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MATHEMATICAL MODELING IN PEM FUEL CELLS

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Abstract. *In proton exchange membrane (PEM) fuel cells, the transport of the fuel to the active zones, and the removal of the reaction products are realized using a combination of channels and porous diffusion layers. In order to improve existing mathematical and numerical models of PEM fuel cells, a deeper understanding of the coupling of the flow processes in the channels and diffusion layers is necessary. We will discuss mathematical models for PEM fuel cells, the work will focus on the description of the coupling of the free flow in the channel region with the filtration velocity in the porous diffusion*

Key words: *Stokes and Darcy equations, Beaver-Joseph condition, proton exchange membrane*

1. INTRODUCTION

Numerical simulation of coupled flows in plain and porous media is essential for many industrial and environmental problems: *proton exchange membrane (*PEM*) fuel cells*, flow through (oil) filters [7], contaminant transport from lakes by groundwater, CO_2 sequestration in the subsurface, salt water intrusion, etc..

We will focus on coupling conditions between the pure liquid flow and the flow in the porous media. Coupling conditions are well studied only in the simple case of parallel flow over a porous media. In general, we distinguish two types of PEM fuel cells: H_2PEM fuel cells ($H_2 PEMFC$) driven by gaseous hydrogen, and *direct methanol fuel cells (DMFC)* operating on methanol in an aqueous solution. Both anode and cathode consist of supply channels, a porous diffusion layer and an active zone. They are connected by a proton conducting membrane. For details we refer the interested reader to [4], [8].

As an application, we present we may have Proton exchange membrane (PEM) fuel cells. In Proton exchange membrane (PEM) fuel cells, the transport of the fuel to the active zones, and the removal of the reaction products are realized using a combination of channels and porous diffusion layers. In order to improve existing mathematical and numerical models of PEM fuel cells, a deeper understanding of the coupling of the flow processes in the channels and diffusion layers is necessary.

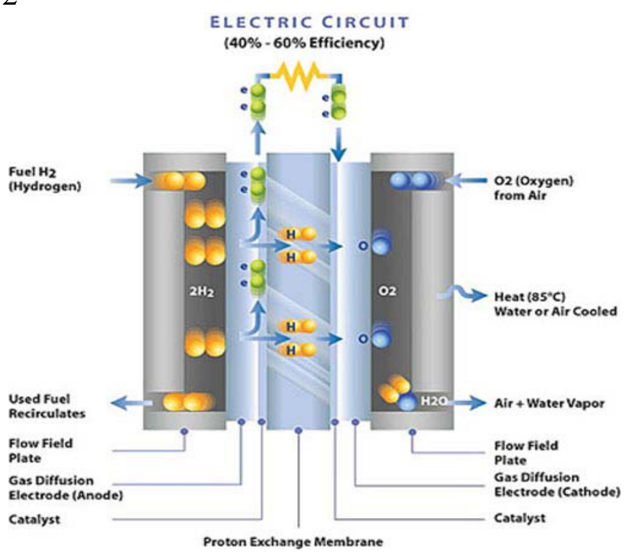
The most important chemical reactions in PEM fuel cells are at the anode

DMFC $CH_3OH + H_2O \rightarrow CO2 + 6H^+ + 6e^-$

PEMFC $3H_2 \rightarrow 6H^+ + 6e^-$

and at the cathode

$$\frac{3}{2}O_2 + 6H^+ + 6e^- \rightarrow 3H_2O .$$



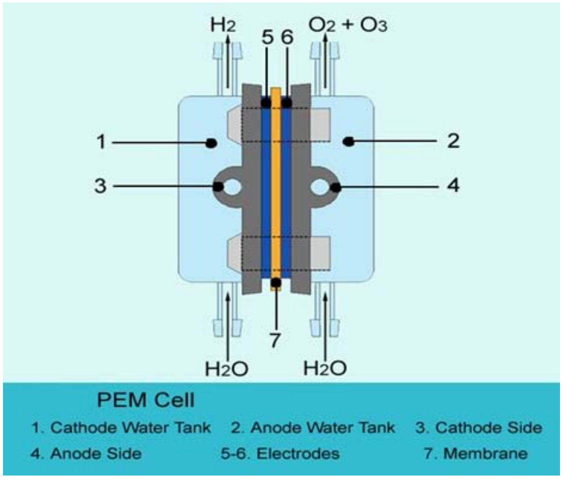


Fig 1 The PEM cell

Consequently, in a H_2PEMFC, ideally, the anode contains only hydrogen, while the cathode contains a mixture of liquid water, water vapor and oxygen resp. air. While for an optimal supply of oxygen, it is desirable to keep the amount of liquid water at the cathode minimal, the optimal proton conductivity of the membrane is reached only if it contains enough water. Hence, the water management is an essential issue.

However for this type of fuel cell, methanol permeation through the membrane, leading to a parasitic reaction on the cathode side, is a key problem. Another problem is clogging of the anodic channels by CO_2 bubbles as in [3].

