

OP 04
Prediction of solubility of organic compound for high-temperature water by machine learning
Authors and affiliation
Mitsumasa Osada ^{*,1} , and Kotaro Tamura ¹
¹ Department of Chemistry and Materials, Faculty of Textile Science and Technology, Shinshu University, 3-15-1, Tokida, Ueda, Nagano 386-8567, Japan
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Abstract (less than 300 words)
<p>In recent years, high-temperature water has attracted attention for processes such as organic reactions and extractions due to its low environmental load and low waste. The experimental data of the solubility of organic compound for high-temperature water is important for designing the processes. However, the data on the solubility of organic compound for high-temperature water is limited due to the difficulty of the experiments. On the other hand, the data on the solubility of organic compound in water under ambient temperature and pressure is abundant. In this study, we developed a prediction model of the solubility by machine learning by combining the experimental data at ambient temperature with those at high temperature.</p> <p>At first, the chemical structure of the organic compound was converted into descriptors using Python RD-kit, which is an open source of chemical informatics and machine learning. Regression of the organic compound solubility was performed using the descriptors, temperature, and water density. As a result, it was found that the model obtained by the regression can predict the solubility of organic compound in high-temperature water.</p>
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