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Modeling Water Sorption Capacity of Silica Gel †

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Abstract: Silica gel is a widely used desiccant with a high water sorption capacity, influenced by factors such as specific surface area, pore volume, and pore size. This study develops mathematical models using multiple linear regression analysis (MLRA) to predict the water sorption capacity of silica gel based on experimental data. The independent variables include the relative humidity (RH), specific surface area (Sp_{BET}), pore volume (Vp), and mean pore diameter (d). The Pearson correlation coefficient reveals strong positive correlations between water sorption capacity (w) and RH, and moderate correlations with Sp_{BET}, Vp, and d. Additionally, Sp_{BET} is strongly correlated with both Vp and d, while Vp and d also show a strong relationship. Two MLRA models are developed to predict sorption capacity: one based on RH and Sp_{BET}, and the other on RH and Vp. The R-squared values for these models are 0.886 and 0.902, respectively, indicating that they are strong predictors of water sorption capacity in silica gel.

Keywords: multiple linear regression analysis (MLRA); water sorption capacity; silica gel; models

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1. Introduction

Silica gel is a widely used desiccant known for its high water sorption capacity, which makes it indispensable in various industrial applications, including moisture control, packaging, and pharmaceuticals. As industries aim to optimize moisture control methods, studying silica gel's water sorption properties has become essential for improving its performance and expanding its applications. Over the years, numerous studies have been conducted to understand and improve the water absorption properties of silica gel. The water sorption capacity of silica gel is influenced by a number of factors, such as the type of silica gel, the incorporation of additives, and the different conditions under which sorption is performed, including variations in humidity, temperature, pressure, and contact time [1–4]. Silica gel comes in different types, which vary in structure, specific surface area, pore size, production method, and specific properties. Today, silica gels are produced with various pore sizes: silica gel with small pores (micropores), which have an average pore diameter below 2 nm; silica gel with medium pores (mesopores), with an average pore diameter between 2 and 50 nm; and silica gel with large pores (macropores), which are larger than 50 nm. Silica gels are also produced with different active centers on their surface, resulting in acidic, neutral, and basic silica gels [5,6]. Some research has focused on enhancing the water capacity of silica gel by modifying its structure or combining it with

other materials to create superabsorbent composites. These materials can potentially absorb even greater amounts of water than traditional silica gel [7,8]. Silica gel is a widely used material in personal protective equipment and is also used in smart textile technologies that enable intelligent thermoregulation. In these applications, understanding the water sorption capacity is crucial [9–12].

In order to quantify the influence of individual factors on the water sorption capacity of silica gel more clearly, the simplest way is to use mathematical modeling to arrive at an appropriate mathematical model that will provide a connection between the sorption capacity of silica gel and its influencing factors.

Mathematical modeling is a powerful tool that bridges theoretical mathematics with practical applications in the physical sciences, engineering, and technology. The integration of mathematical principles into these fields has driven advances across disciplines and continues to provide insights into complex systems, enabling optimization, prediction, and innovation [13,14]. Mathematical modeling involves formulating equations or mathematical structures to represent relationships between variables. A powerful tool in developing models that predict outcomes based on observed data is MLRA (multiple linear regression analysis). MLRA in mathematical modeling is the simplest statistical technique used to model the relationship between a dependent variable (also known as the target variable or output) and two or more independent variables (predictors or input characteristics). In recent years, numerous papers have been published where MLRA is used as an alternative in predicting various variables in the fields of ecology, science, technology, and engineering (e.g., organic pollutants, the prediction of synthetic/natural nanofiber diameters, the viscosity of crude oil, cadmium and lead phytoextraction, and so on) [15–17].

The main objective pursued in this work was to create a mathematical model for the prediction of the water sorption capacity of silica gel depending on influencing factors such as the relative humidity and textural characteristics of the silica gel (specific surface area, pore volume, and pore size).

2. Materials and Methods

To obtain the initial database in this study, four samples of silica gels (Zeochem d.o.o. Zvornik, Bosnia and Herzegovina) were used. The specific surface area (Sp_{BET}), pore volume (Vp) and mean pore diameter (d) of the tested silica gel samples were determined using the low-temperature liquid nitrogen adsorption method on a Micromeritics TriStar 3000 device (Micfrometrics, Norcross, GA, USA). Water sorption capacity (w), or sorbed moisture, is expressed as the mass of water sorbed per unit mass of silica gel (e.g., grams of water per gram of silica gel). It is determined under precisely defined conditions, including a specific temperature, relative humidity (RH), and adsorption time. Therefore, in addition to the sorption capacity value, the following conditions are typically specified: temperature/relative humidity/adsorption time (e.g., W = 3.25% at 25 °C/65% RH/24 h). It is calculated according to the following equation:

$$w = \frac{m_1 - m_0}{m_0} \cdot 100[\%] \quad (1)$$

where

w—sorption capacity (%);
m_0—mass of silica gel before sorption (g);
m_1—mass of silica gel after water sorption (g).

