PB 10

Screening of phase-separation CO_2 absorbent using machine learning combined with molecular information

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Abstract (less than 300 words)

Carbon dioxide capture technologies have been focused to overcome global warming. A chemical absorption process using an aqueous amine solvent is one of the most established technologies of CO_2 capture because of the high absorption rate and high reactivity with CO_2. However, this process operation needs a large amount of energy, causing high regeneration costs. Recently, to reduce energy consumption, phase-separation absorbents have been reported. The phase-separation absorbents are mainly composed of mixed solvents of alkanolamine and organic solvents like glycol ether or alcohol. When the absorbent reacts with CO_2, a single liquid phase of the phase-separation absorbent transforms into two liquid phases, CO_2-rich and -lean phases. This absorbent can reduce the temperature difference between the absorption and desorption operations from 80 ˚C of the conventional chemical absorption process to 40 ˚C [1]. However, it is difficult to know phase behaviors of mixed-solvent absorbents, resulting in the necessity of screening experiments to find phase-separation absorbents [2, 3].

In this work, we developed a screening method of the phase behaviors of the mixed-solvent absorbents using supervised machine learning models: random forest, logistic regression, and support vector machine. There are 61 mixed-solvent absorbents containing alkanolamine/glycol ether or alcohol in a dataset. The dataset was split into a training set and test set, which contains 31 and 30 data of the absorbents, respectively. Extended-connectivity fingerprint [4] or molecular surface charge distributions calculated from a COSMO calculation [5] are used as molecular descriptors in the machine learning models. The machine learning models successfully predicted phase states of the mixed-solvent absorbents before and after CO_2 absorption with accuracies of more than 90 %. Furthermore, we analyzed contributions of explanatory variables to predict the phase states using the learned model.

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