Micro-Macro Simulation of Dumbbells

송선진, 정창권, 김주민[1], 안경현*, 이승종
서울대학교 응용화학부; [1]고려대학교 화공생명공학과
(ahnnet@snu.ac.kr*)

The traditional simulation of polymeric liquid is classified into the macroscopic approach and microscopic approach. The former solves constitutive equation, conservation equation while the latter solves the extra stress using dynamics of a large collection of polymeric molecules in homogeneous flow.

Recently there have been various tries, so-called CONNFFESSIT which combines the microscopic Brownian dynamics simulations with the macroscopic finite element method to get more realistic solution. However, due to massive stochastic calculation, these simulations can get only the solution of a few parameters in simple geometry.

In this study, we simulate 4:1 contraction flow of Hookean, FENE dumbbells as Weissenburg number increases using Brownian Configuration Field method and parallel solver.

Compared to Hookean dumbbell, FENE dumbbell predicts larger stress at the start and smaller stress at the steady state. In both case of Hookean and FENE dumbbell simulation, corner and lip vortex appeared, and the size of vortices are similar but the intensity of FENE dumbbell is weaker than Hookean dumbbell. More accurate modeling is possible through micro-macro simulation.