Transport processes in aqueous sucrose solutions

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Abstract

This work presents the analysis of the transport processes in aqueous polysaccharide solutions based on investigation of sucrose solutions. Its transport properties, such as viscosity and diffusion coefficients, are calculated using molecular dynamics method.

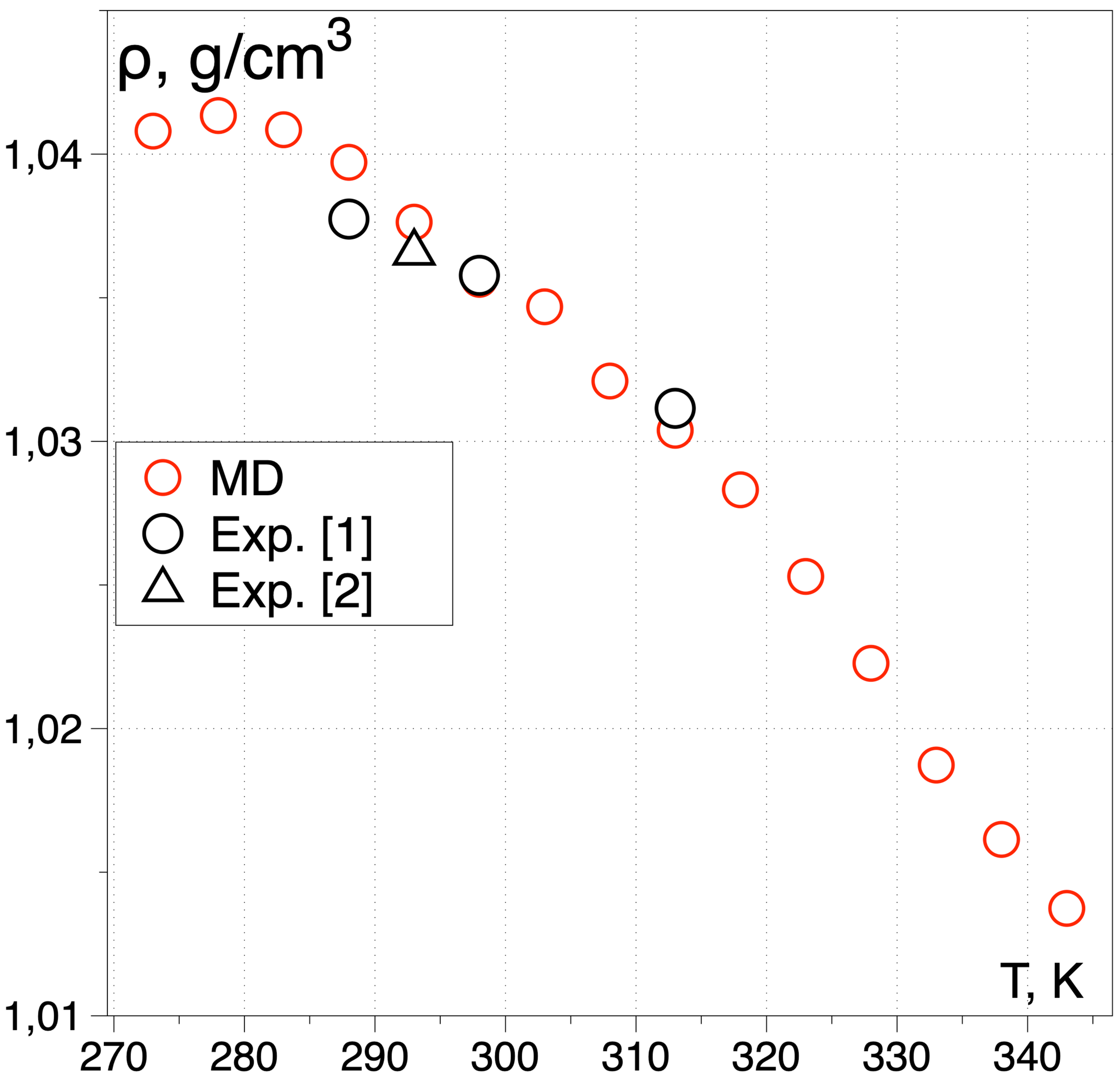
Motivation

Mono- and polysaccharides are widespread in nature: they are of high importance for the functioning of all living cells, performing a variety of biological functions.

