Thermodynamic Properties and Equation of State of Aqueous System with Multi-Walled Carbon Nanotubes

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We present the results of the experimental investigation of the thermodynamic properties and equation of state of a multi-walled carbon nanotube (MWCNT) water system. PVT measurements were carried out using the metallic bellows method with differential inductive sensor of linear shifts in the temperature range from 293 to 375 K and pressure range from 0.1 to 101 MPa. We have found the numerical values of the isothermal modulus of elasticity, isobaric expansion, isothermal deviation of entropy factor, enthalpy, internal energy and isobaric-isothermal Gibbs potential. The molecular structure of pure water and the investigated MWCNT-water system was calculated using molecular dynamics simulation in the NVT ensemble. The thermodynamic properties and molecular structure of the investigated liquid system were analyzed as a function of pressure and temperature. Finally, the equation of state for the investigated MWCNT-water system was obtained. Its parameters were analyzed in detail as a function of temperature.