

EXISTENCE AND UNIQUENESS OF STEADY-STATE SOLUTIONS FOR AN ELECTROCHEMISTRY MODEL

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ABSTRACT. We present a simple proof for the existence and uniqueness of steady-state solutions to an electrochemistry model with multiple species.

In this note we give a simple proof for the existence and uniqueness of steady-state solutions for an electrochemistry model with multiple species. The equations in such a model have been the subject of a series of papers by Choi and Lui (see [1, 2, 3, 4] and references therein). In the steady-state, the species concentrations can be expressed in terms of the electrical potential φ , and thus the problem is equivalent to solving a single integro-differential equation for φ (see, e.g., [4] for details). Let Ω be an open, bounded $C^{0,1}$ domain in R^n ($n = 1, 2$ or 3) and $\partial\Omega = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$ where Γ_1 and Γ_2 are relatively closed. Then the equation for the potential is

$$(1) \quad -\epsilon \Delta \varphi = \sum_{i=1}^m \frac{z_i C_i e^{-z_i \varphi(x)}}{\int_{\Omega} e^{-z_i \varphi(y)} dy} + Q(x)$$

with boundary conditions

$$(2) \quad \varphi = -\alpha/2 \text{ on } \Gamma_1, \quad \varphi = \alpha/2 \text{ on } \Gamma_2 \text{ and } \frac{\partial \varphi}{\partial \nu} = 0 \text{ on } \Gamma_3.$$

Here $Q(x) \in L^2(\Omega)$ represents a possible background charge concentration, and $\epsilon > 0$ is the permittivity. The constant $C_i > 0$ is the prescribed mass for the i th species, and z_i is its signed charge. $\alpha > 0$ is the applied potential difference between the two electrodes. (For convenience, we have translated φ by the constant $\alpha/2$ from the formulation in [4].) The existence/uniqueness of φ in this problem has been shown by Choi and Lui for the case $n = 1$ in [1, 2] and for the case $n \geq 2$ in [3], both under the assumptions that $Q \equiv 0$ and $\sum z_i C_i = 0$. These assumptions were then removed in [4]. Their arguments varied from case to case, and were quite involved, especially for the uniqueness. The proof that we will present in this note is simple and valid for all cases, and provides an explicit L^∞ bound for the solution. In particular, our argument for uniqueness is short and elementary.

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We begin with the weak form of the problem. A weak solution to (1)-(2) is defined as a function $\varphi \in H^1(\Omega) \cap L^\infty(\Omega)$ with $\varphi = -\alpha/2$ on Γ_1 and $\varphi = \alpha/2$ on Γ_2 that satisfies

$$(3) \quad \epsilon \langle \nabla \varphi, \nabla \psi \rangle = \langle f(\varphi) + Q, \psi \rangle$$

for all $\psi \in V = \{\psi \in H^1(\Omega) : \psi = 0 \text{ on } \Gamma_1 \cup \Gamma_2\}$, where we set

$$(4) \quad f(\varphi) = \sum_{i=1}^m \frac{z_i C_i e^{-z_i \varphi}}{\int_{\Omega} e^{-z_i \varphi(y)} dy}.$$

Here $\langle \cdot, \cdot \rangle$ denotes the usual L^2 inner product on Ω .

To show existence, we construct the solution map \mathcal{T} as follows. For each $\tilde{\varphi} \in X = \{\phi \in L^2(\Omega) : |\phi(x)| \leq k\}$ ($k \geq \alpha/2$ is to be chosen below), define $\varphi = \mathcal{T}\tilde{\varphi}$, where $\varphi \in H^1(\Omega)$ with $\varphi = -\alpha/2$ on Γ_1 and $\varphi = \alpha/2$ on Γ_2 is the unique solution to

$$(5) \quad \epsilon \langle \nabla \varphi, \nabla \psi \rangle = \langle \tilde{f}(\varphi) + Q, \psi \rangle, \quad \psi \in V,$$

where

$$\tilde{f}(\varphi) = \sum_{i=1}^m \frac{z_i C_i e^{-z_i \varphi}}{\int_{\Omega} e^{-z_i \tilde{\varphi}(y)} dy}.$$

