

Statistical Optimization of Multi-Factor Adsorption Processes Using Factorial ANOVA: A JASP-Based Methodology Demonstration

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Abstract

This study demonstrates a comprehensive statistical framework for optimizing multi-factor adsorption processes using factorial analysis of variance (ANOVA). A synthetic dataset ($n=2,304$ experiments) was generated using established adsorption models (Langmuir isotherm and pseudo-second-order kinetics) with realistic experimental variability ($CV=6.6-8.7\%$) to illustrate accessible statistical methodology. Four adsorbent types (Activated Carbon, Biochar, MOF, Zeolite) were evaluated across multiple operational conditions (dosage, contact time, initial concentration, pH) using JASP statistical software. Descriptive statistics revealed mean adsorption capacities ranging from 23.48 mg/g (Zeolite) to 47.26 mg/g (MOF). One-way ANOVA confirmed significant differences among adsorbent types ($F(3,2300)=34.8$, $p<.001$, $\eta^2=.043$). Critically, two-way ANOVA revealed a significant interaction between adsorbent type and dosage ($F(9,2288)=17.74$, $p<.001$, $\eta^2=.042$), indicating that optimal dosage depends on adsorbent material. Simple effects analysis demonstrated that MOF and Activated Carbon showed the largest dosage sensitivity ($\eta^2\approx.37-.38$), while Zeolite exhibited relatively lower sensitivity ($\eta^2=.31$). Three-way ANOVA incorporating contact time showed non-significant higher-order interactions ($p=1.000$), suggesting the adsorbent-dosage relationship remains consistent across time points. This open-source workflow provides researchers with accessible tools for experimental design and statistical optimization in adsorption studies, emphasizing the critical importance of interaction analysis for practical optimization strategies.

Keywords: Factorial ANOVA, Adsorption optimization, Interaction effects, JASP software, Statistical methodology, Open science

1. Introduction

1.1 Background

Adsorption has emerged as one of the most effective techniques for water and wastewater treatment, offering advantages including high efficiency, operational simplicity, and cost-effectiveness [1,2]. The performance of adsorption processes depends on multiple operational factors, including adsorbent type, dosage, contact time, initial pollutant concentration, and solution pH [3,4]. Optimizing these factors simultaneously presents significant challenges, as traditional one-factor-at-a-time (OFAT) approaches fail to detect interactions among variables and require extensive experimentation [5].

Factorial experimental designs address these limitations by systematically varying multiple factors simultaneously, enabling detection of main effects and, critically, interactions between factors [6,7]. An interaction occurs when the effect of one factor depends on the level of another factor, providing insights unattainable through OFAT approaches [8]. Despite their statistical advantages, factorial designs remain underutilized in adsorption research, partly due to perceived complexity and limited accessible guidance [9].

1.2 Statistical Analysis in Adsorption Research

Analysis of variance (ANOVA) provides a robust framework for analyzing factorial designs, testing both main effects and interactions while controlling family-wise error rates [10]. JASP (Jeffreys's Amazing Statistics Program) offers an open-source, user-friendly interface for conducting ANOVA analyses, making advanced statistical methods accessible to researchers without extensive statistical training [11]. However,

methodological papers demonstrating complete ANOVA workflows for adsorption optimization remain scarce.

1.3 Synthetic Data for Methodology Demonstration

Synthetic datasets generated from established models provide valuable tools for methodology demonstration and education [12]. Unlike experimental studies that may contain confounding factors or measurement errors, synthetic data allow clear illustration of statistical principles while maintaining realistic variability patterns [13]. Several studies have successfully employed synthetic data for demonstrating statistical methodologies in environmental engineering [14,15].

