Shear Viscosity prediction of Pure Molecules using molecular dynamic method

Tessa Eskander, Joshua Berry, Liqun Zhang
Department of Chemical Engineering Tennessee Technological University

Introduction

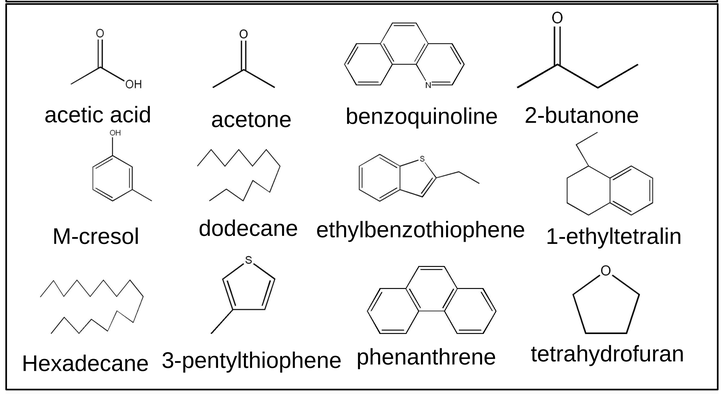
Asphalt pavement is susceptible to extreme temperature failure, such as cold temperature cracking. Pyrolysized swine manure or switchgrass can be mixed with the original asphalt to make bioasphalt, which can improve the low-temperature properties of asphalt on road pavement. In order to understand the relationships between chemical composition, microstructure and major physical and mechanical properties of bioasphalt, molecular dynamics simulations are useful for this. At the starting stage, simulations were performed on 12 simple molecules that contain common functional groups typically found in bio-asphalt: sulfonated, oxygenated, aromatics, aliphatic, etc. Running all atom molecular dynamics simulations using LAMMPS package, density and shear viscosity were predicted at in total eight temperatures on each molecule to understand their property dependence on temperature. Consistent agreement with experimental data was observed.

Goal

Identify molecule types that are contained in bio matter and predict molecules that could enhance asphalt cold-temperature properties.

Simulation Method

Basic Molecules Simulated

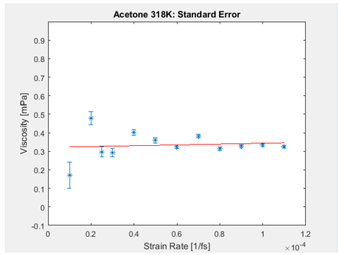


343 of each molecule was generated using Towhee OPLS-aa force field [4]. Simulation was then equilibrated and physical properties were predicted using LAMMPS (Dec 2015) [5].

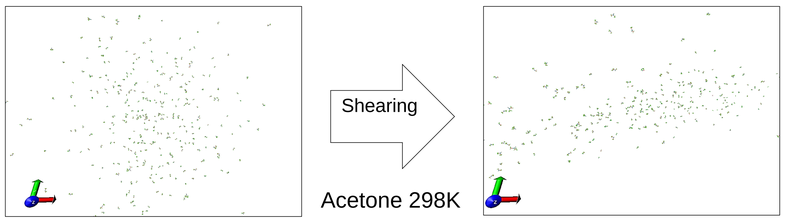
Simulation Method

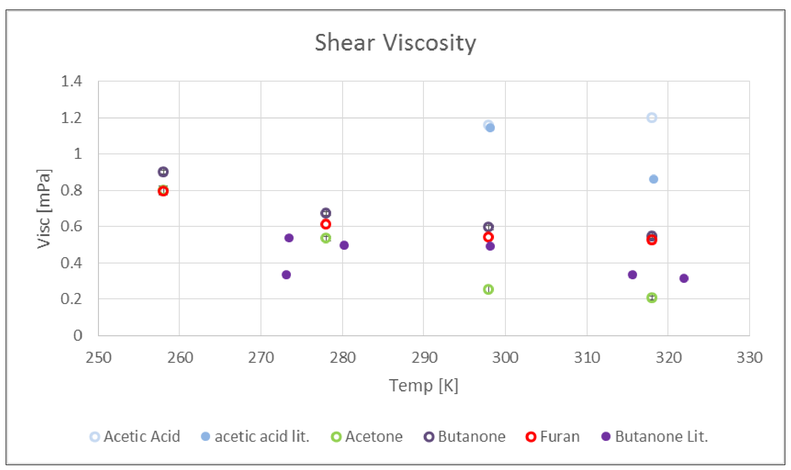
After Equilibrating, several steps are needed to accurately predict viscosity:

