Fluids in random porous media:scaled particle theory

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The scaled particle theory (SPT) is applied to describe thermodynamic properties of hard sphere fluid in random porous media. To this purpose we extended the SPT2 approach which has been developed previously [**?**]. The analytical expression for the chemical potential of a hard sphere fluid in hard spheres and overlapping hard spheres matrices, sponge matrix and hard convex body matrix are obtained and analyzed. A series of new approximations for SPT2 are proposed. The grand canonical Monte-Carlo simulations are performed to verify an accuracy of the SPT2 approach in combination with the new approximations. The possibility of mapping of the thermodynamic properties of hard sphere fluid in random porous media of different types is discussed. It is shown that thermodynamic properties of fluid in the different matrices tend to be equivalent if probe particle porosities and specific surface pore areas of considered matrices are identical. Using the obtained results for a hard sphere fluid in random porous media as a reference systems the possibility of an extension of van der Waals equation of state for a simple fluid in random porous media is discussed. From obtained equation it is shown that with decreasing of porosity of matrix the liquid-vapour coexistence curves stay more narrow and shift to the region of lower fluid densities and temperatures.

References

[1] Patsahan T., Holovko M.,Dong W., J. Chem. Phys, 2011 **134**, 074503.