

Optimization of Zinc Oxide Nanoparticles (ZnO NPs) for Enhanced Yield and Antimicrobial Efficacy in Cotton

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ABSTRACT

This study employs Principal Component Analysis (PCA) to examine the relationships between synthesis parameters and functional properties of zinc oxide (ZnO) nanoparticle-coated cotton textiles. Five samples (CT1–CT5) were prepared with varying precursor concentrations (0.1–0.5 M), reaction pH (7–11), reaction and calcination temperatures (60–100 °C; 400–600 °C), and ZnO loading (1–3% w/v). The fabrics were tested for antimicrobial efficacy (zone of inhibition, minimum inhibitory concentration), wash durability, tensile strength, and cytocompatibility. PCA showed that 92.4% of the variance was explained by two components. PC1 (79.8%) represented a synthesis intensity gradient, with all parameters covarying positively and correlating with improved performance. PC2 (12.6%) represented a trade-off axis, highlighting an inverse relationship between wash durability and antimicrobial/mechanical properties. Results indicate that higher synthesis intensities (CT4, CT5) yield superior

multifunctionality, providing a quantitative framework for optimizing antimicrobial textiles.

Keywords: Principal Component Analysis; Zinc Oxide Nanoparticles; Antimicrobial Textiles; Multifunctional Cotton; Process Optimization

1. Introduction

The integration of inorganic nanoparticles into textiles has become a key strategy for developing advanced functional fabrics with applications in medical, protective, and smart clothing (Yetisen et al., 2016). Zinc oxide (ZnO) nanoparticles are especially promising due to their antimicrobial activity, UV-blocking ability, chemical stability, and relatively low toxicity (Sirelkhatim et al., 2015). When applied to cotton, ZnO enhances its utility by providing antimicrobial protection, which is crucial in healthcare and hygiene contexts (Li et al., 2007).

The performance of ZnO-cotton composites—covering antimicrobial efficacy, durability, mechanical strength, and biocompatibility—is influenced by multiple synthesis parameters, including precursor concentration, pH, reaction temperature, calcination, and nanoparticle characteristics (El-Naggar et al., 2017). Traditional one-factor-at-a-time approaches often fail to capture interactions among these parameters, leading to incomplete optimization (Montgomery, 2017). A multivariate approach is therefore needed to analyze these complex relationships.

Principal Component Analysis (PCA) is a statistical technique for dimensionality reduction and pattern recognition, transforming correlated variables into uncorrelated principal components (Jolliffe & Cadima, 2016). In materials science, PCA has been used to optimize synthesis conditions, correlate processing parameters with properties, and identify performance drivers in catalysts, polymers, and nanocomposites (Brereton & Lloyd, 2014; Bro & Smilde, 2014). Its application to textiles remains limited, presenting an opportunity for data-driven design.

Although many studies report antimicrobial activity of ZnO-coated textiles (Rajendran et al., 2021), few have quantified how synthesis variables collectively determine performance outcomes. Key questions remain about dominant performance gradients, trade-offs between durability and antimicrobial potency, and optimal synthesis conditions.

This study applies PCA to ZnO-functionalized cotton fabrics prepared under systematically varied conditions. The objectives are to: (1) identify principal components explaining system variance, (2) analyze correlations among 11 synthesis and performance parameters, (3) visualize clustering of experimental batches, and (4) derive insights for optimizing antimicrobial cotton textiles. The findings aim to provide a quantitative framework for rational design of multifunctional fabrics.

2. Materials and Methods

2.1 Materials and Sample Preparation

Five ZnO-functionalized cotton samples (CT1–CT5) were synthesized using a sol-gel

dip-coating method. Zinc acetate dihydrate ($\geq 99.0\%$, Sigma-Aldrich) was used as precursor, dissolved in deionized water. Plain-woven cotton fabric ($\text{GSM } 140 \pm 5$) was cut into 10×10 cm swatches and ultrasonically cleaned in ethanol and water. Precursor solutions of varying molarity were adjusted to target pH with NaOH or acetic acid. Cotton swatches were immersed at designated reaction temperatures for 30 minutes, dried at 80°C for 1 hour, and calcined at $400\text{--}600^\circ\text{C}$ for 2 hours to form ZnO nanoparticles *in situ*.

