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Effects of Small Permanent Charge on PNP Models

Guojian Lin

Department of Mathematics, Renmin University of China, Beijing, China
Email: gjlin@ruc.edu.cn

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Abstract

In this paper, a stationary one-dimensional Poisson-Nernst-Planck model with permanent charge is studied under the assumption that $n-1$ positively charged ion species have the same valence and the permanent charge is small. By expanding the singular solutions of Poisson-Nernst-Planck model with respect to small permanent charge, the explicit formulae for the zeroth order approximation and the first order approximation of individual flux can be obtained. Based on these explicit formulae, the effects of small permanent charges on individual flux are investigated.

Keywords

PNP Model, Permanent Charge, Ionic Flow

1. Introduction

The cell membrane is a biological membrane that separates the interior of all cells from the outside environment which protects the cell from its environment. Ion channels are large proteins embedded in cell membranes that have holes open to the inside and the outside of cells. Ion channel opening gives rise to a passageway through which charged ions can cross the cell membrane. It is now well-known that migration of charges for ionic flow through ion channels can be described mathematically by the Poisson-Nernst-Planck model [1] [2].

A stationary one-dimensional Poisson-Nernst-Planck model [3] [4] [5] is

$$\begin{aligned} &\frac{1}{h(x)}\frac{\mathrm{d}}{\mathrm{d}x}\left(\varepsilon_r\varepsilon_0 h(x)\frac{\mathrm{d}\Phi}{\mathrm{d}x}\right) = -e\left(\sum_{j=1}^{n} z_j c_j(x) + Q(x)\right), \\ &\frac{\mathrm{d}\mathcal{J}_i}{\mathrm{d}x} = 0, \quad -\mathcal{J}_i = \frac{1}{kT} D_i h(x) c_i(x) \frac{\mathrm{d}\mu_i}{\mathrm{d}x}, \quad i = 1,2,\cdots,n, \end{aligned} \tag{1.1}$$

where Φ is the electric potential, c_i is the concentration for the *i*th ion species, z_i is the valence, $Q(x)$ is the permanent charge of the channel, $\mu_i(x)$ is the electrochemical potential, $h(x)$ is the area of the cross-section of the channel, $\mathcal{J}_i$ is the flux density, D_i is the diffusion coefficient, ε_r is the relative dielectric coefficient, ε_0 is the vacuum permittivity, k is the Boltzmann constant, T is the absolute temperature, and e is the elementary charge.

The boundary conditions are, for $i = 1, 2, \cdots, n$,

$$\Phi(0) = V,\ c_i(0) = L_i;\quad \Phi(1) = 0,\ c_i(1) = R_i. \tag{1.2}$$

$\mu_i(x)$ in the classical Poisson-Nernst-Planck model takes the following form

$$\mu_i(x) = z_i e\phi(x) + kT\ln\frac{c_i(x)}{c_0} \tag{1.3}$$

with c_0 is a constant.

The Poisson-Nernst-Planck model (1.1) can be viewed as a simplified model which is derived from the Maxwell-Boltzmann equations [6] [7] and the Langevin-Poisson equations [8] [9]. More sophisticated Poisson-Nernst-Planck model has been also developed and analyzed [10] [11]. The dynamics of the classical model (1.1) has been analyzed [12] [13] [14] [15] to a great extent. Especially, the existence and uniqueness of solutions for the boundary value problems (1.1) and (1.2) has been obtained in [16] under the assumption that $Q(x) = 0$. In [17], under the assumption that $Q(x)$ is a piecewise constant function, the general dynamical system framework for studying the boundary value problems (1.1) and (1.2) has been developed by employing the geometric singular perturbation theory [18] [19] [20]. As we know, under the assumption that $Q(x)$ is a piecewise constant function, it is basically difficult to obtain the explicit formula for individual flux with respect to permanent charges, so it is also not easy to analyze the effects of permanent charges on individual flux. In this paper, the effects of permanent charges on ionic flows through ion channels are investigated under the following assumptions.

(A1) $z_1 = \cdots = z_{n-1} = z > 0$ and $z_n < 0$.

(A2) $Q(x) = 0$ for $0 < x < a$, $Q(x) = Q$ for $a < x < b$ and $Q(x) = 0$ for $b < x < 1$, where Q is a constant and Q will be set to be small in the later analysis.

By re-scaling,

$$\phi = \frac{e}{kT}\Phi,\ \bar{V} = \frac{e}{kT}V,\ \varepsilon^2 = \frac{\varepsilon_r\varepsilon_0 kT}{e^2},\ J_i = \frac{\mathcal{J}_i}{D_i}.$$

The model (1.1) is reduced to a standard singularly perturbed system of the following

$$\begin{aligned}
&\frac{\varepsilon^2}{h(x)}\frac{\mathrm{d}}{\mathrm{d}x}\left(h(x)\frac{\mathrm{d}}{\mathrm{d}x}\phi\right) = -\left[zc_1 + \cdots + zc_{n-1} + z_n c_n + Q(x)\right],\\
&h(x)\left(\frac{\mathrm{d}c_1}{\mathrm{d}x} + zc_1\frac{\mathrm{d}\phi}{\mathrm{d}x}\right) = -J_1,\\
&\qquad\vdots\\
&h(x)\left(\frac{\mathrm{d}c_{n-1}}{\mathrm{d}x} + zc_{n-1}\frac{\mathrm{d}\phi}{\mathrm{d}x}\right) = -J_{n-1},
\end{aligned}$$

$$
\begin{aligned}
&h(x)\left(\frac{\mathrm{d}c_n}{\mathrm{d}x}+z_nc_n\frac{\mathrm{d}\phi}{\mathrm{d}x}\right)=-J_n,\\
&\frac{\mathrm{d}J_1}{\mathrm{d}x}=\cdots=\frac{\mathrm{d}J_n}{\mathrm{d}x}=0,
\end{aligned}
\tag{1.4}
$$

with the boundary condition, for $j=1,\cdots,n$.

