Molecular dynamics comparative study of methane–nitrogen and methane–nitrogen–ethane systems

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Abstract :

This work concerns the site–site interaction study of 256 particles using the Buckingham potential model. We have calculated the new parameters of the Buckingham potential using an iterative algorithm with a mean square method. This adapted model allows determining the characteristics for each state point. We have applied this model to study the liquefied natural gas LNG properties for methane-nitrogen and methane–nitrogen–ethane mixtures by molecular dynamics. We have calculated the thermodynamic, dynamic and structural properties for both the microcanonical NVT and the isothermal-isobaric NPT ensembles of binary and ternary systems from the SP1 to SP9 points. Then, we have compared the results between binary and ternary systems. We have obtained a good prediction on transport properties. From the calculated values of self-diffusion coefficient and viscosity, we have confirmed the liquid state of the liquefied natural gas LNG system.

Keywords : Molecular dynamics; Buckingham potential; Binary and ternary mixtures; Structural function;Thermodynamic properties; Transport characteristics.

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