Biophysics

AIMS Biophysics, 9(2): 86–95.
DOI: 10.3934/biophy.2022008
Received: 20 January 2022
Revised: 16 March 2022
Accepted: 21 March 2022
Published: 24 March 2022

http://www.aimspress.com/journal/biophysics

Research article

Density of electric field energy around two surface-charged spheres surrounded by electrolyte I. The spheres are separated from each other

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Appendix 1.

The potential at $D_1 > R_1$ is

$$V(D_1) = \frac{k_e \cdot Q_1 \cdot \lambda_D}{\varepsilon_r \cdot D_1 \cdot R_1} \cdot e^{-\frac{D_1}{\lambda_D}} \cdot sinh\left(\frac{R_1}{\lambda_D}\right) \tag{A1}$$

and the potential at $D_1 < R_1$ is

$$V(D_1) = \frac{k_e \cdot Q_1 \cdot \lambda_D}{\varepsilon_r \cdot D_1 \cdot R_1} \cdot e^{-\frac{R_1}{\lambda_D}} \cdot sinh\left(\frac{D_1}{\lambda_D}\right) \tag{A2}$$

where $Q_1 = 4R_1^2\pi \cdot \rho_1$ is the total charge of the sphere with radius R_1 and surface charge density ρ_1. λ_D is the Debye length in the electrolyte with neutral monovalent ions [11]:

$$\lambda_D = \left(\frac{\varepsilon_0 \varepsilon_r k_B T}{e^2 N_a 2C}\right)^{\frac{1}{2}} \tag{A3}$$

where $\varepsilon_0 = 8.85 \cdot 10^{-12} \mathrm{C^2 J^{-1} m^{-1}}$ is the vacuum permittivity, ε_r is the relative static permittivity of the electrolyte, $k_B = 1.38 \cdot 10^{-23} \mathrm{JK^{-1}}$ is the Boltzmann constant, T is the absolute temperature, $e = 1.6 \cdot 10^{-19}$Coulomb is the charge of a positive monovalent ion, $N_a = 6 \cdot 10^{23} \mathrm{mol^{-1}}$ is the Avogadro's number, C is the monovalent (positive or negative) ion concentration (in $\mathrm{mol/m^3}$) of the electrolyte inside and around the charged sphere. In our calculation we take always $T = 300K$.

Appendix 2. The density of the electric field energy at the connection point of two touching surface-charged spheres

Here the density of the field energy is calculated close to the point where the two charged spheres touch each other. The field strength approaching the connection point from left is (see Eqs.2,3):

$$\underline{E}_{1-} + \underline{E}_{2+} = \left(\left\{-\left[\frac{dV_1}{dD_1}\right]_{D_1=R_{1-}} \cdot (1)\right\}, 0\right) + \left(\left\{-\left[\frac{dV_2}{dD_2}\right]_{D_2=R_{2+}} \cdot (-1)\right\}, 0\right)$$

$$\cong (A\{[G(R_{2+}) - G(R_{1-})] - 2\}, 0) \tag{A4}$$

where $y_p = 0$, $A = 2\pi k_e \rho/\varepsilon_r$ and $G(R) = \frac{e^{-2R/\lambda_D}}{R/\lambda_D} + e^{-2R/\lambda_D} - \frac{1}{R/\lambda_D}$. R_{1-} is the distance between the center of the left sphere and the connection point, when the connection point is approached from the left (i.e. $R_{1-} \lessapprox R_1$). R_{2+} is the distance between the center of the right sphere and the connection point, when the connection point is approached from the right (i.e. $R_{2+} \gtrapprox R_2$). If $R_1 = R_2$ then $G(R_{2+}) \cong G(R_{1-})$ and based on Eqs.5,A4 the density of the field energy approaching the connection point from the left is:

$$u_F\left(x_p = (R_{1-} - R_{2+})/2, y_p = 0\right) = \frac{\varepsilon_r \varepsilon_0}{2}\left([E_{1x-} + E_{2x+}]^2 + \left[E_{1y} + E_{2y}\right]^2\right) \cong \frac{\varepsilon_r \varepsilon_0}{2}([-2A]^2 + [0 + 0]^2) = 2\varepsilon_r \varepsilon_0 A^2 \tag{A5}$$

