UNIVERSITY of DELAWARE

Modeling a Non-Flooding Hybrid Polymer Electrolyte Fuel Cell and Related Diffusion-Migration-Reaction Systems

4 October 2012

Benjamin E. McNealy, Joshua L. Hertz

Center for Fuel Cell Research

Department of Mechanical Engineering

University of Delaware

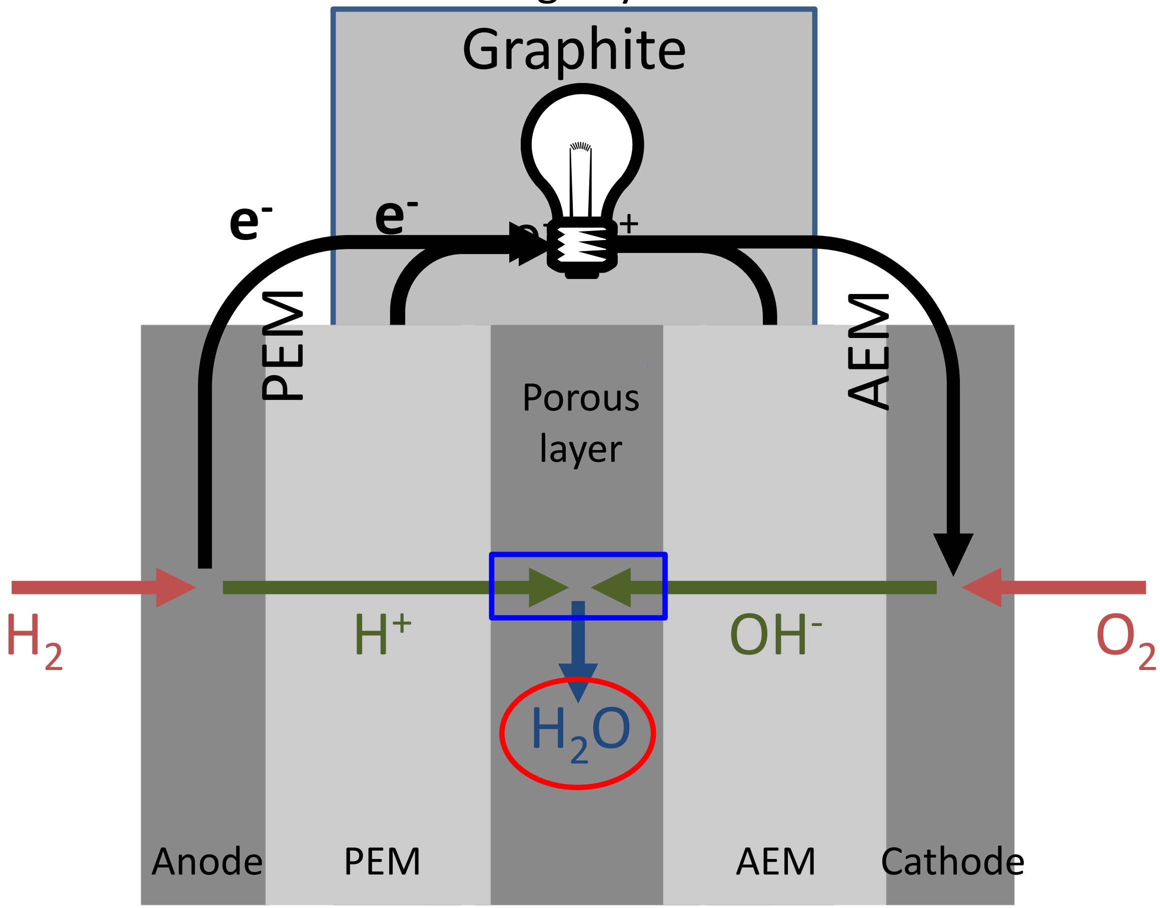
Email: bmcnealy@udel.edu

COMSOL CONFERENCE BOSTON 2012

Excerpt from the Proceedings of the 2012 COMSOL Conference in Boston

Introduction

Proton exchange membrane
(PEM) fuel cell
“Non-flooding” hybrid fuel cell



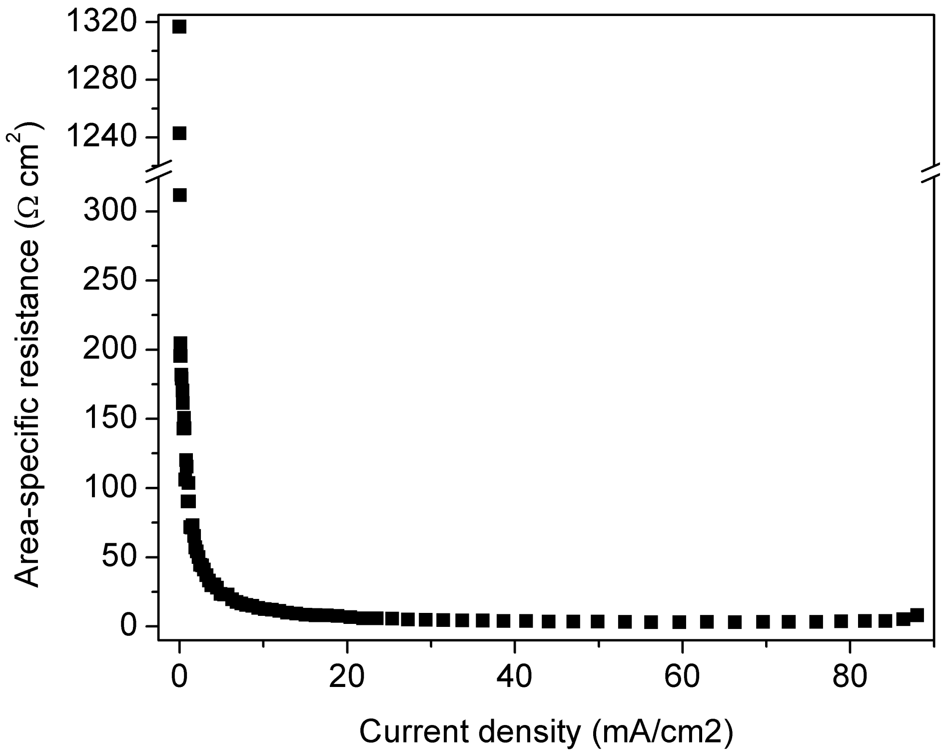
1D, time-dependent model in COMSOL 4.2a

- **Governing equations**
  - Transport of diluted species (Nernst-Planck)
  - Electrostatics (Poisson)
- **Boundary conditions**
  - Inward H^+ flux at $x = 0$
  - Inward OH^- flux at $x = L$
  - Zero flux of other species (H^+, OH^-, e^-, hole$^+$)
  - Electrical ground at $x = 0$, zero charge at $x = L$
- **Initial conditions**
  - Ion concentrations based on neutral pH
  - Electron/hole concentrations from the literature (graphite)[1]
  - Zero voltage

[1] J. W. McClure, *Phys. Rev.*, **112**, 715 (1958).

