Available online at www.sciencedirect.com
ScienceDirect
J. Biochem. Biophys. Methods 70 (2007) 525–530
JOURNAL OF biochemical and biophysical methods
www.elsevier.com/locate/jbbm

# Calculation of transmission coefficients for some permeant molecules in human red cell and resting axolemma squid axon membranes

S.G. Elkomoss [a], A. Pape [b,*]

[a] ULP – UFR de Sciences Physiques, 3-5 Rue de l'Université, 67084 Strasbourg Cedex 2, France
[b] IPHC – UMR 7178 – CNRS – IN2P3/ULP, 23 Rue du Loess, BP 28, F – 67037 Strasbourg Cedex 2, France

Received 22 February 2006; received in revised form 18 July 2006; accepted 14 August 2006

**Abstract**

Quantum mechanical calculations of transmission coefficients for some permeant molecules across the human red cell and resting axolemma squid axon membranes are carried out. The calculations depend on (i) the molecular weight of the molecule and (ii) the depth and width of the potential well of the membrane. In most cases good agreement between calculated and experimental values is found.


*Keywords:* Potential well; Potential barrier; Quantum mechanics; Transmission coefficient; Human red cell; Resting axolemma squid axon

## 1. Introduction

In a thermodynamic treatment, Staverman [1,2] recognized that the reflection coefficient $\sigma$ is an adequate measure of membrane selectivity. When $\sigma = 1$ all the solute is reflected from a membrane, while $\sigma < 1$ means that some of the solute molecules penetrate [3]. The value of $\sigma$ depends on the particular membrane and solute molecule [1,2,4]. For the membranes considered here, the membrane potential [5] is negative (−ve) under physiological conditions. At low ionic strength or excitation, the potential corresponding to other membranes can be positive (+ve). For the simplest one-dimensional case in quantum mechanics (QM), the (−ve) and (+ve) membrane potentials can be represented, respectively, by a rectangular well of finite depth $-V_0$ and a potential barrier of finite height $+V_0$, both with thickness $\delta = 2a$ as shown in Fig. 1. These potentials are treated theoretically in many QM books where one can see that the mathematical development of the two cases is not the same [6–12]. In Fig. 1a the potential is less than that of its surroundings and consequently is attractive while that of Fig. 1b is repulsive. In thermodynamic analysis of biological systems, the negative and positive potentials are both considered indifferently as barriers. Only Danielli [13] has proposed the use of separate potentials in thermodynamic analysis, one of which is somewhat similar to that of Fig. 1a with the difference that his potential applies to molecules such as benzene and propane. Meanwhile, diffusion of non-electrolytes within biological membranes closely resembles diffusion in polymers [14].

In the present report, the red cell and resting axolemma squid axon membranes with a potential well are considered. A particle incident from the left in Fig. 1a is either totally reflected ($\sigma = 1$) or partially transmitted ($\sigma < 1$). In these cases, $\sigma$ has the same meaning and some dependence on the potential as Staverman and others [1–5] have proposed. Once more due to Danielli [13], the membrane can be regarded as constituting the only significant obstacle to diffusion. It is then interesting to carry out QM calculations of the transmission coefficient $T = 1 - \sigma$ for permeant molecules across the potential well and compare the result with experimental values. In these calculations, $T$ depends on the depth of the potential well, its width and the mass of the incident molecule. Consequently, one can get a better idea about the separate role played by the membrane potential and its selectivity in QM. The molecules treated here are formamide, *N*-methylformamide, acetamide, urea, ethylene glycol, *N*-methylacetamide, propionamide, methylurea, thiourea, 1,1-dimethylurea, ethylurea, 1,3-dimethylurea, glycerol

* Corresponding author.
*E-mail addresses:* sabry.elkomoss@laposte.net (S.G. Elkomoss), pape@in2p3.fr (A. Pape).

0165-022X/$ - see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.jbbm.2006.08.004

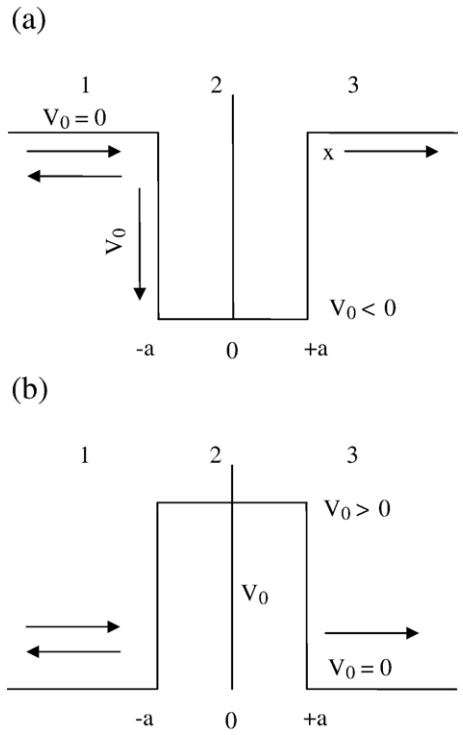


Fig. 1. Rectangular potential well of finite depth (a) and potential barrier of finite height (b), showing the three regions 1, 2 and 3 of integration.

and malonamide for the human red cell. For the resting axolemma squid axon, methanol, formamide, ethanol, urea, ethylene glycol, propionamide, methylurea, glycerol and malonamide molecules are considered. In most of these cases, the $T_{calc}$ are in excellent agreement with the experimental values $T_{exp}$ [15–24], particularly for the resting axolemma squid axon.

