Predicting vapor pressures of components of essential oils using machine learning models

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Essential oils contain a complex mixture of organic compounds with unique scent profiles and therapeutic effects. The increasing market demand for essential oils and their components has led to a growing interest in optimizing batch distillation processes for their fractionation. Since experimental approaches are time-consuming and resource-intensive, researchers are resorting to modeling and simulation methods to improve these separations. To achieve accurate simulations, thermodynamic property data are crucial but challenging to obtain experimentally. Therefore, predictive methods have been proposed to estimate these properties at different temperatures. This study proposes a pathway to develop machine learning models for vapor pressure prediction in essential oil fractionation simulations using data calculated through such predictive methods. The models are trained using the data so calculated and then validated using experimental data. Thirteen machine learning algorithms are employed, and their performance is evaluated using various criteria. The performance of these machine learning models are then compared with that of traditional interpolation techniques. The results demonstrate that machine learning models provide a greater overall accuracy of vapor pressure predictions than interpolation methods. Ensembled machine learning models are found to be effective for some compounds but not superior to using its best performing singular algorithm-based machine learning model counterpart. Though the proposed pathway focuses on vapor pressure prediction for constituents in cinnamon leaf oil, it can also be used to predict properties like enthalpy of vaporization and specific heat capacity relevant to essential oil fractionation, for other types of essential oils as well.

Keywords: Essential oils, vapor pressure prediction, machine learning models, ensembled models, interpolation