Computer Simulation of Osmosis and Reverse Osmosis in Structured Membranes

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Submitted To:

The Division of Chemical Sciences

US Department of Energy

Germantown, MD 20874

By

S. Murad

Department of Chemical Engineering

University of Illinois at Chicago

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Main Accomplishments

The main accomplishments from the grant are described below:

1. We have carried out detailed studies to investigate the separation of two gas mixtures, N_2/O_2 (air) and CO_2/N_2 using a range of zeolite membranes (Faujasite, Chabazite and MFI). These two mixtures were selected because they are known to show contrasting separation characteristics in the membranes selected. The main goal of this work was first to establish the viability of studying such membrane based separations using molecular simulations. After validating the methods used, we used the simulations to understand at the molecular level the controlling mechanisms for these separations, with the ultimate goal of making these processes more efficient. Our results clearly indicated that molecular simulations can realistically model these separations, since they correctly predicted qualitatively all the observed trends reported experimentally, including those in which these mixtures showed contrasting behavior. We were also able to establish the diffusion mechanisms inside the membrane, including clearly determining what molecular mechanisms were ultimately responsible for the observed selectivities of the membrane.

2. We have examined ion-exchange in NaA zeolite membranes by carrying out molecular simulations in which solutions of LiCl, and $CaCl_2$ were made to come in contact with a NaA zeolite ion exchange membrane. Experimental observations indicate that the ion-exchange process is relatively slow for LiCl solutions, but much more rapid for $CaCl_2$ solutions. We were able to show using our simulations, that the exchange process is almost entirely energetically driven, rather than entropically driven. In addition the energetic driving force for Ca^{2+} ions was much larger than for Li^+ ions, and that explained the observed differences in the ion-exchange rate. We were also able to validate the method by examining the hydration of the zeolites by water and comparing with available experimental results, and comparing the positions of the exchanged cations with known experimental data. Our simulations showed qualitative agreement with experimental results. We believe our results have shown that reliable screening studies for determining the suitability of a potential ion exchange process can be carried using molecular simulations.

