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Research Article

On the Existence of a Weak Solution of a Half-Cell Model for PEM Fuel Cells

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A nonlinear boundary value problem (BVP) from the modelling of the transport phenomena in the cathode catalyst layer of a one-dimensional half-cell single-phase model for proton exchange membrane (PEM) fuel cells, derived from the 3D model of Zhou and Liu (2000, 2001), is studied. It is a BVP for a system of three coupled ordinary differential equations of second order. Schauder's fixed point theorem is applied to show the existence of a solution in the Sobolev space H^1.

1. Introduction

The modelling of fuel cells has been an attractive topic in the field of electrochemical theory. In the last decade, models for proton exchange membrane (PEM) fuel cells have been formulated by many scientists (see, e.g., [1]). Among these models, some complicated systems of partial differential equations (PDEs) were constructed from principles of fluid mechanics, electrostatics, and heat transfers; however, most of them were solved by numerical simulations only. We are interested in the mathematical analysis of the system of differential equations and the discussion is restricted on the transport phenomenon of a single-phase model given by [2]. The more complicated two-phase models, like those mentioned in [1, 3], are not in the scope of this paper.

In [4], by reducing space variables to one dimension and making several assumptions, a system of PDEs in [5] was simplified to a boundary value problem (BVP) for a linear system of decoupled ordinary differential equations (ODEs), and an exact solution was constructed. In [6], a 1D half-cell model reduced from [5] is considered; that model is a BVP for a nonlinear system of three ODEs of second order which are no longer decoupled and it seems to be hard to find an exact solution. By Schaefer's fixed point theorem, the study in [6]

is able to show the existence of a solution in the space of continuously twice differentiable functions. In this paper, motivated by [4, 6], we will derive a 1D half-cell model from the 3D model of [2]; it is still a BVP for a nonlinear system of three ODEs of second order; however, the nonlinearity is different from that of [6] and an alternative strategy will be applied; namely, a weak formulation of the BVP will be considered. In this weak formulation, the function space is replaced by the Sobolev space H^1 and an iteration process associated with Schauder's fixed point theorem will be adopted. The result of this paper indicates a direction of attacking the complicated system of PDEs for the modelling of PEM fuel cells.

Now, we briefly describe the contents of this paper. In Section 2, the governed equations and boundary conditions in the cathode catalyst layer for the 1D half-cell model of PEM fuel cells are derived. In Section 3, the weak form of a linear generalized Neumann problem is described. Existence and uniqueness of the generalized Neumann problem is guaranteed by the Lax-Milgram theorem and it will be shown that the solution for the linear problem has an *a priori* bound. In Section 4, Schauder's fixed point theorem is applied to prove the existence of an H^1 solution for the nonlinear system of ODEs.

2. The Model

In this section, we will reduce a 3D model of Zhou and Liu [2, 7] to a 1D half-cell model. This 3D model was a modification of the 2D model given by Gurau et al. [5], so the derivation of the 1D model is quite the same with what we did in [6], we describe the derivation here for the reader's convenience.

Recall (e.g., see [8]) the species equations are

$$0 = \varepsilon\rho D_k^{\text{eff}}\nabla^2 Y_k + \begin{cases} 0, & \text{channel and diffusion layers,} \\ \varepsilon\rho S_k, & \text{catalyst layer,} \end{cases} \tag{2.1}$$

where Y_k is the concentration of kth component gas mixture, and D_k^{eff} is the effective diffusivity of the kth component in the gas mixture, which is given by

$$D_k^{\text{eff}} = \begin{cases} D_k, & \text{channel,} \\ D_k\varepsilon^{1.5}, & \text{porous media.} \end{cases} \tag{2.2}$$

At the cathode, the mass generation source terms S_k for oxygen, water, and protons are $j_c/(2Fc), -j_c/(2Fc)$, and $j_c/(Fc)$, respectively. At the anode, the source terms for hydrogen molecules and protons are $-j_a/(2Fc)$ and j_a/Fc, where j_a and j_c are the transfer current density at anode and cathode, which represent the reaction rates. Note that the value of j_c

is negative and j_a is positive. The relationships between j_a, j_c and the species concentration (Y_{H_2} and Y_{O_2}) are given by the Butler-Volmer equations

$$\begin{aligned} j_a &= \left(\overline{a} i_0^{\text{ref}}\right)_a \left(\frac{Y_{H_2}}{Y_{H_2}^{\text{ref}}}\right)^{1/2} \left[\exp\left(\frac{\alpha^a F}{RT}\eta_a\right) - \exp\left(-\frac{(1-\alpha^a)F}{RT}\eta_a\right)\right], \\ j_c &= \left(\overline{a} i_0^{\text{ref}}\right)_c \left(\frac{Y_{O_2}}{Y_{O_2}^{\text{ref}}}\right) \left[\exp\left(\frac{\alpha^c F}{RT}\eta_c\right) - \exp\left(-\frac{(1-\alpha^c)F}{RT}\eta_c\right)\right], \end{aligned} \tag{2.3}$$

where $\overline{a}$ is the active catalyst surface area per unit volume of the catalyst layer, i_0^{ref} is the exchange current density under the reference conditions, T is the absolute temperature, R is the universal gas constant, α^a and α^c are symmetric factors, and η_a and η_c are the corresponding overpotentials.

