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COMPUTATIONAL SIMULATION OF LITHIUM IONS TRANSPORT THROUGH POLYMER NANOCOMPOSITE MEMBRANES

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INTRODUCTION

We think of membranes as simple devices to facilitate filtration. In fact, membranes play a role in chemical, biological, and engineering processes such as catalysis, separation, and sensing by control of molecular transport and recognition. Critical factors that influence membrane discrimination properties include composition, pore size (as well as homogeneity), chemical functionalization, and electrical transport properties. The membrane community has an increasing interest in using nanomaterials for the production of novel membranes, due to the unique selectivity that can be achieved. Clay-polymer nanocomposites show particular promise due to their ease of manufacture (large sheets), their rigidity (self supporting), and their excellent mechanical properties. However, the process of lithium ion transport through the clay-polymer nanocomposite and mechanisms of pore size selection are poorly understood at the ionic and molecular level. In addition, manufacturing of clay-polymer nanocomposite membranes with desirable properties has proved challenging.

We have built a general membrane-modeling tool (simulation system) to assist in developing improved membranes for selection, electromigration, and other electrochemical applications. Of particular interest are the recently formulated clay-polymer membranes. The transport mechanisms of the lithium ions membranes are not well understood and, therefore, they make an interesting test case for the model.

EXPERIMENTAL

In order to validate the model, we synthesized polymer nanocomposites membranes. One of the membranes studied was prepared from synthetic lithium hectorite (SLH). Preparation of the SLH

clay via hydrothermal crystallization at 100 °C of silica sol, magnesium hydroxide, and lithium fluoride can be found in detail in reference 1. Colloidal suspensions of 1 g SLH/100 ml de-ionized water were stirred for one-half hour. The desired amount of PEO (100 000 average molecular weight, from Aldrich) was then added, and the mixture stirred for 24 hours. Mixtures contained 0.6, 0.8, 1.0, and 1.2 g of PEO/g of clay. Films were prepared by puddle-casting the slurries onto Teflon-coated glass plates and air-drying. Further drying was carried out at 120 °C under an inert atmosphere for at least 48 hours. The typical thickness of the films was found to be about 40 um.

Membrane modeling for electrochemical applications involves non-linear transport processes describing diffusion of ions and their migration under the influence of electric potential fields. For the discretization of the model, we have used finite element methods and spectral element methods for boundary layers to handle the different materials. We have based our model on fundamental transport equations (with a potential function that represents the attractive/repulsive interactions between the solute and the membrane) for mass transfer, conductivity, heat transfer including temperature capability, and migration in the clay polymer matrix. Multi-scale models have shown promise for clay-polymer nanocomposites . We have investigated these and take advantage of membrane modeling with the Nernst-Planck equation.

We have used experimental data from current membranes to verify the computational results. Then, based on simulation predictions, researchers have adjusted the physical properties of the membrane. The results will be presented in detail.

REFERENCES

1. (a) Carrado, K. A.; Winans, R. E.; Botto, R. E. US Patent 5,308,808. (b) Carrado, K. A. *Appl. Clay Sci*., **2000**, *17*, 1.

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