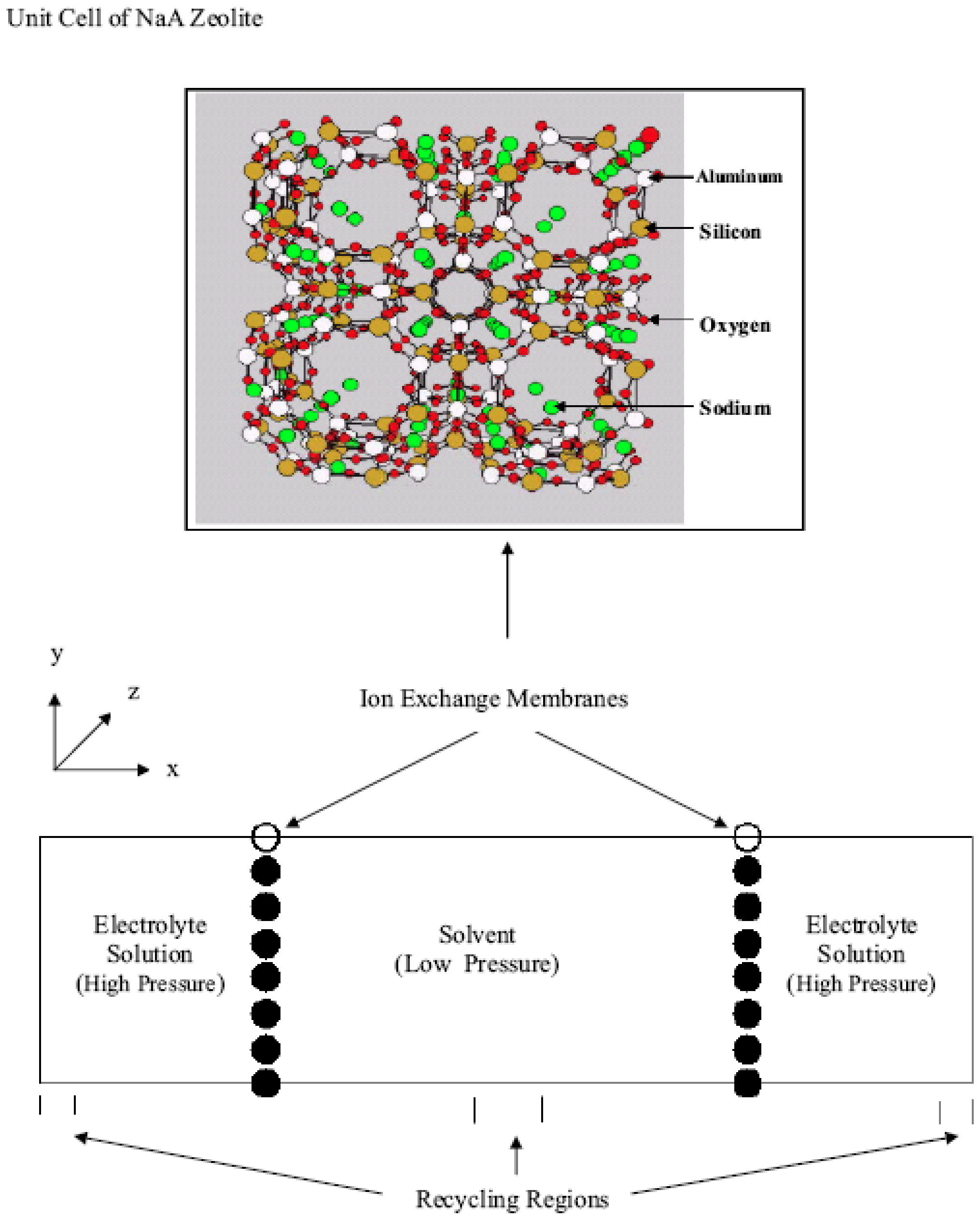

Figure 1: A typical initial system setup for ion-exchange simulations, including a unit cell of the zeolite

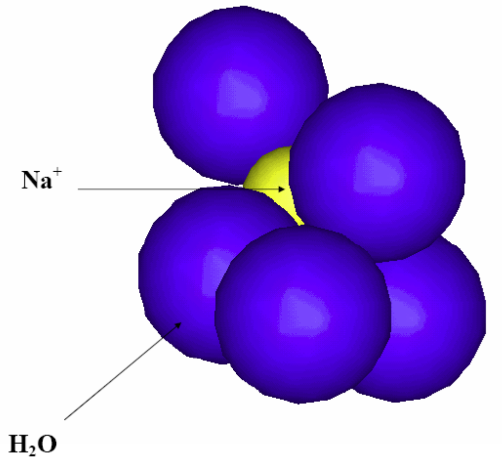

Figure 2: A typical hydrated Na^+ ion, which effectively increases the size of the ion to prevent it from entering the pore of a ZK4 zeolite membranes