The energy equation is

$$0 = k_{\text{eff}} \nabla^2 T + \begin{cases} 0, & \text{channels and diffusion layers,} \\ Q, & \text{catalyst layer and membrane,} \end{cases} \tag{2.4}$$

with

$$k_{\text{eff}} = \begin{cases} k_g, & \text{channels,} \\ -2k_s + \dfrac{1}{\varepsilon/(2k_s + k_g) + (1-\varepsilon)/3k_s}, & \text{porous media,} \end{cases} \tag{2.5}$$

where k_g is the thermal conductivity of the gas while k_s is the thermal conductivity of the solid matrix of the porous media. The heat generation rates Q in different regions are given by

$$Q = \begin{cases} j_a \cdot \eta_a + \dfrac{i^2}{\sigma_{\text{cl}}}, & \text{anode catalyst layer,} \\ \dfrac{i^2}{\sigma_m}, & \text{membrane} \\ j_c \cdot \eta_c + \dfrac{i^2}{\sigma_{\text{cl}}}, & \text{cathode catalyst layer.} \end{cases} \tag{2.6}$$

Note that this is a main difference between the 3D model of [2] and the 2D model of [5].

The phase potential satisfies

$$\nabla \cdot (\sigma \nabla \phi) = \begin{cases} j_c, & \text{cathode catalyst layer,} \\ 0, & \text{membrane,} \\ j_a, & \text{anode catalyst layer,} \end{cases} \tag{2.7}$$

where ϕ is the phase potential, and σ is the ionic/electric conductivity which depends on T:

$$\sigma(T) = \frac{\eta_c}{k_{\text{eff}} l_{\text{cl}}}(0.005139\lambda - 0.00326)\exp\left[1268\left(\frac{1}{303} - \frac{1}{T}\right)\right]. \tag{2.8}$$

The current density is given by

$$i = -\sigma\nabla\phi. \tag{2.9}$$

Next, we assume that T, Φ, Y_k depend on one space variable and restrict to the cathode side of the catalyst layer, following [4], only one species (the oxygen) (i.e., $k = 1$, and let $Y_1 = Y$.) For simplicity, the derivative with respect to x is denoted by $' = d/dx$.

From (2.4), the equation for energy becomes

$$T'' - k(T)Y + \lambda f(T)(\Phi')^2 = 0, \quad x \in (a,b), \tag{2.10}$$

where Φ is the catalyst layer phase potential, T is the energy, and Y is the oxygen mass fraction; $f(T) \in C_b^1(\mathbb{R})$ is a regularization of $1/\lambda \cdot (\sigma(T)/k_{\text{eff}})$ away from $T = 0$ so that $f \geq \delta_1 > 0$ is required, and $k(T) \in C_b^1(\mathbb{R})$ is a regularization of

$$-\frac{\eta_c}{k_{\text{eff}}}\left(\bar{a}i_0^{\text{ref}}\right)_c\left(\frac{1}{Y_{O_2}^{\text{ref}}}\right)\left[\exp\left(\frac{\alpha^c F}{RT}\eta_c\right) - \exp\left(-\frac{(1-\alpha^c)F}{RT}\eta_c\right)\right]. \tag{2.11}$$

By (2.7), in the cathode catalyst layer, we have the following equation for the phase potential

$$\left(f(T)\Phi'\right)' + g(T)Y = 0, \quad x \in (a,b), \tag{2.12}$$

where $g(T) \in C_b^1(\mathbb{R})$ is a regularization of

$$-\frac{\eta_c j_c}{k_{\text{eff}} l_{\text{cl}} Y} = -\frac{\eta_c}{k_{\text{eff}} l_{\text{cl}}}\left(\bar{a}i_0^{\text{ref}}\right)_c\left(\frac{1}{Y_{O_2}^{\text{ref}}}\right)\left[\exp\left(\frac{\alpha^c F}{RT}\eta_c\right) - \exp\left(-\frac{(1-\alpha^c)F}{RT}\eta_c\right)\right]. \tag{2.13}$$

And for the oxygen mass fraction, via (2.2), we obtain the equation in the cathode catalyst layer:

$$Y'' - h(T)Y = 0, \quad x \in (a,b), \tag{2.14}$$

where $h(T) \in C_b^1(\mathbb{R})$ is a regularization of

$$-\frac{j_c}{2FcD_k^{\text{eff}}Y} = \frac{-1}{D_k^{\text{eff}}} \cdot \frac{1}{2Fc} \cdot \left(\bar{a}i_0^{\text{ref}}\right)_c\left(\frac{1}{Y_{O_2}^{\text{ref}}}\right)\left[\exp\left(\frac{\alpha^c F}{RT}\eta_c\right) - \exp\left(-\frac{(1-\alpha^c)F}{RT}\eta_c\right)\right]. \tag{2.15}$$

We can assume that $h \geq \delta_2 > 0$. The boundary conditions for this 1D model are

$$\begin{gathered}\mu_1 T(a) - \mu_2 T'(a) = 1, \quad T'(b) = 0, \\ \Phi(b) + \beta f(T(b)) \cdot \Phi'(b) = 0, \quad \Phi'(a) = 0, \\ \alpha_1 Y(a) - \alpha_2 Y'(a) = 1, \quad Y'(b) = 0,\end{gathered} \tag{2.16}$$

where $\mu_1, \mu_2, \alpha_1, \alpha_2, \beta > 0$. It is convenient to let $l = b - a$ in the following discussions.

Note that the derivation of these boundary conditions can be found in [6]; therefore we do not repeat here.

Now, we formulate a weak form of the boundary value problem (2.10)~(2.16).

Let $\Omega = (a, b)$ and consider $(T, \Phi, Y) \in (H^1(\Omega))^3$; thus it is a *weak solution* of (2.10)~(2.16) if the following equations hold:

$$\begin{gathered}-\left(\frac{\mu_1 T(a) - 1}{\mu_2}\right) \cdot \varphi(a) - \int_a^b T' \cdot \varphi' dx = \int_a^b k(T) Y \varphi dx - \lambda \int_a^b f(T) (\Phi')^2 \varphi dx, \quad \forall \varphi \in H^1(\Omega), \\ -\frac{1}{\beta} \Phi(b) \cdot \varphi(b) - \int_a^b f(T) (\Phi') \cdot \varphi' dx + \int_a^b g(T) Y \varphi dx = 0, \quad \forall \varphi \in H^1(\Omega), \\ -\left(\frac{\alpha_1 Y(a) - 1}{\alpha_2}\right) \cdot \varphi(a) - \int_a^b Y' \cdot \varphi' dx = \int_a^b h(T) Y \varphi dx, \quad \forall \varphi \in H^1(\Omega).\end{gathered} \tag{2.17}$$

For (2.17), we have the following existence theorem.