$$
\phi(0)=\bar{V},\ c_j(0)=L_j,\ \phi(1)=0,\ c_j(1)=R_j. \tag{1.5}
$$

Under the assumptions (A1) and (A2), the existence of the solutions of (1.4) and (1.5) has been studied in [21]. In this paper, it is additionally assumed that the constant Q is small, then by expanding the solutions of (1.4) and (1.5) with respect to small Q, the explicit formulae for the zeroth order approximation and the first order approximation of individual flux can be obtained. Based on these explicit formulae, the effects of small permanent charges on individual flux are investigated. As $n=2$ in (1.4) and (1.5), namely, only one positively charged ion and one negatively charged ion are involved in the Poisson-Nernst-Planck model, the effects of small permanent charges on individual flux has been analyzed in [22]. On the other hand, assuming that the constant Q is large, the effects of large permanent charges on individual flux have been also analyzed in [23].

2. Brief Reviews of Relevant Results in [21]

Let $u=\varepsilon\frac{\mathrm{d}}{\mathrm{d}x}\phi$, $\tau=x$. System (1.4) becomes

$$
\begin{aligned}
&\varepsilon\dot{\phi}=u,\quad \varepsilon\dot{u}=-\left[zc_1+\cdots+zc_{n-1}+z_nc_n+Q(x)\right]-\varepsilon h^{-1}(\tau)h_\tau(\tau)u,\\
&\varepsilon\dot{c}_1=-zc_1u-\varepsilon h_\tau(\tau)J_1,\\
&\qquad\vdots\\
&\varepsilon\dot{c}_{n-1}=-zc_{n-1}u-\varepsilon h_\tau(\tau)J_{n-1},\\
&\varepsilon\dot{c}_n=-z_nc_nu-\varepsilon h_\tau(\tau)J_n,\\
&\dot{J}_1=0,\cdots,\dot{J}_n=0,\quad \dot{\tau}=1.
\end{aligned}
\tag{2.6}
$$

By using the rescaling $x=\varepsilon\xi$, one has

$$
\begin{aligned}
&\phi'=u,\quad u'=-\left[zc_1+\cdots+zc_{n-1}+z_nc_n+Q(x)\right]-\varepsilon h^{-1}(\tau)h_\tau(\tau)u,\\
&c_1'=-zc_1u-\varepsilon h_\tau(\tau)J_1,\\
&\qquad\vdots\\
&c_{n-1}'=-zc_{n-1}u-\varepsilon h_\tau(\tau)J_{n-1},\\
&c_n'=-z_nc_nu-\varepsilon h_\tau(\tau)J_n,\\
&J_1'=0,\cdots,J_n'=0,\quad \tau'=\varepsilon.
\end{aligned}
\tag{2.7}
$$

Define

$$
\begin{aligned}
&B_L=\left\{\left(\bar{V},u,L_1,\cdots,L_n,J_1,\cdots,J_n,0\right)\in\mathbb{R}^{2n+3}:\text{arbitrary } u,J_1,\cdots,J_n\right\},\\
&B_R=\left\{\left(0,u,R_1,\cdots,R_n,J_1,\cdots,J_n,1\right)\in\mathbb{R}^{2n+3}:\text{arbitrary } u,J_1,\cdots,J_n\right\}.
\end{aligned}
\tag{2.8}
$$

Then a solution to Equations (1.4) and (1.5) is to finding an orbit of Equation

(2.6) or (2.7) from B_L to B_R.

Due to the fact that $Q(x)$ is a piecewise constant function, so we analyze the limiting fast and limiting slow orbits of Equations (2.6) and (2.7) on three intervals $[0,a]$, $[a,b]$ and $[b,1]$ respectively.

Let $\phi(a)=\phi^a$, $c_1(a)=c_1^a$, $\cdots$, $c_n(a)=c_n^a$, where ϕ^a, c_1^a, $\cdots$, c_n^a are unknowns to be determined. Let

$$B_a=\left\{\left(\phi^a,u,c_1^a,\cdots,c_n^a,J_1,\cdots,J_n,a\right)\in\mathbb{R}^{2n+3}:\text{arbitrary } u,J_1,\cdots,J_n\right\}.$$

Let $\phi(b)=\phi^b$, $c_1(b)=c_1^b$, $\cdots$, $c_n(b)=c_n^b$, where ϕ^b, c_1^b, $\cdots$, c_n^b are unknowns to be determined. Let

$$B_b=\left\{\left(\phi^b,u,c_1^b,\cdots,c_n^b,J_1,\cdots,J_n,b\right)\in\mathbb{R}^{2n+3}:\text{arbitrary } u,J_1,\cdots,J_n\right\}.$$

Then an singular orbit of Equation (2.6) or (2.7) from B_L to B_R consists of three parts: that is, a singular orbit over the interval $[0,a]$ connecting orbit from B_L to B_a, a singular orbit over the interval $[a,b]$ connecting orbit from B_a to B_b, and a singular orbit over the interval $[b,1]$ connecting orbit from B_b to B_R.