Goals

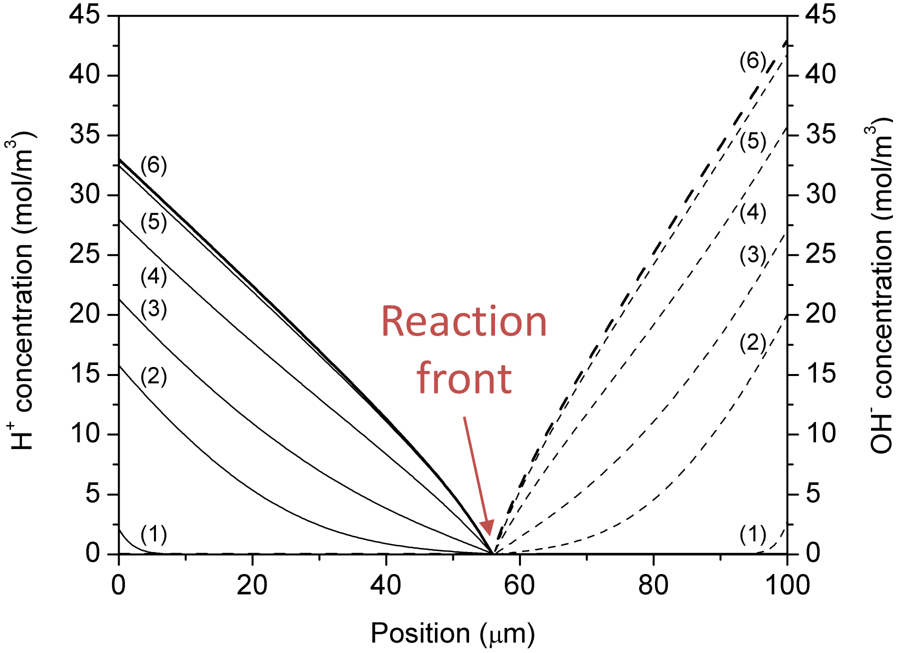
- Comparison with experimental results[1,2]
    - Resistance vs. current
    - Insulating porous layer
- Temperature and thickness effects
- Examine other applications



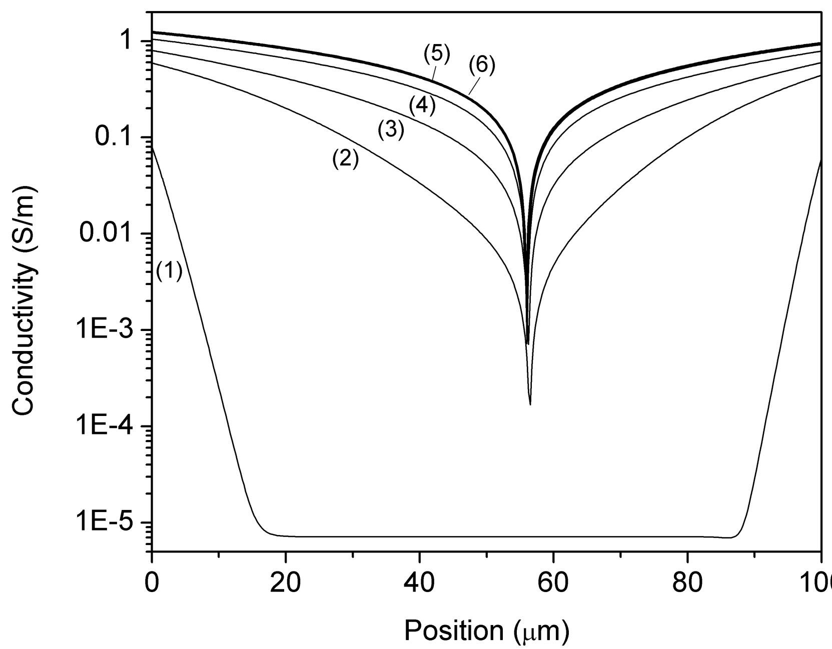
[1] W. Shen, F.-Y. Zhang, A. K. Prasad, and J. L. Hertz, *Electrochem. Soc. Trans.*, **33**, 2011 (2010).
[2] W. Shen, A. K. Prasad, and J. L. Hertz, *Electrochem. Solid-State Lett.*, **14**, B121 (2011).