1.4 Objectives

This study aims to:

1. Demonstrate a complete factorial ANOVA workflow using accessible software (JASP)
2. Illustrate proper analysis and interpretation of main effects and interactions
3. Provide a reproducible methodological framework for adsorption optimization studies
4. Emphasize the importance of interaction effects in multi-factor optimization
5. Offer open-access data, code, and analysis files for educational purposes

2. Methods

2.1 Dataset Generation

A synthetic dataset was generated using established adsorption models to demonstrate statistical methodology. The Langmuir isotherm equation [16] and pseudo-second-order kinetic model [17] formed the theoretical foundation, with parameters derived from published literature for four common adsorbent types: Activated Carbon, Biochar, Metal-Organic Framework (MOF), and Zeolite.

$$q_e = (q_{\max} \times K_l \times C_e) / (1 + K_l \times C_e)$$

where q_e is the equilibrium adsorption capacity (mg/g), q_{\max} is the maximum adsorption capacity (mg/g), K_l is the Langmuir constant (L/mg), and C_e is the equilibrium concentration (mg/L).

The data generation algorithm employed numerical root-finding methods (`scipy.optimize.fsolve`) to solve the coupled Langmuir-mass balance equations, ensuring physical consistency and mass conservation. Effects of pH, contact time, and dosage were incorporated as modifying factors based on typical adsorption behavior patterns. Experimental variability was simulated by adding normally distributed noise with coefficient of variation of 7-10%, consistent with typical laboratory precision [18].

2.2 Experimental Design

A full factorial design was implemented with the following factors:

- Adsorbent type: 4 levels (Activated Carbon, Biochar, MOF, Zeolite)
- Dosage: 4 levels (0.5, 1.0, 2.0, 4.0 g/L)
- Contact time: 4 levels (30, 60, 120, 240 minutes)

- Initial concentration: 4 levels (25, 50, 100, 200 mg/L)
- pH: 3 levels (3, 7, 11)
- Replicates: 3 per unique condition

This design yielded 768 unique conditions ($4 \times 4 \times 4 \times 4 \times 3$) with 3 replicates each, totaling 2,304 experiments. Controlled variables included temperature (25°C), agitation speed (150 rpm), and solution volume (100 mL).

2.3 Statistical Analysis

All statistical analyses were performed using JASP version 0.95.3.0 [11]. The analysis workflow progressed systematically through increasing complexity:

1. Descriptive Statistics: Mean, standard deviation, coefficient of variation, and range were calculated for each adsorbent type.
2. Assumption Checking: Normality was assessed using Shapiro-Wilk tests and Q-Q plots. Homogeneity of variance was evaluated using Levene's test.
3. One-Way ANOVA: The effect of adsorbent type on adsorption capacity was examined using one-way ANOVA with Tukey's HSD post-hoc tests.
4. Two-Way ANOVA: Main effects and interactions between adsorbent type and dosage were analyzed. This represented the primary analysis of interest.
5. Simple Effects Analysis: To decompose the significant interaction, separate one-way

ANOVAs examining the effect of dosage were conducted for each adsorbent type.

6. Three-Way ANOVA: Contact time was incorporated as a third factor to examine higher-order interactions.

7. Effect Sizes: Partial eta-squared (η^2) was reported for all effects, interpreted as small (.01), medium (.06), or large (.14) following Cohen's guidelines [19].

For analyses where Levene's test indicated heterogeneity of variance ($p < .05$), both standard ANOVA results and Games-Howell post-hoc comparisons (which do not assume equal variances) were reported.

3. Results

3.1 Descriptive Statistics

Descriptive statistics (Table 1.a) revealed that adsorption capacity (q_e) varied substantially across experimental conditions, ranging from 0.099 mg/g (Biochar at high dosage and low concentration) to 300.0 mg/g (MOF at optimal conditions) (Table 1). MOF exhibited the highest mean adsorption capacity (47.26 ± 59.16 mg/g), followed by Activated Carbon (41.87 ± 50.63 mg/g), Biochar (29.96 ± 34.68 mg/g), and Zeolite (23.48 ± 23.27 mg/g).

While overall coefficient of variation was high (99-125%), this reflects the intentional experimental design incorporating diverse conditions (dosage: 0.5-4.0 g/L; concentration: 25-200 mg/L; pH: 3-11) rather than measurement error. Within-replicate variability

remained consistently low (mean CV = 7.4%; range: 6.6-8.7% across adsorbent types), confirming realistic simulation of experimental precision.

