Reliable Viscosity from Equilibrium Molecular Dynamics Simulations: A Time Decomposition Method

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January 28, 2015

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Abstract

Keywords:

1 Introduction

2 Simulation Procedure

3 Results and Discussions

Notes:

FOR CORRELATION TIME CUTOFF: There are two reasons to fit the correlation function at as short as possible. One reason is, as shown in the calculated σ, the standard error increases with the increasing correlation time.Secondly, computationally, it is always prefer to run the simulations shorter as long as the results are reliable.

Experimental deviates. There are only four points from simulation, which

The goal of the current work is not to calculate the viscosities for one or two examples, but rather to describe a general method for the calculation of viscosity reliablly. However, for the two examples studied in this work, the calculated viscosity using the proposed procedure do agree with available experimental results reasonable well although only the general Amber force field was used, which was not optimized for the such calculation. If a dedicated force field is used, the results are likely further improved.

4 Concluding Remarks

Supporting Information

Acknowledgment

This material is based upon work supported by the National Science Foundation (NSF) Partnerships for Innovation (PFI) subprogram: Building Innovation Capacity (BIC), award

number 1237829. Computational resources were provided by the Center for Research Computing (CRC) at the University of Notre Dame. **JECSR NERSC**

References

Figure captions

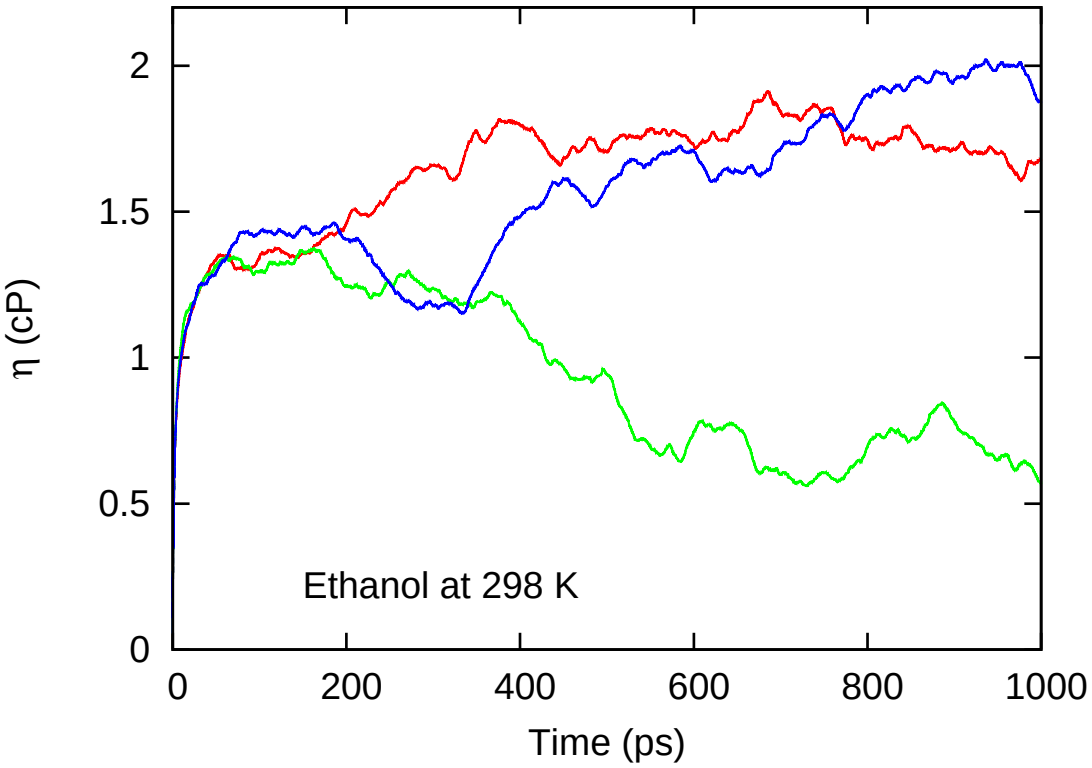

Figure 1: Ethanol

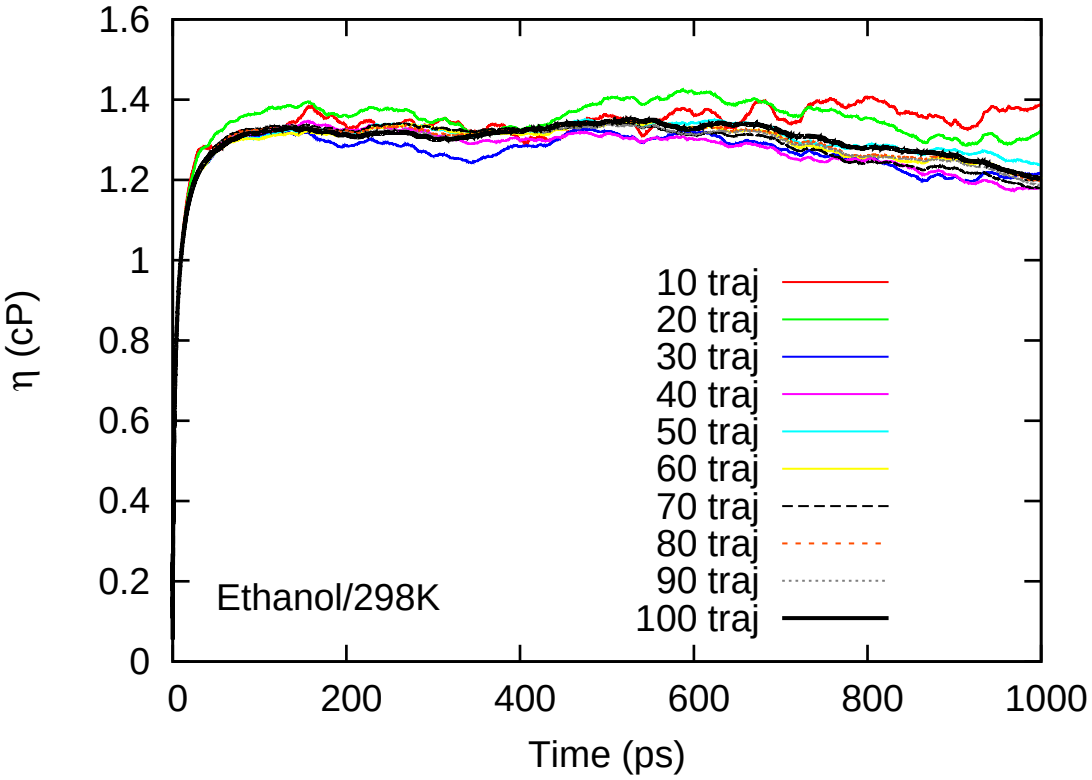

Figure 2: Ethanol

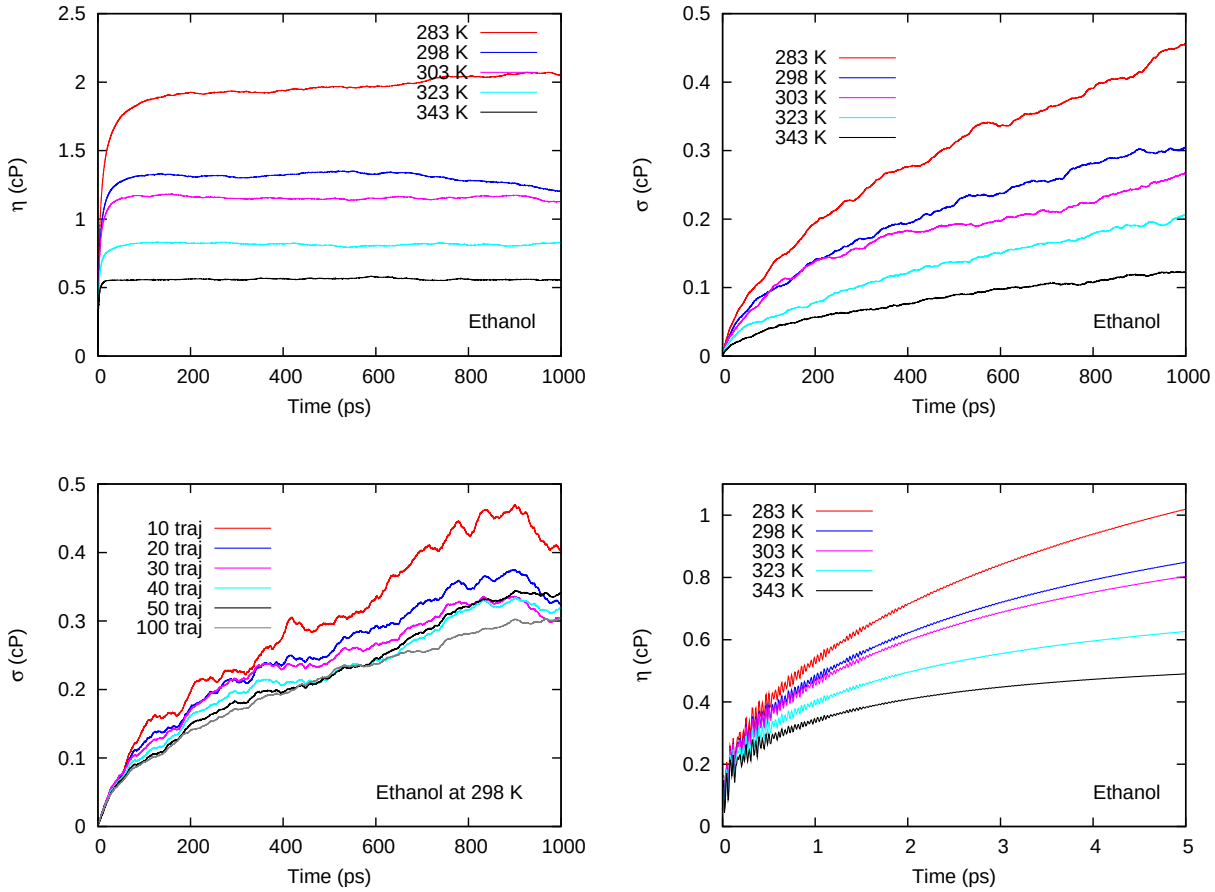

Figure 3: Cutoff for fit.

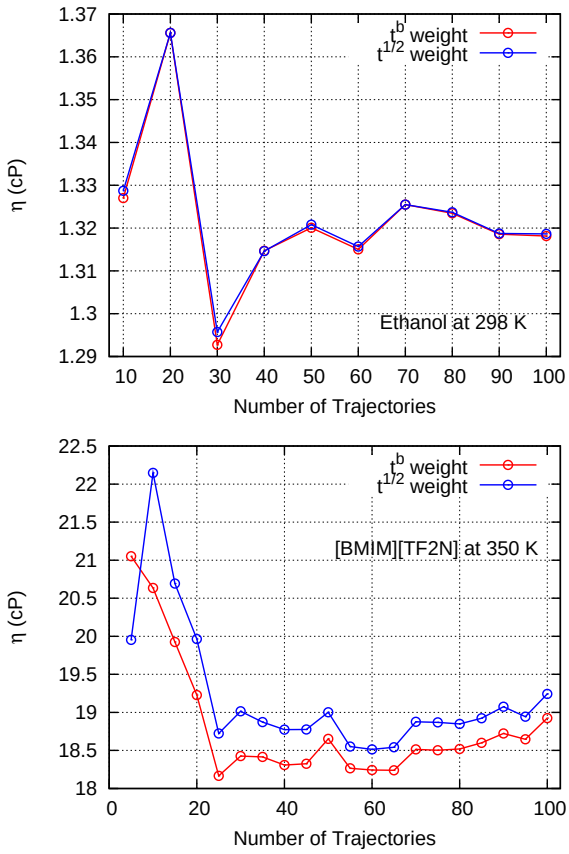

Figure 4: Viscosity convergence.

