Eur Biophys J (1988) 16: 255–257

European Biophysics Journal

The different screening of electric charges and dipoles near a dielectric interface

D. T. Edmonds

The Clarendon Laboratory, Parks Road, Oxford OX1 3PU, United Kingdom

Received July 3, 1987 / Accepted in revised form July 7, 1988

Abstract. The electric fields within a planar slab of material due to both charges and dipoles within the slab and near to its surface are simply calculated using the method of images. If the slab is immersed in a fluid of high dielectric constant the electric field within the slab due to the charge is always reduced but that of a suitably oriented electric dipole is enhanced by as much as a factor of two.

Key words: Electric fields, dielectrics, electric dipoles

Introduction

The important role played by electrostatic forces in biological structure and function is now widely recognized and calculations have been performed for a wide variety of systems as may be seen in a recent review article such as Honig et al. (1986). Effects studied include the possible influence of the large electric dipole moment of the alpha-helix (Hol 1985), the possible effects of electrostatic interactions on enzyme action (Warshel and Levitt 1976; Warwicker and Watson 1982), the possible role of electrostatics on protein stabilization (Fried et al. 1981), the effects of surrounding solvent on electrostatic interactions in globular proteins (Rogers and Sternberg 1984; Gilson et al. 1985) and alternative electrostatic models for gated ion channels, counterports and pumps (Edmonds 1986, 1987).

This short note draws attention to an interesting contrast in the effects of the high dielectric constant fluid surrounding a membrane on the electric fields within the membrane generated by charges on the one hand and electric dipoles on the other which lie within the membrane and close to its surface. The field of the dipole may be enhanced by a factor approaching 2 while that of the charge is much diminished.

Consider a plane interface between a region 1 of relative dielectric constant ε_1 and region 2 of relative dielectric constant ε_2 as shown in Fig. 1 a. The electric field at any point $F(X, Y, Z)$ within the region 1 $(Z > 0)$ due to a single charge q situated within region 2 $(Z < 0)$ may by calculated exactly using the method of images (Smythe 1939) by removing the interface so that all space has a dielectric constant ε_1 and then replacing q by a charge q_2 such that $q_2 = q(2\varepsilon_1)/(\varepsilon_1 + \varepsilon_2)$, as illustrated in Fig. 1 b. Similarly, when the original charge is situated within region 1 the field at any point $F(X, Y, Z)$ within region 1 is obtained by removing the interface such that all space has a dielectric constant ε_1 and placing a second charge q_1 at the position that is the mirror image of q in the original interface. The value of q_1 is given by

$$q_1 = q(\varepsilon_1 - \varepsilon_2)/(\varepsilon_1 + \varepsilon_2).$$

By decomposing an electric dipole into a positive and a negative charge of the same magnitude close together it is possible to calculate in a like manner the field at any point $F(X, Y, Z)$ within region 1 due to an

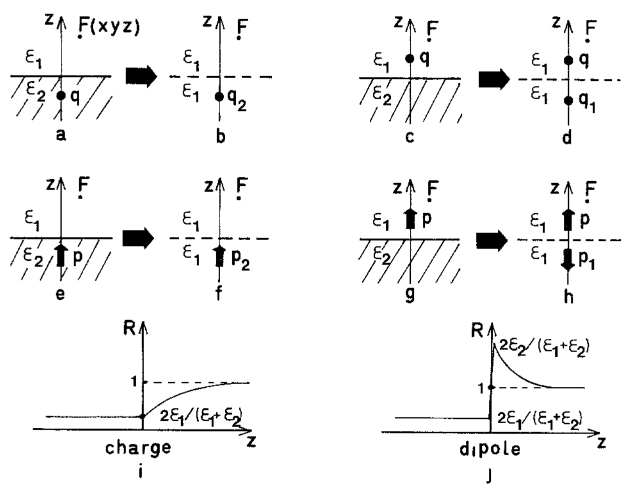

Fig. 1

electric dipole p near the interface. When the dipole is situated in region 2 oriented as in Fig. 1 a the field in region 1 is obtained by removing the interface and replacing the dipole p by one of strength p_2 as in Fig. 1 f. Similarly when the original dipole is situated in region 1 as sketched in Fig. 1 g the field within region 1 is obtained by removing the interface and adding to dipole p a second image dipole p_1 as in Fig. 1 h. Note that the imaging process reverses the direction of the image dipole in this case. The strengths of p_1 and p_2 are given by

$$p_1 = p(\varepsilon_1 - \varepsilon_2)/(\varepsilon_1 - \varepsilon_2); \quad p_2 = p(2\,\varepsilon_1)/(\varepsilon_1 + \varepsilon_2).$$

