

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Complex Pole Approach in Thermodynamic Description of Fluid Mixtures with Small Number of Molecules TIMUR ASLYAMOV, Moscow Inst of Phys & Tech, OLEG DINARIEV, Schlumberger Moscow Research Center — Physically consistent description of equilibrium small molecular systems requires the extension of thermodynamics. The reason is the absence of thermodynamic limit, which is mandatory for the applicability of classical thermodynamics. New theoretical method of complex pole decomposition for the statistical description of small multicomponent molecular systems is implemented. Similar approach has been previously developed and applied in nuclear physics for finite systems of nucleons. We have significantly transformed and extended the original formulation to make it work for multicomponent molecular mixtures in small systems. The aim of this research is to provide new comprehensive description of small equilibrium molecular systems with numerous scientific and industrial applications for artificial and natural materials with nanopores. Several cases for molecular systems in small cavities are studied. In particular size-dependent additional pressure for small systems is evaluated analytically and numerically. The obtained results are in correspondence to published experimental data and molecular dynamics simulations.

Timur Aslyamov
Moscow Inst of Phys & Tech

Date submitted: 10 Nov 2014

Electronic form version 1.4