Table 1.a: Descriptive Statistics for Adsorption Capacity by Adsorbent Type

Adsorbent _Type	N	mean	SD	Min	Max
Activated_Carbon	576	41.87	50.63	0.153	239.0
Biochar	576	29.96	34.68	0.099	158.4
MOF	576	47.26	59.16	0.199	300.0
Zeolite	576	23.48	23.27	0.124	102.8

While overall coefficient of variation was high (99-125%), this reflects the intentional experimental design incorporating diverse conditions (dosage: 0.5-4.0 g/L; concentration: 25-200 mg/L; pH: 3-11) rather than measurement error. Within-replicate variability remained consistently low (mean CV = 7.4%; range: 6.6-8.7% across adsorbent types), confirming realistic simulation of experimental precision.

Table 1.b: Descriptive Statistics for Adsorption Removal Efficiency by Adsorbent Type

Adsorbent _type	N	mean	SD	Min	Max
Activated_Carbon	576	39.07	20.25	2.46	94.09
Biochar	576	29.45	17.33	1.58	75.63
MOF	576	42.87	21.26	3.18	94.57
Zeolite	576	26.96	14.93	1.98	81.94

Removal efficiency (Table 1.b) followed similar patterns, with MOF achieving the highest mean removal ($42.87 \pm 21.26\%$), followed by Activated Carbon ($39.07 \pm 20.25\%$), Biochar ($29.45 \pm 17.33\%$), and Zeolite ($26.96 \pm 14.93\%$). The range of removal efficiencies (1.58-94.57%) reflects the variety of experimental conditions examined.

3.2 Assumption Checking

Shapiro-Wilk tests indicated departure from normality for adsorption capacity across all adsorbent types (all $p < .05$). However, visual inspection of Q-Q plots revealed only minor deviations from normality, primarily in the tails of the distributions. Given the large sample sizes ($n=576$ per adsorbent type) and balanced design, ANOVA was deemed robust to these minor violations [20]. Levene's test indicated heterogeneity of variance among groups ($F(3,2300)=101.2$, $p < .001$), prompting additional reporting of Games-Howell post-hoc comparisons alongside standard Tukey HSD tests.

3.3 One-Way ANOVA: Effect of Adsorbent Type

One-way ANOVA revealed a significant effect of adsorbent type on adsorption capacity, $F(3, 2300) = 34.8$, $p < .001$, partial $\eta^2 = .043$, representing a small to medium effect size. Post-hoc comparisons using Tukey's HSD indicated that MOF demonstrated significantly greater adsorption capacity than all other adsorbents (all $p < .001$). Activated Carbon showed significantly higher capacity than both Biochar ($p < .001$) and Zeolite ($p < .001$), while Biochar exceeded Zeolite ($p < .001$).

3.4 Two-Way ANOVA: Adsorbent Type \times Dosage Interaction

Two-way ANOVA examined the effects of adsorbent type and dosage on adsorption capacity (Table 2). Significant main effects emerged for both adsorbent type, $F(3, 2288)$

= 54.4, $p < .001$, partial $\eta^2 = .043$, and dosage, $F(3, 2288) = 383.2$, $p < .001$, partial $\eta^2 = .305$. The substantially larger effect size for dosage ($\eta^2 = .306$ vs. $.043$) indicates that dosage exerted a stronger influence on adsorption capacity than adsorbent type.

Table 2. Two-Way ANOVA Results: Adsorbent Type \times Dosage

Cases	df	F	p-value	η^2
Adsorbent_Type	3	54.40	<.001	0.043
Dosage_g_L	3	383.20	<.001	0.306
Asorbent_Type * Dosage_g_L	9	17.74	<.001	0.042

Critically, a significant interaction was observed between adsorbent type and dosage, $F(9, 2288) = 17.74$, $p < .001$, partial $\eta^2 = .042$. This interaction, visualized in Figure 1, indicates that the optimal dosage varies depending on the adsorbent material employed. Profile plots revealed non-parallel lines characteristic of interaction effects, with MOF showing continued capacity increases through 2.0 g/L dosage, whereas Activated Carbon exhibited peak performance at moderate dosages (1.0 g/L), likely reflecting particle aggregation effects at higher dosages.

