[pex57] Poly-electrolyte gel: double layer of charges at interface

Consider a gelled polymer with ionic groups immersed in a polyelectrolyte solution. We focus on a region near the interface between gel and solution. Suppose the interface is flat and the x-axis perpendicular to it with the gel at x < 0 and the solution at x > 0. This setup represents an application of [pex56], somewhat generalized. The number densities of (positive) bound charges, and mobile ions have specific profiles: $n_b(x), n_+(x), n_-(x)$, which, in turn, determine the profile of the charge density: $\rho_e(x) = e_0[n_b(x) + n_+(x) - n_-(x)]$.

(a) The electric potential $\psi(x)$ and the charge density $\rho_e(x)$ are then related via the following 1D rendition of the Poisson equation:

$$\epsilon \frac{d^2 \psi}{dx^2} = -\rho_e(x),$$

where $\epsilon \doteq \epsilon_r \epsilon_0$ is the permittivity constant (assumed uniform). Show that this relation can be inverted as follows:

$$\psi(x) = -\frac{1}{2\epsilon} \int_{-\infty}^{+\infty} dx' |x - x'| \rho_e(x').$$

(b) Given the charge neutrality condition and the definition of the electric dipole moment,

$$\int_{-\infty}^{+\infty} dx \rho_e(x) = 0, \quad P_e = \int_{-\infty}^{+\infty} dx \, x \rho_e(x).$$

show that the Donnan potential, $\Delta \psi \doteq \psi(-\infty) - \psi(+\infty)$, is related to P_e as follows:

$$\Delta \psi = -\frac{P_e}{\epsilon}$$

(c) Consider the model potential $\psi(x) = c[1 - b \tanh(ax)]$ with adjustable parameters a, b, c. Infer the corresponding model charge density $\rho_e(x)$ and plot the profiles of both functions for judicious choices of the parameters. Explain any features that have to do with double layers of charges and electric dipole moment.

[adapted from Doi 2013]

Solution: