Liquid Methane and Hydrocarbon Mixtures; an Intensive Molecular Dynamics Simulation Study

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Isothermal, isobaric molecular dynamics calculations are performed for liquid methane and hydrocarbons mixtures over a broad range of temperatures and densities (T, ρ) starting from *ab initio* molecular data obtained at the Hartree-Fock level of theory. The numerical model incorporates the Parinnello-Rahman and the Nose algorithms for the pressure and temperature control respectively. Our investigation uses a flexible molecular model where the bodies interact through an intermolecular Lennard Jones potential and the complete intramolecular potential, gathering all forms of related and unrelated interactions, including Coulomb interactions. The thermodynamic, structural and transport properties are calculated over a wide range of state points. Results are compared to experimental and calculated data obtained from different equations of state. The model introduced gives a reasonably satisfactory description of the properties in different points of the phase diagram, particularly close to the triple point.