Ion concentration and conductivity

Ion concentration profiles



Conductivity

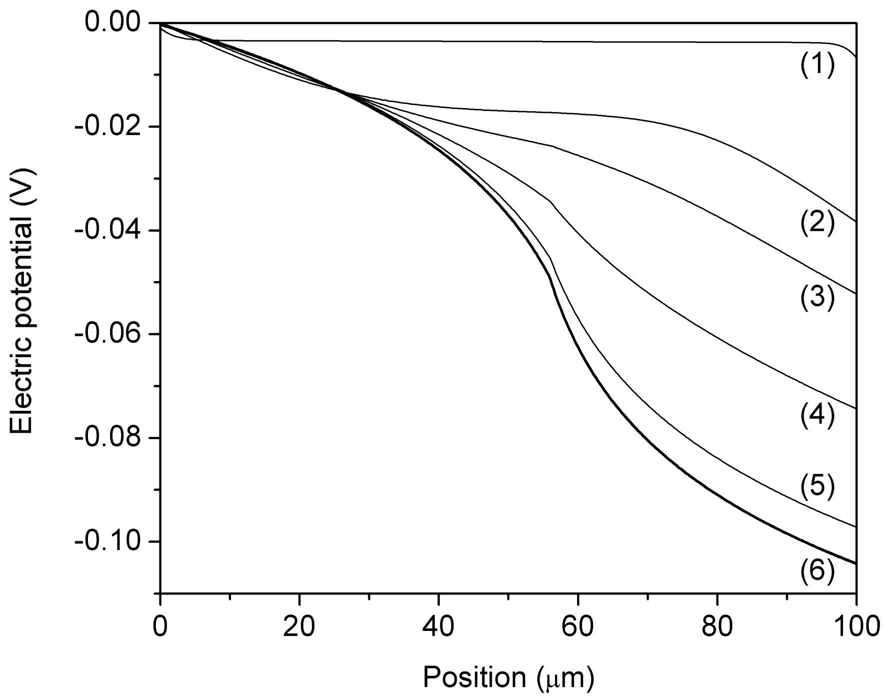


I = 100 mA/cm^2

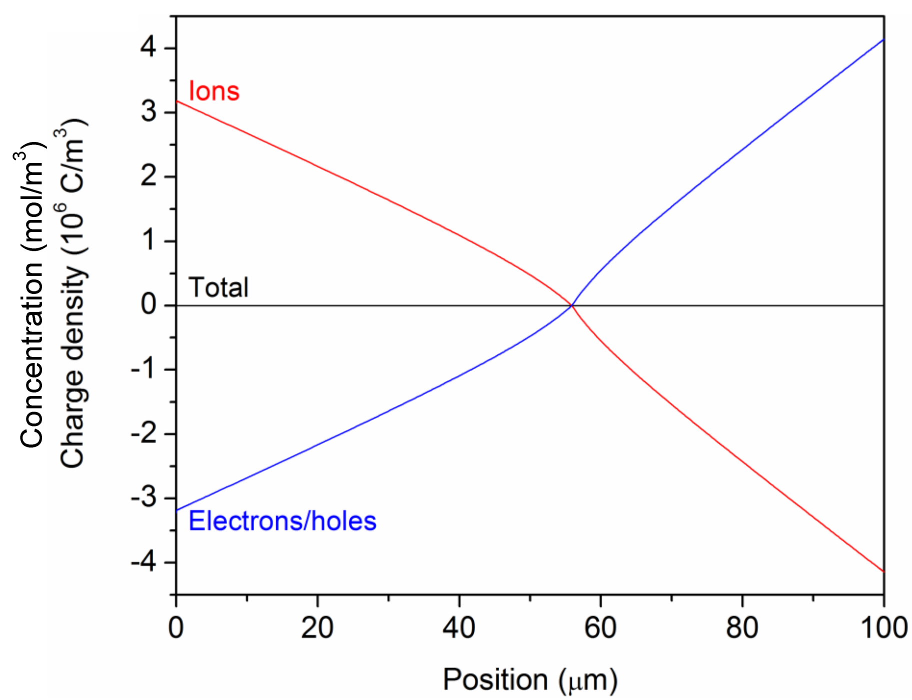
t = (1) 0 s, (2) 0.025 s, (3) 0.05 s, (4) 0.1 s, (5) 0.2 s, (6) 2 s (steady state)

