Novel and accurate mathematical simulation of various models for accurate prediction of surface tension parameters through ionic liquids

ABSTRACT

Ionic Liquids (ILs) as a novel class of liquid solvent simultaneously carry the positive characteristics of both molten salts and organic liquids. Remarkable positive properties of ILs have such as low vapor pressure and excellent permittivity have encouraged the motivation of researchers to use them in various applications over the last decade. Surface tension is an important physicochemical property of ILs, which its experimental-based measurement has been done by various researchers. Despite great precision, some major shortcomings such as high cost and health related problems caused the researchers to develop mathematical models based on artificial intelligence (AI) approach to predict surface tension theoretically. In this research, the surface tension of two novel ILs (bis [(trifluoromethyl) sulfonyl] imide and 1,3-nonylimidazolium bis [(trifluoromethyl) sulfonyl] imide) were predicted using three predictive models. The available dataset contains 45 input features, which is relatively high in dimension. We decided to use AdaBoost with different base models, including Gaussian Process Regression (GPR), support vector regression (SVR), and decision tree (DT). Also, for feature selection and hyper-parameter tuning, a genetic algorithm (GA) search is used. The final R2 -score for boosted DT, boosted GPR, and boosted SVR is 0.849, 0.981, and 0.944, respectively. Also, with the MAPE metric, boosted GPR has an error rate of 1.73E-02, boosted SVR has an error rate of 2.35E-02, and it is 3.36E-02 for boosted DT. So, the ADABOOST-GPR model was considered as the primary model for the research.