Based on [21], an singular orbit of Equation (2.6) or (2.7) from B_L to B_R is equivalent to solving the following algebraic equations:

$$\begin{aligned}
&zc_1^a\mathrm{e}^{z(\phi^a-\phi)}+\cdots+zc_{n-1}^a\mathrm{e}^{z(\phi^a-\phi)}+z_nc_n^a\mathrm{e}^{z_n(\phi^a-\phi)}+Q=0,\\
&zc_1^b\mathrm{e}^{z(\phi^b-\phi)}+\cdots+zc_{n-1}^b\mathrm{e}^{z(\phi^b-\phi)}+z_nc_n^b\mathrm{e}^{z_n(\phi^b-\phi)}+Q=0,\\
&\operatorname{sgn}\left(\phi^a-\phi^{a,l}\right)\sqrt{2\left[c_1^a+\cdots+c_n^a-\left(c_1^{a,l}+\cdots+c_n^{a,l}\right)\right]}\\
&=\operatorname{sgn}\left(\phi^{a,m}-\phi^a\right)\sqrt{2\left[c_1^a+\cdots+c_n^a-\left(c_1^{a,m}+\cdots+c_n^{a,m}\right)-Q\left(\phi^a-\phi^{a,m}\right)\right]},\\
&\operatorname{sgn}\left(\phi^b-\phi^{b,m}\right)\sqrt{2\left[c_1^b+\cdots+c_n^b-\left(c_1^{b,m}+\cdots+c_n^{b,m}\right)-Q\left(\phi^b-\phi^{b,m}\right)\right]}\\
&=\operatorname{sgn}\left(\phi^{b,r}-\phi^b\right)\sqrt{2\left[c_1^b+\cdots+c_b^b-\left(c_1^{b,r}+\cdots+c_n^{b,r}\right)\right]},\\
&J_1+\cdots+J_{n-1}\\
&=\frac{c_1^L+\cdots+c_{n-1}^L-\left(c_1^{a,l}+\cdots+c_{n-1}^{a,l}\right)}{H(a)}\left[1-\frac{z\left(\phi^L-\phi^{a,l}\right)}{\ln\frac{c_1^{a,l}+\cdots+c_{n-1}^{a,l}}{c_1^L+\cdots+c_{n-1}^L}}\right]\\
&=\frac{c_1^{b,r}+\cdots+c_{n-1}^{b,r}-\left(c_1^R+\cdots+c_{n-1}^R\right)}{H(1)-H(b)}\left[1-\frac{z\left(\phi^{b,r}-\phi^R\right)}{\ln\frac{c_1^R+\cdots+c_{n-1}^R}{c_1^{b,r}+\cdots+c_{n-1}^{b,r}}}\right],\\
&J_n=\frac{z\left[c_1^{a,l}+\cdots+c_{n-1}^{a,l}-\left(c_1^L+\cdots+c_{n-}^L\right)\right]}{z_nH(a)}\left[1-\frac{z_n\left(\phi^L-\phi^{a,l}\right)}{\ln\frac{c_1^{a,l}+\cdots+c_{n-1}^{a,l}}{c_1^L+\cdots+c_{n-1}^L}}\right]
\end{aligned}\tag{2.9}$$

$$=\frac{z\left[c_1^R+\cdots+c_{n-1}^R-\left(c_1^{b,r}+\cdots+c_{n-1}^{b,r}\right)\right]}{z_n\left(H(1)-H(b)\right)}\left[1-\frac{z_n\left(\phi^{b,r}-\phi^R\right)}{\ln\dfrac{c_1^R+\cdots+c_{n-1}^R}{c_1^{b,r}+\cdots+c_{n-1}^{b,r}}}\right],$$

$$\phi^{b,m}=\phi^{a,m}-\frac{z\left(J_1+\cdots+J_{n-1}\right)+z_nJ_n}{zz_n\left(J_1+\cdots+J_n\right)}$$
$$\times\ln\frac{z\left(J_1+\cdots+J_n\right)\left(c_1^{b,m}+\cdots+c_{n-1}^{b,m}\right)+Q\left(J_1+\cdots+J_{n-1}\right)}{z\left(J_1+\cdots+J_n\right)\left(c_1^{a,m}+\cdots+c_{n-1}^{a,m}\right)+Q\left(J_1+\cdots+J_{n-1}\right)},$$

$$J_1+\cdots+J_n=\frac{\left(z-z_n\right)\left[c_1^{a,m}+\cdots+c_{n-1}^{a,m}-\left(c_1^{b,m}+\cdots+c_{n-1}^{b,m}\right)\right]}{-z_n\left(H(b)-H(a)\right)}-\frac{Q\left(\phi^{a,m}-\phi^{b,m}\right)}{H(b)-H(a)},$$

and

$$\frac{J_i}{J_1+\cdots+J_{n-1}}=\frac{c_i^{a,l}-c_i^L\mathrm{e}^{z\left(\phi^L-\phi^{a,l}\right)}}{c_1^{a,l}+\cdots+c_{n-1}^{a,l}-\left(c_1^L+\cdots+c_{n-1}^L\right)\mathrm{e}^{z\left(\phi^L-\phi^{a,l}\right)}},$$
$$=\frac{c_i^{b,m}-c_i^{a,m}\mathrm{e}^{z\left(\phi^{a,m}-\phi^{b,m}\right)}}{c_1^{b,m}+\cdots+c_{n-1}^{b,m}-\left(c_1^{a,m}+\cdots+c_{n-1}^{a,m}\right)\mathrm{e}^{z\left(\phi^{a,m}-\phi^{b,m}\right)}} \tag{2.10}$$
$$=\frac{c_i^R-c_i^{b,r}\mathrm{e}^{z\left(\phi^{b,r}-\phi^R\right)}}{c_1^R+\cdots+c_{n-1}^R-\left(c_1^{b,r}+\cdots+c_{n-1}^{b,r}\right)\mathrm{e}^{z\left(\phi^{b,r}-\phi^R\right)}},\ i=1,\cdots,n-1,$$