Electron/hole effects

Electric potential



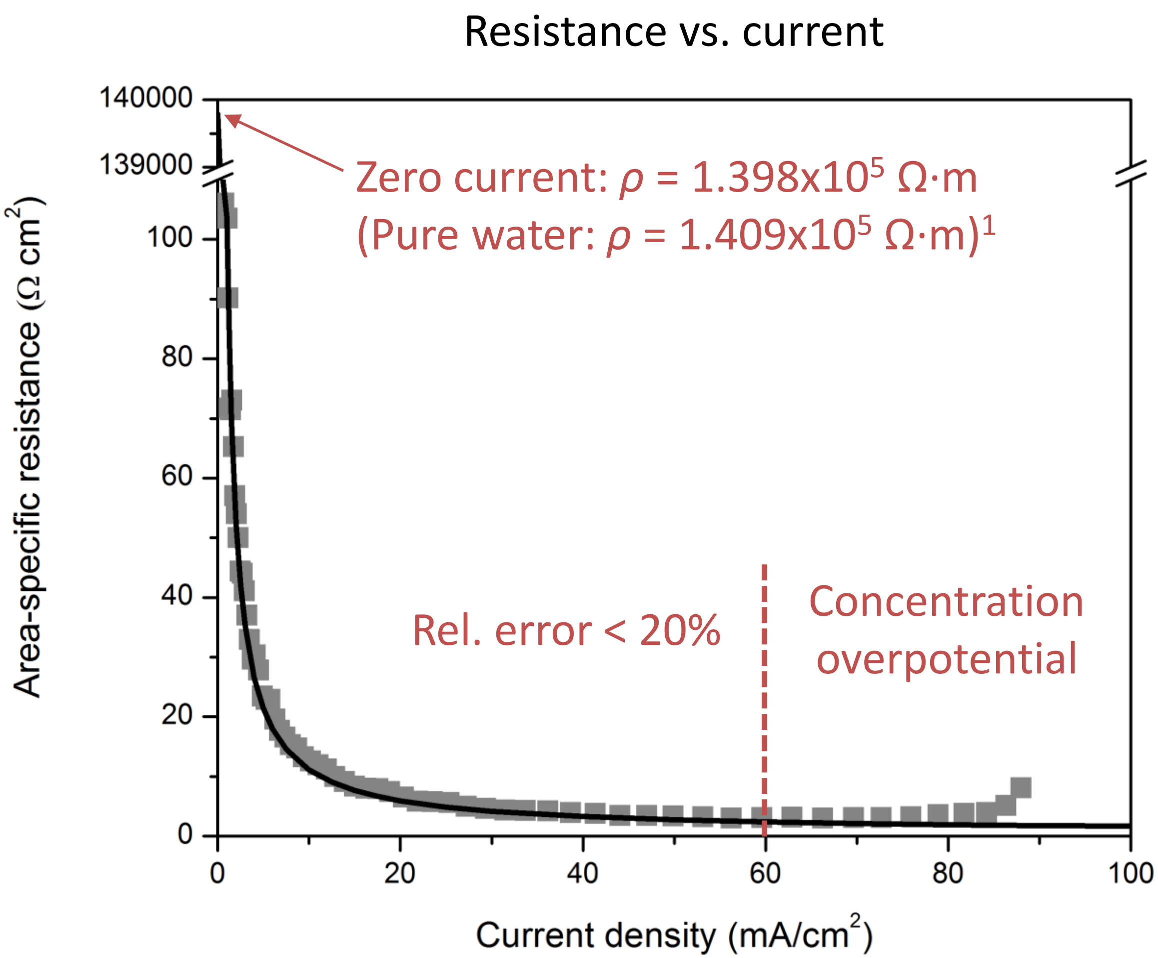
Steady-state charge density



I = 100 mA/cm^2

t = (1) 0 s, (2) 0.025 s, (3) 0.05 s, (4) 0.1 s, (5) 0.2 s, (6) 2 s (steady state)