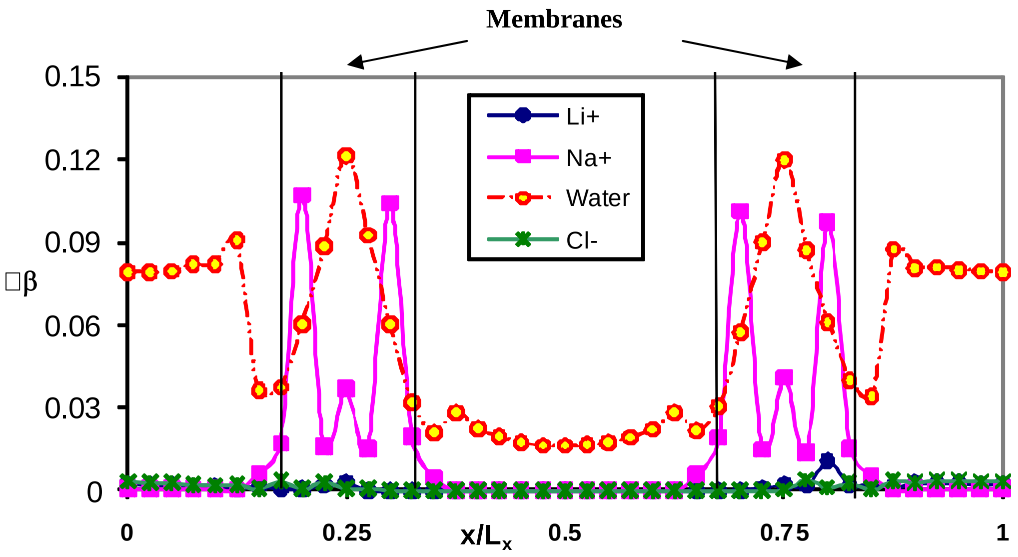

Figure 3: Density profiles of Li^+ and Na^+, Cl^- and water, inside and outside the zeolite membrane for a typical steady state ion exchange simulation with LiCl solution.

3. We have investigated the effectiveness of using NMR chemical shift in determining cross intermolecular potential parameters, needed for simulations and other theoretical studies of range many mixtures. These parameters are particularly difficult to estimate for polar-nonpolar mixtures.

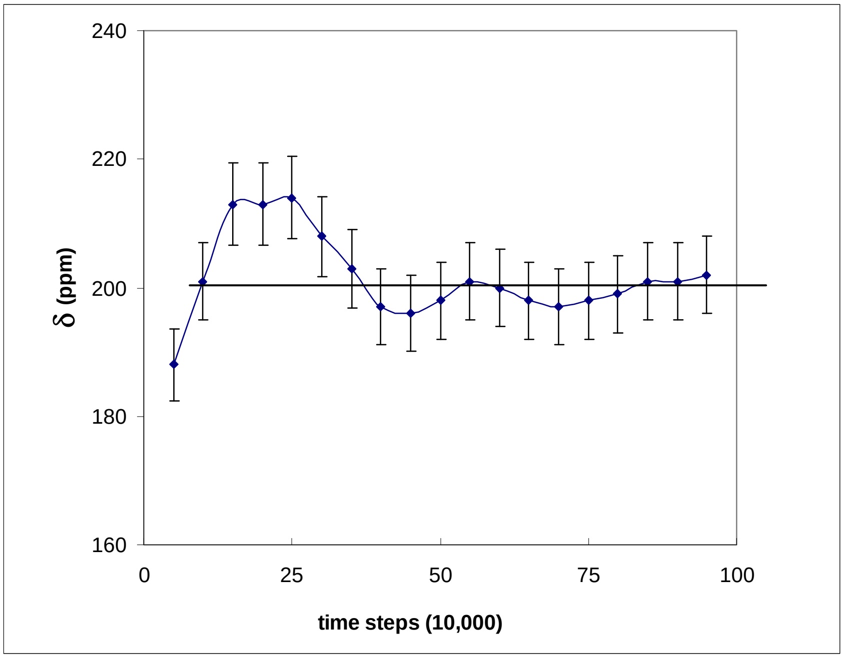

Figure 4: Average Xe chemical shifts as a function of time in molecular dynamics simulations at 298 K. The solid lines guide the eye. The solid line is the experimental value at 298 K.

