

SECTION: FM14

THERMODYNAMIC PROPERTIES OF HOMOGENEOUS STATISTICAL MOLECULAR FLUIDS

Dr. Pradeep Kumar Choudhary

Professor

University Dept of Physics, B.R.A. Bihar University

Email: pkchoudhary1964@gmail.com

Muzaffarpur 842002 Bihar India

ABSTRACT

The development of analytical expression for strongly homogeneous associating homogeneous fluids has proven to be difficult problems that have recently a great deal of attention. An exact statistical- mechanical treatment of homogeneous chain molecules is difficult owing to the large number of internal degree of freedom

The equation of state for the hard –sphere homogeneous chain fluids have been obtained by Hall and co-workers. One approach is to introduce the possibility of molecular association into commonly used integral equation theories. Thus Cumming and Steel have solved the Percus-Yevick (PY) approximation for the chemical association by using a spherical symmetric bonding potential. The highly directional hydrogen bonding is introduced in fluids by the geometry of the interaction at an early stage of the theory. Wertheim's theory, however, is based on a resumed cluster expansion, which is made in terms of two densities, the total number of density ρ , and the monomer density ρ_0 . Wertheim was able to simplify the complex graphical expansions by assuming that the repulsive core of each molecule restricts the orientation ally dependent attractive site..

Key words: spherical symmetry, cluster expansion, associating monomer [1]

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