Title: **Development of Nanofiller-Modulated Polymeric Oxygen Enrichment Membranes for Reduction of Nitrogen Oxides in Coal Combustion**

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OBJECTIVE(s)

The overall goal of this project is to further improve upon our existing technology and further optimize the nanofiller-modulated polymer formula for the oxygen-enrichment for the coal combustion and gasification applications. The major objectives are: (1) Develop a multipurpose filled polymer material system that incorporates functional nanofillers to achieve novel oxygen-enrichment properties; (2) Document the fundamental microstructure-property relationship of the nanofiller-modulated polymer material system.

ACCOMPLISHMENTS TO DATE

We are making progress slowly. We anticipate several instrumental issues with our custom-built inverse gas chromatography. We are conducting additional theoretical study on the membrane diffusional mechanisms using molecular dynamics simulations.

Molecular models of Single-walled carbon nanotubes PDMS membrane and nano fumed silica PDMS membrane were built by Material Studio 4.0 and the resulting output coordinate files were modified to make them compatible with GROMACS. All Molecular dynamics simulations were performed using the GROMACS 3.3 simulation package on a 40-node IBM xSeries Linux Cluster. Modified OPLS-AA force field was used. Diffusion coefficients, solubility and permeability of oxygen, nitrogen and nitrogen oxides were calculated from molecular dynamics simulations and were very good agreement with the experimental values. In the simulations, the leapfrog algorithm was used to integrate Newton's equations of motion with a time step of 2 fs. Periodic boundary conditions were applied and nonbonded force calculations employed a grid system for neighbor searching. In this system, only the atoms in the neighboring grid cells are considered when building a new neighbor list. A twin-range cutoff was used for both Lennard-Jones and Coulombic calculations. A cutoff radius of 1.0 nm was used for short-range forces, which were calculated every simulation step, and a cutoff radius of 1.0 nm was employed for long-range forces, which were calculated during neighbor list generation. In each simulation, the temperature was controlled by employing a Nose-Hoover extended ensemble and the pressure was controlled by employing a Parrinello-Rahman ensemble. Initial velocities were randomly

assigned from a Maxwell distribution at the selected simulation temperature. The LINCS algorithm was used to constrain all bonds.

FUTURE WORK

An understanding of the "mobility selectivity" relies upon an integrated knowledge of thermodynamics, phase separation kinetics, and interphase mass transfer. Integration of non-equilibrium thermodynamics and non-Fickian transport phenomena would be essential for molecular modeling and simulation of the relative transport of components through polymeric membranes.

LIST OF PAPER PUBLISHED

J. Lou, V. Harinath, "Separation of polysaccharides from industrial syrup using tubular membranes", Journal of Liquid Chromatography & Related Technologies. 2005 28(3), 357-367.

Irulappan, S., Roberts, C., Ilias, S., "Developments of Pt-based Ternary and Quaternary Metal Catalysts for PEM Fuel Cell," Chem. Eng. Trans., 2004 (4) 397-402.

U.S. PATENT/PATENT APPLICATION(S) n/a

CONFERENCE PRESENTATIONS n/a

AWARDS RECEIVED AS A RESULT OF SUPPORTED RESEARCH n/a

STUDENTS SUPPORTED UNDER THIS GRANT James Zhang – PhD candidate