All these effects are due to the charges induced at the interface by the electric field of the charge or dipole. The effects of the nearby interface may be judged by calculating the scaling factor R which is the ratio of the electric field at F in region 1 with the interface present to the field that would be found at the same field point F with the charge or dipole remaining at $(0, 0, Z)$ but with the whole region having a dielectric constant ε_1. For the case illustrated in Figs. 1 a and b, R is clearly a constant everywhere in region 1 given by $R = q_2/q$, which is very small when $\varepsilon_2 \gg \varepsilon_1$. For the cases illustrated in Figs. 1 c and d the situation is a little more complicated in that the original single charge q remains but a second charge q_1 is added so that the shape of the electric field is changed. However the limiting situations are clear. When q approaches the interface ($Z \to 0$) then so does q_1 from the other side so that the two charges tend to merge. The field in region 1 becomes that of a single charge of magnitude $q + q_1 = q_2$, so that R is again given by q_2/q. When q is remote from the interface the field in region 1 approximates to that due to q alone as q_1 is remote and $R = 1$. In Fig. 1 i is sketched R as a function of Z illustrating this kind of behaviour, with R small ($\varepsilon_2 \gg \varepsilon_1$) for all negative values of Z, and rising from this low value to 1 as the original charge moves away from the interface. Taking $\varepsilon_1 = 3$ to represent the membrane and $\varepsilon_2 = 80$ to represent the water around it, $R = 0.072$ for a charge close to the membrane surface which illustrates the powerful screening effect of the high dielectric fluid on the electric field of a charge just within a membrane.

Turning now to the dipole, the situation illustrated in Fig. 1 e and f clearly leads to a constant value of R given by $R = p_2/p$. For the case shown in Fig. 1 g and h the situation is again slightly complicated by the presence of two dipoles, the original dipole p and a second dipole p_1, so that the shape of the electric field is again altered. However, as the original dipole approaches the interface, so does its image dipole, and the field in region 1 becomes that of a single dipole of strength $(p - p_1)$. With $\varepsilon_2 > \varepsilon_1$, p is negative so that the combined dipole has a strength larger than the original dipole leading to a value for R of $2\,\varepsilon_2/(\varepsilon_1 + \varepsilon_2)$ which approximates to the value 2 if $\varepsilon_2 \gg \varepsilon_1$. The other limiting case is when the dipole is remote from the interface in which case the field in its vicinity is due effectively to p alone when $R = 1$ everywhere. Figure 1 j is a sketch of R as a function of Z for the dipolar case and illustrates these limits. Whilst the dipole is in the higher dielectric constant fluid the screening factor for a field within region 1 is the same for the dipole as for the charge with $R < 1$ given by

$$R = 2\,\varepsilon_1/(\varepsilon_1 + \varepsilon_2).$$

However with the dipole at the interface $R = 1$ and just within the low dielectric constant region ($Z > 0$) the field in region 1 is enhanced by the presence of the dielectric constant fluid by a factor

$$r = 2\,\varepsilon_2/(\varepsilon_1 + \varepsilon_2).$$

To take a particular case let $\varepsilon_1 = 3$ represent the membrane and $\varepsilon_2 = 80$ the water which bathes it. We will compare the electric field at a point just on the membrane side of the interface and a distance of 0.5 nm from the Z-axis, due to a charge on the one hand and an electric dipole on the other, when they are each situated close to the interface and on the Z-axis. We will use a single electron as the charge and a single water molecule with its dipole moment of 1.84 Debye oriented as in Fig. 1 g as the dipole. Using the expressions given above, the magnitude of the field due to the dipole is 2.05 times as strong as that due to the charge. On the other hand, away from the interface with no screening and at a point the same distance of 0.5 nm away, the electric field of the charge is 13.0 times larger than that of the dipole.

Of course a calculation such as this, which assumes plane interfaces and ideal continuous fluids that display their full bulk relative dielectric constants even at very short range, must be applied with caution, but it does represent a first approximation upon which more elaborate models may improve.

The electrostatic self-energy of charges is very much higher than that of dipoles in regions of low dielectric constant such as membranes (Parsegian 1969; Edmonds 1980). This fact together with the differential effects of the interface screening discussed in this note may mean that electric fields within membranes may often have as their sources electric dipoles rather than electric charges.

References

Edmonds DT (1980) Membrane ion channels and ionic hydration energies. Proc R Soc London [Biol] 211:51–62

Edmonds DT (1986) A two-channel electrostatic model of an ionic counterpart. Proc R Soc Lond [Biol] 228:71–84

Edmonds DT (1987) A physical model of sodium channel gating. Eur Biophys J 14:195–201
Friend SH, Matthew JB, Gurd FRN (1981) Protein-protein interactions: Nature of electrostatic stabilization of deoxyhemoglobin tetramer formation. Biochemistry 20:580–586
Gilson MK, Rashin A, Fine R, Honig B (1985) On the calculation of electrostatic interactions in proteins. J Mol Biol 183:503–516
Hol WG (1985) The role of the α-helix dipole in protein function and structure. Prog Biophys Mol Biol 43:149–195
Honig BH, Hubbell WL, Flewelling RF (1986) Electrostatic interactions in membranes and proteins. Annu Rev Biophys Chem 15:163–193
Parsegian A (1969) Energy of an ion crossing a low dielectric membrane: solutions of four relevant electrostatic problems. Nature 221:844–846
Rogers NK, Sternberg MJE (1984) Electrostatic interactions in globular proteins: different dielectric models applied to the packing of alpha-helices. J Mol Biol 174:527–542
Smythe WR (1939) Static and dynamic electricity. McGraw Hill, New York, p 113
Warshel A, Levitt M (1976) Theoretical studies of enzymic reactions: dielectric, electrostatic and steric stabilization of carbonium ion in the reaction of lysozyme. J Mol Biol 103:227–249
Warwicker J, Watson HC (1982) Calculation of the electric potential in the active site cleft due to α-helix dipoles. J Mol Biol 157:671–679