Theorem 2.1. *There exists at least one solution* (T, Φ, Y) *of* (2.17) *in* $(H^1(\Omega))^3$.

3. Linear Results

Before we prove Theorem 2.1, some linear results should be proved and we still use the notation (T, Φ, Y) for the solution of the following (weak) linear generalized Neumann problem:

$$-\left(\frac{\alpha_1 Y(a) - 1}{\alpha_2}\right) \cdot \varphi(a) - \int_a^b Y' \cdot \varphi' dx = \int_a^b h(T_*) Y \varphi dx, \quad \forall \varphi \in H^1(\Omega), \tag{3.1}$$

$$-\frac{1}{\beta} \Phi(b) \cdot \varphi(b) - \int_a^b f(T_*) (\Phi') \cdot \varphi' dx + \int_a^b g(T_*) Y_* \varphi dx = 0, \quad \forall \varphi \in H^1(\Omega), \tag{3.2}$$

$$-\left(\frac{\mu_1 T(a) - 1}{\mu_2}\right) \cdot \varphi(a) - \int_a^b T' \cdot \varphi' dx = \int_a^b k(T_*) Y_* \varphi dx - \lambda \int_a^b f(T_*) (\Phi_*')^2 \varphi dx, \quad \forall \varphi \in H^1(\Omega), \tag{3.3}$$

where $T_*, Y_*, \Phi_* \in H^1(\Omega)$. Since the equations for (T, Φ, Y) are decoupled, they can be treated separately.

The existence and uniqueness of the solution for the linear generalized Neumann problem (3.1)~(3.3) is guaranteed by the following Lax-Milgram Theorem (see [9]).

Theorem 3.1 (A theorem on linear monotone operators). *Let $\mathcal{A} : X \to X^*$ be a linear continuous operator on the real Hilbert space X. Suppose that $\mathcal{A}$ is strongly monotone, that is, there is a $c > 0$ such that*

$$\langle \mathcal{A}u, u\rangle \geq c\|u\|^2 \quad \forall u \in X, \tag{3.4}$$

then for each given $\widetilde{b} \in X^*$, the operator equation

$$\mathcal{A}u = \widetilde{b}, \quad u \in X, \tag{3.5}$$

has a unique solution.

Next, we show that the solution for the linear problem has an *a priori* bound which can be shown to be independent of (T_*, Φ_*, Y_*) so that a domain for the iteration process exists.

Theorem 3.2. *Suppose that (Y, Φ, T) is a weak solution for* (3.1)~(3.3)*, then one has*

$$\|Y\|_{H^1(\Omega)} \leq N_1, \tag{3.6}$$

$$\|\Phi\|_{H^1(\Omega)} \leq N_2\|Y_*\|_\infty, \tag{3.7}$$

$$\|T\|_{H^1(\Omega)} \leq N_3\left\|\Phi_*'\right\|_2^2 + N_4\|Y_*\|_\infty + N_5, \tag{3.8}$$

where N_1, N_2, N_3, N_4, N_5 are positive constants, and they depend on $\|f\|_\infty, \|g\|_\infty, \|h\|_\infty$.

Proof. (1°) Equation (3.6) holds. Since

$$-\left(\frac{\alpha_1 Y(a) - 1}{\alpha_2}\right) \cdot \varphi(a) - \int_a^b Y' \cdot \varphi' dx = \int_a^b h(T_*) Y \varphi dx, \quad \forall \varphi \in H^1(\Omega), \tag{3.9}$$

let $\varphi = Y \in H^1(\Omega)$; therefore we have

$$-\frac{\alpha_1}{\alpha_2} Y^2(a) + \frac{1}{\alpha_2} Y(a) = \int_a^b \left|Y'\right|^2 dx + \int_a^b h(T_*) Y^2 dx \geq \min(\delta_2, 1)\|Y\|_{H^1}^2. \tag{3.10}$$

By (3.10), we can get that

$$\|Y\|_{H^1}^2 \leq \frac{1}{\min(\delta_2, 1)}\left(-\frac{\alpha_1}{\alpha_2} Y^2(a) + \frac{1}{\alpha_2} Y(a)\right) \leq \frac{1}{\min(\delta_2, 1)} \cdot \frac{1}{4\alpha_1\alpha_2}. \tag{3.11}$$

Set $N_1 = ((1/\min(\delta_2, 1)) \cdot (1/4\alpha_1\alpha_2))^{1/2}$, then (3.6) is proved.

(2°) Equation (3.7) holds. From (3.2),

$$-\frac{1}{\beta}\Phi(b)\cdot\varphi(b)-\int_a^b f(T_*)(\Phi')\cdot\varphi' dx+\int_a^b g(T_*)\Upsilon_*\varphi dx=0,\quad \forall\varphi\in H^1(\Omega). \tag{3.12}$$

Thus let $\varphi=\Phi\in H^1(\Omega)$ so that

$$-\frac{1}{\beta}\Phi^2(b)-\int_a^b f(T_*)(\Phi')^2 dx+\int_a^b g(T_*)\Upsilon_*\Phi dx=0. \tag{3.13}$$

It follows that

$$\int_a^b f(T_*)(\Phi')^2 dx=-\frac{1}{\beta}\Phi^2(b)+\int_a^b g(T_*)\Upsilon_*\Phi dx\le \|g\|_\infty\|\Upsilon_*\|_\infty\|\Phi\|_2\cdot l^{1/2}. \tag{3.14}$$

Since $0<\delta_1\le f$, we have

$$\delta_1\int_a^b(\Phi')^2 dx\le \|g\|_\infty\|\Upsilon_*\|_\infty\|\Phi\|_2\cdot l^{1/2}. \tag{3.15}$$

To prove (3.7) we need a lemma (see [10]).