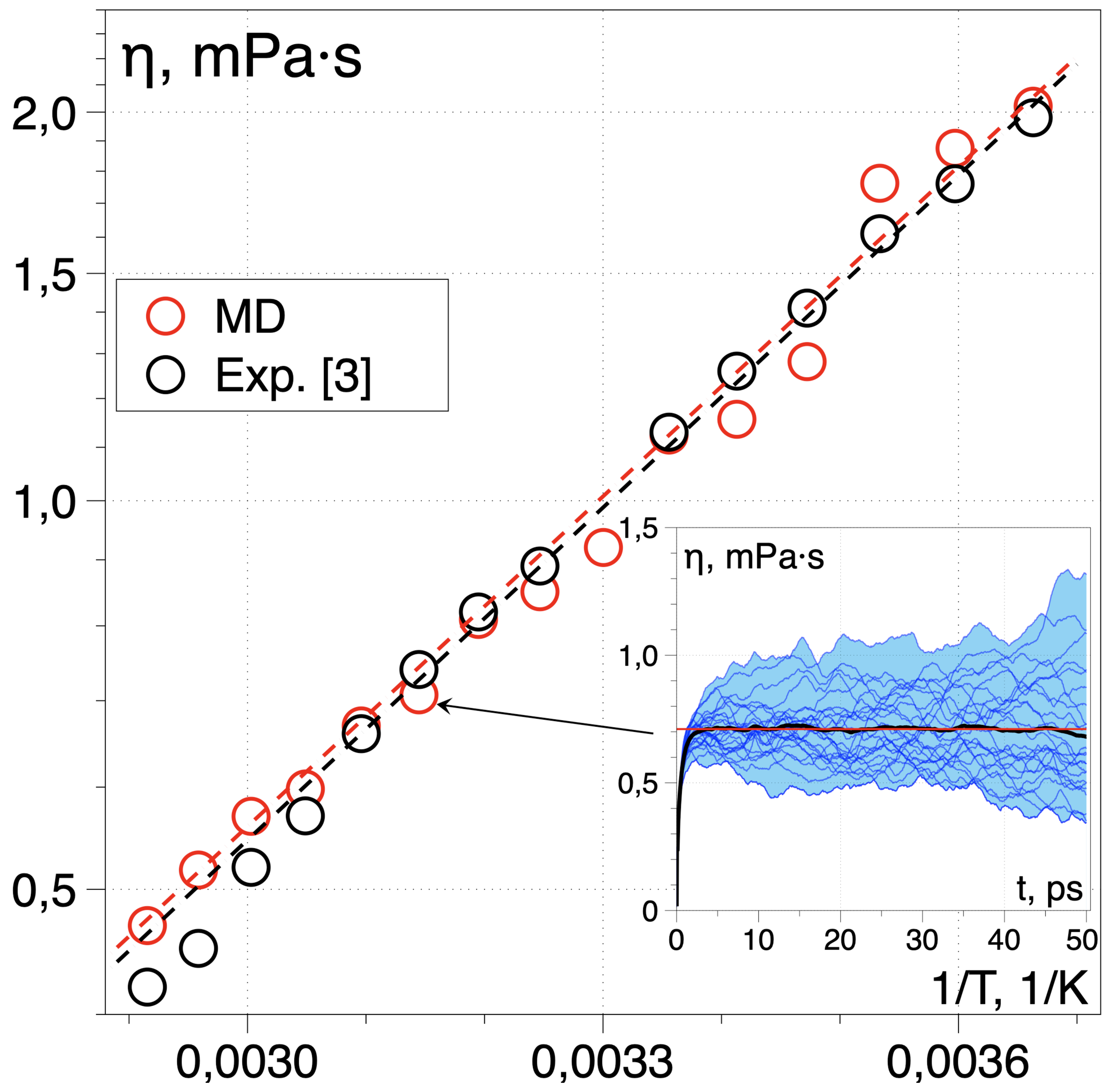
In addition, materials based on polysaccharides, primarily cellulose, are widely used in technology. Membranes based on cellulose ethers, most frequently cellulose acetate, are used in seawater desalination by reverse osmosis, water purification from high-molecular impurities and impurities of heavy metals. Cellulose ester-based membranes can also be of interest as separating membranes in electrochemical power supplies such as Red / Ox cells.

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. For such studies the molecular dynamics method can be used. The accuracy and reliability of molecular modeling is determined by how well the used force fields reproduce the interactions of the studied molecules with each other and with water molecules.

