

CHEMICALS

Project Fact Sheet



MOLECULAR SIMULATION FOR CHEMICALS INDUSTRY

BENEFITS

- Significant reductions in separation energy
- Improved membrane separation analysis techniques
- More user-friendly computer interface

APPLICATIONS

The software tools can be utilized to design materials used in devices that depend upon controlled, molecular transport, such as plastics, biomaterials and modern fuel cell production. Some examples include the production of polyester films, resins and fibers.

COMPUTATIONAL TOOLS WILL PROVIDE ENHANCED MOLECULAR SIMULATION FOR MEMBRANE SEPARATION DESIGN

Commercial software packages with molecular-scale dense phase simulation methods are not currently available for the chemical industry. Commercial software with these capabilities could be applied industry-wide, particularly in the design of new membrane separation methods. Applying this software to membrane technology design could have an enormous impact on energy usage in the production of biomaterials. For instance, replacing steam-driven separation of trimethylene glycol with membrane driven separation could save about 1.4 trillion Btu per plant per year, a 70% reduction. A multitude of other applications in both chemical and biochemical processing is possible.

The development of new software tools will allow the chemical industry to greatly improve the design of separation technology, reducing energy consumption and enabling greater use of renewable feedstocks. Software tools will be developed for the following simulation methods: molecular dynamics for steady state nonequilibrium flow; Gibbs ensemble method for fluid phase equilibria; and general force fields development (collections of inter-molecular potential functions and their parameters). Easy-to-use web-enabled tools can reduce production time leading to significant efficiencies in separations.

MOLECULAR INTERACTIONS



Models will simulate physical/chemical phenomena, such as the absorption of methane in zeolite shown here.



Project Description

Goal: To develop commercial software tools for molecular simulation of physical and thermodynamic phenomena during chemical processing.

Commercial software packages are still not available for molecular-scale simulation methods with wide applicability in the chemical industry, even though many of these methods are well established. This project will provide simulation tools in three main areas. The first is the implementation, evaluation, and further development of Monte Carlo algorithms for dense phase simulation, with particular emphasis on adequate conformational sampling of large and complex molecules. The second is the systematic evaluation of existing force fields and the development of new force fields where the current ones are lacking. The third is the development of a web-based interface that will help the new user set up the input files and understand the implications of various combinations of settings for both simulation codes.

Progress & Milestones

Project partners have extensive experience in developing force fields and simulation methods. Work is now progressing on refining Monte Carlo algorithms for dense phase simulation.

Future research will focus on achieving the following milestones:

- Develop methods and force fields
- Apply molecular dynamics codes and new force fields to the adsorption and tribology of lubricants and lubricant additives confined between surfaces
- Validate molecular dynamics methodology and results relative to actual experimental data and mutual diffusion transport theory
- Apply newly developed force fields and configurational-bias Monte Carlo codes to determine the phase envelopes of liquid/vapor and liquid/liquid mixtures of practical interest
- Code testing and feedback to improve their practical use in industry.

Commercialization

Fifty of the top chemical producers are estimated to have enough resources invested in separations-based research and development to find the software codes appropriate for their work. Ten companies in allied fields concerned with lubrication would benefit from the software. Ten university based research groups would also gain from the codes. The software codes will be transferred to the chemical industry at no cost. As a result, a strong penetration into the potential market is expected.



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