A climate chamber of the "Binder" brand was used to perform the experiment (Figure 1). This chamber allowed for the maintenance of constant relative humidity and temperature during the experiment, i.e., water vapor sorption.



Figure 1. The climate chamber of the "Binder" brand.

3. Results and Discussion

The results obtained from the analysis of the textural characteristics of these silica gels showed that the gels have different specific surface areas (431.2; 516.4; 589.9; and 682.9 g/m^2), pore volumes (0.41; 0.66; 0.85; and 0.74 cm^3/g) and mean pore diameters (2.3; 4.2; 0.74; and 0.85 nm). The surface of the silica gels was not modified, and the analyses of textural characteristics indicate that it was a gel with medium pores (mesopores). Water adsorption on the silica gel samples was conducted in a climate chamber at a temperature of 25 °C and relative humidities of 20%, 40%, and 60%, with an adsorption time of 24 h. The results, including the textural characteristics of the silica gels and their corresponding water sorption capacities, are presented in Table 1.

Table 1. Textural characteristics of silica gels and their corresponding water sorption capacities at 25 °C and relative humidities of 20%, 40%, and 60% RH.

N	W (g/g)	Sp_{BET} (g/m^2)	Vp (cm^3/g)	d (nm)	RH (%)
1.	7.01	682.90	0.41	2.3	20.00
2.	18.90	682.90	0.44	2.3	40.00
3.	27.30	682.90	0.41	2.3	60.00
4.	4.60	589.90	0.66	4.2	20.00
5.	9.00	589.90	0.66	4.2	40.00
6.	20.50	589.90	0.66	4.2	60.00
7.	4.10	431.20	0.85	7.6	20.00
8.	6.40	431.20	0.85	7.6	40.00
9.	11.80	431.20	0.85	7.6	60.00
10.	4.15	516.40	0.74	5.5	20.00
11.	7.86	516.40	0.74	5.5	40.00
12.	16.70	516.40	0.74	5.5	60.00

A correlation matrix helps to understand the relationships between independent variables and the dependent variable. A high correlation between predictors may lead to multicollinearity, making it difficult to interpret the individual effect of each predictor on

the dependent variable. High correlation between predictors can make it hard to interpret the individual effect of each predictor on the dependent variable.

The Pearson correlation coefficient provides a quick and easy way to quantify the linear relationship between two continuous variables. Table 2 shows the Pearson correlation coefficients for all observed variables (Sp_{BET}, Vp, RH, d, and w).

Table 2. Pearson correlation coefficients for all observed variables (Sp_{BET}, Vp, RH, d, and w).

N		W (g/g)	Sp_{BET} (g/m^2)	Vp (cm^3/g)	d (nm)	RH (%)
Pearson Correlation Coefficient	w	1.000	0.508	−0.524	−0.503	0.792
	Sp_{BET}	0.508	1.000	−0.977	−0.997	0.000
	Vp	−0.524	−0.977	1.000	0.970	0.000
	d	−0.503	−0.997	0.970	1.000	0.000
	RH	0.792	0.000	0.000	0.000	1.000
Sig. (1-tailed)	w		0.046	0.040	0.048	0.001
	Sp_{BET}	0.046		0.000	0.000	0.500
	Vp	0.040	0.000		0.000	0.500
	d	0.048	0.000	0.000		0.500
	RH	0.001	0.500	0.500	0.500	
N	w	12	12	12	12	12
	Sp_{BET}	12	12	12	12	12
	Vp	12	12	12	12	12
	d	12	12	12	12	12
	RH	12	12	12	12	12

The Pearson correlation coefficient indicates that the dependent variable, the water sorption capacity of silica gel (w), has a strong positive correlation with RH (0.792), showing a significant positive relationship between the two variables. This relationship is highly statistically significant at the 1% significance level, as evidenced by the one-tailed *p*-value of 0.001. The Pearson correlation coefficient also reveals that the dependent variable, the water sorption capacity of silica gel (w), has a moderate correlation with Sp_{BET}, Vp, and d (0.508, −0.524, −0.503). These relationships are statistically significant at the 5% level, as indicated by the one-tailed *p*-values (0.046, 0.040, 0.048). Additionally, the Pearson correlation shows a strong relationship between Sp_{BET} and both Vp and d (−0.977, −0.997), as well as a strong correlation between Vp and d (0.970). This confirms what is generally known, that the relationship between specific surface area, pore volume, and mean pore diameter can be expressed mathematically using various models, which are derived based on geometric considerations. Two mathematical models were developed by applying MLRA to the experimental data to predict the water sorption capacity of silica gel. The first model (Model 1) predicts sorption capacity based on RH and Sp_{BET}, while the second model (Model 2) predicts it using RH and Vp. The coefficients obtained for the models are presented in Table 3.

