

When mixing two liquids, depending on their properties, we can obtain homogenous solutions or mixtures which separates into two clearly visible non-miscible liquid phases. If two liquids mix with each other at given composition, which depends also on external conditions such a temperature and pressure. The determination of the mixing conditions, thus so-called phase diagram, are particularly important from the point of view of practical application of the liquids. It is necessary in many branches of industry such as cosmetic, pharmaceutical, food product, automotive, dyes and printer ink industries should we think about the stability of the obtained products. In the case of cosmetic, drugs or food the product cannot exhibit phase separation when environmental conditions are changed. Also during the production and purification of different substances the mixed solvents are used and the conditions for their mixing or separation are crucial. Limited miscibility of liquid solutes which can be used to separate other compounds in the process of two-phase extraction.

Ionic liquids are relatively new group of solvents. They are a group of salts which melt below 100°C. They consist ions, contrary to molecular liquids like water, which are electrically neutral molecules. Their possible application seems to be very promising, especially that they can be synthesized to exhibit expected properties. Systems containing ionic liquids are considered as environmental friendly and belong to so-called “*green chemistry*”. From this point of view is seems desirable to use them instead the traditional solvents. However, there is a lack of experimental data of the mixing conditions of those liquids, and available data frequently differs between themselves. Especially the data about the influence of the pressure on the mixing of ionic liquids are missing. Due the unlimited possibilities of the synthesis of the new compounds it seems reasonable to create the data base for the most possible large amount of the compounds, find the correlations between them and with the use of the appropriate mathematical model to predict the properties of the mixtures and the condition for mixing.

In the literature there is practically no data concerning the influence of pressure on the mixing conditions of ionic liquids. From the only few available articles, which deal with this topic, it seems that this influence is much bigger than in the case of mixtures of “classic” solvents. This is the topic, in which there is still much to discover.

The aim of this project is to determine the phase diagram for chosen mixtures of ionic liquids using two combined experimental methods and the use of the mathematical models to describe and predict properties of the mixtures of ionic liquids including technique of machine learning and artificial neural networks – the elements of the artificial intelligence. One of the techniques utilize the change in the heat flow in calorimeter during change of the temperature related to the phase separation. The second is traditional method which uses the change in the intensity of the light passing the sample caused by appearance of the turbidity of the sample. Our project assumes modification of the apparatus which allows for simultaneous determination of the phase separation temperature.

We are planning to investigate the influence of the pressure on the mixing of ionic liquids, using technique which eliminates the use of inert gases to generate pressure, which is commonly used in commercial apparatuses, and causes dissolution of the gases in liquids, which can change conditions of mixing.

Application of the mathematical models, based on the experimental data and thermodynamical relations allows for estimation of properties of liquids and phase equilibria. On the basis of obtained experimental data and those already available we assume calculation of the parameters, which allow for prediction of the mixing conditions for ionic liquids without necessity of the experimental measurements.

Machine learning technique will allow also for determination of the properties of ionic liquids, particularly the phase equilibria, on the basis of finding the regularity and correlations in already available data sets. As the result with this technique it will be possible to construct the phase diagram of the chosen liquids on the basis of the provided parameters of the pure liquids.

In summary, the subject of the proposed project is the unique synergy of 1) thermodynamic modelling of liquid-liquid equilibria based on the equation of state combined with 2) determination of LLE diagrams using machine learning and artificial neural network methods and 3) experimental determination of LLE diagrams for a selected group of ionic liquids at atmospheric and elevated pressure (up to 7000 bar) based on a proprietary measuring device. The combination of these three approaches will not only enable the discovery of an undiscovered area - pressure diagrams of ionic liquid systems, but the modifications made to the optimisation of the equations of state and the proposed machine learning solutions will shed new light on the thermodynamic modelling of liquid-liquid equilibria.