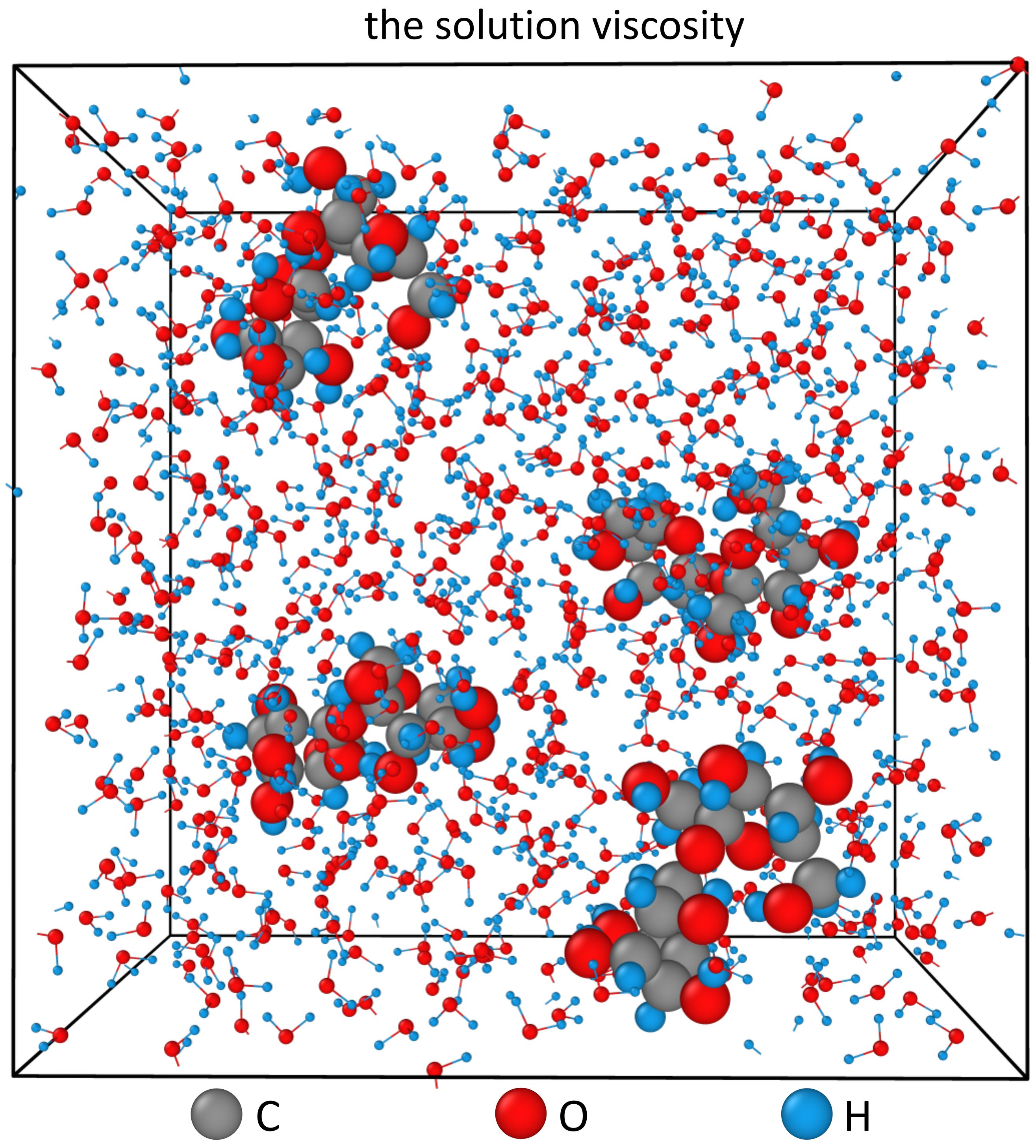
In addition, studying the properties of sucrose and glucose solutions may be of separate interest, since these characteristics are important for estimating the ability of living cells to survive at low temperatures.



Temperature dependence of the equilibrium density of solution



Temperature dependence of the solution viscosity



Snapshot of the simulation cell containing 10% mass fraction of sucrose

Viscosity

$$\eta = \eta_0 exp(E_a/(RT))$$

Arrhenius equation

	η_0, 10^{-3} mPa s	E_a ,kJ/mole
MD	1.56 ± 0.03	16.31 ± 0.04
Experiment	1.45 ± 0.02	16.43 ± 0.03

