Random Forest Model Development for Predicting CO_2 Adsorption on Biochar and Activated Biochar

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Biochar has become a highly versatile carbon-based material, finding use in carbon sequestration, gas separation, soil remediation, and water purification. This widespread adoption of biochar stems from the abundance and availability of the biomass and organic wastes used in its production making biochar, in many cases, more cost-effective and sustainable than fossil-derived carbons. To improve the function of biochar in CO_2 adsorption, for example, the low-porosity carbon is commonly activated which significantly increases biochar surface area and porosity and alters biochar surface functionality to favor interactions with CO_2. However, optimizing thermochemical conversion and activation conditions to produce biochar and activated biochar with the necessary physicochemical characteristics to achieve high CO_2 adsorption is challenging owing to the complex network of relationships between these variables. In this work, a random forest (RF) machine learning model was developed to discover the principal features responsible for maximizing CO_2 adsorption capacity on biochar and activated biochar adsorbents. Feedstock choice, thermochemical conversion/activation conditions, physicochemical characteristics, and adsorption settings were chosen as input variables to train and test the model for CO_2 adsorption capacity prediction. Highly correlated inputs (>0.8 and <-0.8) were removed, datapoints were standardized, and hyperparameter tuning was conducted to develop the RF model. After training, the model was tested and achieved a r^2 of 0.75 and RMSE of 0.72 demonstrating a satisfactory performance in estimating CO_2 adsorption capacity on biochar and activated biochar. Feature importance was then performed to identify the key features impacting CO_2 adsorption capacity prediction.