Prediction of the adsorption capacityof activated carbons using physicochemical parameters, mechanical properties and elemental composition.

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Abstract : Pollutants removal from human's daily activities is one of the most widely known environmental applications of activated carbons. In order to guarantee the successful removal of contaminants and pollutants on activated carbons, the development of new adsorbents has been increasing in the last few years. In this work the effects of different chemical-physical parameters and the elemental composition of precursors for the modeling of specific surface area development in activated carbons synthetized by physical activation is investigated. Three types of data were used in this study, a first data with 24 precursors a second consisting of 24 carbons and a third joining the previous data I and II. The obtained Quantitative Specific Surface Area (QSSA) prediction models give adequate and interpretable results with determination coefficient values in all cases above 80% for the training set. It was also demonstrated that the most of the precursors studied here are feasible alternatives for activated carbons preparation adequate for pollutants removal. The surface area development of the synthetized activated carbons can be successfully described through a multiple linear regression model and a structural interpretation of the factor affecting the Specific Surface Area is showed. This type of models could be useful for the prediction of the adsorption capacity of new materials based on the parameter of the chemical compositions to efficient removal of pollutants in purification process.

Keywords : Activated Carbons, Adsorption and Adsorbents, Physicochemical Parameters, Multiple Linear Regression, QSSAR.

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