where

$$c_i^L=L_i\left[\frac{-z_nL_n}{z\left(L_1+\cdots+L_{n-1}\right)}\right]^{\frac{z}{z-z_n}},\ c_n^L=L_n\left[\frac{-z_nL_n}{z\left(L_1+\cdots+L_{n-1}\right)}\right]^{\frac{z_n}{z-z_n}},$$
$$\phi^L=\bar{V}-\frac{1}{z-z_n}\ln\frac{-z_nL_n}{z\left(L_1+\cdots+L_{n-1}\right)},$$
$$c_i^{a,l}=c_i^a\left[\frac{-z_nc_n^a}{z\left(c_1^a+\cdots+c_{n-1}^a\right)}\right]^{\frac{z}{z-z_n}},\ c_n^{a,l}=c_n^a\left[\frac{-z_nc_n^a}{z\left(c_1^a+\cdots+c_{n-1}^a\right)}\right]^{\frac{z_n}{z-z_n}},$$
$$\phi^{a,l}=\phi^a-\frac{1}{z-z_n}\ln\frac{-z_nc_n^a}{z\left(c_1^a+\cdots+c_{n-1}^a\right)},$$
$$c_i^{a,m}=c_i^a\mathrm{e}^{z\left(\phi^a-\phi^{a,m}\right)},\ c_n^{a,m}=c_n^a\mathrm{e}^{z_n\left(\phi^a-\phi^{a,m}\right)},$$
$$c_i^{b,m}=c_i^b\mathrm{e}^{z\left(\phi^b-\phi^{b,m}\right)},\ c_n^{b,m}=c_n^b\mathrm{e}^{z_n\left(\phi^b-\phi^{b,m}\right)}, \tag{2.11}$$
$$c_i^{b,r}=c_i^b\left[\frac{-z_nc_n^b}{z\left(c_1^b+\cdots+c_{n-1}^b\right)}\right]^{\frac{z}{z-z_n}},\ c_n^{b,r}=c_n^b\left[\frac{-z_nc_n^b}{z\left(c_1^b+\cdots+c_{n-1}^b\right)}\right]^{\frac{z_n}{z-z_n}},$$
$$\phi^{b,r}=\phi^b-\frac{1}{z-z_n}\ln\frac{-z_nc_n^b}{z\left(c_1^b+\cdots+c_{n-1}^b\right)},$$

$$c_i^R = R_i\left[\frac{-z_n R_n}{z\left(R_1+\cdots+R_{n-1}\right)}\right]^{\frac{z}{z-z_n}}, c_n^R = R_n\left[\frac{-z_n R_n}{z\left(R_1+\cdots+R_{n-1}\right)}\right]^{\frac{z_n}{z-z_n}},$$

$$\phi^R = -\frac{1}{z-z_n}\ln\frac{-z_n R_n}{z\left(R_1+\cdots+R_{n-1}\right)}, i=1,\cdots,n-1,$$

$$H(x) = \int_0^x h^{-1}(s)\,\mathrm{d}s.$$

3. Taylor Expansions of (2.9)-(2.11) with Respect to Small $|Q|$

In this section, it is assumed that $|Q|$ is small. All unknown quantities in (2.9)-(2.11) are expanded in Q as follows

$$\begin{aligned}
&\phi^a = \phi_0^a + \phi_1^a Q + \phi_2^a Q^2 + o\left(Q^2\right), \phi^b = \phi_0^b + \phi_1^b Q + \phi_2^b Q^2 + o\left(Q^2\right),\\
&c_i^a = c_{i0}^a + c_{i1}^a Q + c_{i2}^a Q^2 + o\left(Q^2\right), c_i^b = c_{i0}^b + c_{i1}^b Q + c_{i2}^b Q^2 + o\left(Q^2\right),\\
&J_i = J_{i0} + J_{i1} Q + J_{i2} Q^2 + o\left(Q^2\right), i=1,2,\cdots,n.
\end{aligned} \tag{3.12}$$

Let

$$\alpha = \frac{H(a)}{H(1)}, \beta = \frac{H(b)}{H(1)}. \tag{3.13}$$

Inserting the formulae (3.12) into (2.9)-(2.11) and expanding the algebraic equations (2.9)-(2.11) in Q, then by comparing the terms of like-powers in Q, one has

