FINITE SYSTEM SIZE CORRECTION IN MICRORHEOLOGICAL ANALYSIS UNDER PERIODIC BOUNDARY CONDITIONS : A DIRECT NUMERICAL SIMULATION APPROACH

Yasuya Nakayama[1], Yuki Matsuoka[2], Toshihisa Kajiwara[1]

[1]Dept. Chemical Engineering, Kyushu University, Fukuoka 819-0395, Japan
[2]Corporate Engineering Center, Sumitomo Bakelite Co., Ltd., Shizuoka 426-0041, Japan

ABSTRACT

To investigate the Brownian motion of particles suspended in viscoelastic fluids, stochastic Smoothed Profile method (SPm) as a direct numerical simulation is developed by extending deterministic SPm for suspensions in viscoelastic media. To solve the viscoelastic flow driven by thermal fluctuations in the suspending medium, the random stress in the fluid momentum equation as well as the random driving force for the conformation tensor in the Oldroyd-B model are incorporated according to the fluctuating hydrodynamics and fluctuating viscoelasticity formalisms. Thermal equilibrium and dynamical properties calculated by numerical simulations successfully reproduce the analytic predictions, validating the direct simulation for the coupled fluctuating Navier.Stokes and Oldroyd-B equations, and for the coupling between the stochastic viscoelastic medium and particles. As an application of the stochastic SPm, we investigate a finite system size effect under periodic boundary conditions (PBC) on the passive microrheological relationship between the mean-square displacement (MSD) of a Brownian particle and the medium dynamic modulus. Comparing the modulus microrheologically calculated from MSD with the input one reveals that the effect of periodic image cell interaction appears not only in the long-time diffusive regime but also in the short-time region. A frequency-dependent finite system size correction is implemented by phenomenologically extending the long-time diffusive regime correction, allowing the passive microrheology analysis under PBCs. This result can be directly applied to other different mesoscale numerical simulations including coarse-grained molecular dynamics and dissipative particle dynamics.

ACKNOWLEDGEMENTS

The numerical calculations were mainly carried out using the computer facilities at the Research Institute for Information Technology at Kyushu University. This work was supported by Grants-in-Aid for Scientific Research (JSPS KAKENHI) under Grant No. JP18K03563.