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Effect of boundary condition on the viscosity of olefins: A molecular dynamics study LING TI KONG, COLIN DENNISTON, MARTIN MUSER, University of Western Ontario, YUE QI, General Motor — The viscosity of hexene was examined by means of non-equilibrium molecular dynamics simulations under different wall-liquid boundary conditions, namely over-smooth wall, more or less realistic wall, and over-adhesive wall. It is found that the wall-liquid interaction plays an important role in the ordering/layering of liquid, and consequently affects the behavior of olefins upon different normal pressures. With the same moving speeds of walls, the shear-rate (the slope of velocity profile) in the liquid is found to decrease with the increasing of normal pressure under over-smooth wall condition, while it is found to increase under the over-adhesive wall condition. The viscosity, in turn, shows a linear dependence on the normal pressure under over-smooth condition while exhibits an exponential dependence under the over-adhesive wall condition. The underlying mechanism of these observations will be presented and discussed in this talk.

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