One hundred years for Enskog theory: application to fluids in porous media

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The theory proposed by D. Enskog [1] one hundred years ago was the first extension of the Boltzmann transport equation to higher densities. In this report, we present the extension of the Enskog theory for the description of the self-diffusion coefficients of hard sphere fluid and hard sphere mixture in disordered porous media. The theory includes the contact values of fluid-fluid and fluid-matrix pair distribution functions which are used as the input in the theory. In contrast to the bulk case they are modified to include the dependence from the so-called probe particle porosity in order to describe correctly the effects of trapping the fluid particles by a matrix [2]. Such semi-empirical improvement of the Enskog theory corresponds to SPT2b1 approximation for the description of thermodynamic properties and it predicts correct trends for the influence of porous media on the diffusion coefficient of a hard sphere fluid in disordered porous media. For hard-sphere mixture the generalisation is done on the bases of the revised version of Enskog theory developed in bulk case during the last decades. Good agreement with computer simulations is illustrated.
Finally, we present the extension of the Enskog theory for patchy colloidal fluids in disordered porous media. We present two different approaches. On the one of them [4] we modify the contact values of fluid-fluid and fluid matrix pair distribution functions due to clustering. In result the pair distribution functions include three terms. Namely, a hard sphere contribution, the depletion contribution connected to the cluster-cluster and cluster-matrix repulsion and the intermolecular correlation inside the cluster. It is shown that the last term leads to a remarkable decrease of the self-diffusion coefficient at a low fluid density. With a decreasing matrix porosity this effect becomes weaker. For intermediate fluid densities the depletion contribution leads to an increase of the self-diffusion coefficient in comparison with the hard sphere fluid. For a sufficiently dense fluid, the self-diffusion coefficient strongly decreases due to a hard-sphere effects. In other description we consider clusters, as additional particles and the description of patchy colloidal particles in disordered porous media reduces to the hard-sphere mixture in disordered porous media [5]..

REFERENCES

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