In spite of our remark on the validation of current coupling models, most models either focus on the processes in the membrane electrode assembly (MEA), or in the fluidic channels, simplifying the other process, respectively. A further complication comes from the fact that in both cases, the general process includes two phase flow of a fluid and a gas mixture.

The difficulty in finding effective coupling conditions at the interface between the channel flow and the porous layer lies in the fact that, when using stationary (Navier–) Stokes and Darcy's equations to model flow in the two regions, the structures of the corresponding differential operators are different. We have an incompressible fluid in a region Ω_f can flow both ways across an interface Γ into a domain Ω_p which is a porous medium saturated with the same fluid. The mathematical theory and numerical analysis of each sub problem is well developed, and reliable codes are available. Nevertheless, the mathematical theory of the coupled problem seems to be not completely understood. The model of this situation which is most accessible to large scale computations consists of the Navier-Stokes equations (or Stokes equations) in the fluid region coupled across an interface with the Darcy equations for the filtration velocity in the porous medium. For more information we refer [10]

One goal of this report is to find a variational formulation (section 2) for which weak solutions can be guaranteed to exist (section 3) and which can be used as a basis for a domain decomposition strategy for its approximate solution. The method we study imposes the interface conditions using Lagrange multipliers as [9].

Thus, it can be used in a heterogeneous domain decomposition procedure in which each sub problem is alternately or simultaneously solved with codes (possibly "legacy" codes) developed and optimized for the physics of fluid motion and of porous media flow. In section 4 we give a complete analysis of this convergent finite element procedure. Because of the importance of the coupled problem, there are many computations of coupled surface water-groundwater flows in the applied literature, using various ad hoc interface decoupling strategies.

The coupling strategy via Lagrange multipliers we consider herein has been proven in other applications and we are working towards practical tests of our ideas.

2. THE MODEL

The model we consider consists of Stokes flow in the fluid region Ω_f and Darcy's law in the porous medium domain Ω_p. These are separated by an interface Γ. Here $\Omega_f, \Omega_p \subset \mathbb{R}^d$ (d = 2 or 3) are bounded domains with outward unit normal vectors n_j, j = f, p. For simplicity we note by *n*. Each interface and boundary is assumed to be polygonal (d = 2) or polyhedral (d = 3).

The fluid velocities and pressures in Ω_f and Ω_p are denoted by $u_f : \Omega_f \to \mathbb{R}^d$ fluid velocities in Ω_f $p_f : \Omega_f \to \mathbb{R}$ fluid pressure in Ω_f and $u_p : \Omega_p \to \mathbb{R}^d$ fluid velocities in Ω_p, $p_p : \Omega_p \to \mathbb{R}$ fluid pressure in Ω_p.

It is important to keep in mind that the velocities and pressures play different mathematical (and physical) roles in the fluid region and in the porous medium.

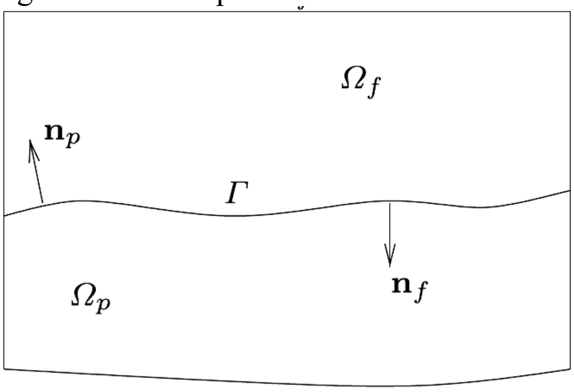


Fig. 2 Le domain for computation

Recall that the deformation rate tensor D and stress tensor T associated with (u_f, p_f) are defined by

$D(u_f) = \frac{1}{2}(\nabla u_f + \nabla^T u_f)$,

$T(u_f, p_f) = 2\nu D(u_f) - p_f I$

where ν is the viscosity.

Assuming Stokes flow, (u_f, p_f) satisfies on Ω_f

$\partial_t u_f - \nabla \cdot T(u_f, p_f) + (u_f \nabla) u_f = f \; in \; \Omega_f$ (conservation of momentum),

$\nabla \cdot u_f = 0 \; în \; \Omega_f$ (conservation of mass),

$u_f = 0 \; on \; \Gamma$ (no slip). (1)

Assuming Darcy's law and no flow through Γ, (u_p, p_p) satisfies on Ω_p

$u_p = -K \nabla p_p$ în Ω_p (Darcy's law),

$\nabla \cdot u_p = 0$ în Ω_p (conservation of mass),

$u_p = 0 \; on \; \Gamma$ (no flow), (2)

where K is a symmetric and uniformly positive definite tensor representing the rock permeability divided by the fluid viscosity. The source f_2 is assumed to satisfy the solvability condition

$$\int_{\Omega_p} f_2 dx = 0 \quad (3)$$

which makes physical sense due to the no-flow boundary condition on $\partial\Omega$ and to (4) below. The mixed formulation (2) is the most natural one for computations in the porous medium region since it leads to direct approximation of the velocity.

