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(Invited) Continuum Mathematical Modeling of Water Electrolysis: A Tutorial

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Abstract

Widespread use of hydrogen energy is contingent on the development of reliable and economical sources of hydrogen. Electrolysis from renewably-derived low-carbon electricity is a potentially viable method of hydrogen generation. Prime among the electrolysis technologies are those utilizing ion-conducting polymers (ionomers) including proton-exchange-membrane water electrolyzer (PEMWE). However, these technologies need to exhibit increased efficiency, performance, and durability to become commercially viable. Like most electrochemical devices, PEMWEs involve multiple components (e.g., catalyst, ionomer, transport layers, membrane, plates) and multiple phases, with phenomena occurring across different time and length scales. Furthermore, it is difficult to experimentally probe many of the species and phenomena during operation. Thus, mathematical modeling at the continuum level has been an invaluable aid in exploring, understanding, and optimizing PEMWE cell and components. This is especially true in the highly coupled and complex physics and chemistries that occur with the membrane-electrode assembly (MEA). The physics in a typical volume-averaged non-isothermal model include multiphase transport in porous media, concentrated-solution theory, Ohm's Law, and Butler-Volmer kinetics, and ion, gas, and water transport in the ionomer.

In this talk, different modeling approaches, governing equations, and constitutive relationships will be described, including the benefits and limits of modeling. While focus will be on continuum equations and macroscale effects, detailed submodels and approaches for scaling to full cells and specific components, respectively, will be introduced. For example, as shown in Figure 1, one can perform an applied voltage breakdown and describe the different mechanisms resulting in the necessary applied overpotentials, which is useful in identifying opportunities for improving cell performance by quantifying the potential losses associated with a specific mechanism. In the talk, the generation of such analysis will be discussed including various approaches. Also shown in Figure 1 is how modeling can be used to elucidate safety concerns and identify issues to be resolved, in this case, nonlinear hydrogen crossover. Finally, future directions for multiscale modeling and multi-model coupling will be discussed.

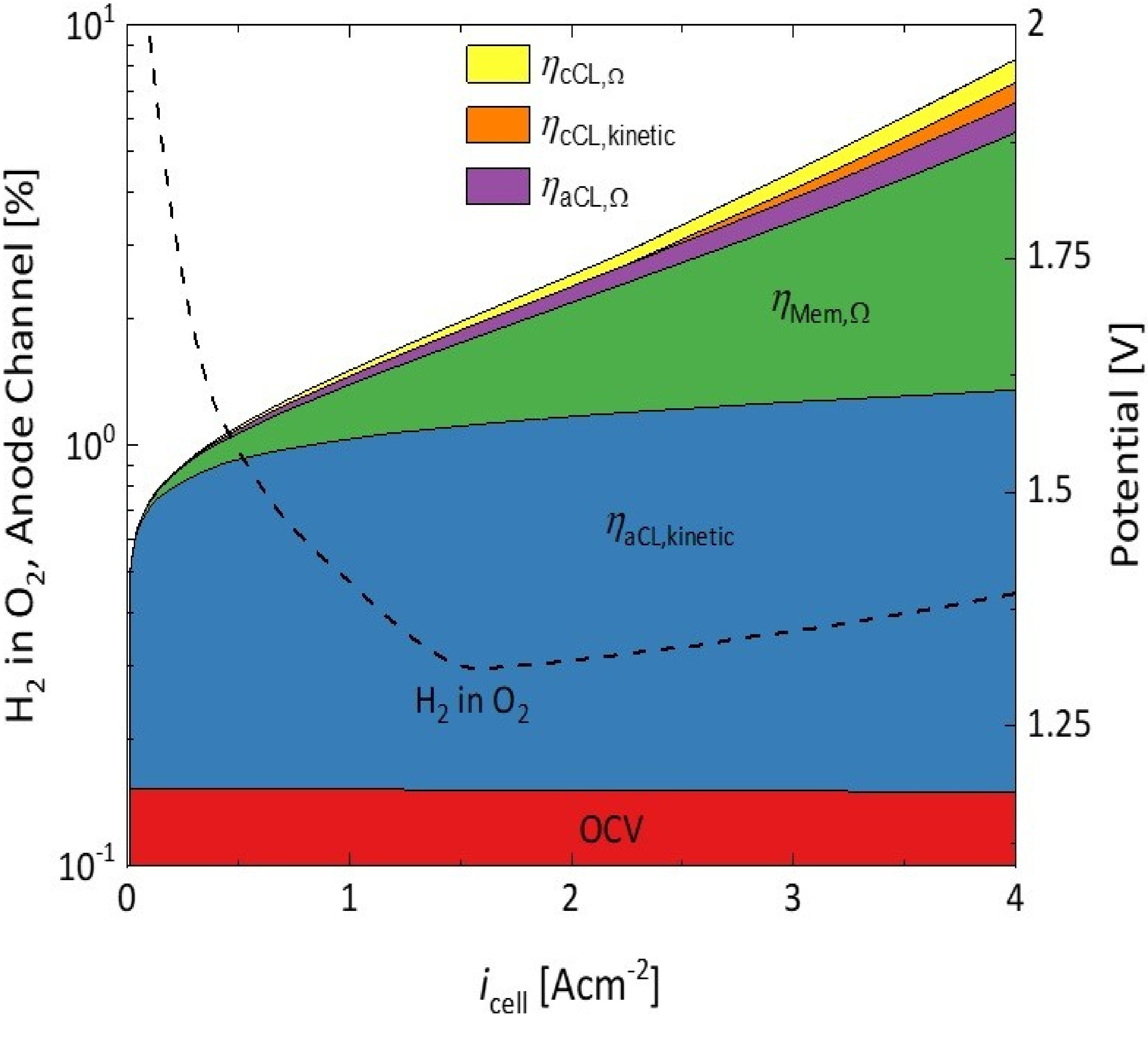
10^1
10^0
10^{-1}
0
1
2
3
4
2
1.75
1.5
1.25
$\eta_{cCL,\Omega}$
$\eta_{cCL,kinetic}$
$\eta_{aCL,\Omega}$
$\eta_{Mem,\Omega}$
$\eta_{aCL,kinetic}$
H_2 in O_2
OCV
H_2 in O_2, Anode Channel [%]
Potential [V]
i_{cell} [Acm^{-2}]

Figure 1