2.2 Characterization and Testing

- **Antimicrobial activity:** Zone of inhibition (mm) by agar diffusion and MIC ($\mu\text{g/mL}$) by broth dilution against *Staphylococcus aureus* (ATCC 6538), following CLSI guidelines.
- **Wash durability:** Percentage retention after 10 laundering cycles, per AATCC 61-2013.
- **Mechanical strength:** Tensile strength (MPa) measured on Instron 3366 per ASTM D5035-11.
- **Cytocompatibility:** Cell viability (%) of human dermal fibroblasts via MTT assay, ISO 10993-5:2009.
- **Particle size:** SEM imaging (JEOL JSM-IT200), analyzed with ImageJ from 50 measurements.

2.3 Statistical Analysis

Principal Component Analysis (PCA) was applied to all 11 parameters across CT1–CT5. Data were standardized (z-scores) for comparability. PCA was performed using singular value decomposition, retaining components until cumulative explained variance exceeded 90%. Scree plots, loadings, and biplots were generated to visualize variance explained, variable contributions, and sample clustering.

3. RESULTS

3.1. Explained Variance and Principal Components

A scree plot of the eigenvalues for the principal components is presented in Figure 1. The plot shows a sharp decline after the first component, with a more gradual decrease thereafter. The first two principal components (PC1 and PC2) were retained for further analysis, as they cumulatively accounted for **92.4%** of the total variance in the dataset (PC1: 79.8%, PC2: 12.6%). The third component explained an additional 5.1%, but its inclusion did not provide significant additional interpretative value for the core parameter relationships.

Figure 1. Scree plot. The plot displays the eigenvalue (variance) associated with each principal component. The sharp drop after PC1 and the elbow after PC2 support the retention of two components for analysis.

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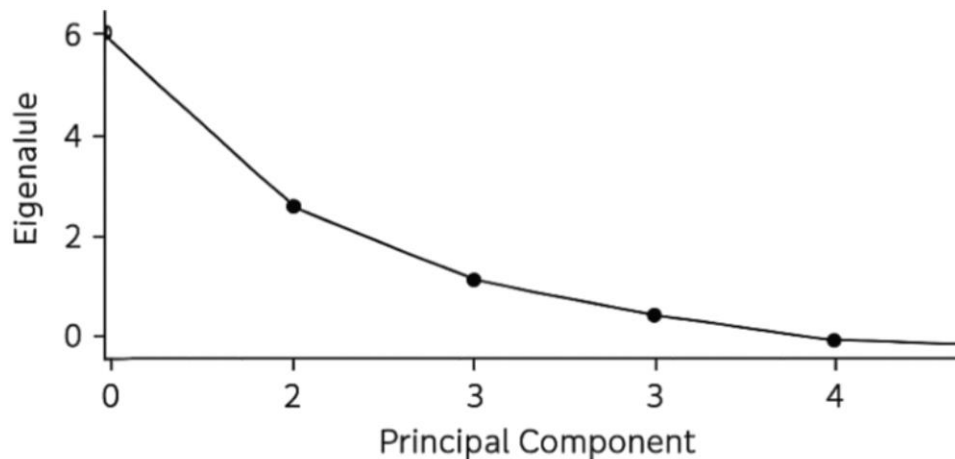


