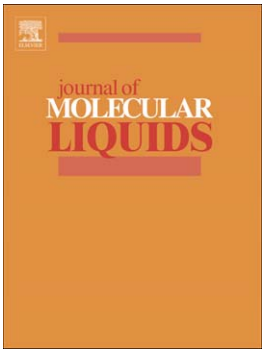

Integral equation and thermodynamic perturbation theory for a two-dimensional model of chain-forming fluid

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PII: S0167-7322(17)31203-5
DOI: doi: 10.1016/j.molliq.2017.04.095
Reference: MOLLIQ 7251

To appear in: *Journal of Molecular Liquids*

Received date: 18 March 2017
Accepted date: 19 April 2017

Please cite this article as: Tomaz Urbic, Integral equation and thermodynamic perturbation theory for a two-dimensional model of chain-forming fluid, *Journal of Molecular Liquids* (2017), doi: 10.1016/j.molliq.2017.04.095

Integral equation and thermodynamic perturbation theory for a two-dimensional model of chain-forming fluid

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Abstract

In this paper we applied analytical theories for the two dimensional chain-forming fluid. Wertheims thermodynamic perturbation theory (TPT) and integral equation theory (IET) for associative liquids were used to study thermodynamical and structural properties of the chain-forming model. The model has polymerizing points at arbitrary position from center of the particles. Calculated analytical results were tested against corresponding results obtained by Monte Carlo computer simulations to check the accuracy of the theories. The theories are accurate for the different positions of patches of the model at all values of the temperature and density studied. The IET's pair correlation functions of the model agree well with computer simulations. Both TPT and IET are in good agreement with the Monte Carlo values of the energy, chemical potential and ratios of free, once and twice bonded particles.

Keywords: Integral equation theory, association, thermodynamic perturbation theory, chain forming fluid

1. Introduction

Important part of the computational physics and chemistry is to develop analytical solution which require less computation time in comparison to computer simulations. Molecular dynamics and Monte Carlos simulations can take long time to yield one reliable single point on a phase diagram. Analytic theories