2.1 Interface conditions

The problems (1)-(2) must be coupled across Γ by the correct interface conditions. Mass conservation across Γ is expressed by

$$u_f \cdot n + u_p \cdot n = 0 \text{ on } \Gamma \quad (4)$$

The second interface condition is balance of normal forces across Γ. Recall from, e.g., Serrin [13], that the Cauchy stress vector or traction vector t is the force on $\partial\Omega_f$ acting on the fluid volume inside Ω_f and that

$\vec{t} = n \cdot T(u_f, p_f)$

(see Figure 3). Thus, the force on Γ exerted by the fluid volume is -t. The only force in Ω_p acting on Γ is the Darcy pressure p_p. Continuity of forces gives

$-\vec{t}(u_f, p_f) \cdot n = p_p$

This gives the interface condition

$$-n \cdot T(u_f, p_f) \cdot n = p_p \text{ on } \Gamma \quad (5)$$

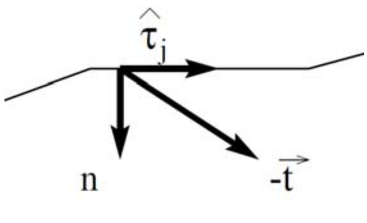


Fig. 3 System of tangent vectors on Γ

Finally, since the fluid model is viscous, a condition on the tangential fluid velocity on Γ must be given. Let τ_j ,j = 1,d-1, denote an orthonormal system of tangent vectors on Γ. The simplest assumption is no-slippage along Γ, i.e., $u_f \cdot \tau_j = 0$, *j=1,d-1*. This is not in good accord with experiment. The boundary condition in best agreement with experimental evidence evolved from the work of Beavers and

Joseph [1] and states that (slip velocity along Γ) is proportional to (shear stress along Γ). Mathematically, this can be represented by

$$\frac{\upsilon\alpha_{BJ}}{\sqrt{K}}\left(u_f - u_p\right)\tau_j - \tau_j \cdot T(u_f, p_f)\cdot n = 0 \quad (6)$$

Here the form $\frac{\upsilon\alpha_{BJ}}{\sqrt{K}}$ for the friction constant arises from dimensional analysis and experimental evidence. The parameter α_{BJ} must be experimentally determined; it seems to depend on many particular features of Γ, including its geometry.

3. WEAK FORMULATION OF THE COUPLED PROBLEM

This section is devoted to developing suitable weak formulations of the problem (1)-(6). The weak formulations have two important purposes. One formulation is used to show well-posedness of (1)-(6). This is already nontrivial because of the incompatibility of the boundary and interface conditions. Thus, the conditions at these points must be interpreted correctly. A second closely related weak form is developed which is suitable for efficiently splitting the coupled problem into two sub problems. In this formulation the coupling conditions (4)-(5) are viewed as constraints and imposed via Lagrange multipliers. For the finite element we refer the readers to [5], [6].

The Sobolev spaces $H^k(\Omega) = W^{k,2}(\Omega)$ are defined in the usual ways with the usual norm and half norm $\|\cdot\|_{k,\Omega}$ and $|\cdot|_{k,\Omega}$ respectively. Let

$$X_1 := \left\{v_f \in \left(H^1\left(\Omega_f\right)\right)^d : v_f = 0 \ on\ \Gamma\right\},$$

$$M_1 = L^2(\Omega_f)$$

denote the usual velocity-pressure spaces on Ω_f. The norm on X_1 is given by

$$\|v\|_{X_1} := |v|_{1,\Omega_f} := \|\nabla v\|_{\Omega_f}$$

The velocity space X_2 on Ω_p [12, 7, 2] is the subspace of

$$H(div;\Omega_p) = \left\{v_p \in \left(L^2\left(\Omega_p\right)\right)^d : \nabla\cdot v_p \in L^2\left(\Omega_p\right)\right\}$$

consisting of functions with zero normal trace on Γ and equipped with the norm

$$\|v_p\|_{H(div;\Omega_p)} := \left(\|v_p\|^2_{\Omega_p} + \|\nabla\cdot v_p\|^2_{\Omega_p}\right)^{1/2}$$

It is well known [12, 7, 2] that for all $v_p \in H(div;\Omega_p)$, $v_p \cdot n \in H^{-1/2}(\Gamma)$ and there exists a positive constant C such that

$$\|v_p \cdot n\|_{-1/2,\partial\Omega_p} \le C\|v_p\|_{H(div;\Omega_p)} \quad (7)$$

We define the velocity-pressure spaces on Ω_p as follows [14], [2, sect. III].