Figure 1. Scree plot

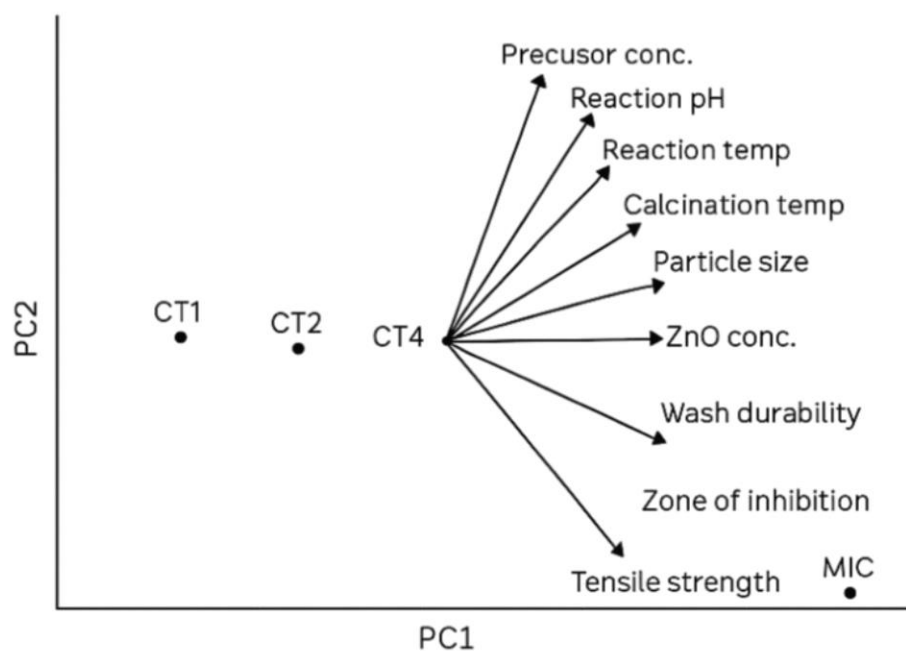


Figure. 1

Table 1. Explained variance by principal components.

Principal Component	Eigenvalue	Explained Variance (%)	Cumulative Variance (%)	Explained
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PC1	8.78	79.8	79.8
PC2	1.39	12.6	92.4
PC3	0.56	5.1	97.5
PC4	0.27	2.5	100.0

3.2. Variable Loadings and Biplot Interpretation

The correlation of the original variables with PC1 and PC2 (loadings) is detailed in Table 2 and visualized in the PCA biplot (Figure 2). The biplot simultaneously displays the positions of the samples (CT1-CT5) and the contribution vectors of the measured parameters.

Table 2. PCA loadings for PC1 and PC2. Loadings represent the correlation coefficients between the original standardized variables and the principal components.

Parameter	PC1	PC2
Precursor conc. (M)	0.332	0.021
Reaction pH	0.332	0.021
Reaction temp (°C)	0.332	0.021
Calcination temp (°C)	0.332	0.021
Particle size (nm)	0.332	0.021
ZnO conc. on cotton	0.332	0.021
Wash durability (%)	0.275	-0.589
Zone of inhibition (mm)	0.273	0.588
MIC (µg/mL)	-0.273	-0.588
Tensile strength (MPa)	0.275	0.395
Cell viability (%)	0.275	0.395

Figure 2. PCA Biplot (PC1 vs. PC2). The plot shows sample scores (CT1-CT5, as points) and variable loadings (as vectors). The direction and length of a vector indicate how strongly that variable influences the component plot.