Proposition 3.1. *Zeroth order solution in* Q *of* (2.9)-(2.11) *is given by*

$$\begin{aligned}
c_{10}^{a,l} + \cdots + c_{n-1,0}^{a,l} &= c_{10}^{a,m} + \cdots + c_{n-1,0}^{a,m} = c_{10}^{a} + \cdots + c_{n-1,0}^{a}\\
&= c_1^L + \cdots + c_{n-1}^L + \alpha\left[c_1^R + \cdots + c_{n-1}^R - \left(c_1^L + \cdots + c_{n-1}^L\right)\right],\\
&z\left(c_{10}^a + \cdots + c_{n-1,0}^a\right) = -z_n c_{n0}^a,\\
c_{10}^{b,r} + \cdots + c_{n-1,0}^{b,r} &= c_{10}^{b,m} + \cdots + c_{n-1,0}^{b,m} = c_{10}^{b} + \cdots + c_{n-1,0}^{b}\\
&= c_1^L + \cdots + c_{n-1}^L + \beta\left[c_1^R + \cdots + c_{n-1}^R - \left(c_1^L + \cdots + c_{n-1}^L\right)\right],\\
&z\left(c_{10}^b + \cdots + c_{n-1,0}^b\right) = -z_n c_{n0}^b,\\
\phi_0^{a,l} = \phi_0^{a,m} = \phi_0^a &= \frac{\ln\left(c_1^R + \cdots + c_{n-1}^R\right) - \ln\left(c_{10}^a + \cdots + c_{n-1,0}^a\right)}{\ln\left(c_1^R + \cdots + c_{n-1}^R\right) - \ln\left(c_1^L + \cdots + c_{n-1}^L\right)}\phi^L\\
&+ \frac{\ln\left(c_{10}^a + \cdots + c_{n-1,0}^a\right) - \ln\left(c_1^L + \cdots + c_{n-1}^L\right)}{\ln\left(c_1^R + \cdots + c_{n-1}^R\right) - \ln\left(c_1^L + \cdots + c_{n-1}^L\right)}\phi^R,\\
\phi_0^{b,r} = \phi_0^{b,m} = \phi_0^b &= \frac{\ln\left(c_1^R + \cdots + c_{n-1}^R\right) - \ln\left(c_{10}^b + \cdots + c_{n-1,0}^b\right)}{\ln\left(c_1^R + \cdots + c_{n-1}^R\right) - \ln\left(c_1^L + \cdots + c_{n-1}^L\right)}\phi^L\\
&+ \frac{\ln\left(c_{10}^b + \cdots + c_{n-1,0}^b\right) - \ln\left(c_1^L + \cdots + c_{n-1}^L\right)}{\ln\left(c_1^R + \cdots + c_{n-1}^R\right) - \ln\left(c_1^L + \cdots + c_{n-1}^L\right)}\phi^R,
\end{aligned} \tag{3.14}$$

$$J_{10}+\cdots+J_{n-1,0}=\frac{c_1^L+\cdots+c_{n-1}^L-\left(c_1^R+\cdots+c_{n-1}^R\right)}{H(1)\left[\ln\left(c_1^L+\cdots+c_{n-1}^L\right)-\ln\left(c_1^R+\cdots+c_{n-1}^R\right)\right]}\times\left[z\bar{V}+\ln\left(L_1+\cdots+L_{n-1}\right)-\ln\left(R_1+\cdots+R_{n-1}\right)\right],$$

$$J_{n0}=\frac{c_n^L-c_n^R}{H(1)\left(\ln c_n^L-\ln c_n^R\right)}\left(z_n\bar{V}+\ln L_n-\ln R_n\right),$$

$$J_{i0}=\frac{c_i^R-c_i^L\mathrm{e}^{z\left(\phi^L-\phi^R\right)}}{c_1^R+\cdots+c_{n-1}^R-\left(c_1^L+\cdots+c_{n-1}^L\right)\mathrm{e}^{z\left(\phi^L-\phi^R\right)}}\left(J_{10}+\cdots+J_{n-1,0}\right),$$

$$c_{i0}^a=\mathrm{e}^{z\left(\bar{V}-\phi_0^a\right)}\frac{L_i\left(R_1+\cdots+R_{n-1}\right)-R_i\left(L_1+\cdots+L_{n-1}\right)}{R_1+\cdots+R_{n-1}-\left(L_1+\cdots+L_{n-1}\right)\mathrm{e}^{z\bar{V}}}+\frac{\left(R_i-L_i\mathrm{e}^{z\bar{V}}\right)\left(c_{10}^a+\cdots+c_{n-1,0}^a\right)}{R_1+\cdots+R_{n-1}-\left(L_1+\cdots+L_{n-1}\right)\mathrm{e}^{z\bar{V}}},$$

$$c_{i0}^b=\mathrm{e}^{z\left(\bar{V}-\phi_0^b\right)}\frac{L_i\left(R_1+\cdots+R_{n-1}\right)-R_i\left(L_1+\cdots+L_{n-1}\right)}{R_1+\cdots+R_{n-1}-\left(L_1+\cdots+L_{n-1}\right)\mathrm{e}^{z\bar{V}}}+\frac{\left(R_i-L_i\mathrm{e}^{z\bar{V}}\right)\left(c_{10}^b+\cdots+c_{n-1,0}^b\right)}{R_1+\cdots+R_{n-1}-\left(L_1+\cdots+L_{n-1}\right)\mathrm{e}^{z\bar{V}}},\ i=1,2,\cdots,n-1.$$

Corollary 3.2. *Under electroneutrality boundary conditions* $z\left(L_1+L_2+\cdots+L_{n-1}\right)=-z_nL_n=L$ *and* $z\left(R_1+R_2+\cdots+R_{n-1}\right)=-z_nR_n=R$, *one has* $c_1^L=L_1,\cdots,c_n^L=L_n$, $c_1^R=R_1,\cdots,c_n^R=R_n$, $\phi^L=\bar{V}$, $\phi^R=0$, *and*

