2004 Vol. 41 No. 3 pp. 400-404 DOI:

Three Semi-empirical Analytic Expressions for the Radial Distribution Function of Hard Spheres

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Abstract: Three simple analytic expressions satisfying the limitation condition at low densities for the radial distribution function of hard spheres are developed in terms of a polynomial expansion of nonlinear base functions and the Carnahan--Starling equation of state. The simplicity and precision for these expressions are superior to the well-known Percus--Yevick expression. The coefficients contained in these expressions have been determined by fitting the Monte Carlo data for the first coordination shell, and by fitting both the Monte Carlo data and the numerical results of Percus-Yevick expression for the second coordination shell. One of the expressions has been applied to develop an analytic equation of state for the square-well fluid, and the numerical results are in good agreement with the computer simulation data.

PACS: 05.70.Ce, Key words: radial distribution function, hard spheres, equation of state, squarewell fluids

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