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A review of cell-scale multiphase flow modeling, including water management, in polymer electrolyte fuel cells

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HIGHLIGHTS

- The transport expressions inside PEFC GDLs are developed to describe significantly different systems.
- Insight into the fundamental processes of liquid water evolution and transport in the GDL and GC is still lacking.
- One important feature is the possibility to track the front between the liquid and the gas phases.
- The two phase micro channels pressure drop correlations may not be applicable for GCs since one wall being porous.

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ABSTRACT

The PEFC has emerged as the most viable fuel cell type for automotive and some portable applications, and also has potential back-up power unit applications due to its low operating temperature, comparative simplicity of construction, high power density, and ease of operation. In spite of tremendous scientific advances, as well as engineering progress over the last few decades, the commercialization of PEFCs remains unrealized, owing primarily to economic viability associated with the high prices of materials and components and technical problems relating primarily to water management. The difficulty in addressing the water management issues lies mostly in the two-phase multi-component flow involving phase-change in porous media, coupled heat and mass transfer, interactions between the porous layers and gas channel (GC) and the complex relationship between water content and cell performance. Due to the low temperature of operation, water generated by the electrochemical reactions often condenses into liquid form, potentially flooding the gas diffusion layer (GDL), GC or other components. Insight into the fundamental processes of liquid water evolution and transport is still lacking, preventing further enhanced PEFC development.

The aim of this paper is to give a comprehensive introduction to PEFC modeling inside GCs and GDLs, with a focus on two-phase flow and related phase-change and transport processes. Relevant momentum, mass and heat transport processes are introduced and the microstructural effects on the transport processes inside the porous GDL are extensively discussed.

The selection of a computational approach, for the two-phase flow within a GDL or GC, for example, should be based on the computational resources available, concerns about time and scale (microscale, cell scale, stack scale or system scale), as well as accuracy requirements. One important feature, included in some computational approaches, is the possibility to track the front between the liquid and the gas phases. To build a PEFC model, one must make a large number of assumptions. Some assumptions have a negligible effect on the results and reliability of the model. However, other assumptions may significantly affect the result. It is strongly recommended in any modeling paper to clearly state the assumptions being implemented, for others to be able to judge the work.

It is important to note that a large fraction of the expressions that presently are used to describe the transport processes inside PEFC GDLs were originally developed to describe significantly different systems, such as sand or rocks. Moreover, the flow pattern maps and pressure drop correlations of two phase

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flow in micro channels may not be applicable for GCs due to one side wall being porous, with the resulting interaction between the GDL and GC.

Nomenclature

A	area, m^2 or control parameter for inter-particle and adhesion forces
a	VOF function (fraction of liquid), –
AAV	area-to-volume ratio, m^2/m^3
a_z	species-dependent parameter
b	ratio of actual area of contact of the surface to projected area, –
b_z	species-dependent parameter
c	heat capacity, J/(kg K) or speed, m/s
C_D	drag coefficient, –
c_p	heat capacity at constant pressure, J/(mol K)
c_z	species-dependent parameter
D	characteristic length, m
d	maximum droplet diameter, m
D_h	hydraulic diameter, m
D_i	diffusion coefficient, m^2/s
e_0	internal energy, J/kg
E	internal energy, J
$\mathbf{e}_a$	linked velocities for inter-particle forces, lu/ts
F	force, N or source term, N/(m^3 s)
f	volume fraction, –
g	gravity, m/s^2
H	channel height, m or mean radius of curvature of the interface, 1/m
h	droplet diameter, m
h_{fg}	enthalpy of phase change, J/kg
h_v	heat transfer coefficient between the solid and fluid phases, W/(m^2 K)
$\boldsymbol{i}$	direction vector of the gas flow
$\boldsymbol{I}$	unit tensor
$J(S)$	Leverett function, –
k	permeability, m^2 or thermal conductivity, W/(m K)
$K(S)$	modified Leverett function, –
k_B	Boltzmann constant, J/K
K_{kq}	inter-phase exchange term
k_r	relative permeability, –
k_{rel}	known function of saturation
L	length, m
M	molar mass, kg/mol or M-factor (describes the microstructural influence), –
$\dot{m}$	mass transfer rate, mol/s or kg/s
$\boldsymbol{n}$	normal vector
p	pressure, Pa
p_c	saturation-dependent capillary pressure, Pa
P	percolation factor, –
q	switch function, –
Q	heat transfer rate, W/m^3
R	gas constant, J mol^{-1} K^{-1}
R	local curvature of the gas-liquid interface
r	pore radius, m
$\boldsymbol{r}$	position (in SPH)
R_k	fluid-to-solid conductivity ratio, -
R_l	reaction rate, mol/(m^3 s)
s	fluid or solid domain parameter, –
S	saturation, - or source term, W/(m^3 s) or kg/(m^3 s)
T	temperature, K
t	thickness, m or time, s
$\boldsymbol{t}$	unit vector
u	velocity, m/s or velocity in x direction, m/s
$\boldsymbol{u}$	velocity vector
$\mathbf{\acute{u}_0}$	Reynolds stress
$\mathbf{v}$	mass-averaged velocity, m/s or velocity vector
v	velocity in y direction, m/s
V	volume, m^3
W	interpolating kernel (in SPH)
w	velocity in z direction, m/s or mass fraction, –
x	mole fraction, –
Y	molar concentration, mol/m^3
∇a_n	original normal vector
∇a_t	transformed normal vector
$1/\alpha$	pore size distribution index, –
α	observed volume fraction, –
β	constriction factor, –
θ	contact angle, ° or rad
γ	surface tension, N/m or ratio of specific heats, –
ρ	density, kg/m^3
μ	dynamic viscosity, Pa s
ν	kinematic viscosity, m^2/s
λ	mean free path, m
ϕ	physical (transport) property
ε	porosity, - or rate of strain tension
κ	surface curvature
τ	tortuosity, –
$\boldsymbol{\tau_0}$	deviatoric stress, N/m^2
θ_c	effective contact angle, ° or rad
ε_p	percolation threshold, –
ρ_w	equivalent density of solid wall material, mu/lu^3
ψ	potential function, –
ω_a	weighting factor, –
Γ	exchange coefficient

Dimensionless numbers

Bi	Biot number, –
Bo	Bond number (also known as Eötvös number [Eö or Eo]), –
Ca	Capillary number, –
Kn	Knudsen number, –
M	Viscosity ratio, –
N_M	MacMullin number, –
Nu	Nusselt number, –
Re	Reynolds number, –
Sc	Schimdt number,–
Sh	Sherwood number, –
Pr	Prandtl number, –
We	Weber number, –

Subscripts and superscripts

0	initial, bulk
1	fiber
a	non-wetting phase, adhesion (force), particle an or advancing
ads	adhesion
b	wetting phase or particle b
cond	condensation