Lemma 3.3. *Let X denote a real Banach space, and let $u\in W^{1,p}([0,\tau];X)$ for some $1\le p\le\infty$. Then*

(i) $u\in C([0,\tau];X)$ *(after possibly being redefined on a set of measure zero), and*

(ii) $u(t)=u(s)+\int_s^t u'(x)dx$ *for all* $0\le s\le t\le\tau$.

By Lemma 3.3, we get

$$\|\Phi\|_{H_1}^2=\int_a^b|\Phi(x)|^2dx+\int_a^b|\Phi'(x)|^2dx\le\int_a^b\left[\int_x^b|\Phi'(t)|dt+|\Phi(b)|\right]^2dx+\int_a^b|\Phi'(x)|^2dx. \tag{3.16}$$

By (3.15), for (3.16), we arrive at

$$\begin{aligned}\|\Phi\|_{H_1}^2&\le 2\int_a^b\left[\int_x^b|\Phi'(t)|dt\right]^2dx+2\int_a^b|\Phi(b)|^2dx+\frac{1}{\delta_1}\|g\|_\infty\|\Upsilon_*\|_\infty\|\Phi\|_2\cdot l^{1/2}\\&\le\left(\int_a^b|\Phi'(t)|dt\right)^2\cdot 2l+2(\Phi(b))^2l+\frac{1}{\delta_1}\|g\|_\infty\|\Upsilon_*\|_\infty\|\Phi\|_2\cdot l^{1/2}.\end{aligned} \tag{3.17}$$

On the other hand, for (3.2), we take $\varphi = 1 \in H^1(\Omega)$, so we know that

$$\Phi(b) = \beta \int_a^b g(T_*) Y_* dx. \tag{3.18}$$

Substituting (3.18) into (3.17), we arrive at

$$\begin{aligned} \|\Phi\|_{H_1}^2 &\le 2\int_a^b |\Phi'(t)|^2 dt \cdot l^2 + 2\beta^2 \left(\int_a^b g(T_*) Y_* dx\right)^2 \cdot l + \frac{1}{\delta_1} l^{1/2} \|g\|_\infty \|Y_*\|_\infty \|\Phi\|_2 \\ &\le \frac{2}{\delta_1} l^{5/2} \|g\|_\infty \|Y_*\|_\infty \|\Phi\|_{H^1} + \frac{1}{\delta_1} l^{1/2} \|g\|_\infty \|Y_*\|_\infty \|\Phi\|_{H^1} + 2\beta^2 l^2 \|g\|_\infty^2 \|Y_*\|_\infty^2. \end{aligned} \tag{3.19}$$

Set $x = \|\Phi\|_{H^1}$, $\widetilde{B} = (2/\delta_1) l^{5/2} \|g\|_\infty \|Y_*\|_\infty + (1/\delta_1) l^{1/2} \|g\|_\infty \|Y_*\|_\infty$, $\widetilde{C} = 2\beta^2 l^2 \|g\|_\infty^2 \|Y_*\|_\infty^2$ so that we have

$$x^2 - \widetilde{B} x - \widetilde{C} \le 0. \tag{3.20}$$

Hence, we get that

$$\begin{aligned} x &\le \frac{\widetilde{B} + \sqrt{\widetilde{B}^2 + 4\widetilde{C}}}{2} \\ &= \frac{1}{2}\left(\frac{2}{\delta_1} l^{5/2} + \frac{1}{\delta_1} l^{1/2} + \sqrt{\left(\frac{2}{\delta_1} l^{5/2} + \frac{1}{\delta_1} l^{1/2}\right)^2 + 8\beta^2 l^2}\right) \|g\|_\infty \|Y_*\|_\infty. \end{aligned} \tag{3.21}$$

Take $N_2 = (1/2)((2/\delta_1) l^{5/2} + (1/\delta_1) l^{1/2} + \sqrt{((2/\delta_1) l^{5/2} + (1/\delta_1) l^{1/2})^2 + 8\beta^2 l^2}) \|g\|_\infty$, and from (3.21), we get (3.7).

(3°) Equation (3.8) holds. For (3.3), take $\varphi = T \in H^1(\Omega)$; thus we have

$$-\frac{\mu_1}{\mu_2} T^2(a) + \frac{1}{\mu_2} T(a) - \int_a^b (T')^2 dx = \int_a^b k(T_*) Y_* T dx - \lambda \int_a^b f(T_*) (\Phi_*')^2 T dx. \tag{3.22}$$

Now we introduce the following lemma (see [9]).

Lemma 3.4. *Let G be a bounded region in $\mathbb{R}^N$ with $N \ge 1$, and $u \in H^1(G)$, set*

$$\begin{aligned} \|u\|_{H^1} &= \left(\int_G \left(u^2 + \Sigma_{j=1}^N (D_j u)^2\right) dx\right)^{1/2}, \\ \|u\|_{H^1}^* &= \left(\int_G \Sigma_{i=1}^N (D_i u)^2 dx + \int_{\partial G} u^2 d\sigma\right)^{1/2}, \end{aligned} \tag{3.23}$$

then the two norms in (3.23) *are equivalent on $H^1(G)$.*

Hence we consider the $H^1(G)$ norm with the type

$$\|u\|_{H^1}^* = \left(\int_G \Sigma_{i=1}^N (D_i u)^2 dx + \int_{\partial G} u^2 d\sigma\right)^{1/2}, \tag{3.24}$$