The field strength approaching the connection point from right is:

$$\underline{E}_{1+} + \underline{E}_{2-} = \left(\left\{-\left[\frac{dV_1}{dD_1}\right]_{D_1=R_{1+}} \cdot (1)\right\}, 0\right) + \left(\left\{-\left[\frac{dV_2}{dD_2}\right]_{D_2=R_{2-}} \cdot (-1)\right\}, 0\right)$$

$$\cong (A\{[G(R_{2-}) - G(R_{1+})] + 2\}, 0) \tag{A6}$$

R_{1+} is the distance between the center of the left sphere and the connection point, when the connection point is approached from the right. R_{2-} is the distance between the center of the right sphere and the connection point, when the connection point is approached from the left. If $R_1 = R_2$ then $C(R_{2-}) \cong C(R_{1+})$ and based on Eqs.5,A6 the density of the field energy approaching the connection point from the left is:

$$u_F\left(x_p = \frac{R_{1+} - R_{2-}}{2}, y_p = 0\right) = \frac{\varepsilon_r \varepsilon_0}{2}\left([E_{1x+} + E_{2x-}]^2 + \left[E_{1y} + E_{2y}\right]^2\right)$$

$$\cong \frac{\varepsilon_r \varepsilon_0}{2}([2A]^2 + [0 + 0]^2) = 2\varepsilon_r \varepsilon_0 A^2 \tag{A7}$$

Thus in the case of $R_1 = R_2$ the density of the field energy is the same either approaching the connection point from the left or right (see Eqs.A5,A7). However when $R_1 \neq R_2$ the density of the field energy is different when approaching the the connection point from the left:

$$u_F\big(x_p = (R_{1-} - R_{2+})/2, y_p = 0\big) = \frac{\varepsilon_r\varepsilon_0}{2}\Big([E_{1x-} + E_{2x+}]^2 + \big[E_{1y} + E_{2y}\big]^2\Big) \cong \frac{\varepsilon_r\varepsilon_0}{2}(A^2[G(R_{2+}) - G(R_{1-}) - 2]^2 + [0+0]^2) \tag{A8}$$

and when approaching the the connection point from the right:

$$u_F\big(x_p = (R_{1+} - R_{2-})/2, y_p = 0\big) = \frac{\varepsilon_r\varepsilon_0}{2}\Big([E_{1x+} + E_{2x-}]^2 + \big[E_{1y} + E_{2y}\big]^2\Big) \cong \frac{\varepsilon_r\varepsilon_0}{2}(A^2[G(R_{2-}) - G(R_{1+}) + 2]^2 + [0+0]^2). \tag{A9}$$

Based on Eqs.A8,A9 if the right sphere is larger than the left sphere (i.e. $R_2 > R_1$) then u_F near the right side of the connection point is larger than u_F near the left side of the connection point. However, the difference between these field energy densities decreases with decreasing electrolyte ion concentration. Actually, the difference becomes zero at zero electrolyte ion concentration (i.e. at $\varepsilon_r = 1$ and $\lambda_D = \infty$). This is the case because according to Newton's Shell Theorem [6,7] or Eq.3 at $\lambda_D \to \infty$:

$$E_{1x-} = 0,\ E_{2x+} = \left[\frac{dV_2}{dD_2}\right]_{D_2=R_{2+}} = -\frac{k_eQ_2}{(R_{2+})^2} = -\frac{k_e4\pi\rho(R_2)^2}{(R_{2+})^2} \cong -k_e4\pi\rho \tag{A10}$$

$$E_{2x-} = 0,\ E_{1x+} = -\left[\frac{dV_1}{dD_1}\right]_{D_1=R_{1+}} = \frac{k_eQ_1}{(R_{1+})^2} = \frac{k_e4\pi\rho(R_1)^2}{(R_{1+})^2} \cong k_e4\pi\rho \tag{A11}$$

