

Transport processes in aqueous sucrose solutions

Deshchenia V I^{1,2,@}, **Kondratyuk N D**^{3,2}, **Lankin A V**^{1,2}
and **Norman G E**^{1,2,3}

¹ Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia

² Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

³ National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia

@ deshchenia.vi@phystech.edu

Mono- and polysaccharides are widespread in nature, but at the same time they are of great industrial importance. Of particular interest are membranes based on cellulose esters, which are used in the desalination of seawater or its purification from high-molecular impurities and heavy metal impurities. Cellulose ester-based membranes may also be promising considered as separation membranes in electrochemical current sources such as Red/Ox elements. This results in the importance of studying the properties of aqueous solutions of mono- and polysaccharides, as well as the interaction of insoluble polysaccharides with water. Some of the defining characteristics are the transport properties: diffusion and viscosity. To study transport processes in solution, we can use the method of molecular dynamics. The accuracy and reliability of its results is determined by how well the used force fields reproduce the interactions of the studied molecules with each other and with water molecules. In this paper, the model of an aqueous sucrose solution is studied and investigated for the dependence of the viscosity and diffusion coefficients on temperature. The viscosity coefficient is determined by the Green-Kubo method, and the diffusion coefficient is derived using Einstein–Smoluchowski relation. In addition, the equilibrium density of the system in wide temperature range is calculated.