Thermodynamic properties of van Hove fluids with a downward concavity attractive parabolic-well

Mariano López de Haro[a], Álvaro Rodríguez-Rivas[b]

[a]*Instituto de Energías Renovables, Universidad Nacional Autónoma de México (U.N.A.M.), Temixco, Morelos 62580, Mexico*
[b]*Department of Physical, Chemical and Natural Systems, Universidad Pablo de Olavide, Sevilla, E-41013, Spain*

E-mail: arodriguezrivas@upo.es

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Van Hove fluids[1] with a relatively short ranged attractive parabolic-well of downward concavity are examined for their thermodynamic properties, including their second virial coefficient, Boyle temperature, and equation of state. The second virial coefficient for this fluid is analytically determined and utilized to calculate the fluid's Boyle temperature based on the potential's range. Additionally, leveraging the second-order thermodynamic perturbation theory by Barker and Henderson[2] and the macroscopic compressibility approximation, an equation of state is deduced, with the hard-sphere fluid serving as the reference. For the latter, the fully analytical expression of the radial distribution function, aligned with the Carnahan-Starling equation of state and derived via the rational function approximation method up to a range twice the hard-core diameter, is employed. The results of the theory for the reduced pressure as a function of packing fraction with two ranges of potential wells and for different isotherms agree with the data from NPT Monte Carlo simulations. Predictions for the critical temperature values using the Vliegenthart and Lekkerkerker criterion[3] are also provided. Our study introduces a new potential that can be linked to real systems. In essence, by understanding model fluids such as van Hove's, we aim to improve the general understanding of real fluid dynamics and catalyse new research in this field.

Referencias

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