overline{\sigma}'_{a,\mathrm{ch}} = \frac{1}{\tau_0} \int_0^{\tau_0} \sigma'_{a,\mathrm{ch}}(l, t) dt, \qquad [7]$$

where $\sigma'_{a,\mathrm{ch}}(l, t)$ denotes the right hand member of Eq. [6].

As a consequence of this dissipation, information is lost at a mean rate (bits/s) given by (see Morowitz (7))

$$\overline{I}_{a,\mathrm{ch}} = \frac{\overline{\sigma}'_{a,\mathrm{ch}}}{k \ln 2}. \qquad [8]$$

So, if a system exists in the channel capable of coupling fluctuations in concentration to fast molecular conformational changes, it will have at least to be able to process the information given by Eq. [8].

To calculate the error function in Eq. [6] we used the subroutines erf, gser, gcf, gammln, and gammp, and to perform the integration in Eq. [7] we used the subroutines qsimp and trapzd (see Press *et al.* (8) for details).

CONCLUSION

In Fig. 2, $\overline{I}_{a,\mathrm{ch}}$ is shown as a function of c_a, for given values of ϵ, and τ_0 for Na$^+$ ion from a symmetrical monovalent electrolyte at room temperature (298 K). We can observe that for common values of biological concentrations, if this system exists, it will have to process information at a rate of about 10^6 bits/s for a fluctuation with $\epsilon = 0.1$. This value is not large as compared with some of the already existent man-made ones which process information at a rate of 10^{10} bit/s (Peled (9)).

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