$$\begin{gathered}
z\left(c_{10}^{a,l}+\cdots+c_{n-1,0}^{a,l}\right)=z\left(c_{10}^{a,m}+\cdots+c_{n-1,0}^{a,m}\right)=z\left(c_{10}^a+\cdots+c_{n-1,0}^a\right)=(1-\alpha)L+\alpha R,\\
z\left(c_{10}^a+\cdots+c_{n-1,0}^a\right)=-z_nc_{n0}^a,\\
z\left(c_{10}^{b,r}+\cdots+c_{n-1,0}^{b,r}\right)=z\left(c_{10}^{b,m}+\cdots+c_{n-1,0}^{b,m}\right)=z\left(c_{10}^b+\cdots+c_{n-1,0}^b\right)=(1-\beta)L+\beta R,\\
z\left(c_{10}^b+\cdots+c_{n-1,0}^b\right)=-z_nc_{n0}^b,\\
\phi_0^{a,l}=\phi_0^{a,m}=\phi_0^a=\frac{\ln\left[(1-\alpha)L+\alpha R\right]-\ln R}{\ln L-\ln R}\bar{V}\\
\phi_0^{b,r}=\phi_0^{b,m}=\phi_0^b=\frac{\ln\left[(1-\beta)L+\beta R\right]-\ln R}{\ln L-\ln R}\bar{V}\\
J_{10}+\cdots+J_{n-1,0}=\frac{L-R}{zH(1)(\ln L-\ln R)}\left(z\bar{V}+\ln L-\ln R\right),\\
J_{n0}=\frac{L-R}{-z_nH(1)(\ln L-\ln R)}\left(z_n\bar{V}+\ln L-\ln R\right),\\
J_{i0}=\frac{z\left(R_i-L_i\mathrm{e}^{z\bar{V}}\right)}{R-L\mathrm{e}^{z\bar{V}}}\left(J_{10}+\cdots+J_{n-1,0}\right),
\end{gathered}\tag{3.15}$$

$$c_{i0}^a = \mathrm{e}^{z\left(\bar{V}-\phi_0^a\right)} \frac{L_i R - R_i L}{R - L\mathrm{e}^{z\bar{V}}} + \frac{z\left(R_i - L_i\mathrm{e}^{z\bar{V}}\right)\left[(1-\alpha)L + \alpha R\right]}{R - L\mathrm{e}^{z\bar{V}}},$$

$$c_{i0}^b = \mathrm{e}^{z\left(\bar{V}-\phi_0^b\right)} \frac{L_i R - R_i L}{R - L\mathrm{e}^{z\bar{V}}} + \frac{z\left(R_i - L_i\mathrm{e}^{z\bar{V}}\right)\left[(1-\beta)L + \beta R\right]}{R - L\mathrm{e}^{z\bar{V}}}, i = 1,2,\cdots,n-1.$$

Proposition 3.3. *First order terms of the solution in Q of* (2.9)-(2.11) *are given by*

$$c_{11}^a + \cdots + c_{n-1,1}^a = \frac{z_n\alpha}{z_n - z}\left(\phi_0^a - \phi_0^b\right) + \frac{1}{2\left(z_n - z\right)},$$

$$c_{11}^b + \cdots + c_{n-1,1}^b = -\frac{z_n(1-\beta)}{z_n - z}\left(\phi_0^a - \phi_0^b\right) + \frac{1}{2\left(z_n - z\right)},$$

$$c_{n1}^a = -\frac{z\alpha}{z_n - z}\left(\phi_0^a - \phi_0^b\right) - \frac{1}{2\left(z_n - z\right)},$$

$$c_{n1}^b = \frac{z(1-\beta)}{z_n - z}\left(\phi_0^a - \phi_0^b\right) - \frac{1}{2\left(z_n - z\right)},$$

$$\begin{aligned} \phi_1^a = {} & \frac{(1+z\lambda)(1+z_n\lambda)\left[c_{10}^a + \cdots + c_{n-1,0}^a - \left(c_{10}^b + \cdots + c_{n-1,0}^b\right)\right]}{z\left(z - z_n\right)\left(c_{10}^a + \cdots + c_{n-1,0}^a\right)\left(c_{10}^b + \cdots + c_{n-1,0}^b\right)} \\ & \times \frac{\ln\left(c_1^L + \cdots + c_{n-1}^L\right) - \ln\left(c_{10}^a + \cdots + c_{n-1,0}^a\right)}{\ln\left(c_1^L + \cdots + c_{n-1}^L\right) - \ln\left(c_1^R + \cdots + c_{n-1}^R\right)} \\ & + \frac{1}{2z\left(z - z_n\right)\left(c_{10}^a + \cdots + c_{n-1,0}^a\right)} + \frac{z_n\alpha\left(\phi_0^b - \phi_0^a\right)\lambda}{\left(z - z_n\right)\left(c_{10}^a + \cdots + c_{n-1,0}^a\right)}, \\ \phi_1^b = {} & \frac{(1+z\lambda)(1+z_n\lambda)\left[c_{10}^a + \cdots + c_{n-1,0}^a - \left(c_{10}^b + \cdots + c_{n-1,0}^b\right)\right]}{z\left(z - z_n\right)\left(c_{10}^a + \cdots + c_{n-1,0}^a\right)\left(c_{10}^b + \cdots + c_{n-1,0}^b\right)} \\ & \times \frac{\ln\left(c_1^R + \cdots + c_{n-1}^R\right) - \left(\ln c_{10}^b + \cdots + \ln c_{n-1,0}^b\right)}{\ln\left(c_1^L + \cdots + c_{n-1}^L\right) - \ln\left(c_1^R + \cdots + c_{n-1}^R\right)} \\ & + \frac{1}{2z\left(z - z_n\right)\left(c_{10}^b + \cdots + c_{n-1,0}^b\right)} + \frac{z_n(1-\beta)\left(\phi_0^a - \phi_0^b\right)\lambda}{\left(z - z_n\right)\left(c_{10}^b + \cdots + c_{n-1,0}^b\right)}, \\ c_{i1}^a = {} & -z\phi_1^a\mathrm{e}^{z\left(\bar{V}-\phi_0^a\right)} \frac{L_i\left(R_1 + \cdots + R_{n-1}\right) - R_i\left(L_1 + \cdots + L_{n-1}\right)}{R_1 + \cdots + R_{n-1} - \left(L_1 + \cdots + L_{n-1}\right)\mathrm{e}^{z\bar{V}}} \\ & + \frac{\left(R_i - L_i\mathrm{e}^{z\bar{V}}\right)\left(c_{11}^a + \cdots + c_{n-1,1}^a\right)}{R_1 + \cdots + R_{n-1} - \left(L_1 + \cdots + L_{n-1}\right)\mathrm{e}^{z\bar{V}}}, \\ c_{i1}^b = {} & -z\phi_1^b\mathrm{e}^{z\left(\bar{V}-\phi_0^b\right)} \frac{L_i\left(R_1 + \cdots + R_{n-1}\right) - R_i\left(L_1 + \cdots + L_{n-1}\right)}{R_1 + \cdots + R_{n-1} - \left(L_1 + \cdots + L_{n-1}\right)\mathrm{e}^{z\bar{V}}} \\ & + \frac{\left(R_i - L_i\mathrm{e}^{z\bar{V}}\right)\left(c_{11}^b + \cdots + c_{n-1,1}^b\right)}{R_1 + \cdots + R_{n-1} - \left(L_1 + \cdots + L_{n-1}\right)\mathrm{e}^{z\bar{V}}}, i = 1,2,\cdots,n-1, \end{aligned} \tag{3.16}$$