- Equilibrate in NVT (controlled volume and temperature)
- Apply Shear Strain Rate
- Determine Steady State Region (Temperature, Pressure, and Energy)
- Calculate and Average
- Simulate multiple strain rates for a linear fit (between noise and temp spike)
- Intrinsic Viscosity: Y-intercept (0 strain rate)



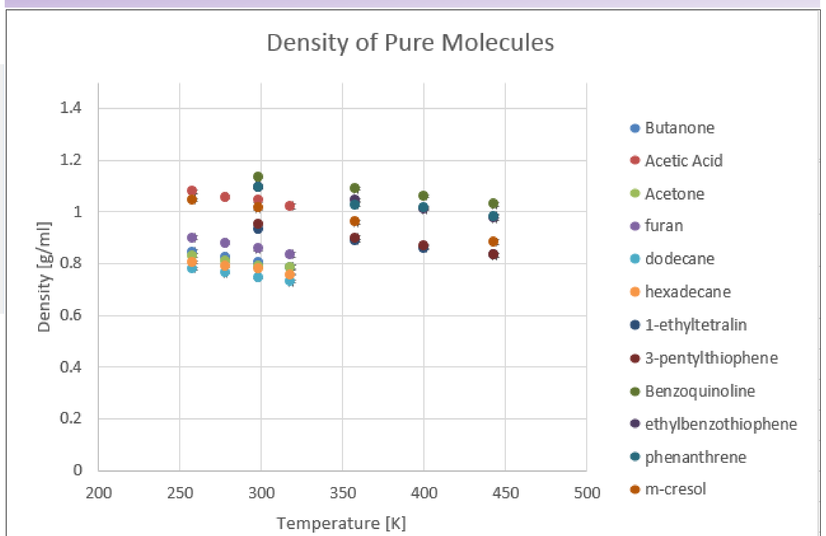
- Muller-Plathe Formulas [1]: $j_z(p_x) = -\eta \frac{\delta x}{\delta z} = \frac{P_x}{2tL_xL_y}$
- Can be Interpreted as[2]: $\eta = \frac{-P_{xy}}{\dot{\gamma}_{xy}}$
- Standard Error (precision) [3] $SE = \frac{\sigma}{\sqrt{n}}; n = \#\ of\ data\ points$





Literature Values from: International Critical Tables [1930] Volume 7 pg.211-222

Results and Discussion



Conclusions and Future Work

Findings:

- Density was successfully predicted
- Viscosity has an inverse relation, but results are not consistent

Plan:

- Continue simulating Basic Molecules
- Combine molecules into asphalt mixture and test effects
- Predict molecules effect on physical properties

Acknowledgements

•Michel Renfro – CAE operator
•CAE- Tennessee Technological University's Computer Aided Engineering System
•LAMMPS User Forum

References

1. "A Reverse Nonequilibrium Molecular Dynamics Method for Calculating the Mutual Diffusion Coefficient for Binary Fluids", H. Yang, J. Zhang, F. Müller-Plathe, and Y. Yang, Chem. Eng. Sci. 130, 1–7 (2015). [DOI: 10.1016/j.ces.2015.03.006]
2. http://www.swinburne.edu.au/ict/success/cms/documents/disertations/jzChap3.pdf
3. Garland, Carl W. (2009) Experiments in Physical Chemistry. New York, New York. McGraw-Hill p. 40
4. http://towhee.sourceforge.net/forcefields/oplsaa.html
5. http://lammps.sandia.gov/