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Development of a new computational method for calculation of viscosity of complex liquids

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Introduction

Viscosity is one of the important factors in the characterization of liquids so that molecular simulation of fluid viscosity is powerful method in order to minimize experimental work and guiding the search for the structural characteristics of the molecule that produce the desired macroscopic properties. Recently, we have developed a new computational chemistry approach for the viscosity prediction of liquids that based on the "Falling-ball" principles using classical molecular dynamics method, in order to establish a new screening method for characterization of complex liquids even under extreme conditions. The developed method has been applied to the evaluation of viscosities of water, electrolyte solutions and simple hydrocarbon structures. Calculated viscosities showed good agreement with experimentally reported values. The developed method has a potential of being an effective tool for evaluating viscosity of complex liquids.

Method

Our method for the viscosity calculation of liquids is based on the classical falling-ball principles and this method is evaluated with a program based on our integrated classical molecular dynamics program "New-RYUDO" which has been developed in our laboratory. Viscosity coefficients (μ) of the liquids can be calculated by analyzing the speed and the force of a monatomic measurement ball inserted to the simulation cell (Figure 1) according to the Stokes' equation.

$$\mu = \frac{F}{3\pi D_p \zeta u_t}$$

where, F is the force on the ball, D_p is diameter of measurement ball, ζ is correction coefficient and u_t is the speed of the ball.

Results and Discussion

The viscosities of water, electrolyte solutions and simple hydrocarbon structures have been calculated. For instance, a cubic model with 272 water molecules with the inserted viscosity measurement ball, where the density was set to 0.99 g/cm^3 at 293.15 K and 100 kPa, was used for the viscosity evaluation of water. Speed of the measurement ball was determined by analyzing the moved distance of the measurement ball via the simulation time. The viscosity of water was calculated as 1.0321 mPa.s at 293.15 K and 1 atm that in agreement with the experimentally known viscosity of water (1.002 mPa.s) at the same conditions within 3% error. Further viscosity calculations were performed for electrolytes of simple ions at different concentrations and the results are also in good agreement with experimental ones (Table 1). Besides, our new computational method for viscosity prediction have been applied to simple hydrocarbon liquids, such as hexane, benzene, acetone, toluene and more complex lubricants even under high pressure conditions.

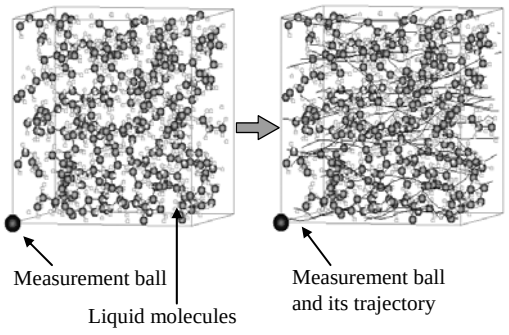

Fig. 1. Process of the viscosity calculation a) Measurement ball is inserted to the simulation cell. b) Compulsory movement is given to the measurement ball applying a constant force.

Table 1. Calculated viscosities of simple electrolyte solutions comparing to the experimental values at different concentrations

Electrolyte	Concentration *[mol/l]*	Viscosity *Calc. [mPa.s]*	Viscosity *Exp. [mPa.s]*
LiCl	*0.2*	0.96	1.02
	1.6	1.17	1.23
	3.0	1.63	1.52
NaCl	*0.2*	0.96	1.01
	1.6	1.09	1.16
	3.0	1.32	1.38
KCl	*0.2*	0.93	0.99
	1.6	1.05	0.99
	3.0	1.10	1.01
CsCl	*0.2*	0.88	0.97
	1.6	0.98	0.93
	3.0	1.03	0.93