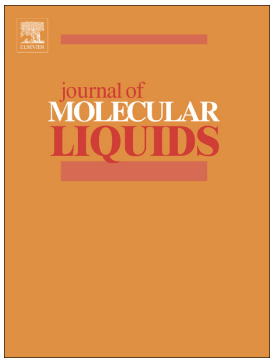

Coarse graining of the fully atomic methane models to monatomic isotropic models using relative entropy minimization

Chuntao Jiang, Jie Ouyang, Lihua Wang, Qingsheng Liu, Wuming Li

PII: S0167-7322(17)30310-0
DOI: doi: 10.1016/j.molliq.2017.07.112
Reference: MOLLIQ 7691

To appear in: *Journal of Molecular Liquids*

Received date: 23 January 2017
Revised date: 17 July 2017
Accepted date: 25 July 2017

Please cite this article as: Chuntao Jiang, Jie Ouyang, Lihua Wang, Qingsheng Liu, Wuming Li , Coarse graining of the fully atomic methane models to monatomic isotropic models using relative entropy minimization, *Journal of Molecular Liquids* (2017), doi: 10.1016/j.molliq.2017.07.112

Coarse graining of the fully atomic methane models to monatomic isotropic models using relative entropy minimization

Chuntao Jiang, Jie Ouyang*, Lihua Wang, Qingsheng Liu, Wuming Li

Department of Applied Mathematics, Northwestern Polytechnical University, Xi'an 710129, China

**Corresponding author*: Jie Ouyang; e-mail: jieouyang@nwpu.edu.cn

Abstract

This work presents the relative entropy minimization method for the construction of a series of coarse grained (CG) methane models based on the four popular methane atomistic models (RISM, LJ (12-6), OPLS and MOPLS). Each CG methane molecule is represented by one bead that interacts through short-ranged isotropic interactions. The calculated dynamic and structural properties of CG model show reasonable agreement with the results of the corresponding atomistic model or experiment. To evaluate the predictive power of the CG model for prediction of mass transfer and the structural properties, the relative error of diffusion coefficient RE_D and the residuals of radial distribution function RES_{RDF} are introduced. Numerical results demonstrate that the CG models can quantitatively reproduce the structural and dynamic properties of the methane fluid. Furthermore, the CGMOPLS could reproduce quite well the radial distribution function, velocity autocorrelation function and diffusion coefficient. Interestingly, we find that the CG potential not only depends on the reference thermodynamic state conditions but also relies on the corresponding atomistic model.

Keywords relative entropy minimization, coarse grained, radial distribution function, diffusion coefficient, residuals, relative error