and based on Eqs.A5,A7

$$u_F\left(x_p = \frac{R_{1+}-R_{2-}}{2}, y_p = 0\right) = \frac{\varepsilon_r\varepsilon_0}{2}\Big([E_{1x+} + E_{2x-}]^2 + \big[E_{1y} + E_{2y}\big]^2\Big) \cong \frac{\varepsilon_r\varepsilon_0}{2}(-k_e4\pi\rho)^2 \tag{A12}$$

$$u_F\left(x_p = \frac{R_{1-}-R_{2+}}{2}, y_p = 0\right) = \frac{\varepsilon_r\varepsilon_0}{2}\Big([E_{1x-} + E_{2x+}]^2 + \big[E_{1y} + E_{2y}\big]^2\Big) \cong \frac{\varepsilon_r\varepsilon_0}{2}(k_e4\pi\rho)^2 \tag{A13}$$

Appendix 3. The electric field energy density of N charged spheres surrounded by electrolyte

The coordinates of the center of the i-th sphere are (x_i, y_i, z_i). The density of the electric field energy at point P_1 with coordinates (x_P, y_P, z_P) is:

$$u_F(x_P, y_P, z_P) = \frac{\varepsilon_r\varepsilon_0}{2}\underline{E}\cdot\underline{E} = \frac{\varepsilon_r\varepsilon_0}{2}\Big(\{\textstyle\sum_{i=1}^N E_{ix}\}^2 + \big\{\sum_{i=1}^N E_{iy}\big\}^2 + \{\sum_{i=1}^N E_{iz}\}^2\Big) \tag{A14}$$

where the electric field created by the i-th sphere at point P_1 is:

$$\underline{E_i} = \big(E_{ix}, E_{iy}, E_{iz}\big) = -\frac{dV_i}{dD_i}\left(\frac{x_P-x_i}{D_i}, \frac{y_P-y_i}{D_i}, \frac{z_P-z_i}{D_i}\right) \tag{A15}$$

where $D_i = \sqrt{(x_P - x_i)^2 + (y_P - y_i)^2 + (z_P - z_i)^2}$ is the distance between point P_1 and the center of the i-th charged sphere and

$$\frac{dV_i}{dD_i} = \begin{cases} \frac{k_e Q_i \lambda_D}{\varepsilon_r R_i} sinh(R_i/\lambda_D) \left[-\frac{e^{-\frac{D_i}{\lambda_D}}}{D_i^2} - \frac{e^{-\frac{D_i}{\lambda_D}}}{D_i \lambda_D} \right] & if\ D_i > R_i \\ \frac{k_e Q_i \lambda_D}{\varepsilon_r R_i} e^{-\frac{R_i}{\lambda_D}} \left[-\frac{sinh\left(\frac{D_i}{\lambda_D}\right)}{D_i^2} + \frac{cosh\left(\frac{D_i}{\lambda_D}\right)}{D_i \lambda_D} \right] & if\ D_i < R_i \end{cases} \tag{A16}$$

where $\sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2} > R_i + R_j$ where $i \neq j$.

Appendix 4. Electric field density around a charged sphere and a charged flat surface surrounded by electrolyte

Eq.A17 is the general solution of the Screened Poisson Equation

$$V(\underline{r}) = \iiint d^3\underline{r}' \frac{\rho_{ex}(\underline{r}')}{4\pi\varepsilon_0\varepsilon_r} \frac{e^{-|\underline{r}-\underline{r}'|/\lambda_D}}{|\underline{r}-\underline{r}'|} \tag{A17}$$

where $\rho_{ex}(\underline{r}')$ is the density of the external charge at position $\underline{r}'$, ε_0 is the electric constant and ε is the relative static permittivity, λ_D is the Debye length. Note, that Eq.A17 is valid if the electrolyte itself is electrically neutral.