and estimate by

$$\begin{aligned}
&\int_a^b (T')^2 dx + \varepsilon' T^2(b) + \varepsilon' T^2(a) \ \left(\varepsilon' \text{ is a small positive number to be determined}\right) \\
&\quad = -\frac{\mu_1}{\mu_2} T^2(a) + \frac{1}{\mu_2} T(a) + \lambda \int_a^b f(T_*)(\Phi_*')^2 T dx - \int_a^b k(T_*) Y_* T dx + \varepsilon' T^2(b) + \varepsilon' T^2(a) \\
&\quad \le -\frac{\mu_1}{\mu_2} T^2(a) + \frac{1}{\mu_2} T(a) + \lambda \int_a^b f(T_*)(\Phi_*')^2 T dx + \left(\varepsilon \int_a^b T^2(x) dx + C_\varepsilon \int_a^b |k|^2 |Y_*|^2 dx\right) \\
&\qquad + \varepsilon' T^2(b) + \varepsilon' T^2(a) \\
&\quad \le -\frac{\mu_1}{\mu_2} T^2(a) + \frac{1}{\mu_2} T(a) + \lambda \left(\frac{\varepsilon}{2}\|T\|_\infty^2 + \frac{1}{2\varepsilon}\left(\int_a^b f(T_*)(\Phi_*')^2 dx\right)^2\right) + \varepsilon \|T\|_{H^1}^2 \\
&\qquad + C_\varepsilon \|k\|_\infty^2 \|Y_*\|_\infty^2 \cdot l + \varepsilon' T^2(b) + \varepsilon' T^2(a).
\end{aligned} \tag{3.25}$$

By Lemma 3.3, we have that

$$|T(x)| \le \int_a^x |T'(t)| dt + |T(a)|, \quad \forall x \in [a, b]. \tag{3.26}$$

Substituting (3.26) into the bound (3.25), we arrive at

$$\begin{aligned}
&\int_a^b (T')^2 dx + \varepsilon' T^2(b) + \varepsilon' T^2(a) \\
&\quad \le -\frac{\mu_1}{\mu_2} T^2(a) + \frac{1}{\mu_2} T(a) + \lambda \left(\frac{\varepsilon}{2}\|T\|_\infty^2 + \frac{1}{2\varepsilon}\left(\int_a^b f(T_*)(\Phi_*')^2 dx\right)^2\right) + \varepsilon \|T\|_{H^1}^2 \\
&\qquad + C_\varepsilon \|k\|_\infty^2 \|Y_*\|_\infty^2 \cdot l + \varepsilon' \left(2\left(\int_a^b |T'| dt\right)^2 + 2|T(a)|^2\right) + \varepsilon' T^2(a) \quad (\varepsilon \ll \varepsilon') \\
&\quad \le -\frac{\mu_1}{\mu_2} T^2(a) + \frac{1}{\mu_2} T(a) + \frac{\lambda\varepsilon}{2} c_1^2 \|T\|_{H^1}^2 + \frac{\lambda}{2\varepsilon}\left(\int_a^b f(T_*)(\Phi_*')^2 dx\right)^2 + \varepsilon \|T\|_{H^1}^2 \\
&\qquad + C_\varepsilon \|k\|_\infty^2 \|Y_*\|_\infty^2 \cdot l + 2\varepsilon' \int_a^b (T'(t))^2 dt \cdot l + 2\varepsilon' T^2(a) + \varepsilon' T^2(a).
\end{aligned} \tag{3.27}$$

By (3.27), we have that

$$\begin{aligned}
&(1-2\varepsilon' l)\int_a^b (T'(t))^2 dt + \varepsilon' T^2(b) + \varepsilon' T^2(a) \\
&\quad \le \left(-\frac{\mu_1}{\mu_2} + 3\varepsilon'\right) T^2(a) + \frac{1}{\mu_2} T(a) + \frac{\lambda\varepsilon}{2} c_1^2 \|T\|_{H^1}^2 + \frac{\lambda}{2\varepsilon}\left(\int_a^b f(T_*)(\Phi_*')^2 dx\right)^2 \\
&\qquad + \varepsilon \|T\|_{H^1}^2 + C_\varepsilon \|k\|_\infty^2 \|Y_*\|_\infty^2 \cdot l,
\end{aligned} \tag{3.28}$$

where c_1 is the constant that appeared in the Sobolev inequality (see [11] and note that $\Omega \subset \mathbb{R}$)

$$\|u\|_\infty \le c_1 \|u\|_{H^1(\Omega)} \tag{3.29}$$

for all $u \in H^1(\Omega)$.

Hence,

$$\begin{aligned}
\varepsilon' \|T\|_{H^1}^2 &\le C_1\left(\varepsilon' \int_a^b (T'(t))^2 dt + \varepsilon' T^2(b) + \varepsilon' T^2(a)\right) \\
&\le C_1\left((1-2\varepsilon' l)\int_a^b (T'(t))^2 dt + \varepsilon' T^2(b) + \varepsilon' T^2(a)\right) \\
&\le C_1\left[\left(-\frac{\mu_1}{\mu_2} + 3\varepsilon'\right) T^2(a) + \frac{1}{\mu_2} T(a) + \frac{\lambda\varepsilon}{2} c_1^2 \|T\|_{H^1}^2 \right. \\
&\qquad \left. + \frac{\lambda}{2\varepsilon}\left(\int_a^b f(T_*)(\Phi_*')^2 dx\right)^2 + \varepsilon \|T\|_{H^1}^2 + C_\varepsilon l \|k\|_\infty^2 \|Y_*\|_\infty^2\right],
\end{aligned} \tag{3.30}$$

where $C_1 > 0$, and ε' is chosen to satisfy $\varepsilon' < \min\{(1/1+2l), (\mu_1/3\mu_2)\}$.