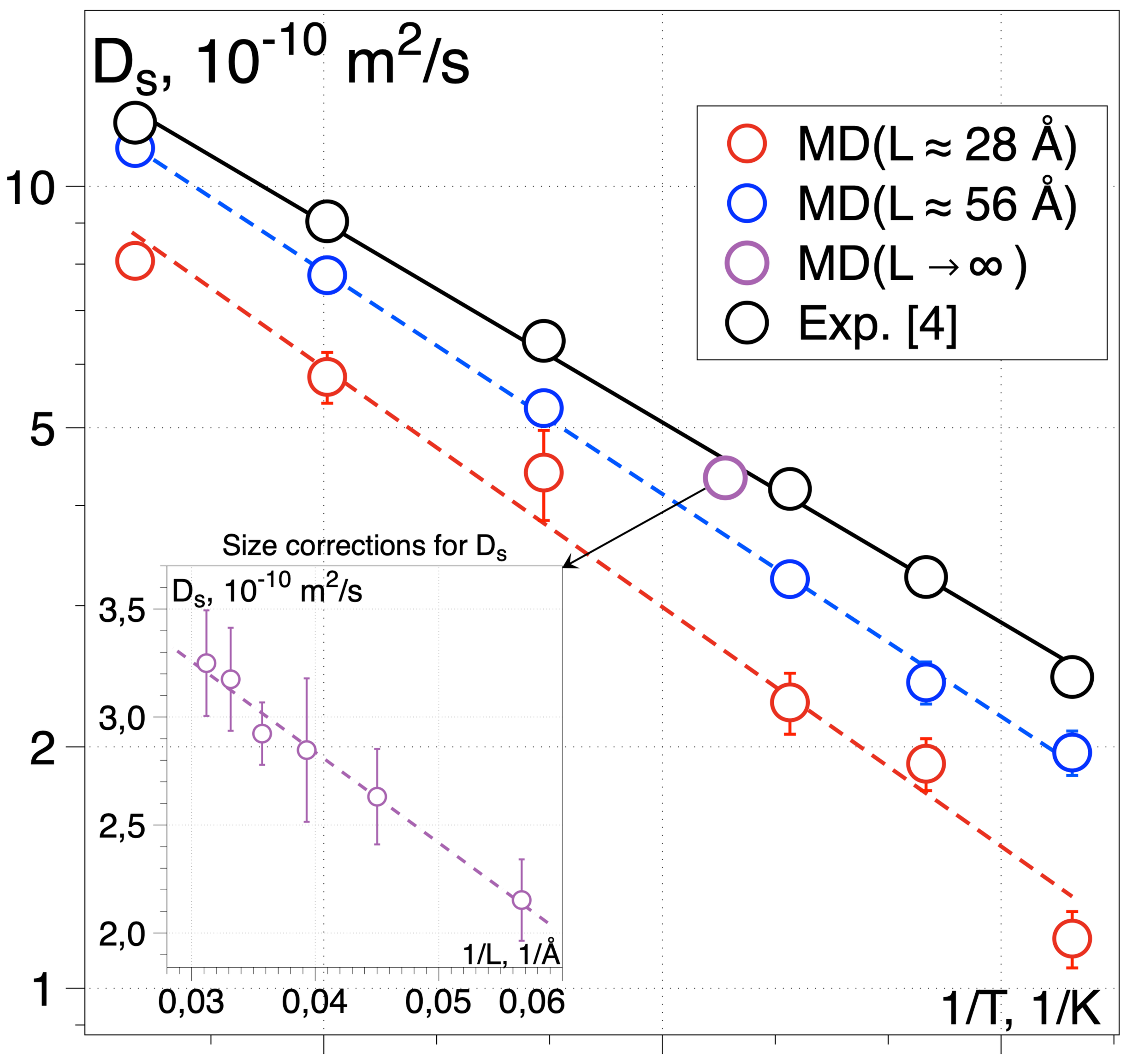
Diffusion

$$D = D_0 exp(-E_a/(RT))$$

Arrhenius equation

	D_0, 10^{-7} m²/s	E_a ,kJ/mole
MD($L \approx 28$Å)	5.7 ± 1.0	19.0 ± 0.5
MD($L \approx 56$Å)	4.24 ± 0.15	17.4 ± 0.1
Experiment	2.81 ± 0.17	15.9 ± 0.2

Note that both activation energies are close



Temperature dependence of the self-diffusion coefficient of sucrose molecules in solution for different simulation cell sizes

Conclusions

- Molecular dynamic model of an aqueous sucrose solution has been considered
- Equilibrium density of the solution has been measured at different temperatures
- Self-diffusion coefficient of sucrose molecules and viscosity coefficient of the solution have been calculated
- Temperature dependences of the transport coefficients has been found
- Self-diffusion and viscosity activation energies have been calculated
- Both activation energies are rather similar
- Good agreement is obtained with experimental data for all types of properties

Acknowledgments

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