Resistance



At I = 60 mA/cm^2
r = 2.5 Ω cm^2

For comparison:

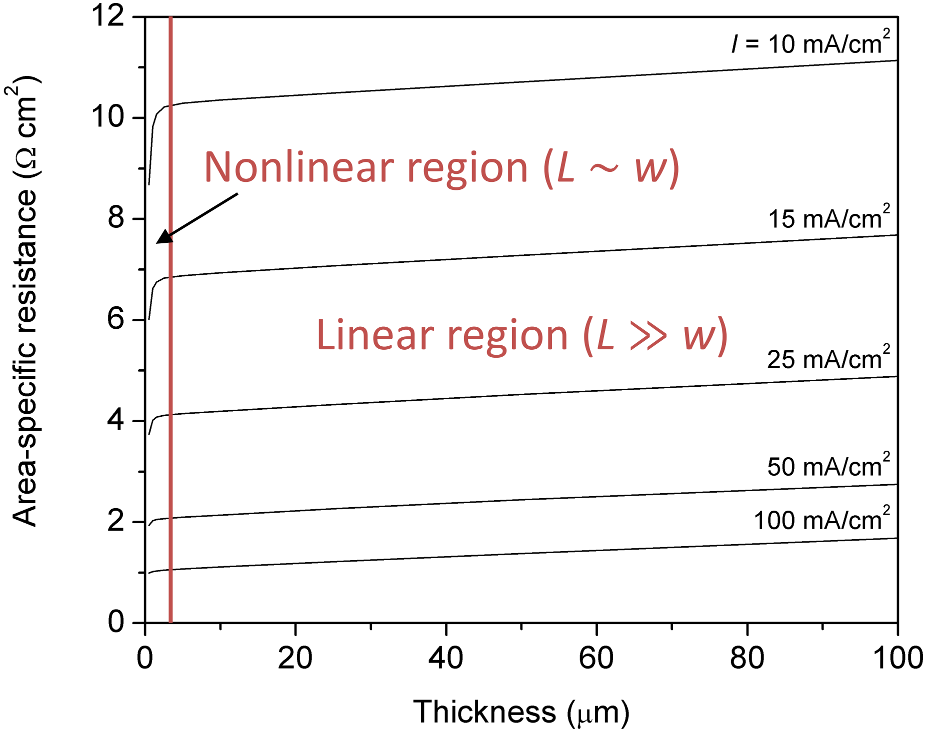
Nafion (50 µm):
r ≈ 0.05 Ω cm^2

Fumapem FAA (50 µm):
r ≈ 0.66 Ω cm^2

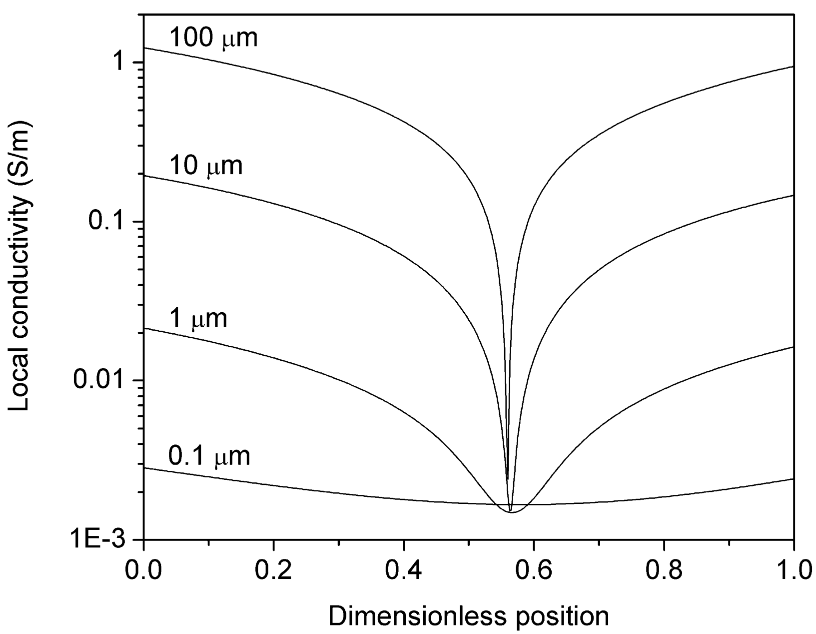
[1] T. S. Light, S. Licht, A. C. Bevilacqua, and K. R. Morash, *Electrochem. Solid-State Lett.*, **8**, E16 (2005).