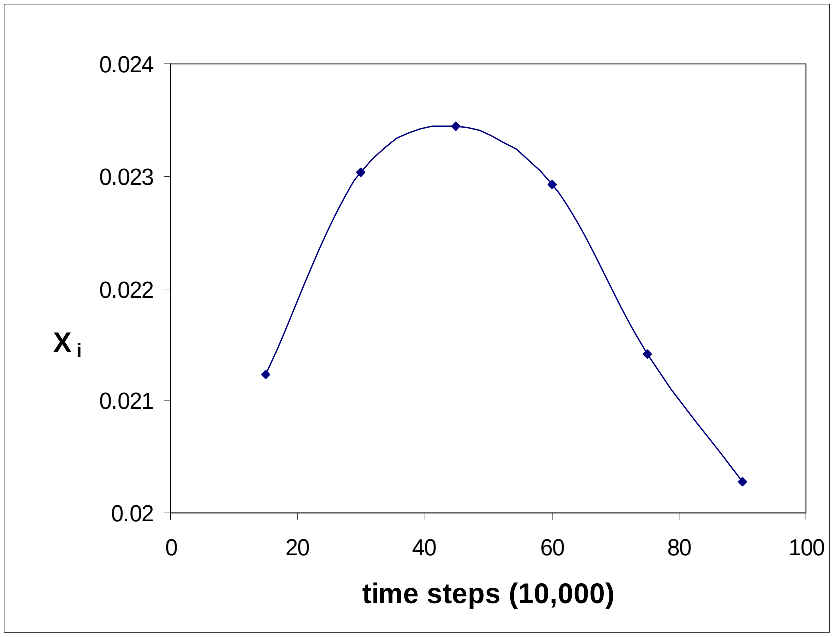

Figure 5: Solubility of xenon in water (mole fractions) as a function of time in molecular dynamics simulations. The solid lines guide the eye. The estimated solubility at this state condition (T, P) is approximately 0.017

We have found out that since in a molecular simulation the NMR chemical shift only involves local equilibrium of a solute surrounded by solvent molecules (e.g. a methane molecule surrounded by water molecules), we were able to develop a simulation scheme to evaluate it almost an order of magnitude more efficiently than via other possibilities such as Henry's constants. Once the parameters for the cross parameters are established via the NMR chemical shift, longer simulations can be carried out to obtain results for properties such as gas solubilities which require global equilibrium. Our studies also showed that for many polar-nonpolar systems, the Lennard-Jones repulsive term ($\mathbf{r}^{-12}$) does not realistically represent the repulsive forces, and the exp-6 (Buckingham) potential ($\mathbf{e}^{\mathbf{br}}$) does a much better job. This is because unlike in pure liquids, in dilute solutions of polar-nonpolar systems, a solute molecule can get rather close to the solvent molecules, and therefore an accurate representation of the repulsive part of the potential becomes rather important.

4. We started a new collaboration with an experimental group in New Mexico to investigate the possibility of using zeolites as sensors for a wide range of chemical contaminants. Our initial experimental results have shown that zeolite-fiber integrated optical chemical sensors are effective for rapid detection of dissolved organics in water. We are now planning to conduct simulation studies to determine the adsorption characteristics of these organic contaminants in zeolites, so that we can investigate possibilities for increasing the efficiency of these sensors for a wider range of contaminants (see accompanying proposal for further details).

5. We have carried out preliminary simulations to investigate the possible role of external magnetic fields on the transport of polar fluids in membranes. Such transport is of great importance for example in the reverse osmosis based separation of water from electrolyte solutions such as brine. We believe this is the first study to examine these effects in such systems. Our results have showed that magnetic fields can increase the transport rate across membranes considerably, and could thus be used to make reverse osmosis based separation processes more efficient. Magnetic fields make water and hydrated ionic clusters slightly less stable, which then allows water to permeate the membrane more readily, while not still allowing ions to break from their hydrated clusters. This increases the flux of water for a given pressure, while not adversely affecting the selectivity of the membrane.

6. We have also used simulations to examine the effect of pore size and structure of pores in membranes on the flux and selectivity. Our results indicated that permeation occurs within a Knudsen like regime where close confinement in these pores precludes significant water-water interactions, leaving water-pore interactions to determine hydraulic resistance. Results show the solvent flux to be rather insensitive to an appropriately defined tortuosity. Ion selectivity seems to correlate primarily with overall hydraulic resistance, irrespective of the number of membrane layers.

7. Our molecular simulation studies have indicated that zeolites show considerable promise for use in a wide range of membrane based processes involving the separation of aqueous electrolyte solutions. These include processes as diverse as desalination, to the cleanup of chemical or radioactive wastes. The pore size in zeolites investigated by us varied from 4 - 6 Å.