## 2. Calculations

### 2.1. Transmission coefficient $T_{calc}$

The potential of Fig. 1a has been treated mathematically by many authors in more or less detail [6–12]. Here the procedure developed in [8] has been used because of its clarity and simplicity. When $V_0$ is negative, the wave functions which are solutions to the Schrödinger equations in the three regions 1, 2 and 3 (Fig. 1a) for a particle of mass $m$ incident from the left are:

$$\varphi_1 = D\exp(ixp_1/\hbar) + F\exp(-ixp_1/\hbar) \qquad x<-a \tag{1}$$

$$\varphi_2 = B\exp(ixp_2/\hbar) + C\exp(-ixp_2/\hbar) \qquad -a<x<a \tag{2}$$

$$\varphi_3 = A\exp(ixp_1/\hbar) \qquad x>a \tag{3}$$

$$\text{where} \quad p_1 = (2mE)^{1/2} \quad \text{and} \quad p_2 = [2m(E+V_0)]^{1/2}. \tag{4}$$

The constants $D$, $F$ and $A$ represent, respectively, the amplitudes of the incident, reflected and transmitted waves. The reflection $\sigma$ and transmission $T$ coefficients are given by the absolute values of the squares of $F/D$ and $A/D$, respectively. The boundary conditions for $\varphi$ and $d\varphi/dx$ being continuous at $x=a$ and $x=-a$ determine these constants and hence $\sigma$ and $T$, keeping in mind that $\sigma+T=1$. Following the same procedure as in [8], one obtains the expression for the transmissivity $T_{calc}$:

$$T_{calc} = 1/[1 + (1/4)(p_1/p_2 - p_2/p_1)^2 \sin^2(2p_2\ a/\hbar)] \tag{5}$$

which is the same as Eq. (6.63) of [8] after some mathematical transformation.

### 2.2. Bound states

The wave functions $\varphi$ corresponding to eigenvalues of the bound states in the region where $x>a$ must be finite as $x$ tends to $+\infty$. They decrease as $x$ increases. Thus:

$$\varphi = A\exp(-x\ p_1/\hbar) \qquad \text{with} \quad p_1 = (2m|E|)^{1/2} \tag{6}$$

where $E$ is the energy of the bound state which is negative. This means that $E=-|E|$. Inside the square well the wave function is:

$$\varphi = B\exp(ixp_2/\hbar) + C\exp(-ixp_2/\hbar) \quad \text{where} \quad p_2 = [2m(V_0-|E|)]^{1/2}. \tag{7}$$

Continuity at $x=a$ determines the constants $B$ and $C$ in terms of $A$. For $x=-a$, the solution is the exponential function $\varphi=D\exp(xp_1/\hbar)$ that decreases as $x$ tends to $-\infty$. Since it is convenient to place the origin of the $x$-axis at the center of the potential well, one has two classes of solutions, symmetric and antisymmetric. Using the boundary conditions at $x=-a$ and after some manipulation, one gets:

$$[|E|/(V_0-|E|)]^{1/2} = \begin{cases} \tan[(2m(V_0-|E|))^{1/2}(a/\hbar)] & \text{symmetric} \\ -\cot[(2m(V_0-|E|))^{1/2}(a/\hbar)] & \text{antisymmetric} \end{cases} \tag{8}$$

Replacing $|E|$ by $-E$ in Eq. (8) gives exactly Eq. (6.49) of [8]. Up to this stage, the procedure of [8] has been followed. Eq. (8) can be solved graphically or numerically. Most authors [6–12] have employed different graphical methods even though a graphical solution is approximate. Since the problem treated here is quite sensitive to the values of $V_0$ and $\delta$, a better result is obtained numerically.

Squaring both sides of Eq. (8), one gets:

$$[|E|/(V_0-|E|)] = \begin{cases} \tan^2[(2m(V_0-|E|))^{1/2}(a/\hbar)] & \text{symmetric} \\ \cot^2[(2m(V_0-|E|))^{1/2}(a/\hbar)] & \text{antisymmetric} \end{cases} \tag{9}$$

The numerical solution of this equation gives the eigenvalues of $|E|$ corresponding to the bound states inside the well. The number of these bound states depends on the values of $V_0$ and $\delta$. Using this value of $|E|$ in Eq. (5), one gets the best agreement between $T_{calc}$ and $T_{exp}$. The values of $|E|$ are determined such that the difference between the left- and right-hand sides of