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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.

1.Introduction

Adsorption is a widely used purification process as an effective physical method of separation in order to elimination or lowering the concentration of wide range of dissolved pollutants (organics, inorganics) in an effluent. It is big news that activated carbons are a well-known adsorbent that can be used efficiently for removal of a broad spectrum of pollutants from air, soil and liquids.[1, 2, 3]

Activated carbons can be obtained from different precursors, with probed benefits to the environment. Due to its chemical composition, forestall biomasses are valuable sources in the synthesis of adsorbents materials. Various examples of activated carbons preparation can be found in the open literature. They have been used among others in the purification of pollutants gases such as carbon dioxide, sulfur dioxide, hydrogen sulfide, nitrogen oxides, mercury and other harmful heavy metals, etc.[4, 5, 6]

Besides, to develop adsorbent with desired adsorbent properties, it is necessary to know the chemical, morphological and textural features of the starting materials. Furthermore, the determination of the optimal conditions for activated carbons synthesis usually involves several experiments. For practical and less time-consuming during adsorbents preparation, design and control, it is important to minimize the lab tests and optimize the influence of the experimental conditions and the raw materials composition on the adsorptive properties of the final materials.[7, 8]

The adequation of theoretical models to the available experimental information will be helpful in order to rationalize time and experiments.[9, 10, 11] However due to the complexity of the correlation between input and output variables on the adsorbent properties, it is difficult to be studied using traditional mathematical modeling.[12, 13, 14]Multiple linear regression models based on genetic algorithms processing, can be successfully applied in many areas of sciences because of their multiple linearity, simplicity, reliability and robustness in modeling those complex systems.[10, 15]

Therefore, the objectives of the present investigation were: (1) use multiple linear regression models to predict the adsorptive characteristics of activated carbons; (2) select the initial precursor composition as the independent variable, whereas the specific surface area of the synthetized materials will be considered as the output variable for the developed networks; (3) incorporate the resulting structure-property relationship into the model to predict the adsorptive characteristics of the activated carbons studied.

2 Material and Methods

The raw materials selected for the study are presented in Table 1.

Table 1.Common and scientific names of the precursors studied.

Common Name	Scientific Name	Common Name	Scientific Name
Woods:		**Seeds:**	
White Algarroba	Prosopis Alba	Olives Stones	OleaEuropaea
Spanish Lime	MelicoccusBijugatus	Guava	PsidiumGuajava
Sickle Bush	Dichrostachyscinerea	MameyZapote	Mammea Americana
Brasiletto	CaesalpiniaBahamensis	**Seed shells:**	
South American Mahogany	Jacaranda Semiserrata		
Casuarina or River Oak	CasuarinaCunninghamiana	American Mahogany	KhayaSpp
Cedar	CedrelaBalansae	Honduran Mahogany	SwieteniaMacrophylla
Eucalyptus	Eucalyptus Robusta	Coconut	CocosNucifera
Marabou Stork	LeptoptilusCrumeniferus	**Agro-industrial wastes:**	
Bronco Lumber	MalpighiaFucata		
Holy Wood	BulnesiaSarmientoi	Sugar Cane Bagasse	SaccharumOfficinarum
Pine	Araucaria Angustifolia	Tropical Bamboo	BambusoideaeBambuseae
Red Quebracho/Iron Tree	SchinosisBalansae	Sugar Cane Straw	SaccharumOfficinarum
Teak	TectonaGrandis	Common Corncobs	Zea Mays

2.1. Preparation of activated carbons

The starting raw materials were cut up in small pieces and then subjected to pyrolysis. This process was carried out in a tubular reactor in nitrogen atmosphere. The samples were heated at the rate of 10°C/min from room temperature to the final pyrolysis temperature of 500°C. In the final pyrolysis temperature, samples were kept for 60 minutes and then cooled down. The solid products of pyrolysis were then physically activated. The experimental conditions used here were: activation time of 60min, activating agent: H_2O. The heating speed from room temperature to the final activation temperature of 800°C was 10°C/min.[16, 17]