and

$$J_{11}+\cdots+J_{n-1,1}=\frac{A\left[1+(1-B)z_n\lambda\right](1+z\lambda)}{(z-z_n)H(1)},$$
$$J_{n1}=\frac{A\left[1+(1-B)z\lambda\right](1+z_n\lambda)}{(z_n-z)H(1)}, \quad (3.17)$$
$$J_{i1}=\frac{\left[c_i^R-c_i^L\mathrm{e}^{z(\phi^L-\phi^R)}\right](J_{11}+\cdots+J_{n-1,1})}{c_1^R+\cdots+c_{n-1}^R-(c_1^L+\cdots+c_{n-1}^L)\mathrm{e}^{z(\phi^L-\phi^R)}}, i=1,2,\cdots,n-1,$$

where

$$\lambda=\frac{\phi^L-\phi^R}{\ln(c_1^L+\cdots+c_{n-1}^L)-\ln(c_1^R+\cdots+c_{n-1}^R)},$$
$$A=\frac{c_{10}^b+\cdots+c_{n-1,0}^b-(c_{10}^a+\cdots+c_{n-1,0}^a)}{(c_{10}^a+\cdots+c_{n-1,0}^a)(c_{10}^b+\cdots+c_{n-1,0}^b)}\times\frac{c_1^L+\cdots+c_{n-1}^L-(c_1^R+\cdots+c_{n-1}^R)}{\ln(c_1^L+\cdots+c_{n-1}^L)-\ln(c_1^R+\cdots+c_{n-1}^R)}, \quad (3.18)$$
$$B=\frac{\ln(c_{10}^b+\cdots+c_{n-1,0}^b)-\ln(c_{10}^a+\cdots+c_{n-1,0}^a)}{A}.$$

4. Effects of Small Permanent Charge

In this section, the effects of small permanent charges on individual fluxes are analyzed under electroneutrality conditions $z(L_1+L_2+\cdots+L_{n-1})=-z_nL_n=L$ and $z(R_1+R_2+\cdots+R_{n-1})=-z_nR_n=R$.

For $|Q|$ small, the individual flux $\mathcal{J}_i$ of the *i*th ion species are

$$\mathcal{J}_i=D_iJ_{i0}+D_iJ_{i1}Q+O(Q^2), i=1,2,\cdots,n.$$

From Proposition 3.3, it follows that

$$J_{11}+\cdots+J_{n-1,1}=(z\bar{V}+\ln L-\ln R)\left(\frac{A\left[(1-B)z_n\bar{V}+\ln L-\ln R\right]}{(z-z_n)H(1)(\ln L-\ln R)^2}\right),$$
$$J_{n1}=(z_n\bar{V}+\ln L-\ln R)\left(\frac{A\left[(1-B)z\bar{V}+\ln L-\ln R\right]}{(z_n-z)H(1)(\ln L-\ln R)^2}\right), \quad (4.1)$$
$$J_{i1}=\frac{z(R_i-L_i\mathrm{e}^{z\bar{V}})}{R-L\mathrm{e}^{z\bar{V}}}(J_{11}+\cdots+J_{n-1,1}), i=1,2,\cdots,n-1.$$

where, in terms of α,β defined in (3.13), A and B defined in (3.18) become

$$A(L,R)=-\frac{(\beta-\alpha)(L-R)^2}{\left[(1-\alpha)L+\alpha R\right]\left[(1-\beta)L+\beta R\right](\ln L-\ln R)}, \quad (4.2)$$
$$B(L,R)=\frac{\ln\left[(1-\beta)L+\beta R\right]-\ln\left[(1-\alpha)L+\alpha R\right]}{A}.$$

Remark 4.1. *Note that* $\lim_{\bar{V}\to\frac{1}{z}\ln\frac{R}{L}}\frac{z\bar{V}+\ln L-\ln R}{R-L\mathrm{e}^{z\bar{V}}}=-\frac{1}{R}\neq 0$, *it means that*

$\bar{V}=\frac{1}{z}\ln\frac{R}{L}$ *is not a zero point of* J_{i1}, *also, it can be easily seen that there are only two values* $\bar{V}_1=\frac{1}{z}\ln\frac{R_i}{L_i}$ *and* $\bar{V}_2=\ln\frac{\ln R-\ln L}{z_n(1-B)}$ *such that* $J_{i1}=0, i=1,2,\cdots,n-1$.