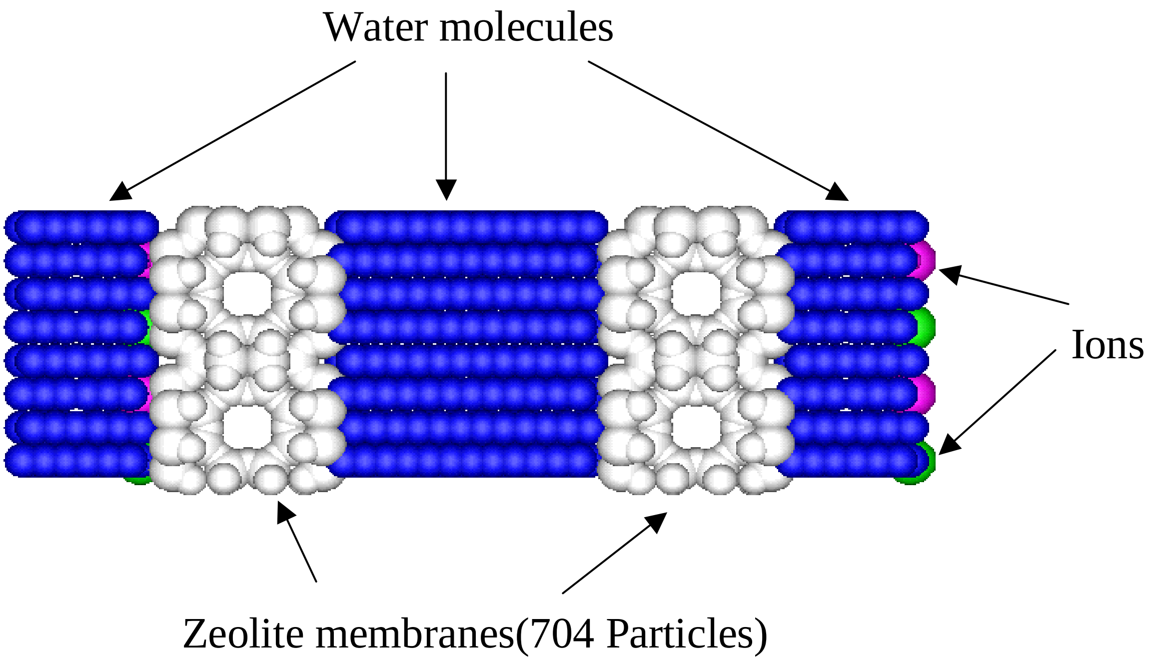

Figure 6: A schematic of the simulation system

We found that ions formed rather stable hydrated clusters, which effectively increased their size to about 10 Å. The energy of desolvation of such ions is about 400 kJ/mole, which is almost 20 times larger than the hydrogen bond energy of water . This makes these clusters rather stable and prevents the ions from being able to permeate the membrane. Our research also showed that if the temperature of the solution was increased, or an external electric field was used (both of which tend to make the clusters less stable), the ions begin to permeate the membrane. There has been considerable recent progress in the manufacture of zeolite membranes; they can therefore be realistically viewed as potential candidates for many membrane processes.

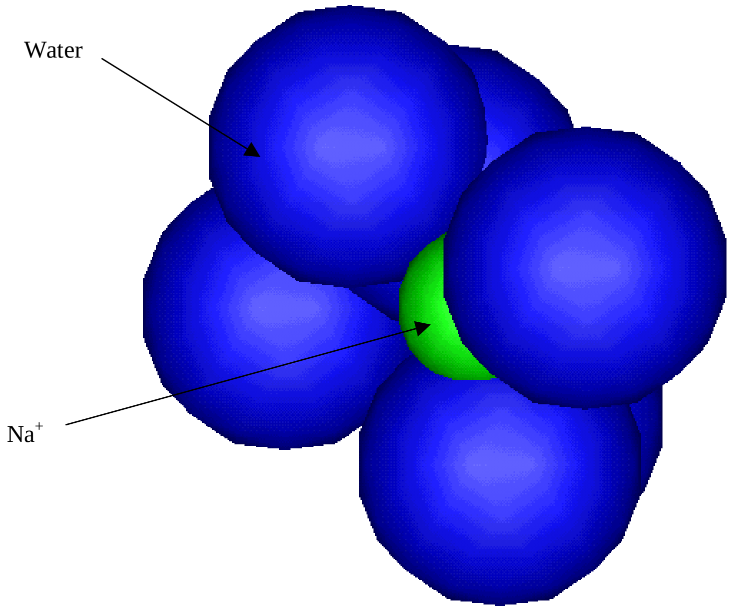

Figure 7: Example of an ionic cluster formed by ions being surrounded by molecules of polar solvent molecules (such as water). Such clusters increase the effective size of ions.