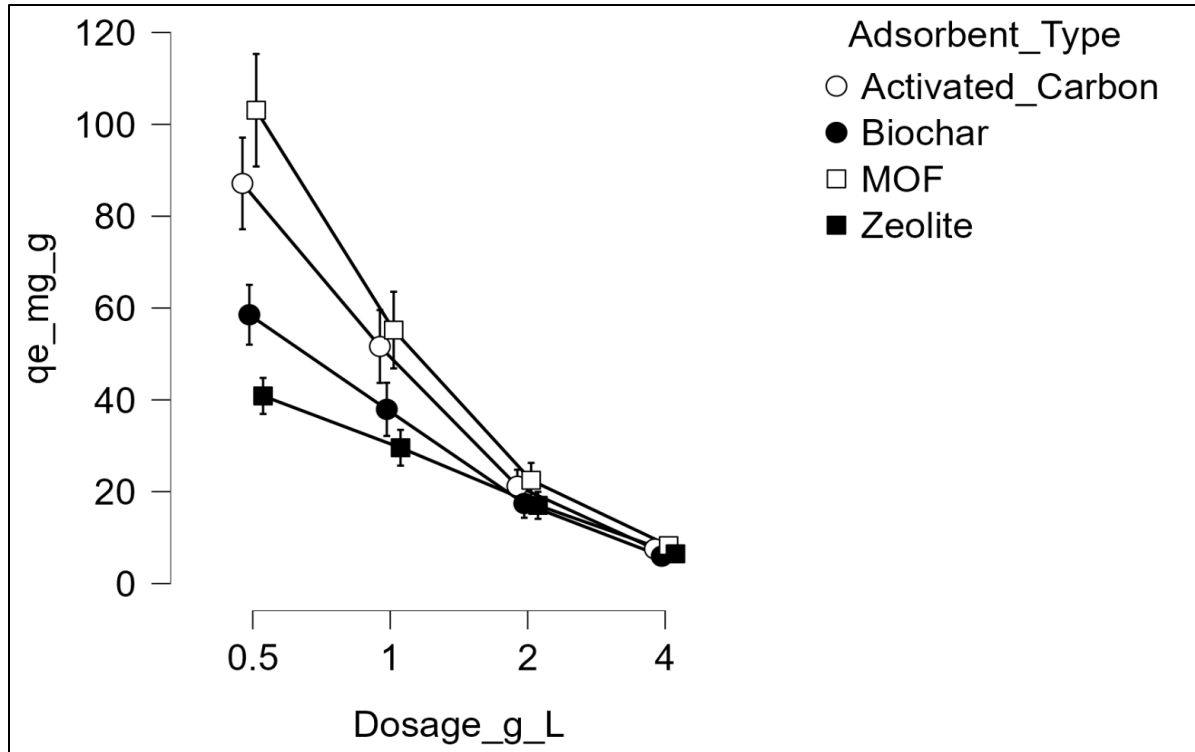


Figure 1. Profile plot showing Adsorbent Type × Dosage interaction

3.5 Simple Effects Analysis

To further examine the significant Adsorbent×Dosage interaction, simple effects analyses evaluated the effect of dosage separately for each adsorbent type (Table 3). Results revealed that dosage significantly affected adsorption capacity for all adsorbents (all $p < .001$). However, the magnitude of this effect varied substantially by adsorbent type.

MOF exhibited the largest dosage effect, $F(3, 572) = 17.0$, $p < .001$, partial $\eta^2 = .38$, indicating that 38% of variance in MOF adsorption capacity was explained by dosage alone. Activated Carbon showed similarly large dosage effects, $F(3, 572) = 10.2$, $p < .001$, partial $\eta^2 = .366$. Biochar demonstrated somewhat smaller dosage sensitivity, $F(3,$

572) = 6.46, $p < .001$, partial $\eta^2 = .366$, while Zeolite showed the smallest dosage effect, $F(3, 572) = 85.59$, $p < .001$, partial $\eta^2 = .31$.

