

KUNWOO HAN

HAN, KUNWOO

Address Texas A&M University
Department of Chemical Engineering
TAMU 3122, College Station, TX 77843-3122
1103 Holik Dr. #D
College Station, TX 77840

Phone (979)862-1079
(979)694-9769, (979)571-6578(cell)

e-mail kunwoo.han@gmail.com, k0h6639@chemail.tamu.edu

Career Goals

- To exploit the molecular simulation technique to understand and predict phenomena of complex molecules at interfaces such as the fabrication of nanocomposite and protein behavior near lipid bilayers
- To extend the horizon combining both experiment and molecular simulation

Summary of Qualifications

- Strong background in molecular simulation, statistical mechanics, heat transfer, and combustion engineering
- 6-year professional research experience as research engineer in industry
- Specialty for molecular simulations using MD(molecular dynamics) and MC(Monte Carlo) techniques, gas separation technology using membranes, and design of industrial burners
- Computer/Software skills
 - Languages/Systems : FORTRAN, C, C++, UNIX/LINUX
 - Software skills : MAPLE, Matlab, Excel, SigmaPlot, VMD, VideoMach
 - Simulation tools : LAMMPS(MD), Cerius²(MD), MC codes

Professional Experience

07/96 – 07/01 Research Engineer, Energy & Chemical Process Research Team
Research Institute of Industrial Science & Technology (RIST)

01/95 – 07/96 Research Engineer, Environment & Energy Research Team
Technical Research Laboratories, POSCO (POSLAB)

Education

08/01 – present Graduate Student (Ph.D. candidate), expected graduation in May, 2006
Department of Chemical Engineering, Texas A&M University

03/93 – 02/95 M.S. Chemical Engineering, POSTECH

03/89 – 02/93 B.S. Chemical Engineering, Pohang University of Science & Technology(POSTECH),
Republic of Korea

Current Research Summary

I am currently being advised by Dr. David M. Ford at the department of chemical engineering, Texas A&M University. I have been involved with two projects (Dendrimer-clay nanocomposite and $A\beta$ research). All those works are purely computational (no experiment by myself) and require high computational load. The machines I am using are SGI, unix-machines (DEC), linux machines, G5 clusters and supercomputers (Origins).

[Dendrimer-clay nanocomposite]

As the polymer-clay nanocomposite shows superior physical properties such as higher mechanical strength, thermal resistance, much attention has been drawn. There are two well-known morphologies of the nanocomposite, the intercalated and exfoliated structures. One way of fabricating a polymer-clay nanocomposite is to modify the clay surface by performing cationic exchange to enhance the interaction between the clay surface and polymer and mix it with the polymer melt. Several research groups such as Giannelis at Cornell University have tried to interpret the partitioning process based on the free energy behavior associated with the process, mainly of the modified clay-polymer melt.

We are interested in understanding and interpreting the whole fabrication process including the partitioning of surfactant into clay surface, the tethering (anchoring) of surfactant to clay, and the interaction between the modified surface and polymer.

As a first step to the ultimate goal, our research focused on examining the partitioning process of single surface-modifier or dendritic surfactant into clay surface. We performed molecular dynamics simulations using a software called LAMMPS (developed by Sandia National Laboratories). Confinement forces associated with this process have been obtained directly from the simulations, and the free energies at each clay layer separation (6 to 500 Å) were calculated by integrating the forces. Based on the free energy profiles the partitioning process has been analyzed. Also, the process has been interpreted by the energy-entropy interplay, since it can be viewed from the competition between energetic and entropic contributions. We studied four different types of melamine-based dendrimers and their partitioning process into the montmorillonite clay. We found that small and linear molecules showed frustrated intercalation where portion of dendrimer is extended into clay dimension, while large molecules exhibited complete intercalation (Acosta et al., *Chem. Mater.* 2003). Simulation study result comes into agreement with the experimental findings in the sense that the dendritic surfactants are expected to intercalate into the clay gallery.

Simulations on higher loading of dendrimers (multiple molecules) and tethered dendrimer are to be performed. Also, the tethering process of dendrimer to clay surface is under study from the theoretical and simulation viewpoints. Theoretical and simulation study associated with the ion exchange process including the partitioning, tethering of surfactants, and solvent rearrangement will be done. We plan to study the fabrication process of nanocomposite with polymer and surface modified clay, which will be our final task of this research.