$$X_2 = \left\{v_p \in H(div;\Omega_p) : \left\langle v_p \cdot n, w\right\rangle_{\partial\Omega_p} = 0 \ w \in H^1_{o,\Gamma}(\Omega_p)\right\}$$

$$M_2 = L^2(\Omega_f)$$

Where

$$H^1_{o,\Gamma}(\Omega_p) = \left\{w \in H^1(\Omega_p) : w = 0 \ on\ \Gamma\right\}.$$

Defining $X = X_1 \times X_2$, a typical $v \in X$ takes the form (v_f, v_p). The norm on X is, as usual,

$$\|v\|_X := \left(\|v_f\|^2_{X_1} + \|v_p\|^2_{X_2}\right)^{1/2}$$

If $V \subset X$ is any closed subspace, then $\|\cdot\|_x$ is also the induced norm on V. Similarly, Let

$$M = \left\{q = (q_f, q_p) \in (M_1, M_2) \ \sum_{i=f,p}(q_i, 1) = 0\right\}$$

with norm

$$\|q\|_M := \left(\|q_f\|^2_{M_1} + \|q_p\|^2_{M_2}\right)^{1/2}$$

The coupling across Γ between the sub problems in Ω_f and Ω_p occurs in the interface conditions (1.4)-(1.5). The procedure for uncoupling the two sub problems is to pick one (we pick the second) and introduce the Lagrange multiplier:

$l \in \Lambda,\ l = -n \cdot T(u_f, p_f)\cdot n = p_p$ on Γ (8)

Considering l to be known data for each sub problem, the weak formulation is then derived in the usual manner as follows. Beginning with a classical solution of (1.1), multiplying by a sufficiently smooth $v_f \in X_1$ and integrating by parts gives

$$(f_1, v_f)_{\Omega_f} = \left(-2\nu\nabla\cdot D(u_f) + \nabla p_f, v_f\right)_{\Omega_f}$$

$$\left(-2\nu\nabla\cdot D(u_f)D(u_f)\right)_{\Omega_f} - \left(p_f, \nabla\cdot v_f\right)_{\Omega_f}$$

$$+\left\langle\left\{-n\cdot T(u_f, p_f)\cdot n\right\}, v_f\cdot n\right\rangle_\Gamma$$

$$\sum_{j=1}^{d}\left\langle\left\{-2\nu n\cdot T(u_f, p_f)\cdot\tau_j\right\}, v_f\cdot\tau_j\right\rangle_\Gamma$$

The first term in the braces $\{\cdot\}$ is replaced by l using (8) and (6). Therefore, introducing the bilinear forms

$$a_f(v,w) = \int_{\Omega_f} 2\nu(\nabla u + \nabla^T u)\cdot(\nabla v + \nabla^T v)$$

$$+\int_\Gamma \sum_{j=1}^{d-1}\frac{\nu\alpha_{BJ}}{\sqrt{K}}(u\cdot\tau_j)(v\cdot\tau_j)$$

$$+\int_\Gamma \sum_{j=1}^{d-1}\frac{\nu\alpha_{BJ}}{\sqrt{K}}(K\nabla p_p\cdot\tau_j)(v\cdot\tau_j)$$

and

$$b_f(v,q) = -\int_{\Omega_f} q\nabla\cdot v$$

we obtain

$$a_f(u_f, v_f) + b_f(v_f, p_f) + \left\langle l, v_f\cdot n\right\rangle$$

$$= \int_{\Omega_f} f_1\cdot v_f \,\forall v, u\in X_1$$

$$b_f(u_f, p_f) = 0$$

In the porous medium region, multiplication of the first equation in (1.2) by $v_p \in X_2$, integration over and integration by parts gives

$$0 = (K^{-1}u_p + \nabla p_p, v_p)_{\Omega_p} =$$

$$(K^{-1}u_p, v_p)_{\Omega_p} - (p_p, \nabla\cdot v_p)_{\Omega_p} + \left\langle l, v_p\cdot n\right\rangle_\Gamma$$

where, by (8), p_p is replaced by l in the last term. Introducing

$$a_p(u_p, v_p) = \int_{\Omega_f} K^{-1}u_p v_p$$

$$b_p(v_p, p_p) = -\int_{\Omega_f} p_p\nabla\cdot v_p$$

we have

$$a_p(u_p, v_p) + b_p(v_p, p_p) + \left\langle l, v_p\cdot n\right\rangle_\Gamma = 0$$

$$b_p(u_p, p_p) = 0$$

The linking across Γ occurs through the condition $u_f\cdot n + u_p\cdot n = 0$ on Γ and the definition (8) of l. This linkage is the key to the well-posedness of the coupled problem and it hinges on the choice of the space Λ for the Lagrange multipliers. Define

$$b_\Gamma : X\times\Lambda \to \mathbb{R},\; b_\Gamma(\underline{v}, l) = \left\langle v_1\cdot n + v_2\cdot n, l\right\rangle_{|\Gamma}$$

