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Evaporation, two phase flow, and thermal transport in porous media with application to low-temperature fuel cells

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ABSTRACT

A pore level model of the vapor transport, heat transfer, and evaporation are incorporated into a network model to study the mass transport inside a porous transport layer of proton exchange membrane (PEM) fuel cell. Viscous models are used for the flow of liquid water and for the air–vapor mixture. Thermal transport is included by performing an energy balance at each pore. Existing models for vapor transport and evaporation are adapted for incorporation into the network model.

The effect on the water transport of different gas channel conditions such as temperature and relative humidity is studied. Effective thermal conductivities and vapor diffusivities are calculated from the simulation and compared against published values.

1. Introduction

During operation of a proton exchange membrane (PEM) fuel cell, water, heat, and electricity are produced. Fuel cell product water is removed through the reactant flow channels in either liquid or vapor state after passing through the porous transport layer (PTL), also referred to as the gas diffusion layer (GDL). The heat generated will be partially dissipated by evaporating a portion of the water mass generated and the balance of thermal energy is removed by an external cooling system. A combined state of liquid water, and water vapor, and gaseous reactants coexist inside the PTL. The displacement of the liquid and vapor water within the PTL is not well characterized, but water transport is known to be an important factor affecting the fuel cell efficiency at high current density [1,2].

PEM fuel cell operating conditions can vary significantly. For example, at startup mostly liquid water is expected to percolate through the PTL due to the low temperature. In contrast, a significant amount of water vapor content is expected during steady operation at 80°C. The inlet air humidity and the cooling temperature also significantly affects mass transport. Making this problem even more challenging is that many of these transport phenomena are coupled. Isolating each effect is difficult not only experimentally, but also from a modeling perspective.

The presence of liquid water in the PTL affects thermal and mass (reactant and vapor) transport as compared to a dry PTL. Due to the complexity of the problem at the local pore level, mass and thermal transport is most often modeled through effective properties in cell-level models [3,4]. These properties are normally obtained through in situ [5] and ex-situ [6,7] experimental measurements and related to liquid saturation in the PTL. Effective properties are used in cell-level models of fuel cell performance, the results from which are then compared to fuel cell stack testing.

The inability to effectively manage water transport is due in part to technical limitations in observing liquid water and water during in situ or ex-situ measurements. Among the unknown effects is the evaporation rate within a PTL. Recent studies have shown a discrepancy between different evaporation models when applied to fuel cell studies [8–14]. Associated with the evaporation phenomena is the thermal conductivity of the PTL, which also plays a significant role on the mass transport via the temperature gradient through the PTL. This coupling of thermal and mass transport requires an accurate values of the PTL thermal conductivity and thermal contact resistant under different condition such as water content, compression pressure, and thickness [15–17].

There has been recent progress and success in local modeling of liquid water transport in fuel cell porous media using network simulations [18–24]. Yet, evaporation, which is the most prominent mechanism for removal of product water has not been effectively incorporated into pore network simulations. Incorporation of evaporation into a network simulation of liquid water transport in fuel cell porous media is complicated by the coupling of the liquid, vapor, and heat transport equations [25].

Modeling of evaporation in porous media has been attempted in applications unrelated to fuel cells [26–28]. In most cases, those

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Nomenclature

GDL	gas diffusion layer, referred to as PTL
PEM	proton exchange membrane
PTL	porous transport layer
PTFE	polytetrafluoroethylene
A^*	non-dimensional wetted area
C	vapor concentration
c_p	specific heat
D	binary diffusivity of water vapor on air
F	Faraday constant
H	simulated domain height
I_a	current density
k	thermal conductivity
L	simulated domain length
l	pore length
M_w	molar mass of water
m	mass
P_e	power per unit area
P_{sat}	saturation pressure
p^c	capillary pressure
p	pressure
$\dot{Q}$	rate of heat conduction
q	volumetric flow rate
R	thermal resistance
r	pore radius
s	fraction of water–air inside the pore
T	temperature
t	time
V_c	voltage
V^*_{ev}	non-dimensional evaporated volume of water
v	pore volume
x	meniscus position inside the pore
γ	surface tension
Δh^{ev}	phase change enthalpy
ε	porosity
θ	contact angle
κ	proportionality constant
μ	viscosity
ρ	density
ϕ	relative humidity
ω	humidity ratio

models where developed to study drying in fully saturated soils at relatively low temperatures of *20* to 25°C. Under normal fuel cell operating conditions, the PTL is never fully saturated with liquid water and there will be a balance between water generation and evaporation during steady operation.