8. We have also carried out a comprehensive investigation of the effect of the nature and strength of the electric field on the flux of the solvent molecules across semi-permeable membranes. This could be an effective method for increasing the efficiency of such processes. For ionic systems, in general, direct fields are not desirable, since they tend to accumulate the ions near the membrane, which then leads to pore blockage. In our studies we examined both direct and alternating fields. Several types of alternating fields were examined including square, saw-tooth, and sinusoidal. We studied the effect of field strength and frequency for several model systems in which the solute was ionic and solvent nonpolar. Our results showed that direct fields do not increase the solvent flux rates in such systems (for reasons stated above), but indirect fields can significantly increase the flux. In addition the frequency of the field also

affects the flux rate. If the magnitude of the field is increased, at low values, the effect is almost linear, but then becomes nonlinear as a result of dielectric saturation.

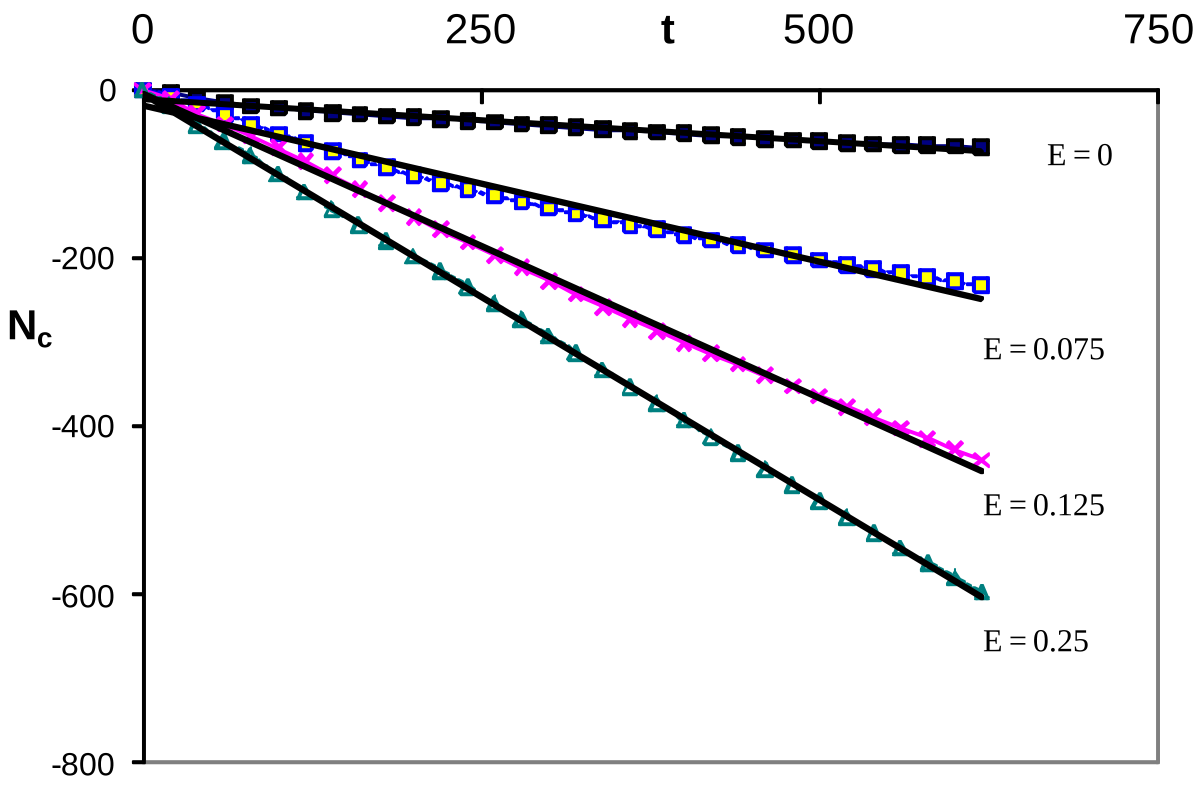

Figure 8: Effect of external electric field on the number of the solvent molecules permeating the membrane as a function of time. The negative value of N_c implies reverse osmosis.