with $\underline{v} = (v_1, v_2)$

The flux continuity condition (1.4) on Γ is then

$$b_\Gamma(\underline{v}, l) = 0$$

Since $v_p \in H(div;\Omega_p)$, it holds that. $v_p\cdot n \in H^{-1/2}(\partial\Omega_p)$ We wish to pick $\Lambda\subset L^2(\Gamma)$ to be the largest space for which the pairing $\left\langle v_p\cdot n, l\right\rangle_\Gamma$ is well defined. We show in Lemma 2.1 below (see also [20]) that

$$v_p\cdot n_\Gamma \in (H_{00}^{1/2}(\Gamma))$$

where $(H_{00}^{1/2}(\Gamma))$ is the completion of the smooth functions with compact support in Γ with respect to the norm

$$\|\mu\|_{1/2,\partial\Omega_2} := \left(\|\mu\|_{\partial\Omega_2}^2 + \int_{\partial\Omega_2}\int_{\partial\Omega_2}\frac{\left|\mu(t_1)-\mu(t_2)\right|^2}{\left|t_1 - t_2\right|}\right)^{1/2}$$

It is well known that $(H_{00}^{1/2}(\Gamma_I))$ is the interpolation space

$$(H_{00}^{1/2}(\Gamma)) = \left[L^2\left(\Gamma_1, H_0^1\left(\Gamma_1\right)\right)\right]_{1/2}$$

Any function $\mu\in(H_{00}^{1/2}(\Gamma_I))$ has the property that its extension by zero to $\partial\Omega_f$ gives a function $\tilde{\mu}_j \in (H^{1/2}(\partial\Omega_f))$ with

$$\left\|\tilde{\mu}_j\right\|_{1/2,\partial\Omega_j} \le C\|\mu\|_{(H_{00}^{1/2}(\Gamma_I))},\quad \text{j=f,p.} \qquad (9)$$

See Lions and Magenes [11] for background information on $(H_{00}^{1/2}(\Gamma_I))$. Accordingly, choose

$$\Lambda := H_{00}^{1/2}(\Gamma_I)\left(\subset L^2\left(\Gamma_I\right)\right).$$

Lemma 3.1. The bilinear form $b_\Gamma(\cdot,\cdot)$ is continuous on X x Λ.

Proof. First note that $v_j \cdot \hat{n}_j \in H^{-1/2}(\partial\Omega_j)$ =f,p. Let $\mu \in H_{00}^{1/2}(\Gamma_I)$ and let $\hat{\mu}_j$ be its extension by zero to $\partial\Omega_j$. We have

$$\int_{\Gamma_1} v_j \cdot \hat{n}_j \mu \, ds = \int_{\partial\Omega_j} v_j \cdot \hat{n}_j \mu_j ds$$
$$\le \|v_j \cdot \hat{n}_j\|_{-1/2\partial\Omega_j} \|\hat{\mu}_j\|_{1/2\partial\Omega_j}$$
$$\le C\|v\|_X \|\mu\|_\Lambda$$

using (7) and (9) in the last inequality.

Further, define

$$a(u,v) := \sum_{i=1}^{2} a_i(u_i, v_i) : X \times X \to \mathbb{R}$$
$$b(v,p) := \sum_{i=1}^{2} b_i(v_i, p_i) : X \times M \to \mathbb{R}$$
$$l(v) := (f_1, v_1)\Omega_1$$
$$g(q) := -(f_2, q_2)_{\Omega_2}$$

Then, (1)-(6) has the following weak formulation: find $(u,p,\lambda) \in X \times M \times A$ satisfying

$$\begin{cases} a(u,v) + b(v,p) + b_I(v,l) = l(v) \ \ \forall v \in X \\ b(u,q) = g(q) \ \ \forall q \in M \\ b_I(u,\mu) = 0 \ \ \forall \mu \in \Lambda \end{cases} \quad (10)$$

We next derive another weak formulation using the space V of functions in X with trace-continuous normal velocities:

$$V := \{v \in X : b_I(v,\mu) = 0 \ \ \textit{for all } \mu \in \Lambda\}$$

The connection between the two formulations (2.4) and (2.5) is considered in Remark 3.1 in section 3. Note that, due to Lemma 2.1, V is a closed subspace of X, e.g., Brezzi and Fortin [2]. The next lemma indicates that a trace-continuous normal velocity has a well-defined divergence on the whole domain. Let

$$\Omega := \mathrm{int}\,\textit{erior}\left(\overline{\Omega_1} \cup \overline{\Omega_2}\right)$$

For a given $v = (v_f, v_p) \in X$, define $\tilde{v}\big|_{\Omega_j} := v_j$, j= f, p.

Lemma 3.2. If $v \in V$, then $v \in H(div;\Omega)$.

