A hard sphere fluid in a random porous media: new approximations in the scaled particle theory

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The scaled particle theory (SPT) [1] is applied for a description of the thermodynamic properties of a hard sphere (HS) fluid confined in random porous media. Recently, the SPT2 approach was developed by us and the corresponding equations of state of a HS fluid in two types of porous matrices were derived [2]. From the obtained analytical expressions the chemical potential of a fluid was calculated and compared with the simulation data. It is observed that the results of SPT2 are in a good agreement with the simulations in low and intermediate regions of the fluid density. In the same time, at high fluid densities a remarkable error of the theory is noticed, especially when the fluid and matrix particle sizes are equal.

We present several new approximations (SPT2b1, SPT2b2, SPT2b3), which are successfully applied within the SPT2 approach and they lead to the essential improvement of the results for thermodynamic properties of a confined fluid. Previously, it was already shown for the case of one-dimensional systems that these new approximations give a very good description of the chemical potential of a hard rod fluid in a random matrix up to the highest fluid densities [3]. Also in the case of small sizes of matrix particles we get satisfied results. Now we consider three dimensional systems, i.e. a hard sphere fluid in hard sphere and overlapping hard sphere matrices. The obtained results show a very good agreement with computer simulations as well, therefore it proves the applicability of them to the considered systems up to the highest densities of a HS fluid and in the wide range of matrix parameters.

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[2] T. Patsahan, M. Holovko, W. Dong. J. Chem. Phys. 134, 074503 (2011).
[3] M. Holovko, T. Patsahan, W. Dong. Condens. Matter Phys. (2012).