The unique existence of such φ is standard since $\tilde{f}(\varphi)$ is monotone decreasing in φ and hence the unique solution φ is the minimizer of the convex, lower-semicontinuous functional

$$J(\varphi) = \frac{\epsilon}{2} |\nabla \varphi|_2^2 + \sum_{i=1}^m C_i \frac{\int_{\Omega} e^{-z_i \varphi(y)} dy}{\int_{\Omega} e^{-z_i \tilde{\varphi}(y)} dy} - \langle Q, \varphi \rangle$$

in a convex set of $H^1(\Omega)$. Clearly \mathcal{T} is compact due to the compact embedding of H^1 to L^2 , and it can be easily shown that \mathcal{T} is continuous with respect to the L^2 norm. Next we choose k so that \mathcal{T} maps X into itself. Notice that

$$z_i |\Omega| e^{-z_i k} \leq z_i \int_{\Omega} e^{-z_i \tilde{\varphi}(y)} dy \leq z_i |\Omega| e^{z_i k}$$

and thus

$$\frac{1}{|\Omega|} \sum_{i=1}^m z_i C_i e^{-z_i(\varphi+k)} \leq \tilde{f}(\varphi) \leq \frac{1}{|\Omega|} \sum_{i=1}^m z_i C_i e^{-z_i(\varphi-k)}.$$

Hence by setting $\psi = \varphi_k \equiv (\varphi - k)^+ \in V$ in (5) we obtain

$$(6) \quad \epsilon \langle \nabla \varphi_k, \nabla \varphi_k \rangle = \langle \tilde{f}(\varphi) + Q, \varphi_k \rangle \leq \langle q, \varphi_k \rangle,$$

where

$$(7) \quad q(x) = \frac{1}{|\Omega|} \sum_{i=1}^m z_i C_i + Q(x).$$

Here q measures the total charge concentration in the system. Under the assumptions in [1, 2, 3], $q \equiv 0$ and the usual maximum principle applies to yield $|\varphi| \leq \alpha/2$. In the general case when $q \not\equiv 0$, we apply a more general version of the maximum

principle, which is stated in Lemma A below. From this result, inequality (6) yields that $\varphi(x) \leq k^*$ for all $x \in \Omega$, where

$$(8) \quad k^* = \frac{\alpha}{2} + \frac{4\alpha_6^2 |\Omega|^{1/6}}{\epsilon} |q|_2.$$

Similarly, by choosing $\psi = (\varphi + k)^- = -(-\varphi - k)^+ \in V$ in (5) we can show that $-\varphi(x) \leq k^*$. Thus, we have established the L^∞ bounds for $\varphi = \mathcal{T}\tilde{\varphi}$:

$$(9) \quad |\varphi(x)| \leq k^* \quad \text{for } x \in \Omega.$$

Therefore, when we choose $k = k^*$ in the definition of X , the solution map \mathcal{T} is from X into X . Hence, by Schauder's fixed point theorem, \mathcal{T} has a fixed point in X , which is a solution to (3).

As for uniqueness, it suffices to simply show that f in (4) is monotone decreasing:

$$\langle f(\varphi) - f(\hat{\varphi}), \varphi - \hat{\varphi} \rangle \leq 0$$

for all admissible φ and $\hat{\varphi}$. In fact *each* term in f is monotone decreasing. To see this, let

$$\delta_i = -\ln \left(\int_{\Omega} e^{-z_i \varphi(y)} dy \right) \quad \text{or} \quad e^{-\delta_i} = \int_{\Omega} e^{-z_i \varphi(y)} dy$$

and similarly for $\hat{\delta}_i$. Then

$$\frac{e^{-z_i \varphi(x)}}{\int_{\Omega} e^{-z_i \varphi(y)} dy} = e^{\delta_i - z_i \varphi(x)}, \quad \frac{e^{-z_i \hat{\varphi}(x)}}{\int_{\Omega} e^{-z_i \hat{\varphi}(y)} dy} = e^{\hat{\delta}_i - z_i \hat{\varphi}(x)}$$

and

$$\int_{\Omega} e^{\delta_i - z_i \varphi(x)} dx = \int_{\Omega} e^{\hat{\delta}_i - z_i \hat{\varphi}(x)} dx = 1.$$