In Figure A1(A) there is a homogeneously charged flat surface (with surface charge density $\rho_{ex} = \rho_2$) surrounded by electrolyte. By using Eq.A17 one can calculate the potential at point P_1 (located at a distance Z_0 from the charged flat surface). The potential caused by the charges in the black ring (of radius r and thickness dr) at point P_1 is:

$$V(\propto, Z_0)d \propto = \frac{\rho_2 2r\pi \cdot dr(\propto)}{4\pi\varepsilon_0\varepsilon_r} \frac{e^{-R(\propto)/\lambda_D}}{R(\propto)} \tag{A18}$$

After substituting into Eq.A18 $R = Z_0/\cos(\alpha)$ $r = Z_0 \cdot tg(\alpha)$ and $dr = Z_0 \cdot d[tan(\alpha)] = d\alpha \cdot Z_0/cos^2(\alpha)$ we get:

$$V(\propto, Z_0)d \propto = \frac{\rho_2 Z_0}{2\varepsilon_0\varepsilon_r} \cdot \frac{\sin(\alpha)}{cos^2(\alpha)} \cdot e^{-Z_0/[\lambda_D \cdot \cos(\alpha)]} d\alpha \tag{A19}$$

Let us make the substitutions in Eq.A19: $u = cos^{-1}(\propto)$ and $du = \sin(\propto) \cdot cos^{-2}(\alpha) \cdot d\alpha$ and integrate from $u(\propto = 0) = 1$ to $u(\propto = \pi/2) = \infty$ and we get the potential at a distance Z_0 from the charged flat surface

$$V(Z_0) = \int_{u(\propto=0)}^{u\left(\propto=\frac{\pi}{2}\right)} V(u, Z_0)\, du = \int_{u(\propto=0)}^{u\left(\propto=\frac{\pi}{2}\right)} \frac{\rho_2 Z_0}{2\varepsilon_0\varepsilon_r} \cdot e^{-\frac{Z_0 u}{\lambda_D}}\, du$$

$$= \left[\frac{\rho_2 Z_0}{2\varepsilon_0\varepsilon} \cdot \left(-\frac{\lambda_D}{Z_0}\right) e^{-Z_0 u/\lambda_D}\right]_1^{\infty} = \frac{\rho_2\lambda_D}{2\varepsilon_0\varepsilon_r} e^{-Z_0/\lambda_D} \tag{A20}$$

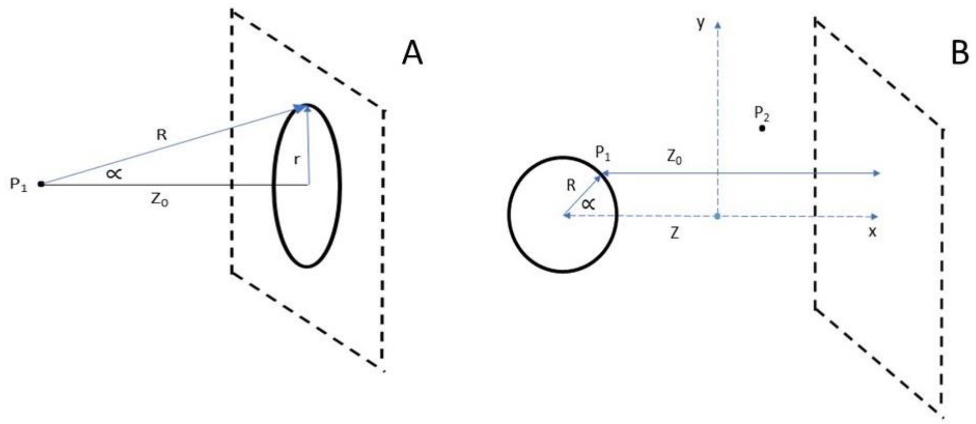

Figure A1. Modelling cell electrophoresis.

A) Location of a point charge (P_1) from a charged flat surface. B) Location of a surface-charged sphere from a charged flat surface. The origin of the coordinate system (x,y) is attached to the middle of the distance between the center of the sphere and the flat surface (see blue dot), and the coordinates of point P_2 (marked by black dot) are x_p and y_p.

