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Abstract of the dissertation thesis entitled: „Modelling the fate of selected ionic liquids in the aquatic environment”

Due to the rising amount of new applications of Ionic Liquids (ILs) proposed over the last years, the importance of these compounds in science and industry has increased significantly. However, despite the huge application potential, compounds from this group may be dangerous to the environment as well as human health and life. Studies have shown that some ionic liquids are characterized by, for example, high toxicity, ecotoxicity, environmental sustainability or bioaccumulative potential. Therefore, in order to ensure the maximal safety of ecosystems and human health, there is a need for a comprehensive risk assessment for ionic liquids being introduced to the market. My Ph.D. thesis focuses on the exposure assessment for ionic liquids – one of the aspects of risk assessment.

One way to assess exposure for chemical compounds is to use computer-based deterministic models, called Multimedia Mass-balance models (MM). This name is closely related to the construction of models which, in their theoretical space, contain selected elements of the environment, called components (such as water, soil, organic matter, air, etc.). The operation of the MM models is based on an equation (or equation system) called the mass balance equation. Once solved, it allows to calculate the concentration of test chemical in individual components, with respect to the assumed thermodynamic state. By using this type of tools, one can assess the extent to which living organisms will be exposed to a substance after its possible deposition into the environment. At the moment, however, there are no existing MM models developed for ionic liquids. Moreover, the use of existing models developed for other groups of compounds (and thus possibly not taking the ionic nature of IL into account) is associated with the risk of inaccurate results. Another important problem is the low availability of experimental data describing the physicochemical properties of ionic liquids, important from the point of view of the environmental fate of these compounds, which are inputs to these deterministic models. These include properties such as partition coefficients, water solubility, or persistence in individual components of the environment.

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The hypothesis placed in my study assumes that current knowledge on ionic liquids, supported by chemoinformatic methods, already allows the development of a deterministic model describing the environmental fate of IL. That's why my research project focuses on solving problem of the low availability of experimental data for ILs as well as on the lack of a MM model for testing ionic liquids. My research is focused on developing a computational tool: the MM model for ionic liquids, coupled with a series of probabilistic models (describing the physicochemical properties of ionic liquids), to generate the input data required for MM model operation.

In order to develop the MM model, basing on the analysis of available scientific literature, I selected environmental components prone to the exposition on ionic liquids. These include water, bottom sediments and aquatic organisms. Then, I determined the ILs properties relevant for the fate of these compounds in the abovementioned components. These are: n-octanol-water partition coefficient, sediment-water partition coefficient, solubility in water, critical micellisation concentration and biodegradability.

To solve the problem of low availability of experimental data I have developed five Quantitative Structure-Activity Relationship (QSPR) models. All models have been properly validated in the terms of internal and external validation process. Such approach allowed to deliver data describing physicochemical properties of ionic liquids by chemoinformatic methods, without the need for experimental measurements. In addition, I have developed a MM model that evaluates the fate of ionic liquids in aqueous environments. It allows to estimate concentrations of ILs in particular environmental components (water, sediment, and organic matter), assuming equilibrium in the closed system (for the evaluative environment). I have also performed a sensitivity analysis of the developed model, which showed that biodegradability is the physicochemical property, that has the greatest impact on the fate of ionic liquids in the environment.

By using the QSPR-MM coupled method in my tool, it is possible to investigate the environmental fate of ionic liquids solely on the basis of their chemical structure. Such approach provides great application potential for the proposed tool. It is the world's first computer model to estimate the environmental fate of ionic liquids. The case study presented in the paper shows examples of application of the developed tool. Model allows for classification of ionic liquids in terms of their potential threat they pose to the environment (on qualitative level).

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The results obtained in my dissertation are the first important step in the development of computational methods for evaluating the exposure to ionic liquids. They also summarize the needs of exposure assessment in current ionic liquid chemistry, setting the pathway to maximize the environmental safety of these compounds.

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