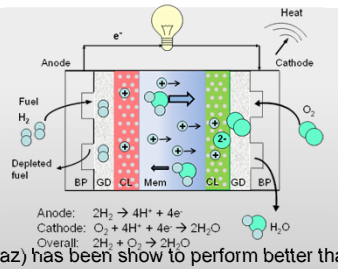
Molecular Modeling of Novel Fuel Cell Membranes

Tessa Brown, Ram Devanathan
Fundamental & Computational Sciences Directorate, Pacific Northwest National Laboratory, Richland, WA 99352, USA

Pacific Northwest NATIONAL LABORATORY
Proudly Operated by Battelle Since 1965

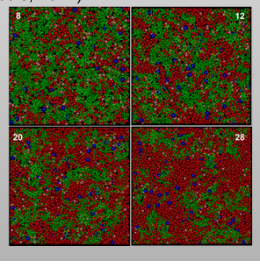
Introduction

Fuel cells are clean and efficient energy conversion devices. The fuel cells of interest contain polymer electrolyte membranes (PEMs) that inhibit the conduction of electrons and facilitate the transport of protons. Nafion® is the most widely used membrane for fuel cell applications. However, alternatives are desired because Nafion is expensive, allows significant amounts of methanol crossover, and functions poorly at low humidity or high temperature. An acid-base blend membrane composed of both acidic sulfonated poly(ether ether ketone ketone) (Ph-SPEEKK) and basic polysulfone tethered with 5-amino-benzotriazole (PSf-BTraz) has been show to perform better than traditional acidic PEMs such as Nafion and Ph-SPEEKK. We used molecular dynamics to study the PEM morphology and the transport of water, hydronium, and methanol in Ph-SPEEKK/PSf-BTraz blend membranes. Our aim is to understand the fundamental science behind the enhanced properties of the blend membrane.

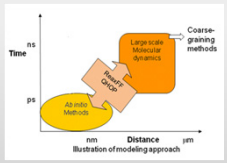


Previous Research

- There is no membrane that meets the performance, durability, and cost requirements for widespread adoption of fuel cell technology.
- Nafion®, the most widely used PEM, sets the standard for comparative analysis.
- Aromatic membranes based on the poly(ether ether keetone) (PEEK) family show promise (Devanathan, Idupulapati, & Dupuis, 2012) .



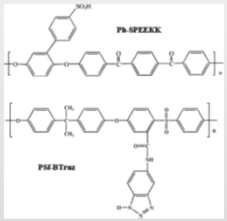
Multiscale Modeling



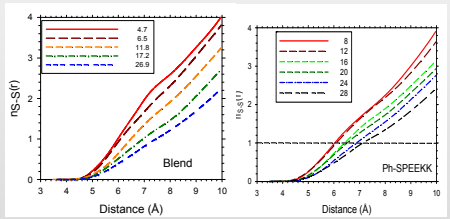
- Experimental studies cannot adequately describe nonoscale morphology and transport mechanisms (Devanathan, 2008).
- Multiscale modeling helps us understand the interplay between microscopic and macroscopic phenomena.
- Multiscale modeling reduces research and development costs, increases product quality, and leads to the development of new materials (Horstemeyer, 2009).
- Present work used ab initio molecular dynamics (AIMD) and molecular dynamics (MD). MD results are presented here.

SPEEK/PSf-BTraz Blend Membrane

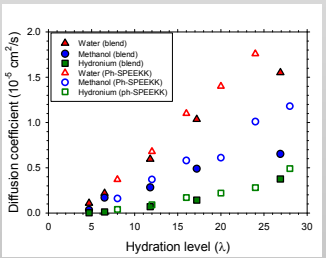
- Experiment shows that this acid-base blend membrane has higher proton conductivity and lower methanol crossover vs. Ph-SPEEKK (Li et al., 2010).



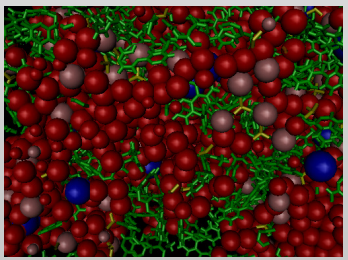
Chemical structure



Sulfur (SO_3^-) coordination number (MD) in Blend vs. Ph-SPEEKK



Diffusion coefficient at various hydration levels



Projection of SPEEK/PSf-Btraz with λ=11

Summary

- The sulfonate groups are farther apart in the blend membrane at similar hydration levels.
- Water and methanol diffuse slower in the blend membrane.
- The superior performance of the blend membrane may be due to reduced methanol crossover.
- Further studies are needed to relate the structure to transport properties.

References

Devanathan, R. (2008). Recent developments in proton exchange membranes for fuel cells. *Energy& Environmental Science*(1), 101-119.

Devanathan, R., Idupulapati, N., & Dupuis, M. (2012). Molecular modeling of the morphology and transport properties of two direct methanol fuel cell membranes: Phenylated sulfonated poly(ether ether ketone ketone) versus Nafion. *Journal of Materials Research, 27*(0).

Horstemeyer, M. (2009). Mutiscale Modeling: A Review. In J. Leszczynski, & M. Shukla (Eds.), *Practical Aspects of Computational Chemistry* (pp. 87-135). New York: Springer.

Li, W., Manthiram, A., Guiver, M., & Liu, B. (2010). High performance direct methanol fuel cells based on acid-base blend membranes containing benzotriazole. *Electrochemistry Communications*, 607-610.

Acknowledgment

RD was supported by the US Department of Energy, Office of Basic Energy Sciences, Chemical Sciences, Geosciences and Biosciences Division.

About Pacific Northwest National Laboratory

The Pacific Northwest National Laboratory, located in southeastern Washington State, is a U.S. Department of Energy Office of Science laboratory that solves complex problems in energy, national security and the environment, and advances scientific frontiers in the chemical, biological, materials, environmental and computational sciences. The Laboratory employs 4,000 staff members, has a $760 million annual budget, and has been managed by Ohio-based Battelle since 1965.

For more information about the science you see here, please contact:

Ram Devanathan
Pacific Northwest National Laboratory
P.O. Box 999, MS K2-01
Richland, WA 99352
(509) 371-6487
ram.devanathan@pnnl.gov

Blend PSfT | August 03, 2012 | PNNL-SA-89661

www.pnl.gov

This material is based upon work supported by the S.D. Bechtel, Jr. Foundation and by the National Science Foundation under Grant No. 0952013. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the S.D. Bechtel, Jr. Foundation or the National Science Foundation. This project has also been made possible with support of the National Marine Sanctuary Foundation. The STAR program is administered by the Cal Poly Center for Excellence in Science and Mathematics Education (CESaME) on behalf of the California State University (CSU). PNNL-SA-89661