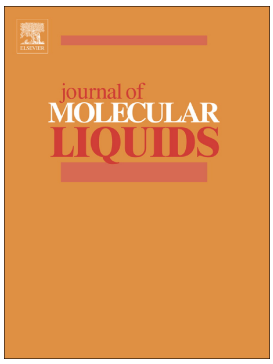

The dependence of the size of confined water fluid molecules on the radius of carbon nanotube

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The dependence of the size of confined water fluid molecules on the radius of carbon nanotube

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Abstract

A recently-derived perturbation-theory-based equation of state (EoS) has been used for describing the *p*-*v*-*T* behavior of water confined inside a carbon nanotube (CNT). The one-center united atom model (OCUA) was employed for modeling of water molecules inside the CNT with temperature-dependent effective diameter, σ_{eff}. The interaction between two nearest-neighbor molecules was taken into account as an effective pair potential (EPP) which is an average effective extended Lennard-Jones (12, 6, 3) (AEELJ) pair interactions in the framework of thermodynamic perturbation theory (TPT). A new concept as effective molecular diameter tensor (EMDT) was introduced to consider the anisotropic character of compression factor in the EoS. The values of $\sigma_{eff,zz,}$ and $\sigma_{eff,xy}$ of the EMDT for the axial and radial directions, respectively, in both filled and unfilled states of the CNT, were estimated by using the simulated *p*-*v*-*T* data in the EoS. The results mirror the fact that the $\sigma_{eff,zz,}$ and $\sigma_{eff,xy}$ values of water molecule increase with the radius of CNT (*R*). Moreover, the values of $\sigma_{eff,zz}$ for the different radii of CNT are nearly close to those of