From (3.30), we arrive at

$$\begin{aligned}
&\left(\varepsilon' - \frac{\lambda\varepsilon}{2} c_1^2 C_1 - \varepsilon C_1\right) \|T\|_{H^1}^2 \\
&\quad \le C_1\left(-\frac{\mu_1}{\mu_2} + 3\varepsilon'\right) T^2(a) + \frac{1}{\mu_2} C_1 T(a) + \frac{\lambda}{2\varepsilon} C_1 \left(\int_a^b f(T_*)(\Phi_*')^2 dx\right)^2 + C_\varepsilon C_1 \|k\|_\infty^2 \|Y_*\|_\infty^2 \cdot l.
\end{aligned} \tag{3.31}$$

Now we choose $\varepsilon > 0$ such that $\varepsilon' - (\lambda\varepsilon/2) c_1^2 C_1 - \varepsilon C_1 > 0$. Note that, in (3.3), if we choose test function $\varphi = 1 \in H^1(\Omega)$, then

$$-\left(\frac{\mu_1 T(a) - 1}{\mu_2}\right) = \int_a^b k(T_*) Y_* dx - \lambda \int_a^b f(T_*)(\Phi_*')^2 dx. \tag{3.32}$$

Hence, we obtain that $T(a)$ is bounded by a number depending on $\|Y_*\|_\infty$, l, $\|\Phi_*\|_{H^1(\Omega)}$, $\|k\|_\infty$ and $\|f\|_\infty$, and is independent of T_*. So

$$\|T\|_{H^1}^2 \leq \frac{C_1}{(\varepsilon' - (\lambda\varepsilon/2)c_1^2 C_1 - \varepsilon C_1)}\left[\frac{\lambda}{2\varepsilon}\|f\|_\infty^2\|\Phi_*'\|_2^4 + C_\varepsilon\|k\|_\infty^2\|Y_*\|_\infty^2 \cdot l - \frac{1}{-4\mu_1\mu_2 + 12\varepsilon'\mu_2^2}\right], \tag{3.33}$$

where $-(1/\mu_2^2)/4(-\mu_1/\mu_2+3\varepsilon')$ is the maximum of $(-\mu_1/\mu_2+3\varepsilon')T^2(a)+(1/\mu_2)T(a)$. By (3.33), we have that

$$\|T\|_{H^1} \leq C_2\left[\sqrt{\frac{\lambda}{2\varepsilon}}\|f\|_\infty\|\Phi_*'\|_2^2 + \sqrt{C_\varepsilon l}\|k\|_\infty\|Y_*\|_\infty + \left(\frac{1}{4\mu_1\mu_2 - 12\varepsilon'\mu_2^2}\right)^{1/2}\right], \tag{3.34}$$

where $C_2 = (C_1/(\varepsilon' - (\lambda\varepsilon/2)c_1^2 C_1 - \varepsilon C_1))^{1/2}$.

Let

$$N_3 = C_2\sqrt{\frac{\lambda}{2\varepsilon}}\|f\|_\infty, \qquad N_4 = C_2\sqrt{C_\varepsilon l}\|k\|_\infty, \qquad N_5 = C_2\left(\frac{1}{4\mu_1\mu_2 - 12\varepsilon'\mu_2^2}\right)^{1/2}, \tag{3.35}$$

so (3.8) is proved. □

4. Proof of Theorem 2.1

Now, we show the proof of Theorem 2.1.

Step 1. Under the assumptions made in Section 3, for each $(T_n, \Phi_n, Y_n) \in (H^1(\Omega))^3$, $n \in \mathbb{N} \cup \{0\}$, we first consider the linear generalized Neumann problem,

$$\begin{aligned}
-\left(\frac{\mu_1 T_{n+1}(a) - 1}{\mu_2}\right)\cdot\varphi(a) - \int_a^b T_{n+1}'\cdot\varphi' dx &= \int_a^b k(T_n)Y_n\varphi dx - \lambda\int_a^b f(T_n)(\Phi_n')^2\varphi dx,\\
-\frac{1}{\beta}\Phi_{n+1}(b)\cdot\varphi(b) - \int_a^b f(T_n)(\Phi_{n+1}')\cdot\varphi' dx + \int_a^b g(T_n)Y_n\varphi dx &= 0,\\
-\left(\frac{\alpha_1 Y_{n+1}(a) - 1}{\alpha_2}\right)\cdot\varphi(a) - \int_a^b Y_{n+1}'\cdot\varphi' dx &= \int_a^b h(T_n)Y_{n+1}\varphi dx,
\end{aligned} \tag{4.1}$$

for all $\varphi \in H^1(\Omega)$.

Denote by $Rv \equiv (Y_{n+1}, \Phi_{n+1}, T_{n+1}) = (RY_n, R\Phi_n, RT_n)$ the unique solution of problem (4.1), where $v = (Y_n, \Phi_n, T_n) \in (H^1(\Omega))^3$.

From Theorem 3.2, we know that

$$\begin{aligned}
&\|Y_{n+1}\|_{H^1(\Omega)} \le N_1 \equiv M_1,\\
&\|\Phi_{n+1}\|_{H^1(\Omega)} \le N_2\|Y_n\|_\infty \le N_2c_1\|Y_n\|_{H^1(\Omega)} \le N_2c_1M_1 \equiv M_2,\\
&\|T_{n+1}\|_{H^1(\Omega)} \le N_3\left\|\Phi_n'\right\|_2^2 + N_4\|Y_n\|_\infty + N_5\\
&\qquad\qquad \le N_3\|\Phi_n\|_{H^1}^2 + N_4c_1\|Y_n\|_{H^1(\Omega)} + N_5\\
&\qquad\qquad \le N_3M_2^2 + N_4c_1M_1 + N_5 \equiv M_3.
\end{aligned} \tag{4.2}$$

Now we consider the convex set

$$S = \left\{(v_1,v_2,v_3) \in \left(H^1(\Omega)\right)^3 : \|v_1\|_{H^1} \le M_1,\ \|v_2\|_{H^1(\Omega)} \le M_2,\ \|v_3\|_{H^1(\Omega)} \le M_3\right\}. \tag{4.3}$$

By the estimate (4.2), we know that R maps S into S.