Proof. Define

$$g(x) = \nabla \cdot v_j(x) \ \ \textit{for } x \in \Omega_j, \ \ j\textit{=f,p.}$$

We will show that $g = \nabla \cdot v$. Since $v_j \in H(div;\Omega_j)$, *j=f,p.*, we can apply the divergence theorem in each Ω_j. This gives, for all $\phi \in C_0^\infty(\Omega)$,

$$\int_\Omega v\nabla\phi \, dx = \int_{\Omega_1} v_1\nabla\phi \, dx + \int_{\Omega_2} v_2\nabla\phi \, dx$$
$$= -\int_{\Omega_1} (\nabla \cdot v_1)\phi \, dx - \int_{\Omega_2} (\nabla \cdot v_2)\phi \, dx$$
$$+ \int_{\Gamma_1} \left(v_1 \cdot \hat{n}_1 + v_2 \cdot \hat{n}_2\right)\phi \, dx$$

The last term vanishes since $\phi \in C_0^\infty(\Omega)$. Thus,

$$\int_\Omega v\nabla\phi \, dx = -\int_\Omega g\phi \, dx$$

Since $\nabla \cdot v_j \in L^2(\Omega_j)$, $g \in L^2(\Omega)$, and hence g is the weak L^2 divergence of $v \in V$.

We next define the subspace Z,

$$Z := \{v \in V : b(v,q) = 0 \ \ \textit{for all } q \in M\}$$

Lemma 3.3. The space Z is a closed subspace of V and X. Moreover, if $v \in Z$, then $\nabla \cdot v = 0, \ \textit{a.e. } x \in \Omega$.

Proof. Let $v \in Z$. Since $Z \subset V$, we know by Lemma 2.2 that $v \in H(div;\Omega)$. Thus, for any $q \in M$

$$b(v,q) = -\int_\Omega \nabla \cdot v \, q \, dx$$

We claim that $\nabla \cdot v \in M$. Indeed $\nabla \cdot v \in L^2(\Omega)$, and $\nabla \cdot v$ has zero mean value over Ω:

$$\int_\Omega \nabla \cdot v \, dx = \int_{\partial\Omega} v \cdot \hat{n} \, ds = 0$$

The space Z is a closed subspace of V since

$$b(v,p) = -\int_\Omega \nabla \cdot vq dx \le \|\nabla \cdot v\|_\Omega \|q\|_M$$

i.e., $b(\cdot,\cdot)$ is continuous on V x M.

Since V is a closed subspace of X, we can write the following variational formulation: find $(u,p) \in V \times M$ satisfying

$$\begin{cases} a(u,v) + b(v,p) = l(v) \ \ \textit{for all } v \in X \\ b(u,q) = g(q) \ \ \textit{for all } q \in M \end{cases}$$

We end this section noting that, under the solvability condition (3), any solution of (11) satisfies the mass conservation equations in (1) and (2). Indeed, define $f \in L^2(\Omega)$ such that $f = 0$ on and $f = f_2$ on Ω_p. If *(u,p)* is a solution to (11), then $\nabla \cdot u \in L^2(\Omega)$ due to Lemma 3.2. The second equation in (11) implies that $\nabla \cdot u - f = c$, where c is a constant. The divergence theorem gives

$$C|\Omega| = \int_\Omega (\nabla \cdot u - f)dx = \int_{\partial\Omega} u \cdot n dx - \int_\Omega f dx = \int_\Omega f_2 dx$$

using (3). There are $\nabla \cdot u = 0$ on Ω_f and $\nabla \cdot u = f_2$ on Ω_p.

4. ANALYSIS OF THE WEAK FORMULATION

This section is devoted to a proof of existence of weak solutions to (1)-(6) based on the weak formulations (10) and (11). Existence depends on our choice of the Lagrange multiplier space $\Lambda = H_{00}^{1/2}(\Gamma)$ so that the problem is neither over nor under constrained.

We begin with a few simple but useful estimates. Let

$W_p := \{v_p \in X_2 : \nabla \cdot v_p = 0 \ a.e. \ x \in \Omega_p\}$

denote the (closed) subspace of div-free functions in X_2.

Lemma 4.1. For $v_i \in H^1(\Omega_i)^d \cap X_i$ *(i = v, p)* we have

$$C_1 \|v_i\|_{\Omega_i} \le \|v_i\|_{X_i} \le C_2 \|v_i\|_{1,\Omega_i} \qquad (12)$$

Furthermore, for *(i = v, p)* there holds

$$|a_i(u_i, v_i)| \le C_3 \|u_i\|_{X_i} \|v_i\|_{X_i} \quad \forall u_i, v_i \in X_i \qquad (13)$$

$$a_1(v_f, v_f) \ge \frac{C_4}{2} \|v_f\|_{X_i}^2 \quad \forall v_f \in X_1 \qquad (14)$$

$$a_1(v_p, v_p) \ge C_4 \|v_p\|_{X_2}^2 \quad \forall v_p \in X_p \qquad (15)$$

$$|b_i(v_i, p_i)| \le C_6 \|v_i\|_{X_i} \|p_i\|_{M_i} \quad \forall v_i \in X_i, p_i \in M_i \qquad (16)$$

$$|a(u,v)| \le C_3 \|u\|_X \|v\|_X \quad \forall u_i, v_i \in X_i \qquad (17)$$

$$|b(v,p)| \le C_6 \|v\|_X \|p\|_M \quad \forall v \in X, p \in M \qquad (18)$$

$$a(v,v) \ge \min\left\{\frac{C_4}{2}, C_5\right\} \|v\|_X^2 \quad \forall v \in X_1 \times W_2 \qquad (19)$$