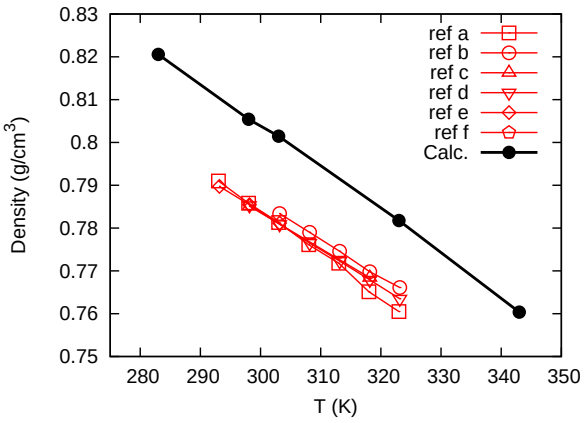

Figure 5: Ethanol

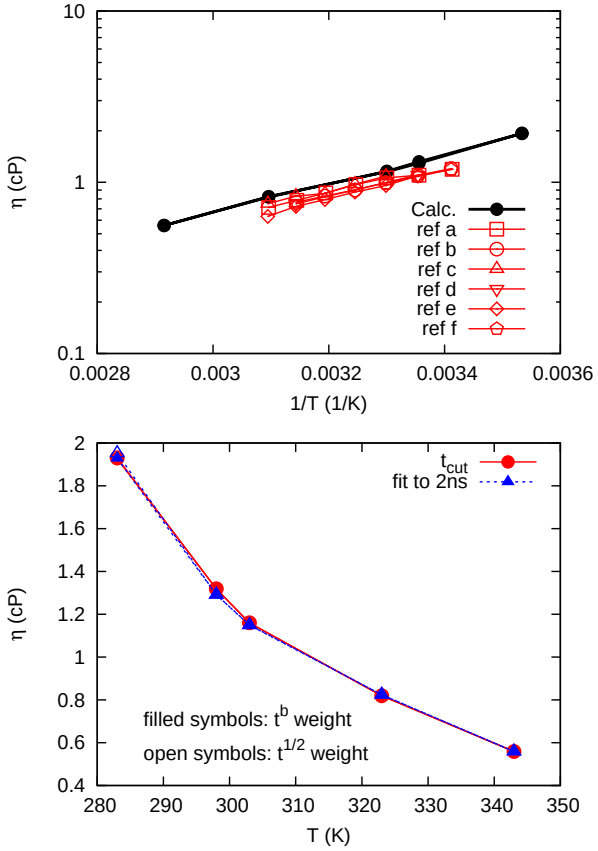

Figure 6: Ethanol

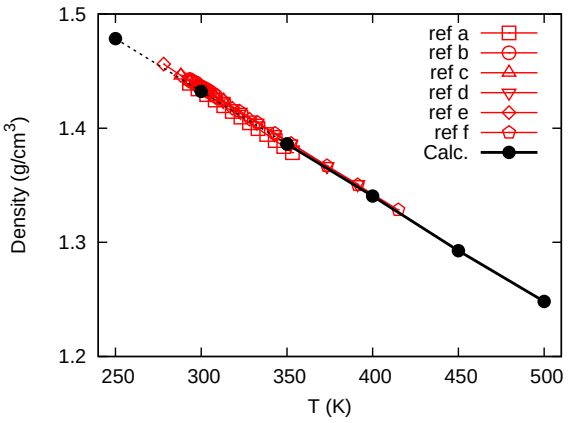

Figure 7: Bmim-TF2N

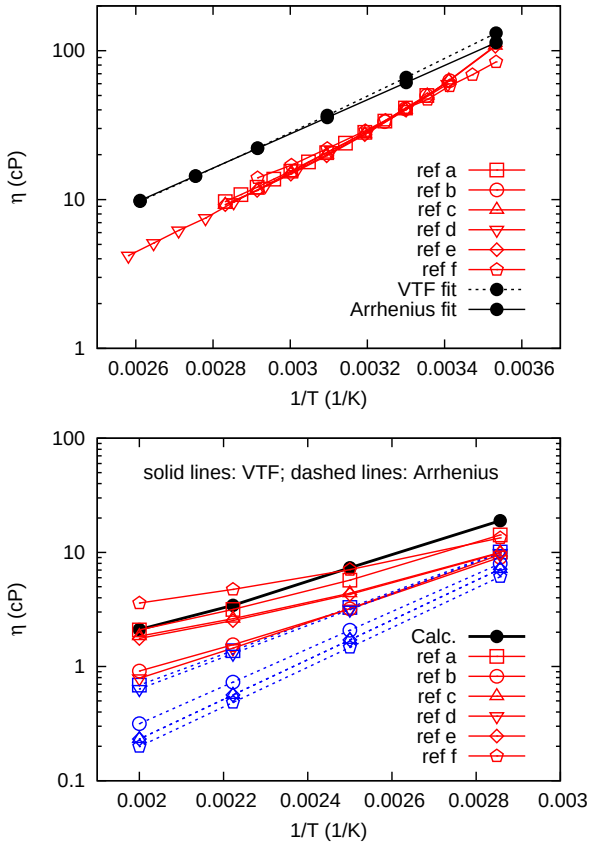

Figure 8: Top: BMIM-TF2N viscosity extrapolation from simulation data. Bottom: BMIM-TF2N viscosity extrapolation from experimental data.