Step 2. We show that R is continuous on S, that is,

$$\lim_{j\to\infty}\left(\left\|R\tilde{T}_j - R\tilde{T}\right\|_{H^1} + \left\|R\widetilde{\Phi_j} - R\tilde{\Phi}\right\|_{H^1} + \left\|R\widetilde{Y_j} - R\tilde{Y}\right\|_{H^1}\right) = 0 \tag{4.4}$$

if $(\tilde{T}_j, \widetilde{\Phi_j}, \widetilde{Y_j}) \to (\tilde{T}, \tilde{\Phi}, \tilde{Y})$ in S, as $j \to \infty$.

Consider the equations

$$\begin{aligned}
&-\left(\frac{\alpha_1 R\tilde{Y}_j(a) - 1}{\alpha_2}\right)\varphi(a) - \int_a^b \left(R\tilde{Y}_j\right)'\varphi' dx - \int_a^b h\left(\tilde{T}_j\right)\left(R\tilde{Y}_j\right)\varphi dx = 0,\\
&-\left(\frac{\alpha_1 R\tilde{Y}(a) - 1}{\alpha_2}\right)\varphi(a) - \int_a^b \left(R\tilde{Y}\right)'\varphi' dx - \int_a^b h\left(\tilde{T}\right)\left(R\tilde{Y}\right)\varphi dx = 0,
\end{aligned} \tag{4.5}$$

for all $\varphi \in H^1(\Omega)$. The difference (4.5) gives

$$-\frac{\alpha_1}{\alpha_2}\left(R\tilde{Y}_j - R\tilde{Y}\right)(a)\cdot\varphi(a) + \int_a^b \left(R\tilde{Y} - R\tilde{Y}_j\right)'\varphi' dx + \int_a^b \left(h\left(\tilde{T}\right)\left(R\tilde{Y}\right) - h\left(\tilde{T}_j\right)\left(R\tilde{Y}_j\right)\right)\varphi dx = 0. \tag{4.6}$$

By (4.6), we have

$$\begin{aligned}
&-\frac{\alpha_1}{\alpha_2}\left(R\tilde{Y}_j - R\tilde{Y}\right)(a)\cdot\varphi(a) + \int_a^b \left(R\tilde{Y} - R\tilde{Y}_j\right)'\varphi' dx\\
&\qquad + \int_a^b \left[h\left(\tilde{T}_j\right)\left(R\tilde{Y} - R\tilde{Y}_j\right) + R\tilde{Y}\left(h\left(\tilde{T}\right) - h\left(\tilde{T}_j\right)\right)\right]\varphi dx = 0.
\end{aligned} \tag{4.7}$$

Set $D_j = R\widetilde{Y} - R\widetilde{Y}_j$, and let $\varphi = D_j$ in (4.7), then

$$\int_a^b \left(D_j'\right)^2 dx + \delta_2 \int_a^b D_j^2 dx \le \left\|R\widetilde{Y}\right\|_\infty \|h'\|_\infty \|D_j\|_\infty \left\|\widetilde{T} - \widetilde{T}_j\right\|_2 l^{1/2}. \tag{4.8}$$

Since $0 < \delta_2 \le h$, we know that

$$\min(\delta_2, 1)\|D_j\|_{H^1}^2 \le c_1 \left\|R\widetilde{Y}\right\|_\infty \|h'\|_\infty \|D_j\|_{H^1} \left\|\widetilde{T} - \widetilde{T}_j\right\|_{H^1} l^{1/2}. \tag{4.9}$$

Since $\lim_{j\to\infty}\|\widetilde{T}_j - \widetilde{T}\|_{H^1} = 0$, hence we have

$$\lim_{j\to\infty}\left\|R\widetilde{Y}_j - R\widetilde{Y}\right\|_{H^1} = 0. \tag{4.10}$$

The proof of

$$\lim_{j\to\infty}\left\|R\widetilde{\Phi_j} - R\widetilde{\Phi}\right\|_{H^1} = 0, \qquad \lim_{j\to\infty}\left\|R\widetilde{T}_j - R\widetilde{T}\right\|_{H^1} = 0 \tag{4.11}$$

is similar and is omitted. Hence, R is continuous on S.

Before the next step, we first state a regularity theorem, (see [12]). Consider the operator

$$\mathbb{L}u = D_i\left(a^{ij}(x)D_j u + b^i(x)u\right) + c^i(x)D_i u + d(x)u, \tag{4.12}$$

whose coefficients a^{ij}, b^i, c^i, d $(i, j = 1, \ldots, n)$ are continuous on a domain $\Omega \subset \mathbb{R}^n$.

Theorem 4.1. *Let $u \in H^1(\Omega)$ be a weak solution of the equation $\mathbb{L}u = p$ in Ω where $\mathbb{L}$ is strictly elliptic on Ω, the coefficients a^{ij}, b^i $(i, j = 1, \ldots, n)$ are uniformly Lipschitz continuous on Ω, the coefficients c^i $(i = 1, \ldots, n), d$ are essentially bounded on Ω, and the function p is in $L^2(\Omega)$. Also, assume that $\partial\Omega$ is of class C^2 and that there exists a function $\varphi \in H^2(\Omega)$ for which $u - \varphi \in H_0^1(\Omega)$. Then one has also $u \in H^2(\Omega)$ and*

$$\|u\|_{H^2(\Omega)} \le C\left(\|u\|_{L^2(\Omega)} + \|p\|_{L^2(\Omega)} + \|\varphi\|_{H^2(\Omega)}\right) \quad \text{for } C = C\left(n, \widetilde{\lambda}, K, \partial\Omega\right), \tag{4.13}$$

where $K = \max\{\|a^{ij}, b^i\|_\infty, \|c^i, d\|_\infty\}$.