Proof. Inequalities (12) and (13) follow from the Poincaré-Friedrich inequality and the trace theorem. The Korn inequality implies (14) when we have α_{BJ} small enough, while (15) and (16) are immediate. Inequalities (17), (18), and (19) follow by combining earlier ones.

The next lemma establishes the Ladyzhenskaya-Babuska-Brezzi condition required for the formulation (11) in *V x M*.

Lemma 4.2. There is a constant $\beta > 0$ such that

$$\inf_{q \in M \backslash \{0\}} \sup_{v \in V \backslash \{0\}} \frac{b(v,q)}{\|v\|_X \|q\|_M} \ge \beta \qquad (20)$$

Proof. Let q G M \{0} be fixed but arbitrary. We construct $a v \in V$ satisfying

$$b(v,q) \ge \beta \|v\|_X \|q\|_M$$

Given $q = (q_1, q_2) \in M$ the function $\tilde{q}(x)$ defined by $\tilde{q}_{|\Omega_i} = q_i$ has mean value zero over Ω; thus $\tilde{q} \in L_0^2(\Omega)$. Thus, (see, e.g., [7, 10]) there exists $\tilde{v} \in (H_0^1(\Omega))^d$ satisfying

$\nabla \cdot \tilde{v} = \tilde{q}$ in Ω $\tilde{v} = 0$ on $\partial\Omega$, $\|\tilde{v}\|_{1,\Omega} \le C_7 \|\tilde{q}\|_\Omega$

Given this v, define $v = (v_f, v_p) \in X$ by $v_f = \tilde{v}_{|\Omega_f}$, $v_p = \tilde{v}_{|\Omega_p}$. Since $\tilde{v} \in (H_0^1(\Omega))^d$ it follows $v_f = \tilde{v}_{|\Omega_f} = 0$ and $v_p \cdot n_{|\Omega_p} = 0$

Further, $v_{f|\Gamma} = v_{p|\Gamma} \in \Lambda = H_{00}^{1/2}(\Gamma)$ so that $v_f \cdot n \in L^2(\Gamma)$, $v_p \cdot n \in L^2(\Gamma)$ and

$$b_\Gamma(v,l) = \langle v_1 \cdot n + v_2 \cdot n, l \rangle = 0$$

for all $l \in L^2(\Gamma)$. Thus, $v \in V$. Using (3.1) we find

$$\|v\|_X \le C_2 \|\tilde{v}\|_{1,\Omega} \le C_2 C_7 \|\tilde{q}\|_{0,\Omega} = C_2 C_7 \|q\|_M$$

Finally, for this v

$$b(v,q)=\sum_{i=f,p}(-\nabla\cdot v_i,q_i)=-(\nabla\cdot\tilde{v},\tilde{q})_\Omega \qquad (21)$$

$$\|\tilde{q}\|_{0,\Omega}^2 \ge (C_2C_7)^{-1}\|v\|_X\|q\|_M \qquad (22)$$

completing the proof with $\beta=(C_2C_7)^{-1}$.

To apply the abstract theory of mixed problems in, e.g., Girault and Raviart [7], Brezzi and Fortin [2], we must show $a(\cdot,\cdot)$ is coercive on the constraint set Z. This is accomplished in the next lemma.

Lemma 4.3. $a(\cdot,\cdot)$ is coercive on Z: there is an $\alpha>0$ such that
$a(v,v)\ge\alpha\|v\|_X^2$ for all $v\in X$.

Proof. Note that by Lemma 2.3 if $v=(v_f,v_p)\in\ker(B)$, $\nabla\cdot v=0$, a.e. $x\in\Omega$, i.e., $v_p\in W_2$. Coercively now follows from (3.8) of Lemma 4.1. □

Lemmas 3.1, 4.2, and 4.3, together with the abstract theory of mixed problems [7, 2], immediately imply existence of a weak solution $(u,p)\in V\times M$ satisfying (11).

THEOREM 4.1. There exists a unique solution $(u,p)\in V\times M$ to the problem (11). □

To verify that the solution to (11) is also the solution to the formulation (10) in $X\times M\times\Lambda$ using the general saddle point problem theory [7, 2], we must verify the inf-sup condition

$$\inf_{l\in\Lambda}\sup_{v\in V\setminus\{0\}}\frac{b_I(v,l)}{\|v\|_X\|l\|_M}\ge\beta>0 \qquad (23)$$

Due to technical difficulties related to the restriction of $H^{-1/2}(\partial\Omega_p)$ functions to Γ, we are only able to show a modified inf-sup condition:

$$\inf_{l\in\Lambda}\sup_{v\in V\setminus\{0\}}\frac{b_I(v,l)}{\|v\|_X\|l\|_{1/2,\Gamma}}\ge\beta>0 \qquad (24)$$

Lemma 4.4. The inf-sup condition (24) holds.