The obtained models are

$$\text{Model 1}: \ w = -24.711 + 0.353 \cdot RH + 0.040 \cdot Sp_{BET} \quad (2)$$

$$\text{Model 2}: \ w = 13.522 + 0.353 \cdot RH - 24.124 \cdot Vp \quad (3)$$

The relationship between RH and Sp_{BET} with the dependent variable w, represented by Model 1, is statistically significant. Both RH and Sp_{BET} have positive relationships with w, but RH has a stronger effect (larger standardized coefficient).

In Model 2, the coefficient for RH remains unchanged; now, we observe a significant negative effect of Vp on w.

All of the predictors (RH, Sp_{BET}, and Vp) have p-values of less than 0.05, indicating they are statistically significant and have a reliable relationship with the dependent variable w.

The quality and suitability of the multiple linear regression models are assessed using the correlation coefficient (R), R-squared (R^2), and adjusted R-squared, with the corresponding values shown in Table 4.

Table 3. Coefficients for models obtained by applying MLRA.

Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.
		B [a]	Std. Error	Beta		
1	(Constant)	−24.711	5.361		−4.610	0.001
	RH	0.353	0.050	0.792	7.033	0.000
	Sp_{BET}	0.040	0.009	0.508	4.513	0.001
2	(Constant)	13.522	3.774		3.582	0.006
	RH	0.353	0.046	0.792	7.606	0.000
	Vp	−24.124	4.791	−0.524	−5.035	0.001

[a] Dependent Variable: w.

Table 4. Correlation coefficient (R), R squared (R^2), and adjusted R squared for models obtained by applying MLRA (model summary).

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	0.941 [a]	0.886	0.860	2.83731
2	0.950 [b]	0.902	0.881	2.62340

[a] Predictors: (Constant), RH, Sp_{BET}; [b] Predictors: (Constant), RH, Vp.

For Model 1, the correlation coefficient (R) is 0.941, indicating a very strong positive linear relationship between the predictors (RH and Sp_{BET}) and the dependent variable (w). The R-squared (R^2) value of 0.886 means that 88.6% of the variability in the dependent variable (w) can be explained by the independent variables (RH and Sp_{BET}). The adjusted R^2 value of 0.860 suggests that the model is very strong, with most of the variability in w being explained by RH and Sp_{BET}.

For Model 2, the correlation coefficient of 0.950 indicates an even stronger linear relationship between the predictors (RH and Vp) and the dependent variable (w) compared to Model 1. The R-squared (R^2) value of 0.902 means that 90.2% of the variability in w can now be explained by the predictors (RH and Vp), which is a higher percentage than in Model 1. The adjusted R^2 value of 0.881 indicates that, after accounting for the number of predictors in Model 2, 88.1% of the variability in w is explained. This is an improvement over Model 1 (0.860), suggesting that adding Vp helps explain more of the variance in the dependent variable.

Model 2 outperforms Model 1 in terms of correlation (R), explanatory power (R^2), and prediction accuracy (Standard Error of the Estimate). This indicates that including Vp as a predictor in the model enhances its ability to explain the variance in w.

4. Conclusions

By applying multiple linear regression analysis (MLRA) to experimental data on the water sorption capacity of silica gel, two mathematical models (Model 1 and Model 2) were developed, with the dependent variable being water sorption capacity (w) and the independent variables including relative humidity (RH), specific surface area (Sp_{BET}), pore volume (Vp), and mean pore diameter (d). The first model (Model 1) predicts sorption capacity based on RH and Sp_{BET}, while the second model (Model 2) predicts it using RH

and Vp. The R-squared (R^2) values for these models were 0.886 and 0.902, respectively, indicating that both models are strong predictors of water sorption capacity in silica gel based on the independent variables used in the analysis.

In the end, it can be concluded that the presented results are a good initial step in setting up a mathematical model for predicting the water sorption capacity of silica gel depending on the most influential factors that affect it. Although the sample size taken for the study was not large, further research should be directed towards expanding the data, as well as including other factors that affect the sorption capacity, such as temperature.

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