9. We have investigated the effectiveness of zeolites as potential semi-permeable membranes for separating supercritical aqueous electrolyte solutions. Supercritical fluids are becoming increasingly important because they are environmentally friendly and have considerable promise as solvents for a wide range of pollutants. In supercritical aqueous solutions ions pairs are often observed, and thus their behavior is unlike that of liquid solutions. Our simulations have shown however, that even in such systems zeolites show promise. The water molecules were able to easily permeate the zeolite, while the ions were prevented either as a result of ion-pair formation, or ion hydration, both of which effectively

increase the size of the ions. In addition, in such systems, electric fields appear to play a much more significant role in increasing solvent flux rate than in comparable liquid solutions.

10 Molecular simulation studies of electrolyte solutions in polar solvents (other than water) have also been carried out to determine if the formation of ionic clusters also play an important role in membrane transport in such solutions. We have examined polar solvents methanol and ethanol and several ions (Na^+, K^+, Cl^- and Br^-) in our studies, and found that in such solutions, rather stable clusters are also formed as a result of the ions bonding with the solvent molecules. These clusters then seem to prevent the ions from permeating the membranes and may contribute significantly to the observed selectivity of many membranes used for such systems as well.

11 We have also used the molecular simulation method developed by us to study membrane based separation processes (described above), to investigate the solubility of light gases in liquids. The simulation system consists of a gas (specie A) separated from a liquid (specie B) by a semi-permeable membrane, permeable only to specie A. By varying the pressure of the gas, the solubility of A in B can be easily varied. Henry's constant can then be obtained using standard thermodynamic relations from the limiting case, when $x_A \rightarrow 0$. We have confirmed that the results from this method agree with results from traditional Monte-Carlo methods, and have then used it to study the solubility of oxygen in benzene. Our results showed that these simulations give rather accurate results, even when no binary parameters (for the molecular interactions between oxygen and benzene) are used. In equation of state methods, if no binary parameters were used, the results were off by almost a factor of 2 and also showed the wrong temperature dependence.

Publications Resulting From Grant

1. H. Yuan, C. J. Jameson, S. K. Gupta, J. D. Olson and S. Murad, “Prediction of Henry's Constants of Xenon in cyclo-alkanes from Molecular Dynamics Simulations”, Fluid Phase Equilibria, 269, 73-79 (2008)

2. H. Yuan, S. Murad, C. J. Jameson, J. D. Olson, “Molecular Dynamics Simulation of Xe Chemical Shifts and Solubility in n-Alkanes”, Journal of Physical Chemistry C, 111, 15771-15783 (2007)

3. H. Liu, S. Murad, and C. J. Jameson, “Ion Permeation Dynamics in Carbon Nanotubes”, Journal of Chemical Physics, 125, 084713 [1-12] (2006)

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Doctoral Thesis Completed:

Jiansong Lin, “Molecular Dynamics Simulation of Osmosis, Reverse Osmosis, and Electro-Osmosis in Electrolyte Solutions, Ph.D., 2000, University of Illinois at Chicago.

Wei Jia, “Molecular Simulation of Separation of Gas Mixtures Using Zeolite Membranes”, Ph.D., 2004, University of Illinois at Chicago.

Soumik Banerjee, “Molecular dynamics simulations of nanoscale transport phenomena”, Ph.D., 2008, Virginia Tech.

Huajun Yuan, “MD Simulations of Membrane Related Equilibrium and Non-Equilibrium Processes: Gas Permeation and Solubility”, Ph.D., 2009, University of Illinois at Chicago.

Educational Software

The Concord Consortium (Concord, MA), a non-profit research and development organization working for improvements in educational curricula, through the use of information technologies has used our molecular dynamics method for modeling osmosis in its flagship program MW2D^{TM}. MW2D^{TM} is an interactive molecular simulation software tool designed to help students acquire a concrete picture about atomic-scale models that are otherwise static and preset in traditional textbooks. Details of their implementation of our method are given at their website

http://people.concord.org/~qxie/oslet/guide/index.html

in the, "Restrain Particles" section of the chapter, "The Model Builder" at the web address

http://people.concord.org/~qxie/oslet/guide/builder_restrain.html.