2.2. Characterization of the raw materials and synthetized activated carbons

2.2.1. Elemental analysis

The amount of elements (carbon, hydrogen, nitrogen and oxygen) in the raw materials was determined by an Elemental Analyzer that uses flash combustion to completely digest the samples. The analizedsamples were dried, before the measurement was carried out, in a stove at 110°C. The materials was flash burned at the temperature of 1000°C in flowing oxygen (99.99% purity) for the later C, H and N analysis. The CO_2, H_2O and NO_xcombustion gases were passed through a reduction tube with helium as the carrier gas to convert the NO_xnitrogen oxides into N_2 and bind the free oxygen. The CO_2 and H_2O were measured by selective IR detector. After corresponding absorption of these gases, the content of the remaining nitrogen was determined by thermal conductivity detection. The oxygen was calculated by the difference of carbon, hydrogen and nitrogen.

2.2.2. Apparent Density Measurement

Apparent Density is a measure of the mass per unit volume of a material. It is also called Bulk Density and provides a measure of the "fulffiness" of a material in its natural form. In this work the Standard ASTM D1895 was used. According to this standard the materials are poured into a cylinder of known volume (e.g. 100 mL measuring cilinder) and later weight. Apparent density was calculated as the mass of material divided by the volume occupied into the cylinder. [17]

2.2.3. Specific Surface Area Measurement

In order to examine the structure of the synthetized materials, the measurement of the specific surface area was carried out by gas adsorption isotherms using a Sorptometerand applying BET Theoretical Model. All samples were degassed at 200°C prior to N_2 adsorption measurements. Specific surface area was determined by a multipoint BET method using the adsorption data in the relative pressure range: 0.05-0.3.[18]

2.2.4. Mechanical Resistance Measurement

The mechanical resistance of the obtained activated carbons was measured through a simple method. A know mass of the granular material was impacted by six glass balls into a semispherical container of stainless steel. The percentage relation between the fragmented mass retained in a 0.5mm mesh and the initial mass is used to estimate the mechanical resistance. [17]

2.3 Construction of QSSAR models

The adsorption capability was predicted by using a multiple linear regression model. In this case, several QSSAR models were obtained using the different physicochemical parameters and composition of precursors and carbons as independent variables of the model. The quality of the models was established with the most commonly regression's statistical parameters used and a cross-validation analysis of the performance of the prediction equation.[19, 20, 21]

In this case the Multiple Linear Regression (MLR) was the technique chosen and was performed with software packageSTATISTICA.[22]The considered tolerance parameter was the default value for minimum acceptable tolerance, which was 0.01. The strategy for variable selection was the forward stepwise method. Besides the principle of maximal parsimony (Occam's razor) was used at time to model selection variables. Therefore, the model with the highststatistical signification, but having as few features as possible, was selected. The dependent variable was specific surface area (S) where the values are reported in m^2/g.

The validation of the models is another of the main aspects in good QSAR methodologies concerningto the diagnostic of the developedmodels. Therefore, a reliable QSAR model should have suitable measures of

goodness-of-fit and robustness. In the case of the training set, the good-of-fit is proven by the prediction of the cases for the model given by the measure of the response variance for the training set.

For this study the quality of the models was determined by using some statistical regression parameters such as: the correlation coefficient (R), Fisher ratio's p-level and the standard error in calculation for training set. In the cross-validation procedure, the stability of the predictor coefficients of the models when occurs the removal of one or more cases in the TS was also checked. Thisinternal leave-one-out validation method (Q^2_{LOO})proves the validity of the prediction models obtained by the MLR.[23]

3. Results and Discussion

3.1 Data preparation

The parameter used as independent and dependent variables for the construction of the QSSAR models were collected from our laboratory and were published previously.[24]In the Table 2 are showed the chemical composition (percent of carbon, oxygen, nitrogen and hydrogen) and the physicochemical parameters of the precursors studied. In other hand for the activated carbons synthetized at 800°C and 60 min with steam water thechemical composition and some physicochemical and mechanical properties are depicted in Table 3.

Table 2.Chemical composition of the precursors and physical properties studied.