In Figure A1(B) a homogeneously charged sphere (with radius R and surface charge density $\rho_{ex} = \rho_1$) interacts with the charged flat surface. The sphere inside and outside is surrounded by electrolyte. Calculating the interaction energy between the charged sphere and the charged flat surface first let us consider the interaction of a ring of the sphere with the flat surface. The radius of the ring is $R \cdot \sin(\alpha)$, the thickness of the ring is $R \cdot \mathrm{d}\alpha$, and the distance of each point of the ring from the flate surface is Z_o. The total charge of the ring is $\rho_1 \cdot 2R \cdot \sin(\alpha) \cdot \pi \cdot R \cdot d\alpha$ and the potential at each point of the ring is given by Eq.A20. Thus the interaction energy between the ring and the flat surface is

$$E(\alpha, Z)d\alpha = \frac{\rho_2\lambda_D}{2\varepsilon_0\varepsilon_r} e^{-\frac{Z_0}{\lambda_D}} \rho_1 \cdot 2R \cdot \sin(\alpha) \cdot \pi \cdot R \cdot d\alpha$$

$$= \frac{\rho_1\rho_2\lambda_D}{\varepsilon_0\varepsilon_r} e^{-[Z - R\cos(\alpha)]/\lambda_D} \cdot R^2\pi \cdot \sin(\alpha) \cdot d\alpha \tag{A21}$$

where $Z[= Z_0 + R\cos(\propto)]$ is the distance between the charged flat surface and the center of the charged sphere

After the following substitutions in Eq.A21: $u = \cos(\propto)$ and $du = -\sin(\propto) \cdot d\alpha$ in order to get the total interaction energy, $E(Z)$ between the charged sphere and the charged flat surface one has to integrate the ring energy from $u(\propto = 0) = 1$ to $u(\propto = \pi) = -1$

The following integral gives the total interaction energy between the charged sphere and the charged flat surface where the distance between the center of the sphere and the flat surface is Z:

$$E(Z)=\int_0^{\pi}E(\alpha,Z)d\alpha=\int_1^{-1}E(u,Z)du=\int_1^{-1}\frac{\rho_1\rho_2\lambda_D}{\varepsilon_0\varepsilon_r}e^{-[Z-Ru]/\lambda_D}\cdot R^2\pi\cdot(-du)=$$
$$\frac{\rho_1\rho_2\lambda_D}{\varepsilon_0\varepsilon_r}R^2\pi\cdot e^{-Z/\lambda_D}\left[\left(-\frac{\lambda_D}{R}\right)e^{Ru/\lambda_D}\right]_1^{-1}=\frac{\rho_1\rho_2\lambda_D}{\varepsilon_0\varepsilon_r}R^2\pi\cdot e^{-Z/\lambda_D}\frac{\lambda_D}{R}\{e^{R/\lambda_D}-e^{-R/\lambda_D}\}=$$
$$\frac{Q_1\rho_2\lambda_D^2}{2\varepsilon_0\varepsilon_r R}\cdot e^{-Z/\lambda_D}\cdot sh\left(\frac{R}{\lambda_D}\right)\tag{A22}$$

where $Q_1(=\rho_1 4R^2\pi)$ is the total charge of the sphere.

In order to calculate density of electric field energy at point P2 (x_p,y_p) (see Figure A1(B) one has to use Eq.5. where $\underline{E_1}$ (the field strength created by the charged sphere) is given by Eqs.2,3. To calculate the field strength $\underline{E_2}$ (created by the charged flat surface) one has to consider the distance of point P2 from the charged flat surface, i.e: $0.5Z-x_p$ and substituting this to Z_0 in Eq.A20 one gets the potential caused by the charged flat surface at point P2:

$$V(x_p,y_p)=\frac{\rho_2\lambda_D}{2\varepsilon_0\varepsilon_r}e^{-(0.5Z-x_p)/\lambda_D}\tag{A23}$$

Then the electric field strength $\underline{E_2}$ is:

$$\underline{E_2}=(E_{2x},E_{2y})=-grad[V(x_p,y_p)]=-\left(\frac{dV}{dx_p},\frac{dV}{dy_p}\right)$$
$$=(-\frac{\rho_2}{2\varepsilon_o\varepsilon_r}e^{-\frac{0.5Z-x_p}{\lambda_D}},0)\tag{A24}$$