MedeA Viscosity

Reliable Momentum Transport Properties from Classical Simulations

At-a-Glance

Supporting both equilibrium (EMD) and non-equilibrium (NEMD) calculation methods, the *MedeA*®[1] *Viscosity* module automates the setup, simulation, and detailed analysis procedures needed to predict the shear viscosity of fluids and fluid mixtures. *MedeA Viscosity* uses the LAMMPS simulation engine, in conjunction with appropriate force fields, to compute viscosity of both organic and inorganic materials in the liquid state, reducing the need for difficult-to-perform and expensive experiments.

Key Benefits

- Handles the complexity of calculating the viscosity in LAMMPS, letting you focus on the science
- Easily sets up multi-step calculations with *MedeA*'s powerful flowchart interface, and supports recall of these calculations later on, to modify conditions before rerunning.
- Performs automatic graphical analysis of the viscosity and fitting of the results, computing the numerical value of the viscosity and statistical error bars
- Validates calculations using graphs and reporting of all intermediate results through the convenient *MedeA JobServer* web-interface
- Works with the *MedeA JobServer and TaskServer* to run your calculations on the appropriate hardware, centralizing the results
- Integrates with *MedeA Forcefield* for advanced forcefield handling and automated assignment

'Until recently, computing the shear viscosity of complex mixtures, such as those found in oil field reservoirs, was a major research undertaking. The MedeA Viscosity module has begun to change this situation dramatically, by combining access to fast affordable compute clusters with the power of the LAMMPS simulation code, and with MedeA's versatile model building, simulation management, analysis tools, and accurate forcefields. The end result is that such simulations are now more widely accessible than ever before.'

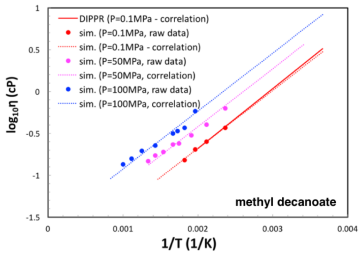
[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

Computational Characteristics

- Uses the LAMMPS forcefield engine for high performance on any computer, whether it is a scalar workstation or a massively parallel cluster
- Compatible with any forcefield handled by *MedeA*
- Scales consistently with system size and the size of the computational cluster. If you double the system, but run on twice as many CPUs, the computational time remains unchanged
- Equilibrium molecular dynamics (EMD) Green-Kubo method:
  - Requires moderate size boxes of fluid
  - Length of simulation required depends on viscosity: the higher the viscosity the longer the calculation needed - typical fluids with viscosities around 1 centipoise require 5-20 ns of simulation time
- Reverse non-equilibrium method (RNEMD):
  - Uses elongated cells, and sometimes large boxes of fluids
  - Calculation time may be less than EMD methods
  - Enables investigation of shear rate effects

Viscosity of esters

- Computation of viscosities using Molecular Dynamics at:
  - P ∈ [1,4000] bar
  - T ranging depending on P
- Fit of η(T) equations to simulation data for each P
- Good agreement with available experimental data, particularly for small to medium sized esters



MedeA®-LAMMPS simulations with pcff+ forcefield

Materials Design - Total, joint presentation Petrophase 2017, Le Havre, 11-15 June 2017

Required Modules

- *MedeA Environment*
- *MedeA LAMMPS*

Recommended Modules

- *MedeA Amorphous Materials Builder*

Find Out More

Learn more about how *Viscosity* can be used to study viscosity of materials ranging from simple liquids to industrially important fluids, such as those used in model biodiesel fuels and fragrance compounds, by contacting info@materialsdesign.com.

12121 Scripps Summit Drive, Suite 160 San Diego CA 92131, USA
P: +1 760 495-4924 - F: +1 760 897-2179 - E: info@materialsdesign.com

materialsdesign.com

materials design