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[Ab in hydrated lipid bilayer]

The deposition of A β (beta-amyloid) is the known cause of Alzheimer's Disease(AD). To investigate the neurotoxicity of A β , we intend to perform molecular simulation of a system of A β protein, water, and lipid bilayers such as DPPC.

We've studied the bulk water system with several sets of model parameters, and successfully reproduced the potential energy and pressure of the system. Currently we are working on the construction of hydrated lipid bilayer(8 \times 8 \times 2) model with the aid of Cerius² and performing test runs with different treatment method of long-range electrostatics, number of CPUs, etc. We are going to simulate a system consisting of A β protein and the hydrated lipids. The free energy as a function of the distance between the protein and the water-lipid interface will be obtained from the potential energy at each separation using free energy perturbation method for different starting conformation of A β protein and membrane composition(pure lipids and lipids with cholesterol, etc.). The free energy profiles will provide the most stable structure and position of A β protein in hydrated lipids and effect of membrane composition change.

Honors and Awards

Spring 2005	Recipient of SPE South Texas Section Polyolefin 2005 Conference Scholarship(from The Society of Plastic Engineers, SPE)
2003	Recipient of The Korean Honor Scholarship (from the government of R.O.K.)
Spring 1992	Academic Excellence Award at POSTECH
Fall 1991	Academic Excellence Award at POSTECH

Publications

- Kil Won Cho, Kunwoo Han, Y.K.Lee, D.-S. Noh, H.M. Yoon, K.-J. Riu, K.-H. Lee, Premixed combustion of coke oven gas in a metallic fibre mat, *FUEL*, Vol. 80, No.7(May 2001) 1033-1036
- Kil Won Cho, Kunwoo Han, H.S. Park, Y.K.Lee, K.-H. Lee, On the short-cut calculation of the air ratio in the case of firing fuels containing incombutibles, *FUEL*, Vol. 77, 9-10(July-August 1998) 1129-1130
- Yoon-Kyung Cho, Kunwoo Han, Kun-Hong Lee, Separation of CO₂ by modified γ -Al₂O₃ membranes at high temperature, *J. of Memb. Sci.*, 104 (1995) 219-230

Presentations/Conference Proceedings

- Kunwoo Han, Molecular Simulation of the Partitioning Process of Single Untethered Dendrimers into Clay Gallery, LG Chem Tech Fair USA 2005, Hilton Anaheim Hotel, Anaheim, CA, USA, March 4-6, 2005
- Kunwoo Han, David M. Ford, and Eric Simanek, A Combined Experimental and Molecular Modeling Study of Intercalation in Dendrimer-Clay Nanocomposites, 2004 AIChE Annual Meeting, Austin Convention Center, TX, USA, November 7-11, 2004
- Kunwoo Han, David M. Ford, and Eric Simanek, A Molecular Dynamics Study of Intercalation in Dendrimer/Clay

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Nanocomposite, 2nd Annual TAMUS Pathways Research Symposium, Texas A&M University – Corpus Christi, Corpus Christi, TX, USA, October 15-16, 2004

