



# Multiphase flow through multilayers of thin porous media: General balance equations and constitutive relationships for a solid–gas–liquid three-phase system



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## ABSTRACT

In this work, we propose a new approach to modeling multiphase flow and solute transport through a stack of thin porous layers. Currently, numerical simulation of thin layers involves discretization across the layer thickness. In our new approach, thin porous layers are treated as a bunch of two-dimensional (2D) interacting continua. Macroscale balance laws are formulated in terms of thickness-averaged material properties. A number of exchange terms are employed to account for exchanges of mass, momentum, energy, and entropy between two neighboring layers. The entropy inequality is then exploited for obtaining constitutive equations to close the problem under study. As an example, simplified governing equations are derived for a system of air–water flow and heat transfer through two thin porous layers. In comparison to previous macroscale models, our model possesses the following distinctive advantages: (1) it is rigorous thermodynamics-based model; (2) it is formulated in terms of layer-thickness-averaged material properties which are usually easily measurable; and (3) it reduces 3D modeling to 2D leading to a very significant reduction of computational efforts.

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## 1. Introduction

Multiphase flow and solute transport through thin layers of porous media are encountered in a number of industrial applications [1–4], such as fuel cells, paper printers, filters, and hygiene products (e.g. diapers and wipes). As an example, consider a polymer electrolyte fuel cell (PEFC), schematically shown in Fig. 1, which has been the subject of extensive studies over the past two decades [5,6,32,33]. A typical PEFC unit consists of gas channels (GCs), gas diffusion layers (GDLs), micro porous layers (MPLs), and catalyst layers (CLs) on both cathode and anode sides. The two sides are connected by a solid polymer electrolyte membrane (PEM). In automotive applications, the GDL, MPL, and CL usually have thicknesses of 150–300  $\mu\text{m}$ , 5–20  $\mu\text{m}$ , and 5–30  $\mu\text{m}$ , respectively. In the in-plane directions, they can have dimensions of around  $50 \times 50$  cm. So, they are very thin layers of porous media stacked upon each other. The operating principles of a PEFC are as follows. Streamed humidified hydrogen (or hydrogen-rich gas) and oxygen (or air) are delivered into the GCs on the anode and cathode sides, respectively. At the anode side, hydrogen diffuses through the diffusion layers and enters into the CL, where each hydrogen molecule splits into two electrons and two protons. The protons

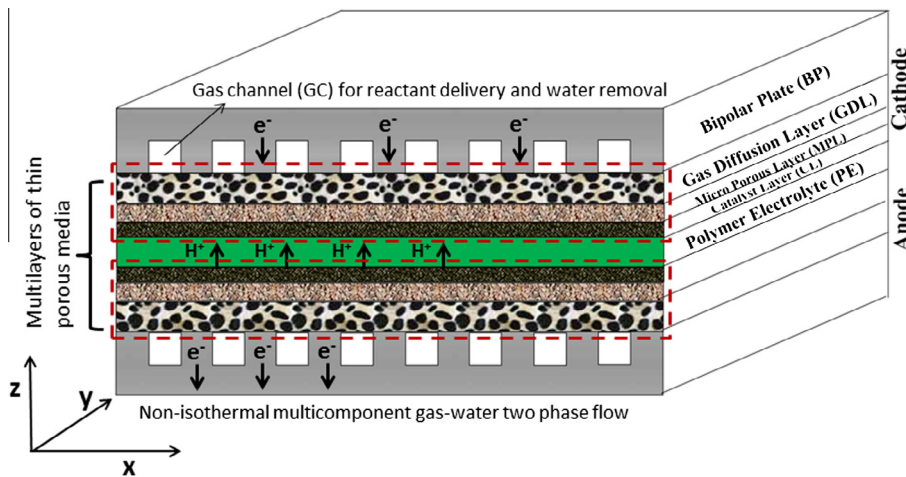
migrate into the cathode CL via the membrane. The electrons cannot enter the membrane and have to travel through an external circuit to the cathode side. There, electrons and oxygen diffuse into the CL where they combine with the protons, which have diffused from the membrane, forming water and generating heat. Though the operating principles are quite simple, several electrochemical and physical processes (e.g. two-phase flow, electrochemical reactions in CL and heat transfer) occur simultaneously. These processes are crucial to the operation of transport PEFCs [7,8]. To increase the performance and durability as well as optimize the material properties for cost reduction, an effective and reliable numerical model for describing water flow and heat transfer in PEFCs is needed. This is the main objective of the present work.

To date, the modeling of flow and transport through such a thin porous medium has been mostly performed in a three-dimensional (3D) discretized domain with many computational cells, based on some macroscale theories like the well-known two-phase Darcy's law [1,9,10]. However, there are a number of problems with this approach. First, currently available macroscale theories are formulated in terms of averaged quantities, which are defined over an average domain known as the representative elementary volume (REV). A major requirement of the REV is that its size must be much larger (10–15 times) than the pore-scale dimensions, but much smaller than the modeling domain size [11]. Obviously, this criterion cannot be satisfied in a thin porous medium. So, the

