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Multiscale simulation for non-isothermal polymeric flow between parallel plates[1] SHUGO YASUDA, University of Hyogo, RYOICHI YAMAMOTO, Kyoto University — A multiscale simulation method for non-isothermal polymeric flow is developed based on the local stress sampling strategy and applied to the flows of a polymer melt in the simple creep motion of the parallel plates. In our multiscale modeling, the macroscopic quantities, e.g., density, velocity and temperature, are calculated by using a usual lattice-mesh based computational fluid dynamic (CFD) simulation, but, instead of using any constitutive equations, the local stresses are generated by performing the molecular dynamics (MD) simulations associated with each mesh interval of the CFD calculation according to the local macroscopic quantities. It is found that, at a rapid creep velocity, the distinct regimes in the velocity field appear between the vicinity and intermediate of the plates because the local viscosity drastically varies due to the temperature variation generated by the local viscous heating. The effect of density variation due to the thermal expansion and compressible flow on the flow field is also investigated.

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