	Chemical Composition					**Physical Properties**		
Sample	**%C**	**%H**	**%O**	**%N**	**O/C**	**d_{ap}(g/cm^3)**	**d_r(g/cm^3)**	**P(%)**
Woods:								
White Algarroba	52.9	6.5	40.3	0.3	0.76	0.371	0.760	0.44
Spanish Lime	51.6	5.4	42.0	1.0	0.82	0.467	0.900	0.13
Sickle Bush	51.3	5.4	42.2	1.1	0.82	0.340	0.565	0.38
Brasiletto	50.8	5.2	43.2	0.9	0.85	0.395	0.857	0.30
South American Mahogany	58.3	5.9	35.0	0.8	0.60	0.570	0.850	0.47
Casuarina or River Oak	48.6	6.1	44.9	0.4	0.62	0.580	0.900	0.32
Cedar	45.8	6.2	47.4	0.6	1.03	0.230	0.480	0.59
Eucalyptus	47.2	5.6	46.7	0.5	0.89	0.440	0.800	0.48
Marabou Stork	51.1	5.4	42.4	1.1	0.83	0.374	0.780	0.46
Bronco Lumber	47.9	5.0	46.0	1.1	0.96	0.324	0.565	0.33
Holy Wood	56.5	6.8	36.4	0.3	0.64	0.710	1.150	0.12
Pine	53.6	5.9	40.4	0.1	0.75	0.409	0.550	0.58
Red Quebracho/Iron Tree	61.4	6.6	30.7	1.3	0.50	0.853	1.200	0.06
Teak	55.3	6.5	37.0	1.2	0.47	0.832	1.100	0.27
Seeds:								
Olives Stones	57.3	6.0	36.1	0.7	0.63	0.764	0.913	0.32
Guava	56.5	3.0	40.1	0.4	0.71	0.408	1.040	0.62
MameyZapote	58.5	5.5	35.1	0.9	0.60	0.750	1.080	0.35
Seed shells:								
South American Mahogany	53.9	5.1	40.0	1.0	0.74	0.382	0.612	0.37
Honduran Mahogany	54.2	5.1	39.7	1.0	0.73	0.371	0.750	0.50
Coconut	69.9	5.0	24.5	0.7	0.35	1.308	1.537	0.14
Agro-industrial wastes:								
Sugar Cane Bagasse	42.6	5.6	50.7	1.1	1.19	0.100	0.700	0.86
Tropical Bamboo	47.3	8.4	43.9	0.4	0.93	0.350	0.604	0.35
Sugar Cane Straw	44.5	5.3	49.0	1.2	1.10	0.176	0.350	0.58
Common Corncobs	42.9	4.9	51.5	0.7	1.20	0.168	0.420	0.79

d_{ap}: Apparent density; dr: Real density; P: Porosity; R_m: Mechanical resistance

Table 3.Chemical Composition and some Physicochemical and Mechanical Properties of the activated carbons synthetized at 800°C and 60 min with steam water.

	Chemical Composition				Physicochemical and Mechanical Properties					
Sample	**%C**	**%H**	**%O**	**%N**	**dap(g/cm^3)**	**Rm(%)**	**η (%)**	**Yp (%)**	**Yt (%)**	**S(m^2/g)**
Woods:										
White Algarroba	86.4	2.8	10.4	0.4	0.275	85.8	41.8	30.6	24.3	867
Spanish Lime	86.5	2.1	10.2	1.2	0.566	94.4	52.8	27.0	20.1	991
Sickle Bush	86.4	2.1	10.3	1.2	0.202	83.1	39.1	31.0	24.7	820
Brasiletto	86.2	2.0	10.6	1.2	0.394	90.2	46.3	30.0	23.6	918
South American Mahogany	89.2	2.3	8.0	0.6	0.219	81.0	39.7	26.7	19.8	832
Casuarina or River Oak	85.3	2.4	11.1	1.2	0.373	90.2	45.5	37.8	32.5	843
Cedar	84.2	2.4	11.9	1.5	0.157	77.6	35.1	25.9	18.9	909
Eucalyptus	84.8	2.2	11.7	1.4	0.223	89.0	42.9	36.6	31.2	791
Marabou Stork	86.3	2.1	10.3	1.3	0.317	86.6	39.9	31.0	26.8	879
Bronco Lumber	85.1	1.9	11.5	1.5	0.362	89.0	45.1	27.0	20.1	905
Holy Wood	88.5	2.6	8.4	0.5	0.571	96.6	53.0	42.0	35.3	994
Pine	87.3	2.3	9.7	0.7	0.108	79.5	35.5	26.6	19.7	796
Red Quebracho/Iron Tree	90.4	2.5	6.6	0.4	0.634	98.9	55.4	44.5	40.2	1020
Teak	88.0	2.5	8.6	0.9	0.420	92.7	47.3	39.6	34.6	929
Seeds:										
Olives Stones	88.8	2.3	8.3	0.6	0.373	89.4	45.5	28.0	21.3	909
Guava	88.7	1.1	8.8	1.4	0.364	86.6	42.7	43.0	38.5	888
MameyZapote	91.1	2.5	6.2	0.2	0.329	91.7	47.9	43.0	39.1	940
Seed shells:										
American Mahogany	86.4	2.3	11.3	0.0	0.257	85.0	39.6	43.0	38.6	847
Honduran Mahogany	87.5	1.8	9.3	1.4	0.292	86.9	43.0	42.0	37.1	889
Coconut	93.4	1.5	5.0	0.1	0.572	96.6	53.0	45.0	39.8	990
Agro-industrial wastes:										
Sugar Cane Bagasse	82.3	2.6	13.1	2.0	0.120	76.9	32.7	22.0	14.4	580
Tropical Bamboo	85.2	2.9	11.4	0.5	0.294	84.4	42.5	30.0	23.2	875
Sugar Cane Straw	84.4	2.1	12.4	1.1	0.050	79.5	25.4	20.0	12.1	554
Common Corncobs	83.3	1.5	12.6	2.6	0.080	71.7	27.3	26.0	17.4	507