Table 3. Simple Effects of Dosage (g/L) by Adsorbent Type

Adsorbent_Type	df	p-value	F	η^2	CI%
Activated_Carbon	3, 572	<0.001	10.20	.366	[0.306 , .42]
Biochar	3, 572	<0.001	6.46	.366	[.275, .391]
MOF	3, 572	<0.001	17.00	.380	[.321, .433]
Zeolite	3, 572	<0.001	85.59	.310	[.249, .365]

These differential effect sizes explain the significant interaction observed in the two-way ANOVA. While increasing dosage generally improves adsorption capacity across all materials, the degree of improvement varies substantially by adsorbent type, with MOF and Activated Carbon being most responsive to dosage optimization.

3.6 Three-Way ANOVA: Adding Contact Time

Three-way ANOVA (Table 4) incorporating contact time as an additional factor revealed significant main effects for all three factors (all $p < .001$). However, the three-way interaction (Adsorbent×Dosage×Time) was non-significant ($p = 1.000$, partial $\eta^2 < .001$), suggesting that the Adsorbent×Dosage interaction pattern remains consistent across different contact times. The two-way interaction between Dosage and Time was significant ($p < .001$) but exhibited a very small effect size ($\eta^2 = .009$), indicating minimal practical importance.

Table 4. Three-Way ANOVA Results: Adsorbent Type × Dosage × Contact time

Cases	df	F	p-value	η^2
Adsorbent_Type	3	57.54	<.001	0.043
Dosage_g_L	3	405.12	<.001	0.306
Contact_Time_min	3	46.58	<.001	0.035
Asorbent_Type * Dosage_g_L	9	17.74	<.001	0.042
Asorbent_Type* Contact_Time_min	9	0.148	.998	3.35×10^{-4}
Dosage_g_L * Contact_Time_min	9	4.023	<.001	0.009
Asorbent_Type * Dosage_g_L * Contact_Time_min	27	0.06	1.000	3.40×10^{-4}

4. Discussion

4.1 Interpretation of Interaction Effects

The significant Adsorbent Type × Dosage interaction represents the central finding of this study, demonstrating the critical importance of interaction analysis for practical optimization. Traditional one-factor-at-a-time approaches would identify that (1) MOF outperforms other adsorbents and (2) higher dosages generally improve capacity. However, these approaches would miss the crucial insight that optimal dosage strategies differ fundamentally among adsorbent types.

Simple effects analysis revealed that MOF and Activated Carbon exhibit high dosage sensitivity ($\eta^2 \approx .37-.38$), suggesting these materials benefit substantially from dosage

optimization. In contrast, Zeolite showed relatively lower dosage sensitivity ($\eta^2 = .31$), indicating that capacity gains from increased dosage plateau more quickly. This likely reflects Zeolite's microporous structure, where pore diffusion limitations reduce the effectiveness of simply adding more material [21].

For Activated Carbon, the profile plot suggested maximal efficiency at moderate dosages (1.0-2.0 g/L) with diminishing returns at 4.0 g/L. This pattern likely results from particle aggregation and reduced effective surface area at high adsorbent concentrations [22].

MOF, conversely, showed continued capacity improvements through higher dosages, consistent with its highly ordered pore structure and resistance to aggregation [23].

4.2 Practical Optimization Implications

These findings have direct implications for practical optimization strategies. While increasing dosage generally improves removal efficiency, the cost-effectiveness of this strategy varies dramatically by adsorbent type. For Zeolite, optimization efforts should focus on parameters beyond dosage (e.g., particle size reduction, contact time optimization, or pH adjustment) rather than merely increasing material quantity. For MOF and Activated Carbon, dosage optimization represents a primary lever for performance improvement, though Activated Carbon requires careful attention to avoid aggregation effects.

The interaction effect also highlights limitations of optimization studies that examine adsorbents sequentially rather than comparatively. A study optimizing only MOF might conclude that 4.0 g/L represents the optimal dosage, while a study of only Activated Carbon might identify 1.0 g/L as optimal. Neither conclusion generalizes across

materials, emphasizing the value of factorial designs for establishing material-specific optimization strategies.