Remark 4.2. Theorem 4.1 continues to hold for sufficiently smooth $\partial\Omega$ with $\varphi \in H^2(\Omega)$ if we assume only that the principal coefficients a^{ij} are in $C^0(\overline{\Omega})$.

Step 3. $R(S)$ is precompact.

By Theorem 4.1, one has the following:

$$\|Y_{n+1}\|_{H^2(\Omega)} \le C\left(\|Y_{n+1}\|_{L^2(\Omega)} + \left\|Y_{n+1}^{\varphi}\right\|_{H^2(\Omega)}\right), \tag{4.14}$$

where $Y_{n+1}^{\varphi} \in H^2(\Omega)$ is a function for which $Y_{n+1} - Y_{n+1}^{\varphi} \in H_0^1(\Omega)$,

$$\|\Phi_{n+1}\|_{H^2(\Omega)} \leq C\left(\|\Phi_{n+1}\|_{L^2(\Omega)} + \|g(T_n)Y_n\|_{L^2(\Omega)} + \left\|\Phi_{n+1}^{\varphi}\right\|_{H^2(\Omega)}\right), \tag{4.15}$$

where $\Phi_{n+1}^{\varphi} \in H^2(\Omega)$ is a function for which $\Phi_{n+1} - \Phi_{n+1}^{\varphi} \in H_0^1(\Omega)$,

$$\|T_{n+1}\|_{H^2(\Omega)} \leq C\left(\|T_{n+1}\|_{L^2(\Omega)} + \left\|k(T_n)Y_n + \lambda f(T_n)\left(\Phi_n'\right)^2\right\|_{L^2(\Omega)} + \left\|T_{n+1}^{\varphi}\right\|_{H^2(\Omega)}\right), \tag{4.16}$$

where $T_{n+1}^{\varphi} \in H^2(\Omega)$ is a function for which $T_{n+1} - T_{n+1}^{\varphi} \in H_0^1(\Omega)$.

For (4.14)~(4.16), set

$$\begin{aligned} Y_{n+1}^{\varphi}(x) &= \frac{Y_{n+1}(b) - Y_{n+1}(a)}{b-a}(x-a) + Y_{n+1}(a), \\ \Phi_{n+1}^{\varphi}(x) &= \frac{\Phi_{n+1}(b) - \Phi_{n+1}(a)}{b-a}(x-a) + \Phi_{n+1}(a), \\ T_{n+1}^{\varphi}(x) &= \frac{T_{n+1}(b) - T_{n+1}(a)}{b-a}(x-a) + T_{n+1}(a), \end{aligned} \tag{4.17}$$

for all $x \in [a,b]$.

By (4.17), we obtain that

$$\begin{aligned} \left|Y_{n+1}^{\varphi}(x)\right| &= \left|\frac{Y_{n+1}(b) - Y_{n+1}(a)}{b-a}(x-a) + Y_{n+1}(a)\right| \\ &\leq \int_a^b \left|Y_{n+1}'\right| dx + |Y_{n+1}(a)| \leq \left(l^{1/2} + c_1\right) M_1, \end{aligned} \tag{4.18}$$

for all $x \in [a,b]$.

From (4.14), (4.18) and by a simple calculation, we obtain

$$\begin{aligned} \|Y_{n+1}\|_{H^2(\Omega)} &\leq C\left(\|Y_{n+1}\|_{L^2(\Omega)} + \left\|Y_{n+1}^{\varphi}\right\|_{H^2(\Omega)}\right) \\ &\leq C\left(M_1 + M_1\sqrt{l^{1/2} + c_1^2 l + \frac{4c_1^2}{l}}\right) \\ &\equiv \gamma_1. \end{aligned} \tag{4.19}$$

Using the same formula, we also obtain that

$$\begin{aligned}
\|\Phi_{n+1}\|_{H^2(\Omega)} &\le C\left(\|\Phi_{n+1}\|_{L^2(\Omega)} + \|g(T_n)Y_n\|_{L^2(\Omega)} + \left\|\Phi_{n+1}^{\varphi}\right\|_{H^2(\Omega)}\right) \\
&\le C\left(M_2 + \|g\|_\infty M_1 + M_2\sqrt{l^{1/2} + c_1^2 l + \frac{4c_1^2}{l}}\right) \\
&\equiv \gamma_2, \\
\|T_{n+1}\|_{H^2(\Omega)} &\le C\left(\|T_{n+1}\|_{L^2(\Omega)} + \left\|k(T_n)Y_n + \lambda f(T_n)(\Phi_n')^2\right\|_{L^2(\Omega)} + \left\|T_{n+1}^{\varphi}\right\|_{H^2(\Omega)}\right) \\
&\le C\left(M_3 + \|k\|_\infty M_1 + \lambda\|f\|_\infty\left(c_1^4\gamma_2^4 l\right)^{1/2} + M_3\sqrt{\left(l^{1/2} + c_1\right)^2 l + \frac{4c_1^2}{l}}\right) \\
&\equiv \gamma_3.
\end{aligned} \tag{4.20}$$

Thus, we have

$$\|RY_n\|_{H^2(\Omega)} \le \gamma_1, \quad \|R\Phi_n\|_{H^2(\Omega)} \le \gamma_2, \quad \|RT_n\|_{H^2(\Omega)} \le \gamma_3, \quad \forall n \in \mathbb{N}. \tag{4.21}$$

So, R maps S into a bounded set in $(H^2(\Omega))^3$, since $H^2(\Omega)$ is compactly imbedded in $H^1(\Omega)$ (see, e.g., [9]); hence, $R(S)$ is precompact in $(H^1(\Omega))^3$.

Hence by Schauder's fixed point theorem, R has a fixed point and there exists a $(T, \Phi, Y) \in (H^1(\Omega))^3$ satisfyng (2.17). Thus, we complete the proof of Theorem 2.1.

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