عنوان مقاله:

NEMD Simulation Prediction for Rheological Behavior of linear long chain hydrocarbons

محل انتشار:

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خلاصه مقاله:

Rheological properties of long chain hydrocarbons can be important in many industrial uses. Application of comutational methhods such as molecular dynamics MD to rhelogy help us to understand the qualitative and quantitative behavior of long chain hydrocarbons by predicting rheological properties such as the viscosity. use of the non-equilibrium molecular dynamics NEMD simulation technique has allowed investigation of the shear-rate dependent rheology of linear chain alkane systems. in this work NEMD simulations were performed on model chain hydrocarbons representing C H,C2H4 and C4H8. the hydrocarbon molecules are represented by a bead-rod model with lennard -jones LJ interations between all beads sites . all interations are described by lennard -jones potential energy funcion. the equation of motion is integrated by velocity -verlet algorithm. results are presented for shear .viscosity and first normal stress differnce versus shear rate

کلمات کلیدی:

non - equilibrium molecular dynamics simulation, rheological properties , linear hydrocarbon, shear viscosity , first normal stress defference