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Development of Computational Approach for Calculation of Hydrogen Solubility in Hydrocarbons for Treatment of Petroleum

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Abstract : For the hydrogenation process, knowing the solubility of hydrogen (H2) in hydrocarbons is critical to improve the efficiency of the process. We investigated the H2 solubility computation in four heavy crude oil feedstocks using machine learning techniques. Temperature, pressure, and feedstock type were considered as the inputs to the models, while the hydrogen solubility was the sole response. Specifically, we employed three different models: Support Vector Regression (SVR), Gaussian process regression (GPR), and Bayesian ridge regression (BRR). To achieve the best performance, the hyper-parameters of these models are optimized using the whale optimization algorithm (WOA). We evaluated the models using a dataset of solubility measurements in various feedstocks, and we compared their performance based on several metrics. Our results show that the WOA-SVR model tuned with WOA achieves the best performance overall, with an RMSE of 1.38 × 10− 2 and an R-squared of 0.991. These findings suggest that machine learning techniques can provide accurate predictions of hydrogen solubility in different feedstocks, which could be useful in the development of hydrogen-related technologies. Besides, the solubility of hydrogen in the four heavy oil fractions is estimated in different ranges of temperatures and pressures of 150 ◦C–350 ◦C and 1.2 MPa–10.8 MPa, respectively

Keywords : temperature, pressure variations, machine learning, oil treatment
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