传递现象

聚合物流动的多尺度模拟

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摘要

基于聚合物分子运动论，提出了一种新的计算聚合物流体的多尺度方法。该方法在宏观尺度上应用无网格方法求解速度场，在微观尺度上应用随机模拟技术计算聚合物对应力的贡献，从而避免需要本构方程来封闭连续性方程和动量守恒方程。对Hooke哑铃模型、FENE哑铃模型、FENE-P哑铃模型，模拟了突然起动平面Couette流动；对Hooke哑铃模型，模拟了方腔驱动流动。从而验证了该方法的有效性和计算结果的可靠性。

关键词

无网格方法　Brown动力学模拟　多尺度方法　聚合物流体

分类号

Micro-macro simulation of polymeric fluid flow

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Abstract

Based on simulation of molecular models of polymeric fluids，a new micro-macro method for numerical calculation of viscoelastic flow is presented in this paper. This method coupled the mass and momentum conservation equations at the macroscopic level，with a stochastic differential equation which models the evolution of the polymer configures at the microscopic level. Accordingly，the velocity filed was determined by solving the conservation equation with a meshless method，and the stress was computed from the molecular configuration rather than from closed-form constitutive equations. Thus this method bypassed the need for a rheological constitutive equation to describe the polymeric fluid. In order to validate this method and to demonstrate its robustness，the start-up planar Couette flow was studied for Hookean，FENE and FENE-P dumbbell models and the lid-driven cavity flow was studied for Hookean dumbbell models.

Key words

meshless method　Brownian dynamics simulation　multiscale method　polymeric flow

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