In this paper, a pore network model [20,29] is extended to include a coupled system of heat transfer, vapor transport, and evaporation models to an existing fluid transport model. Local models of capillary pressure, vapor diffusion, thermal conduction, and evaporation ratio at the pore level are established. The objective behind developing a pore level model of the PTL is to reduce the number of uncertainties associated with using bulk property measurements such as relative permeabilities, effective diffusivities, effective thermal conductivity, and evaporation rates on the fuel cell performance.

2. Liquid water, vapor concentration, heat transfer, and evaporation models

There are two traditional methods for modeling the void space, or pore volume, in regularized pore-network simulations. The first approach considers all volume is assigned to the nodes and the second is that all volume is assigned to the passages between nodes. In the network model developed herein, all the pore volume is assigned to a cylinder or tube that is located between nodes in a similar manner as Aker [30]. The plot inset in Fig. 1, illustrates the schematic of partially saturated pores and the location of the pore volumes. The two-dimensional numerical model presented is an extension of the work by Médici and Allen [20] with the addition of heat transfer, vapor transport, and evaporation coupled to the liquid transport model. Condensation is not considered at this time.

Liquid displacing gas between nodes 'i' and 'j', which constitutes a single pore, is modeled as:

$$q_{ij} = \kappa \frac{r_{ij}^4}{\mu_{ij}^e l}\left(p_i - p_j - p_{ij}^c\right), \tag{1}$$

where l is the length of the pore, r_{ij} is the pore radius, p_i and p_j are the pressure acting on each end of pore, p_{ij}^c is the capillary pressure, and κ is a proportionality constant equal to $\pi/8$ for Poiseuille flow. Eq. (1) is only valid when $p_i - p_j > p_{ij}^c$, otherwise $q_{ij} = 0$. The transition viscosity within a pore, μ_{ij}^e, is a function of the meniscus position inside the pore x_{ij}:

$$\mu_{ij}^e = (\mu_{nw} - \mu_w)\frac{1-\cos(\pi x_{ij}/l)}{2} + \mu_w, \tag{2}$$

where μ_{nw} is the non-wetting (injected) fluid viscosity, and μ_w is the wetting (displaced) fluid viscosity. When only one fluid is present, the viscosity is the value for that fluid.

The capillary pressure p_{ij}^c is also modeled as a function of the meniscus position inside of the pore. The capillary pressure inside each pore is approximated by using cosine functions to smoothly mimic the throat effect present at both ends of the pore:

$$p_{ij}^c = \gamma\cos\theta\left[\left(1-\frac{r_{ij}}{2\bar{r}_i}-\frac{r_{ij}}{2\bar{r}_j}\right)\frac{1-\cos(2\pi x_{ij}/l)}{r_{ij}}+\frac{1+\cos(\pi x_{ij}/l)}{\bar{r}_i}+\frac{1-\cos(\pi x_{ij}/l)}{\bar{r}_j}\right], \tag{3}$$

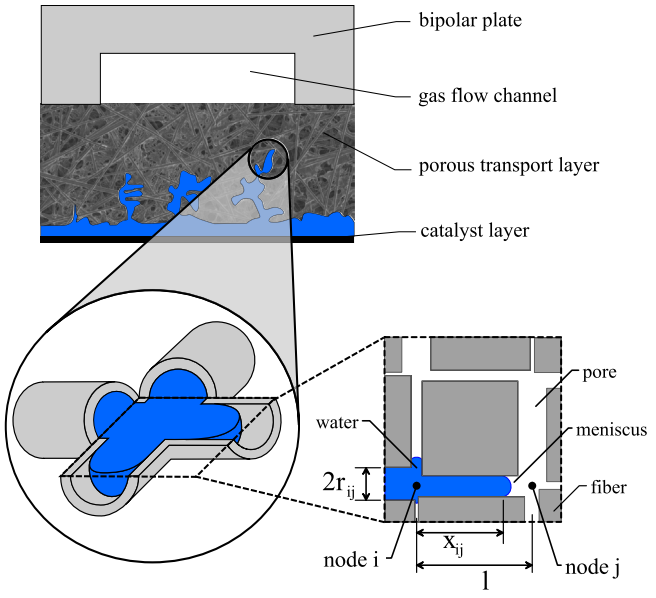

Fig. 1. Schematic representation of the two-dimensional model domain of the fuel cell and pore network. Pores are modeled as cylindrical tubes where the porosity is set by specifying the thickness of tube wall.