d_{ap}: Apparent density; **R_m:** Mechanical resistance; **η:**Crystallinity; **Y_p:** Pyrolysis yield;
Y_t: Yield during the whole activation process; **S:** Specific surface area.

3.2. Development and assessment of QSSAR-MLR models

In this study, seven models in total were obtained, one for the precursors and the remaining six using the activated carbons, all models are shown in Table 4. As can be seen the model for the precursors (model 1 in Table 4) explains 86.42% of the experimental variance of the adsorption capacity and a value of Q^2 (LOO) of 86.84 the cross-validated determination coefficient from this LOO experiment.

The remaining six QSSAR model were built for the carbon activated as cases. For these models, several combinations were proven, by removing variables, with the aim to improve the performance of the models. The first three models for activated carbons, (models 2, 3 and 4 in Table 4), have coefficients of determination of 81.73%; 93.64% and 81.73% for the training set, respectively. For the cross-validation the values of Q2 (LOO) were 79.97%; 92.75% and 79.97%, correspondingly. The interpretation of these models and the rest are commented in the next subsection.

Table 4.Performance of the QSSAR MLR models.

Model	N*	Q_{train} (%)	R^2	F	*p*	Q^2_{LOO}(%)
Precursor	5	92.96	86.42	22.91	0.00	86.84
Carbon(non-Y_t)	6	90.41	81.73	12.68	0.00	79.97
Carbon(non-%C)	6	96.77	93.64	41.74	0.00	92.75
Carbon (non-%C, non-η (%))	5	90.41	81.73	16.11	0.00	79.97
Carbon(Wood) all	**8**	**99.85**	**99.69**	**202.12**	**0.00**	**98.86**
Carbon(Wood) non-Y_t	**7**	**99.84**	**99.68**	**268.18**	**0.00**	**99.10**
Carbon(other materials) Y_t	3	97.82	95.70	44.46	0.00	94.67

N: *Number of attributes in the training model*

Later the carbons were separated into groups, one conformed by carbons from woods and other with carbons from other sources. For these two groups new models were developed are have improved values of performance compared with the previous three models. For the case of the models from woods using all eight variables, the coefficient of determination in training and cross-validation were 99.69% and 98.86%, respectively. In a second step one variable was removed and the experimental variance remains almost equal with a value of 99.68%, surprisingly for the cross-validation an increase of the value up to 99.10% was experimented.

In the case of the model developed for the second group considering the other materials, the model explain the 99.50% and 94.67 of the experimental variance in training set and cross-validation procedure, respectively.

From the results above can be observed more suitable to separate the materials at time to build the QSSAR because occurs an improvement of the performance of the models over those equations that consider all the sources of the activated carbons in one unique model.

