Prediction of transport properties of aqueous sugar solutions by the molecular dynamics method

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Due to the prevalence of mono- and polysaccharides, they have a wide range of applications. They are used in osmotic dehydration processes, as well as in the desalination of seawater and its purification from heavy metal impurities. These make it important to study the properties of aqueous solutions of mono- and polysaccharides. One of the possible methods for studying aqueous sugar solutions is the molecular dynamics method. To obtain accurate and reliable results, the used force fields must correctly reproduce the interactions of molecules with each other. In this paper, the model of an aqueous sucrose solution is studied at temperatures from 273 to 343 K with a sugar concentration of up to 50%. The concentration and temperature dependencies of density, viscosity, and diffusion were calculated. The viscosity coefficient was calculated by the Green-Kubo method, and the diffusion coefficient was obtained using the Einstein–Smoluchowski relation. Temperature dependencies of transport coefficients were approximated by the Arrhenius equation. Activation energies were calculated for each of the studied sugar concentrations. In addition, using the Stokes-Einstein equation, the hydrodynamic radius of the sucrose molecule was calculated. The obtained data were compared with the experimental results.