Popular science summary

One of the basic goals of science is to get to know the reality. The complementation of the description of the observed phenomena and their mechanics are physicochemical constants, which allow for unambiguous characterization of the studied system. A well-known process occurring naturally in nature is diffusion, the rate of which determines the diffusion coefficient. This phenomenon consists in the spontaneous movement of matter or energy under the influence of the driving force, which is the difference in concentration or temperature, respectively. A special case of the environment in which diffusion plays an important role is the air / water system with the addition of amphiphilic substances. These compounds, due to their specific structure, have the property of dissolving in both polar (eg water) and non-polar liquids (eg fats). This behaviour can be described colloquially with the known law of solubility, meaning "similar in a similar". Another feature of amphiphilic substances is the adsorption, i.e. the formation of a monolayer of oriented molecules at the interface, which is described by the size called surface excess. The result of this process is the reduction of the surface tension of the system, which is defined as the minimum necessary amount of work to enlarge the field between two phases by a unit of area. Adsorption of non-ionic amphiphilic compounds at the gas / liquid interface describes two mechanisms - diffusion of compound molecules from the bulk volume to the interface and adsorption of molecules on it. The diffusion-controlled model assumes that the phenomenon of particle accumulation occurs very quickly in relation to the transport process to the interphase layer. It means that the last of these processes limits the whole phenomenon. The diffusion model allowing to determine the change of superficial excess in time is presented in the Ward-Tordai total equation.

The aim of the project is to examine the change in the surface tension of the air / water system with the addition of selected amphiphiles. In addition, the effect of the concentration value of a given compound on surface tension will be determined. From the data received, surface excess values will be determined, which is an immeasurable parameter in the considered system. Then, by determining physicochemical constants to the experimental data, selected adsorption isotherms will be fitted, i.e. curves showing the amount of adsorbed substance on the surface under constant temperature conditions. Critical micellar concentration will be determined, the exceeding of which results in the lack of influence of the increase in the concentration of the compound on the decrease of surface tension of the system. The next step is the computerized solution of the Warda-Tordai integral equation combined with the adsorption isotherms, in order to determine the behavior of the solution depending on the chosen isotherm. In addition, a study will be carried out on the impact of changes in the coefficients occurring in the Ward-Tordai equation to solve it. The last element is defining and then numerically solving the inverse problem comparing the experimental data of the surface excess with the values obtained from the simulation, in order to determine the diffusion coefficient of selected amphiphilic compounds in the air / water system. The set task is a problem in the field of optimization, that is searching for the best solution.

The last of the presented points introduces a special innovation in basic research. In the literature, there is a lack of a clearly determined diffusion coefficient for many compounds with amphiphilic structure. There is a wide range of experimental and approximate methods for determining the diffusion coefficient, however, the values presented by scientists vary widely, due to the simplifications made. The solution of the inverse problem allows to determine this physicochemical constant with the assumed accuracy in a way that does not cause any doubts. An important issue is the introduction of an adsorption isotherm with an appropriate degree of complexity so that the simulation results reflect the experimental data as much as possible. An additional benefit is obtaining solids occurring in the adsorption isotherms equations, which also have their own physical interpretation, and their value is characterized by the given system. Computer analysis of the collected experimental measurements will allow to supplement the literature description of adsorption phenomenon controlled by diffusion at the air / water interface, contribute to the development of an interdisciplinary research area and give a chance to create a unified method of searching for diffusion coefficient.