3.3. Interpretation of QSSAR models

In the case of the precursors the following Equation 1 was obtained (R^2 =86.42):

$$\mathbf{S = 8.36 * \%C - 60.61 * \%N - 324.40 * d_{ap} + 218.48 * d_r - 542.31 * P + 663.36} \quad \text{(Eq. 1)}$$

Elemental composition of the raw materials must be carefully considered in order to obtain an acceptable product that can be used for environmental applications. As can be observed in the model higher values of the physical parameters have negative influence for the Specific surface area, related with the adsorption capacity. The details for the performance of the above model and others in this work are showed in Table 4.

The raw material is important when comparing activated carbons, as the source directly influences the suitability of the carbon to its proposed application. Carbon commonly comes from a variety of sources. Wood based carbons are predominantly microporous and mesoporous but with some macroporous character, which provides a wider range of applications.

The primary goal when carbon is activated is to increase the surface area to allow adsorption of different molecules. The surface area of activated carbons is very important as the larger the surface area, the greater the ability to adsorb contaminants.[25]Porosity is also important to provide proper contact of gases or liquid on activated carbons, and it is also related to the rate of adsorption across the adsorbent. It is a fact that raw materials with high porosity are not good as precursors for activated carbons synthesis; it explains the strong influence of this physical property on the later porosity development.

For carbons using the six attributes the following MLR-QSSAR model was obtained (R^2 =81.73):

$$\mathbf{S = 2.32 * \%C + 1.46 * \%H - 0.005 * \%O - 46.18 * \%N + 561.54 * d_{ap} + 1.63 * Y_p + 432.51} \quad \text{(Eq. 2)}$$

The oxygen content resulted negative; this is expected since heat treatment eliminates some oxygen containing functional groups that are not stable at high temperatures.

The real density of activated carbons is also important when comparing the speed of adsorption of carbons with similar specifications. Activated carbons are dosed by weight so the lower density carbons will be added in greater volume. A higher volume of carbon will deliver a greater surface area for adsorption of micro-pollutants. The higher surface area will usually deliver a higher adsorption rate and thus lower doses of activated carbons may be added to achieve the same result as for high doses of more dense grades.

In order to achieve more accurate equations, the following assumptions could be incorporated into the models:

Removing C and d_{ap} (R^2 =93.64)

$$\mathbf{S = 7.51*\%O - 29.59*\%H + -49.80*\%N + 16.01*\eta - 22.90Y_p + 20.22Y_t + 425.22} \quad \text{(Eq. 3)}$$

Removing C and η (R^2 =81.73)

$$\mathbf{S = 13.14*\%H - 2.32*\%O - 48.50*\%N + 561.54*d_{ap} + 1.63*Y_p + 664.11} \quad \text{(Eq. 4)}$$

It was surprisingly found that removing variable C, better models were obtained. Carbon content is often the most critical parameter of the adsorbents and may be the predominant component of the Model, so its elimination to get better correlation coefficients is not a valid physicochemical assumption.

To analyze the change in physicochemical properties during the activation process, materials were divided in two groups, first one only with woods and second one with the other materials (seeds, seed shells and agro-industrial wastes). It was found that there was a significant difference in performance when activated carbons are produced from wood compared with other precursors.

The surface area of activated carbon can be precisely estimated using the equations here derived; however we should be careful when include or eliminate some variables from the equations.

4. Conclusions

Most of the precursors studied here are feasible alternatives for activated carbons preparation adequate for environmental applications. The surface area development of the synthetized activated carbons can be successfully described through the multiple linear regression model used here, considering the initial precursor's chemical composition as independent variables, such as the specific surface area of the activated carbons as the output variable for the developed systems.

In the present study the better results were obtained with the QSSAR models for the activated carbons using wood as materials with correlation coefficients of 99.69% and 99.68% over the models developed considering the other materials. Finally, from the interpretation of the models could be observed that some removed variables like the percent of carbon are of high importance for the adsorbent material capacity. Hence, an important aspect that should be taken in consideration for any study of this type is the criteria of the experts in the field. This is with the aim to have valid assumptions in the models and discard the construction of trivial models that don't reflect the true nature of the scientific problem.

Conflict of interest: The authors confirm that this article content has no conflicts of interest

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