Proof. Fix $l\in H_{00}^{1/2}(\Gamma)$ and let $\tilde{l}\in H_{00}^{1/2}(\Gamma)$ be its extension by zero to $\partial\Omega_p$. Since $H_{00}^{1/2}(\Gamma)\subset H^{1/2}(\Gamma)$, there exists $l_I\in H^{-1/2}(\Gamma)$ such that

$$\frac{\langle l_I,l\rangle_{|\Gamma}}{\|l_I\|_{-1/2,\Gamma}}\ge\frac{1}{2}\|l\|_{1/2,\Gamma} \qquad (25)$$

We next define $\hat{l}\in H^{-1/2}(\Gamma)$ by

$$\langle\hat{l},w\rangle_{\partial\Omega_p}:=\langle l_I,w\rangle_\Gamma \text{ for } w\in H^{1/2}(\partial\Omega_p)$$

We then have

$$\|\hat{l}\|_{-1/2,\partial\Omega_p}=\sup_{0\ne w\in H^1(\partial\Omega_p)}\frac{\langle\hat{l},w\rangle_{|\Gamma}}{\|w\|_{1/2,\partial\Omega_p}}\le\|l_I\|_{-1/2,\Gamma} \qquad (26)$$

Since the normal trace operator maps $H(div,\Omega_p)$ onto $H^{-1/2}(\partial\Omega_p)$ (see [7, Corollary 2.8]) and it is continuous (see (2.1)), by the open mapping theorem there exists $v_p\in H(div,\Omega_p)$ such that $v_p\cdot n=\tilde{l}$ on $\partial\Omega_p$ and

$$\|v_p\|_{X_2}\le C\|\hat{l}\|_{-1/2,\partial\Omega_p}\le C\|l_I\|_{-1/2,\Gamma} \qquad (27)$$

using (26) for the second inequality. We note that $v_p\in X_2$ since, for all $w\in H_{0,\Gamma}^1(\Omega_p)$

$$\langle v_p\cdot n,w\rangle_{\partial\Omega_p}=\langle\hat{l},w\rangle_{\partial\Omega_p}=\langle l_I,w\rangle_\Gamma=0$$

Choosing $v=(0,v_p)\in X$ and using (25) and (27) we get

$$\frac{b_I(v,l)}{\|v\|_X}=\frac{\langle v_p\cdot n,\tilde{l}\rangle_{\partial\Omega_p}}{\|v_p\|_{X_2}}=\frac{\langle\hat{l},\tilde{l}\rangle_{\partial\Omega_p}}{\|v_p\|_{X_2}}$$

$$\frac{\langle\hat{l},\tilde{l}\rangle_\Gamma}{\|v_p\|_{X_2}}\ge\frac{1}{C}\frac{\langle\hat{l},\tilde{l}\rangle_\Gamma}{\|\hat{l}\|_{-1/2,\Gamma}}\ge\beta_1\|l\|_{1/2,\Gamma}$$

REMARK

If the porous medium is entirely enclosed within the fluid region, then $\Gamma = \partial\Omega_p$. In this case there are no incompatible points and it is easy to extend slightly the proof of Lemma 3.4 to show that the stronger inferior – superior condition (3.12) holds. In this case, the unique weak solution to (2.5) is also the unique weak solution to (2.4) and the two formulations are equivalent.

5. CONCLUSION

We studied the mathematical model of this setting consisting of the Stokes equations in the fluid region coupled with the Darcy equations in the porous medium, coupled across the interface by the Beavers-Joseph conditions. We prove existence of weak solutions. This is important because there are many "legacy" codes available which have been optimized for uncoupled porous media and fluid flow and because using this interface conditions we have a model more appropriate to the reality and for PEM cells.

Having proved the weak formulation this opens us the possibility for good algorithms that will be presented in other work.

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Modelarea matematică în pilele de combustie PEM

Rezumat: În celule de combustibil cu membrană cu schimb de protoni (PEM), transportul de combustibil pentru zonele active, precum şi eliminarea produselor de reacţie sunt realizate folosind o combinaţie de canale şi a straturilor poroase de difuzie. În scopul de a îmbunătăţi modelele existente matematice si numerice de celule de combustie PEM, o înţelegere mai profundă a proceselor de curgere în canale şi straturi de difuzie este necesară. Se va discuta modelul matematic pentru pilele de combustie PEM, activitatea se va concentra pe descrierea de cuplare a fluxului liber în regiune, canal cu viteza de filtrare în stratul de difuzie poros

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