Hence $\langle e^{\delta_i - z_i \varphi(x)} - e^{\hat{\delta}_i - z_i \hat{\varphi}(x)}, c \rangle = 0$ for any constant c . Therefore

$$\begin{aligned} & z_i C_i \left\langle \frac{e^{-z_i \varphi(x)}}{\int_{\Omega} e^{-z_i \varphi(y)} dy} - \frac{e^{-z_i \hat{\varphi}(x)}}{\int_{\Omega} e^{-z_i \hat{\varphi}(y)} dy}, \varphi(x) - \hat{\varphi}(x) \right\rangle \\ &= C_i \langle e^{\delta_i - z_i \varphi(x)} - e^{\hat{\delta}_i - z_i \hat{\varphi}(x)}, z_i \varphi(x) - z_i \hat{\varphi}(x) \rangle \\ &= C_i \langle e^{\delta_i - z_i \varphi(x)} - e^{\hat{\delta}_i - z_i \hat{\varphi}(x)}, (z_i \varphi(x) - z_i \hat{\varphi}(x)) - (\delta_i - \hat{\delta}_i) \rangle \\ &= -C_i \langle e^{\delta_i - z_i \varphi(x)} - e^{\hat{\delta}_i - z_i \hat{\varphi}(x)}, (\delta_i - z_i \varphi(x)) - (\hat{\delta}_i - z_i \hat{\varphi}(x)) \rangle \\ &\leq 0 \end{aligned}$$

since the exponential function is increasing and $C_i > 0$. Therefore f is monotone decreasing in φ and thus we easily obtain the uniqueness of weak solutions.

We complete our presentation by proving the lemma that is used to establish the L^∞ bounds (9). We denote by α_6 the constant in the Poincaré inequality $|\psi|_6 \leq \alpha_6 |\nabla \psi|_2$ for all $\psi \in V$.

Lemma A. Suppose $\phi \in H^1(\Omega)$, and $\phi_\tau = (\phi - \tau)^+ \in V$ for $\tau \geq \bar{\tau}$. If ϕ_τ satisfies

$$\langle \nabla \phi_\tau, \nabla \phi_\tau \rangle \leq \langle F, \phi_\tau \rangle$$

for some $F \in L^2(\Omega)$, then

$$\phi(x) \leq \bar{\tau} + 4\alpha_6^2 |\Omega|^{1/6} |F|_2.$$

Proof. Let $\Omega_\tau = \{x \in \Omega : \phi(x) > \tau\}$. By the Poincaré and the Hölder inequalities,

$$\alpha_6^{-2} |\phi_\tau|_6^2 \leq |\nabla \phi_\tau|_2^2 \leq \langle F, \phi_\tau \rangle \leq |F|_2 |\phi_\tau|_6 |\Omega_\tau|^{1/3},$$

that is,

$$|\phi_\tau|_6 \leq \alpha_6^2 |F|_2 |\Omega_\tau|^{1/3}.$$

For $\hat{\tau} > \tau \geq \bar{\tau}$,

$$|\phi_\tau|_6^6 \geq \int_{\Omega_{\hat{\tau}}} |\phi_\tau|^6 dx \geq (\hat{\tau} - \tau)^6 |\Omega_{\hat{\tau}}|.$$

Therefore

$$|\Omega_{\hat{\tau}}| \leq (\alpha_6^2 |F|_2)^6 (\hat{\tau} - \tau)^{-6} |\Omega_\tau|^2.$$

Then by applying an elementary lemma (see [5, Lemma 2.9]) to the non-increasing function $|\Omega_\tau|$ of τ , we obtain

$$|\Omega_\tau| = 0 \quad \text{for } \tau \geq \tau^*,$$

where

$$\tau^* = \bar{\tau} + 4\alpha_6^2 |\Omega|^{1/6} |F|_2.$$

Therefore we have $\phi_{\tau^*} = 0$ a.e. in Ω . Hence $\phi \leq \tau^*$ as stated.

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