- Kunwoo Han, Kil Won Cho, and Yong Kuk Lee, Combustion characteristics of gases with low calorific values for the stabilizer, Spring Meeting, The Korean Institute of Chemical Engineers, Yonsei University, Seoul, Korea, April 27-28, 2001
- Kil Won Cho, Kunwoo Han, and Yong Kuk Lee, An Experimental Study for the Reduction of Nitrogen Oxides in Oxygen Enriched Combustion, Spring Meeting, The Korea Society for Energy Engineering, Sungkyunkwan University, Suwon, Korea, May 25-26, 2000
- Kunwoo Han, Kil Won Cho, and Yong Kuk Lee, Effect of Fuel Change on the Surface Combustion Characteristics, Spring Meeting, The Korean Institute of Chemical Engineers, Sungkyunkwan University, Suwon, Korea, May 25-26, 2000
- Kunwoo Han, Kil Won Cho, and Yong Kuk Lee, A Study on Performance Enhancement of Boilers through Oxygen Concentration Control, Fall Meeting, The Korean Institute of Chemical Engineers, Kyungnam University, Masan, Korea, October 22-23, 1999
- Kil Won Cho, Kunwoo Han, and Yong Kuk Lee, The emission characteristics and reduction measures of nitrogen oxides in oxygen enriched combustion for reheating furnace burners, Fall Meeting, The Korean Institute of Chemical Engineers, Kyungnam University, Masan, Korea, October 22-23, 1999
- Kunwoo Han, Kil Won Cho, Young Il Kim, Yong Kuk Lee, and Rae Woong Chang, Analysis on the steam pipe network at a steel company, The Korean Institute of Chemical Engineers, Sungkyunkwan University, Suwon, Korea, April 23-24, 1999
- Kunwoo Han, Kil Won Cho, and Yong Kuk Lee, Surface Combustion Characteristics of Gases on a Metallic Fiber Mat, Spring Meeting, The Korean Institute of Chemical Engineers, KOEX, Seoul, Korea (R.O.K.), April 25-25, 1998
- Kunwoo Han, K.W. Cho, O.H. Park, and Y.K. Lee, Surface Combustion Characteristics of LPG and Coke Oven Gas Using Metallic Fiber Burner, Fall Meeting, The Korea Society for Energy Engineering, Seoul National University, Seoul, Korea, November 14, 1997
- Kunwoo Han, K.W. Cho, H.S. Park, and Y.K. Lee, Interchangeability of gaseous fuels at the steel industry – Mixing of by-product gases and city gas, Fall Meeting, The Korean Institute of Chemical Engineers, Kyungbuk National University, Taegu, Korea, October 18-19, 1996
- Kunwoo Han, Tae Jung Kim, and Kun-Hong Lee, A Study on the Separation of Carbon Dioxide Using IS Membranes, Fall Meeting, The Membrane Society of Korea, Taejon, Korea, November 4-5, 1994
- Kunwoo Han, Tae Jung Kim, and Kun-Hong Lee, Separation of CO₂ Using IMS(Immobilized Molten Salt) Membranes, Fall Meeting, The Korean Institute of Chemical Engineers, Chonbuk National University, Jeonju, Korea, October 21-22, 1994

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- Surface combustion burner with diffusion mixing apparatus (No. KR20-1997-40978)

Teaching/Research Experiences

- 01/2004 – 05/2004 ACI(Assistant to Course Instructor) of CHEN 643, TAMU
09/2003 – 12/2003 Grader of CHEN 689 (Applications of Thermodynamics to Chemical Engineering), TAMU
09/2002 – 12/2002 Grader of CHEN 320 (Numerical Methods in Chemical Engineering), TAMU
09/2001 – 12/2001 Grader of CHEN 320 (Numerical Methods in Chemical Engineering), TAMU
09/2001 – present Research Assistant at the Department of Chemical Engineering, TAMU
03/1993 – 06/1993 Teaching Assistant at POSTECH (Mathematical Methods in Chemical Engineering)

Academic/Technical Trainings

- Fall 2003 Supercomputing Short Courses at TAMU Supercomputing Facility(09/03 – 10/03)
Summer 2002 Quantum Mechanics Workshop at LMS, Chemistry Department, Texas A&M University
Spring 2002 UNIX Workshop at LMS, Chemistry Department, Texas A&M University

Academic Affiliations

- 2004 – 2005 Member, The American Institute of Chemical Engineers (AIChE)
1994 – 2000 Member, The Korean Institute of Chemical Engineers (KIChE)
1994 Member, The Membrane Society of Korea

Extracurricular Activities

- 10/2003 - present System administrator of Molecular Simulations and Membrane Technology Group at TAMU
09/2003 – 08/2004 Member of Graduate Student Council at Chemical Engineering Department, TAMU
02/28/2003 Performer of Talent Show of International Week at TAMU
09/2002 Volunteer of Korean Thanksgiving Party by Korean Student Association at TAMU
08/2002 - present Member of a soccer club (KASA, Korean Aggie Soccer Association) at TAMU
President of the club from 08/2004 – 01/2005
08/2002 Counselor of I-Camp (International Student Camp) at TAMU
07/2002 – 06/2003 Representative of Korean Student Association at Chemical Engineering Department, TAMU
1996 YWCA teaching volunteer (unofficial) for under-educated women in Pohang, R.O.K.
03/1991 - 02/1992 Chair of Undergraduate Association of the Department of Chemical Engineering, POSTECH
09/1989 - 02/1995 Member of a soccer club (KAISER) at POSTECH
03/1989 - 02/1990 Staff of Student Club Union at POSTECH