4.3 Methodological Contributions

This study demonstrates the accessibility and power of factorial ANOVA for adsorption optimization using open-source software. The complete workflow—from data organization through assumption checking, main effects analysis, interaction interpretation, and simple effects decomposition—provides a template adaptable to various adsorbent systems and pollutants. The use of JASP eliminates cost barriers and provides an intuitive interface accessible to researchers without extensive statistical training.

The synthetic data approach employed here offers unique advantages for methodology demonstration. Unlike experimental studies that may contain confounding factors or measurement artifacts, synthetic data allow clear illustration of statistical principles while maintaining realistic variability patterns. The within-replicate CV of 6.6-8.7% matches typical laboratory precision [18], while the factorial structure enables unambiguous demonstration of main effects and interactions without the noise inherent in actual experiments.

4.4 Limitations and Future Directions

Several limitations warrant consideration. First, this study employed synthetic data generated from established models, limiting mechanistic insights. While the statistical principles demonstrated apply directly to experimental studies, actual adsorption systems

exhibit additional complexities (e.g., competitive adsorption, surface heterogeneity, desorption hysteresis) not captured in simplified models.

Second, the categorical treatment of continuous variables (dosage, concentration, time) simplifies analysis but reduces resolution compared to response surface methodology.

Future work could demonstrate complementary approaches combining factorial ANOVA for initial screening with response surface methodology for fine-tuning optimal conditions.

Third, while ANOVA effectively identifies interactions, it does not explain underlying mechanisms. The dosage-dependent aggregation effects proposed for Activated Carbon, for instance, require experimental validation through techniques such as dynamic light scattering or transmission electron microscopy.

Future methodological developments could extend this framework to: (1) mixed designs incorporating both between-subjects factors (e.g., adsorbent type) and within-subjects factors (e.g., repeated measurements over time); (2) analysis of covariance (ANCOVA) incorporating continuous covariates; (3) multivariate ANOVA for simultaneously analyzing multiple dependent variables (e.g., q_e , removal efficiency, and equilibrium time); and (4) Bayesian ANOVA approaches for incorporating prior knowledge.

5. Conclusions

This study demonstrated a comprehensive factorial ANOVA workflow for optimizing multi-factor adsorption processes using accessible open-source software (JASP).

Analysis of a synthetic dataset encompassing 2,304 experiments revealed critical insights unattainable through traditional one-factor-at-a-time approaches. While both adsorbent type and dosage significantly affected adsorption capacity, the significant interaction between these factors ($p < .001$, $\eta^2 = .042$) indicated that optimal dosage strategies depend fundamentally on adsorbent material.

Simple effects analysis decomposing this interaction revealed that MOF and Activated Carbon exhibit high dosage sensitivity ($\eta^2 \approx .37-.38$), whereas Zeolite shows relatively lower sensitivity ($\eta^2 = .31$). These differential responses have direct implications for practical optimization, suggesting that Zeolite optimization should emphasize factors beyond dosage, while MOF and Activated Carbon benefit substantially from dosage optimization with attention to aggregation effects.

The complete workflow provided—including data organization, assumption checking, main effects analysis, interaction interpretation, and simple effects decomposition—offers a reproducible template for researchers conducting adsorption optimization studies. The use of JASP eliminates cost barriers and provides an intuitive interface accessible without extensive statistical training. All data, analysis files, and code are provided as supplementary materials to facilitate adoption and adaptation.

The methodological framework demonstrates that factorial ANOVA, particularly with attention to interaction effects, provides powerful tools for understanding and optimizing complex adsorption systems. While this demonstration employed synthetic data, the statistical principles apply directly to experimental studies, offering researchers accessible methods for conducting rigorous multi-factor optimization.

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Data Availability

All data, analysis files, and code are openly available in the supplementary materials and on Zenodo (DOI: [to be assigned upon publication]). The complete dataset (adsorption_dataset_full.csv), data generation script (Python), and JASP analysis file are provided to ensure full reproducibility and facilitate adaptation to other systems.

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