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Nomenclature	
<i>Latin symbols</i>	
$A^\alpha$	Helmholtz free energy function defined by Eq. (32), ( $L^2/T^2$ )
$\delta A$	cross-sectional area of REV, ( $L^2$ )
$b$	layer thickness, (L)
$C^\alpha$	mass-specific heat capacity of the $\alpha$ phase, ( $L^2/T^{2\circ}$ )
$e^\alpha(\rho)$	mass exchange term defined by Eq. (A15), ( $1/T$ )
$e_{\alpha}^T, e_{\alpha}^B$	layer–layer mass exchange terms defined by Eqs. (A16) and (A17), ( $L/T$ )
$E^\alpha$	macroscopic internal energy, ( $L^2/T^2$ )
$\mathbf{E}^s$	planar Lagrangian strain tensor, (-)
$\mathbf{F}^s$	solid phase motion
$\mathbf{g}$	gravity vector, ( $L/T^2$ )
$G^\alpha$	Gibbs free energy defined by Eq. (57), ( $L^2/T^2$ )
$h^\alpha$	external heat supply, ( $L^2/T^3$ )
$\mathbf{j}_i$	diffusive flux, ( $M/L^2 T$ )
$\mathbf{j}_{ih}^\alpha$	volume-averaged nonconvective species flux defined by Eq. (B1), ( $M/L^2 T$ )
$J_i^\alpha$	mass transfer into species $i$ in the $\alpha$ phase, ( $1/T$ )
$J_{ix}^T, J_{ix}^B$	layer–layer mass exchanges for species $i$ in the $\alpha$ phase, ( $L/T$ )
$k$	layer index, (-)
$\mathbf{K}$	heat conductivity tensor, ( $M L^2/T^{3\circ}$ )
$\bar{K}$	energy exchange coefficient between neighboring layers, ( $M/T^{3\circ}$ )
$l^\alpha$	external supply of entropy, ( $L^2/T^{3\circ}$ )
$p$	pressure, ( $M/L T^2$ )
$\mathbf{q}$	heat flux, ( $M/T^3$ )
$Q^\alpha$	energy transfer into the $\alpha$ phase, ( $L^2/T^3$ )
$Q_{\alpha}^T, Q_{\alpha}^B$	layer–layer energy exchanges defined by Eqs. (B11) and (B12), ( $L^3/T^3$ )
$r_i^\alpha$	mass-averaged chemical reaction rate, ( $1/T$ )
$\mathbf{R}^\alpha$	material property in Eq. (62), ( $1/T$ )
$s$	saturation
$S^\alpha$	macroscopic entropy per unit mass, ( $L^2/T^{2\circ}$ )
$\delta S_{\alpha\beta}$	interfacial area between two phases, ( $L^2$ )
$\delta S_{\alpha}^B$	interfacial area of the $\alpha$ phase at the top of the layer, ( $L^2$ )
$\delta S_{\alpha}^T$	interfacial area of the $\alpha$ phase at the bottom of the layer, ( $L^2$ )
$\mathbf{t}_h^\alpha$	in-plane part of macroscopic stress tensor, ( $M/L T^2$ )
$\mathbf{T}^\alpha$	momentum transfer into the $\alpha$ phase through phase interfaces, ( $L/T^2$ )
$\mathbf{T}_{\alpha}^T, \mathbf{T}_{\alpha}^B$	layer–layer momentum exchanges defined by Eqs. (B7) and (B8), ( $L^2/T^2$ )
$\mathbf{v}$	velocity vector for bulk phase, ( $L/T$ )
$\mathbf{w}$	velocity vector for interfaces, ( $L/T$ )
<i>Greek symbols</i>	
$\varepsilon$	porosity of porous medium, (-)
$\varepsilon^\alpha$	volume fraction of the $\alpha$ phase, (-)
$\rho$	mass density, ( $M/L^3$ )
$\psi$	thermodynamic property
$\Psi$	microscopic entropy flux; macroscopic entropy flux if with superscript, ( $M/T^{3\circ}$ )
$\Phi^\alpha$	entropy transfer into the $\alpha$ phase, ( $L^2/T^{3\circ}$ )
$\Phi_{\alpha}^T, \Phi_{\alpha}^B$	layer–layer entropy exchanges, ( $L^3/T^{3\circ}$ )
$\Gamma$	entropy production, ( $L^2/T^{3\circ}$ )
$\Lambda$	total amount of net rate of entropy production, ( $M/T^{3\circ}$ )
$\theta$	temperature, ( $^{\circ}$ )
$\omega$	mass fraction, (-)
$\Omega^\alpha$	wettability potential defined by Eq. (61), ( $M/L T^2$ )
$\Pi_m$	material coefficient in Eq. (63), ( $M T^{\circ}/L^4$ )
$\Pi_b$	material coefficient in Eq. (64), ( $L^2 T/M$ )
$\Pi_s$	material coefficient in Eq. (65), ( $L T/M$ )
<i>Superscripts and subscripts</i>	
$h$	in-plane part
$\alpha, \beta$	phase indicator
$T$	top of layer
$B$	bottom of layer
$l$	liquid phase
$g$	gas phase
$s$	solid phase
$r$	reference



**Fig. 1.** Schematic of a PEFC unit including gas channels (GCs), gas diffusion layer (GDL), micro porous layer (MPL), catalyst layer (CL) on each side; both sides are connected by a solid polymer electrolyte membrane (PEM). Here, GDL, MPL and CL constitute a system of three thin porous layers. The  $z$  is the through-plane direction, and the  $x$  or  $y$  is the in-plane direction.

application of those macroscale theories to thin porous media (at least in the through-plane direction) is questionable. Second, there are problems with the numerical solution of those macroscale

models. For instance, one needs to discretize a thin porous medium into computational cells, whose size may be comparable to the pore sizes. This suggests that the methods are not applicable to

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