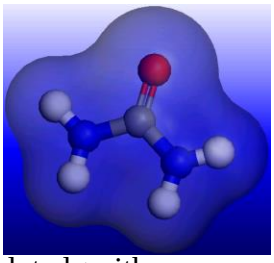
**Research Project**: Nano-Enhanced and Bio-Inspired Composite Materials for Mitigation and Protection of TIH Railcars and Stationary Tanks against High Power Impact

**Research Topic**: Equation of State (EOS) calculations via Molecular Mechanics (MM) and Molecular dynamic (MD) simulations

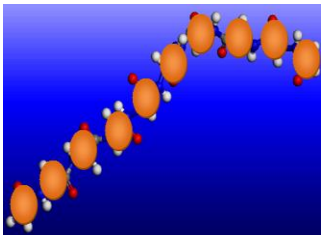
**Problem**

Equation of state (EOS) is a relation between state variables. EOS describes the state of matter under a given set of physical conditions. During the last decades, computer simulations based on molecular mechanics (MM) and molecular dynamics (MD) have initiated several routes, to calculate and predict both equilibrium and nonequilibrium thermophysical properties of small molecules and long polymeric chains as well. Recently the cost of producing one Vapor-Liquid Equilibrium data point for a binary mixture has been estimated to be about 2600$ and an average experiment time of two days. From above one can state that an acute necessity for a computational technique has risen. MM/MD techniques combined with EOS theory were developed to calculate the perturbed hard-sphere chain (PHSC) EOS parameters characteristic surface area (A*), characteristic volume (V*), and characteristic "cohesive" energy (E*), the mentioned characteristic parameters can be performed via the Connolly dot algorithm.



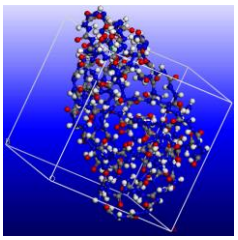
**Approach**

In this study it is proposed to use computational tools (MM/MD) simulations) to predict the EOS of polymers.
The simplified PHSC EOS model considered in this work, in which the polymer molecule is considered to be constituted by chains of freely jointed tangents hard spheres.



The models will be equilibrated by a series of energy minimization and NVT molecular dynamics runs.

The fully relaxed polymer PBC will be submitted to an NPT ensemble at 380 K (a temperature above



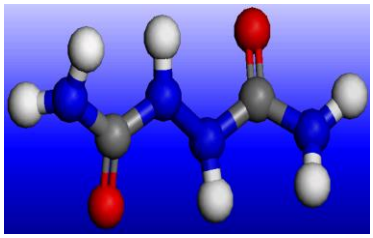
glass transition for the polymer) and then from 350 to 50 K at intervals of 50 K. Each NPT run was started by assigning initial velocity for the atoms according to a Boltzmann distribution at 2xT. For the NPT dynamic simulations, the relaxation time is 0.10ps and an equilibration time of 50 ps steps with time step =1fs. COMPASS force field is used through the simulation.

The materials that will be studied include:

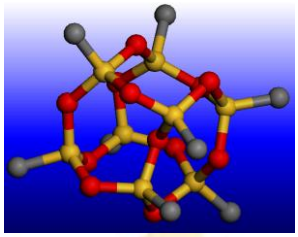
- Polyurea
- POSS: Polyhedral Oligomeric Silsesquioxanes

**Findings**

The work is in progress. A 128-node parallel processing license of Accelrys, a molecular dynamics simulation software is used. Negotiation has been conducted with the Mississippi Center for Supercomputing Research to house and maintain the software, and to allow the simultaneous use of up to 128 SGI and Linux based computers. Simulations of polyurea and polyurea reacted with different percents of POSS will be performed. The results will be used as a bench mark for EOS simulations of other polymeric matrices.



***Polyurea basic structure***



***POSS***

**Impact**

Whereas traditional construction material database (e.g. concrete, reinforced concrete, steel, masonry, timber, polymer concrete, and fiber reinforced polymers) can be easily generated from available literature, material database of emerging new materials (e.g. nano-structured materials) is yet to be developed.

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