Remark 4.2. *Note that* $\lim_{\bar{V}\to\pm\infty}\frac{J_{i1}}{\bar{V}^2}=\frac{z^2 z_n L_i A(1-B)}{(z-z_n)LH(1)(\ln L-\ln R)^2}$, $i=1,2,\cdots,n-1$, *where the sign of* $A(1-B)$ *has been analyzed by in* [22].

Remark 4.3. J_{n1} *in* (3.3) *is exactly similar to* J_{21} *in* [22], *whose properties have been analyzed in* [22].

Let $\max\{\bar{V}_1,\bar{V}_2\}$ denote the larger value between $\bar{V}_1$ and $\bar{V}_2$, $\min\{\bar{V}_1,\bar{V}_2\}$ denote the smaller value between $\bar{V}_1$ and $\bar{V}_1$.

Theorem 4.4. (i) *If* $A(1-B)<0$, *for* $\bar{V}>\max\{\bar{V}_1,\bar{V}_2\}$ *or* $\bar{V}<\min\{\bar{V}_1,\bar{V}_2\}$, *then* $J_{i1}>0$; *for* $\min\{\bar{V}_1,\bar{V}_2\}<\bar{V}<\max\{\bar{V}_1,\bar{V}_2\}$, *then* $J_{i1}<0, i=1,2,\cdots,n-1$.

(ii) If $A(1-B)>0$, for $\bar{V}>\max\{\bar{V}_1,\bar{V}_2\}$ or $\bar{V}<\min\{\bar{V}_1,\bar{V}_2\}$, then $J_{i1}<0$; for $\min\{\bar{V}_1,\bar{V}_2\}<\bar{V}<\max\{\bar{V}_1,\bar{V}_2\}$, then $J_{i1}>0, i=1,2,\cdots,n-1$.

Proof. If $A(1-B)<0$, based on Remark 4.2, then it follows that

$$\lim_{\bar{V}\to\pm\infty}\frac{J_{i1}}{\bar{V}^2}=\frac{z^2 z_n L_i A(1-B)}{(z-z_n)LH(1)(\ln L-\ln R)^2}>0, i=1,2,\cdots,n-1.$$

By Remark 4.1, there are only two values $\bar{V}_1$ and $\bar{V}_2$ such that

$$J_{i1}(\bar{V}_1)=J_{i1}(\bar{V}_2)=0, i=1,2,\cdots,n-1,$$

therefore the statement (i) can be obtained. Similarly, the statement (ii) can be also proved.

Theorem 4.5. *If* $A(1-B)<0$, *for* $\bar{V}>\bar{V}_2$, *then* $J_{i0}J_{i1}>0$; *for* $\bar{V}<\bar{V}_2$, *then* $J_{i0}J_{i1}<0, i=1,2,\cdots,n-1$.

If $A(1-B)>0$, for $\bar{V}>\bar{V}_2$, then $J_{i0}J_{i1}<0$; for $\bar{V}<\bar{V}_2$, then $J_{i0}J_{i1}>0, i=1,2,\cdots,n-1$.

Equivalently, for $A(1-B)<0$ *and* $\bar{V}>\bar{V}_2$, *small positive Q strengthens the individual flux* $|\mathcal{J}_i|$; *for* $A(1-B)<0$ *and* $\bar{V}<\bar{V}_2$, *small positive Q reduces the individual flux* $|\mathcal{J}_i|, i=1,2,\cdots,n-1$.

For $A(1-B)>0$ *and* $\bar{V}>\bar{V}_2$, *small positive Q reduces the individual flux* $|\mathcal{J}_i|$; *for* $A(1-B)>0$ *and* $\bar{V}<\bar{V}_2$, *small positive Q strengthens the individual flux* $|\mathcal{J}_i|, i=1,2,\cdots,n-1$.

Proof. Based on Corollary 3.2 and Equation (4.1), one has

$$\begin{aligned} J_{i0}&=\frac{z\left(R_i-L_i e^{z\bar{V}}\right)}{R-Le^{z\bar{V}}}\frac{L-R}{zH(1)(\ln L-\ln R)}\left(z\bar{V}+\ln L-\ln R\right),\\ J_{i1}&=\frac{z\left(R_i-L_i e^{z\bar{V}}\right)}{R-Le^{z\bar{V}}}\left(z\bar{V}+\ln L-\ln R\right)\left(\frac{A\left[(1-B)z_n\bar{V}+\ln L-\ln R\right]}{(z-z_n)H(1)(\ln L-\ln R)^2}\right). \end{aligned} \tag{4.3}$$

From (4.3), the statement can be obtained. □

5. Conclusion

In this paper, a stationary one-dimensional Poisson-Nernst-Planck model with permanent charge is studied under the assumption that $n-1$ positively charged ion species have the same valence and the permanent charge is small. By expanding an singular orbit of Poisson-Nernst-Planck model (1.1) in small $|Q|$, the explicit formulae for J_{i0} and J_{i1} are obtained. The signs of J_{i1} are discussed in Theorem 4.4, which indicates that as $|\bar{V}|$ is sufficiently large, fixing the other parameters, J_{i1} behaves like $\bar{V}^2$. The effects of small permanent charges on individual flux are investigated in Theorem 4.5, which means that small Q can strengthen or reduce the individual flux under suitable conditions. However, for $|Q|$ that is not small, the regular perturbation analysis does not work, so it seems not easy to analyze the effects of permanent charges on individual flux by directly using (2.9)-(2.11).

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Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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