Thickness effects

Resistance vs. thickness



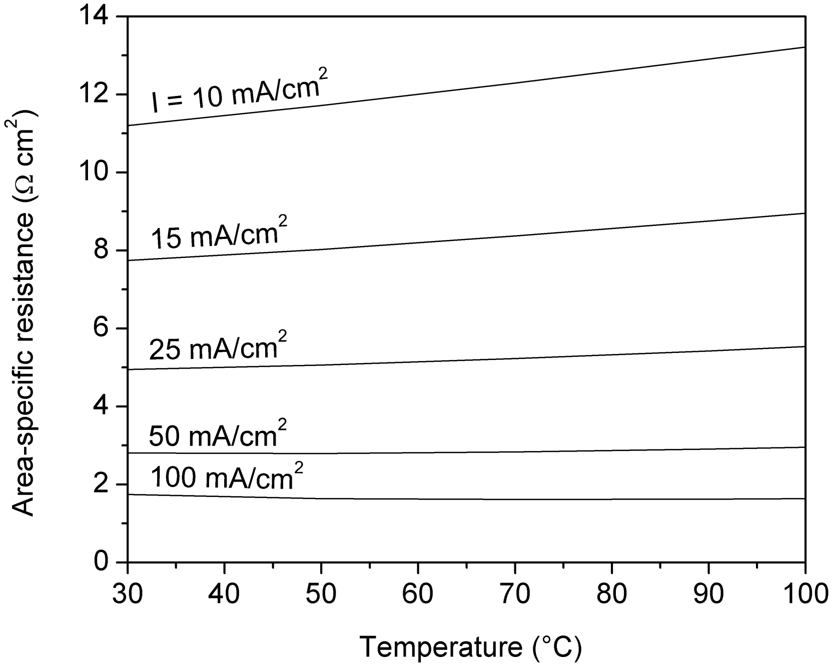
Local conductivity



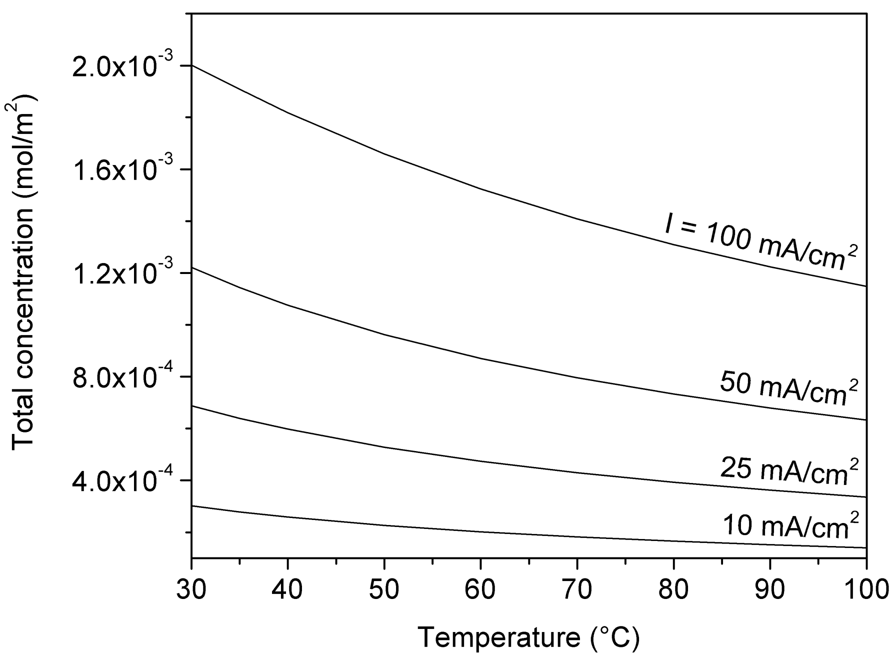
I = 100 mA/cm^2

Temperature effects

Resistance

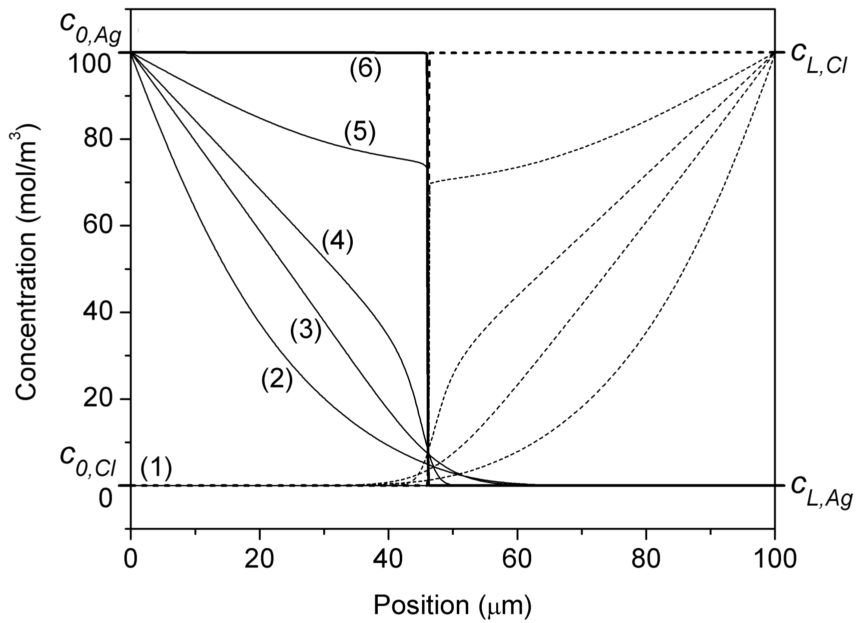


Ion density per area



Related systems

- Model can be extended to more complex cases, e.g. interdiffusion of $AgNO_3$/NaCl solutions
- Buildup of AgCl precipitate at the reaction front impedes diffusion
- Potential applicability to corrosion or biomineralization phenomena



Concentration profiles for Ag^+ (solid line) and Cl^- ions (dashed line) at *t* = (1) 0 s, (2) 0.6 s, (3) 5 s, (4) 125 s, (5) 127 s, (6) 140 s.[1]

[1] B. E. McNealy and J. L. Hertz, *submitted*.

Conclusions

- 1D porous layer model developed in COMSOL Multiphysics
- Unified treatment of heterogeneous electrochemical species in a Poisson-Nernst-Planck framework
- Good match with experimental results
  - Porous layer behaves as non-Ohmic electrolyte
  - Successful operation requires electron/hole conduction in porous layer scaffold
  - Porous layer dominates overall hybrid fuel cell resistance
- Resistance generally increases with thickness and temperature
- Model can be extended to have wider applicability