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Multiscale simulations of polymer melt flow in an abrupt contraction and expansion channel[1] TAKASHI TANIGUCHI, KOHEI HARADA, Department of Chemical Engineering, Kyoto University, T.TANIGUCHI TEAM —
We investigated a flow of a polymer melt with a molecular weight distribution in a channel with 4:1:4 contraction and expansion geometry by using a multi-scale simulation (MSS) method here a macroscopic model and microscopic molecular model are directly connected through the velocity gradient field and stress field. In the MSS method, we introduced Lagrangian particles which contain many chains to precisely maintain the microscopic states. As the microscopic polymer model, a slip-link model is used. As a result, we clarified the relation between the macroscopic flow behavior and molecular level information such as a local polymer configuration and spatial distribution of number of entanglements per chain.

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