Summary of the dissertation

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Theoretical methods for predicting ultrasound velocity under conditions of increased pressure and temperature in selected ionic liquids

The aim of presented dissertation was to demonstrate that four computational methods, based on different theoretical foundations, can be effectively used to predict parameters important from the point of view of the thermodynamics of the condensed phase, such as the speed of sound and density, in a wide range of temperature and pressure variations for selected ionic liquids. The computational approaches analyzed in this work, including the spinodal method, the CP-PC-SAFT equation of state and neural networks, along with classical machine learning methods, made it possible to obtain accurate predictions of the above quantities, taking into account both the potential limitations and benefits associated with each method used. Various aspects such as numerical stability, computational complexity and the ability to account for nonlinear effects were taken into account in the research.

The dissertation is divided into four main parts: introduction, literature part, computational part and summary part. The literature part analyzes the current state of knowledge about ionic liquids, their industrial applications and physicochemical aspects. It also discusses the importance of physicochemical studies with special emphasis on the speed of sound propagation in ionic liquids, including a discussion on the influence of the structure of the liquid on the speed of sound.

The computational section presents four approaches, different in theoretical basis, to predict speed of sound and density over a wide range of pressure and temperature variation, using the spinodal method, the CP-PC-SAFT equation of state, neural networks and a number of classical machine learning methods. Each of these methods is described in detail, along with identification of its advantages and limitations. The results of speed of sound and density prediction for the tested ionic liquids are presented, along with an analysis of the obtained results.

In addition, in the section on computational methods, thermodynamic derivatives were determined and analyzed, with particular emphasis on the coefficient of isobaric thermal expansion. It was shown that when determining speed of sound and density using a neural network and classical machine learning methods, very high prediction accuracy can be achieved. However, the results of thermodynamic derivatives obtained from these methods are subject to significant errors resulting from the assumptions used in machine learning and neural networks methods.

Moreover, the work shows that further thermodynamic research using neural networks and machine learning should be continued and predictive models continuously improved. It was proposed that research using NN/ML should place special emphasis on determining and predicting thermodynamic conditions in conjunction with the fluid structure and other fluid properties such as viscosity, where the fluid under consideration will exhibit undesirable phenomena that negatively affect the speed of sound, such as wave absorption, ultrasonic relaxation and dispersion of speed of sound.