Osmosis: A module to help undergraduate students understand the principles of osmosis and reverse osmosis. http://rheneas.eng.buffalo.edu/wiki/Osmosis. This module is a part of the etomica project, www.etomica.org, sponsored by Computers Aids for Chemical Engineering, www.cache.org, and the National Science Foundation, www.nsf.gov. Project Etomica is housed at University at Buffalo, The State University of New York.

CV: **SOHAIL MURAD**

Department of Chemical Engineering
University of Illinois at Chicago
810 S Clinton Street
Chicago IL 60607-7000

Tel: (312) 996 5593
Fax: (312) 996 0808
www.uic.edu/~murad
E-mail: murad@uic.edu

EDUCATION

Ph.D., Chemical Engineering, Cornell University, Ithaca, N.Y., 1979.

M.S., Chemical Engineering, University of Florida, Gainesville, 1976.

B.S., Chemical Engineering, University of Engineering, Lahore, Pakistan, 1974.

PROFESSIONAL EXPERIENCE

Assistant Professor, 1979 - 86; Associate Professor, 1986 - 91; Professor, 1991 - date; Head, 2004-date; University of Illinois at Chicago.

Research Fellow, U. S. Army Ballistic Research Laboratory, Summer 1985.

Senior Engineer, Exxon Research and Engineering Company, 1981 - 82.

PROFESSIONAL MEMBERSHIPS

Member, American Institute of Chemical Engineers (AIChE), American Chemical Society (ACS) and American Society for Engineering Education (ASEE)

Member, Editorial Board, Computer Applications in Engineering Education, Wiley, New York; Letters in Chemical Engineering, Hindawi, New Yrok.
Affiliate Professor, Project Lead the Way (www.pltw.org)

SELECTED HONORS AND AWARDS

Faculty Research Award, College of Engineering, University of Illinois (1998, 2004).

Teaching Excellence Award, University of Illinois (1998).

Research Fellowship, Army Research Office (1985).

EDUCATIONAL SOFTWARE:

Osmosis: A module to help undergraduate students understand the principles of osmosis and reverse osmosis. http://rheneas.eng.buffalo.edu/wiki/Osmosis (part of a CACHE/NSF project)

SELECTED RECENT PUBLICATIONS

Chapters in Books

I. K. Puri and S. Murad, “Multiscale Methodology to Approach Nanoscale Thermal Transport”, in, Trends in Computational Nanomechanics: Transcending Time and Space, T. Dumitrica (Ed.), Springer, Heidelberg, Chapter 5, p 135-150 (2010)

Selected Recent Refereed Journals

B. Song, H. Yuan, C. J. Jameson and S. Murad, “Permeation of Nanocrystals Across Lipid Membranes”, Molecular Physics, in press (2011)

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N. Sedighi, S. Murad , and S. K. Aggarwal, “Molecular Dynamics Simulations of Spontaneous Spreading of a Nanodroplet on Solid Surfaces”, Fluid Dynamics Research, **43**, 015507 (2011)

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RESEARCH COLLABORATORS

Thesis Advisor: Professor Keith Gubbins (NC State)

Other Recent Collaborators: Professors S. Aggarwal (UIC), G. Ayappa (Indian Institute of Science), J. Dong (NMTech), C. Jameson (UIC), L. Nitsche (UIC), I. K. Puri (Virginia Tech), H. Xiao (NM Tech); Drs. S. Gupta (Dow), J. Olson (Dow), D. Sears (Alberta),C. Gosling, P. Kokayeff (UOP)

Recent PhD-Post-Doc Students: Drs. H. Yuan (UIC), W. Jia (UIC), J. Lin (Motorolla), P. Ravi (Internoc)

SYNERGISTIC ACTIVITIES

Affiliate Professor, Project Lead the Way, A nonprofit group dedicated to improving the quality of engineering education, by focusing on their high school education (www.pltw.org).

Developed the Quaternion Method (in Collaboration with D.J. Evans) Widely Used in Molecular Dynamics Simulations.