Interface characteristics in methane-ethane mixture

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Molecular dynamics is used to study planar interfaces in methane-ethane mixture. Intermolecular interactions are described by TraPPE-UA model [1]. First, Nose-Hoover barostat is used to achieve desired pressure. Then, the system is held at constant temperature and volume until it reaches equilibrium. After that, the values of pressures for every axis and density profiles are averaged for 10 ns.
Surface tension is calculated using the difference between normal and tangential pressure. It is found that TraPPE-UA does not exactly reproduce experimental data [2] on densities. However, the temperature dependence of surface tension of pure ethane on temperature is very close both to experiment [2] and to parachor correlation proposed in [3].
Two peaks were discovered on all methane density profiles near the interfaces. This phenomenon can be explained by adsorption. One can numerically study adsorption by approximating the surfaces and integrating the difference between the approximation and the actual profile. The dependencies of adsorption on temperature, pressure and composition of gas and liquid are obtained this way.
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