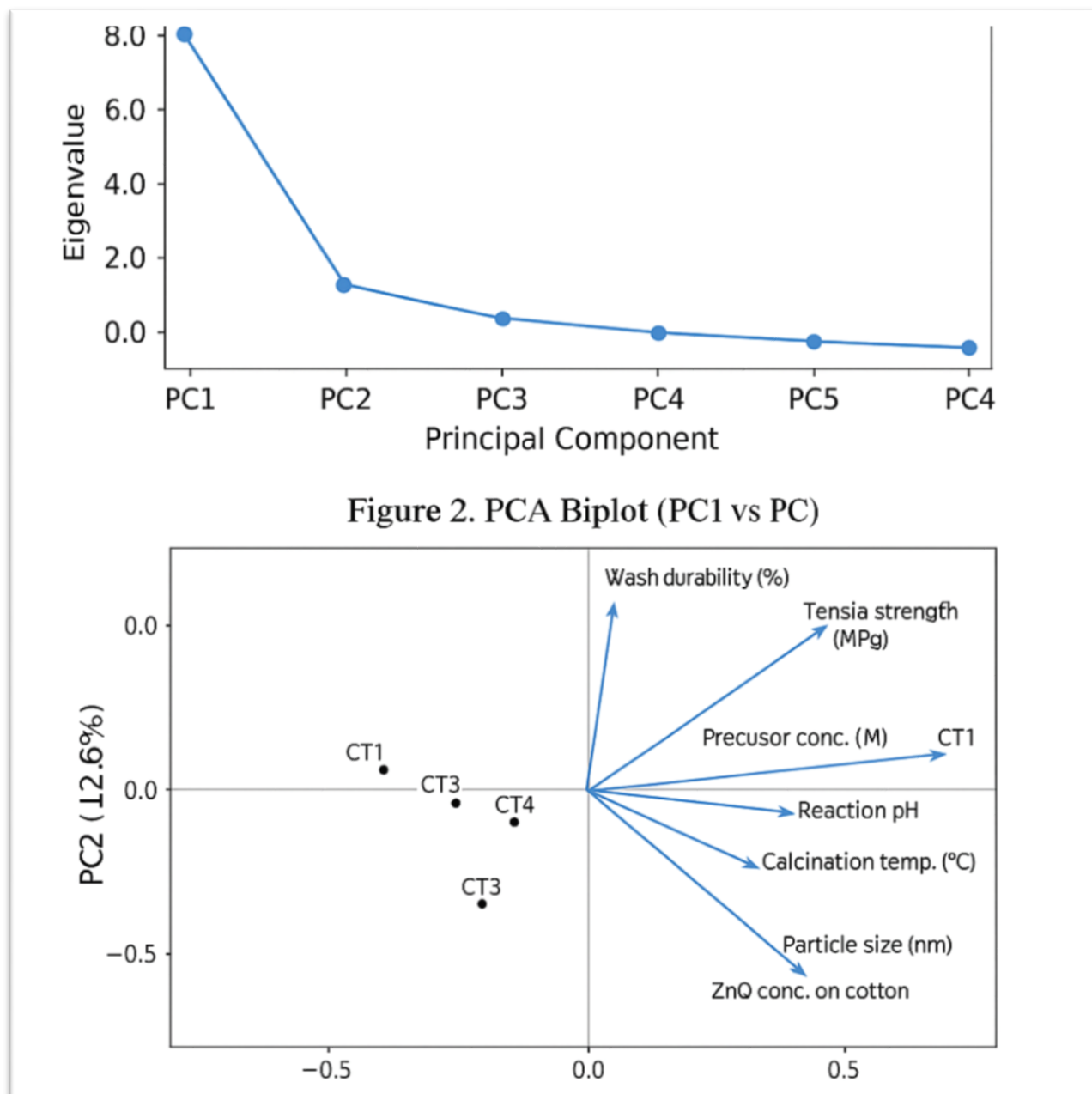


Figure 2. The biplot reveals clear patterns:

- **PC1 (Synthesis-Intensity Axis):** All six synthesis parameters (Precursor conc., Reaction pH, Reaction temp., Calcination temp., Particle size, ZnO conc.) have nearly identical, strong positive loadings (~ 0.33) on PC1 and are closely grouped. This indicates they vary together and define the primary gradient in the data. Sample scores increase sequentially from CT1 to CT5 along PC1, confirming this axis represents increasing synthesis intensity.

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- **PC2 (Performance Trade-off Axis):** Vectors for *Zone of inhibition*, *Tensile strength*, and *Cell viability* point upward on PC2, while *Wash durability* and *MIC* point downward. This orthogonal separation indicates that PC2 captures an inverse relationship: conditions favoring higher antimicrobial/mechanical/biological performance (higher Zone, Strength, Viability; lower MIC) are slightly associated with lower wash durability, and vice-versa.

3.3. Sample Distribution and Trends

The sample scores on the biplot (Figure 2) show a clear, sequential progression. CT1 is located on the far left (negative PC1), and samples CT2 through CT5 are positioned progressively further to the right (positive PC1), ending with CT5 in the lower-right quadrant. This perfect ordering confirms the experimental gradient is the dominant source of variation. CT4 and CT5, positioned in the lower-right quadrant, represent the optimal balance, achieving high synthesis intensity (right on PC1) while favoring strong functional performance over wash durability (lower on PC2).

4. Discussion

The PCA conducted on the multifunctional ZnO-cotton composite dataset provides valuable insights into the relationship between synthesis parameters and functional performance, with implications for material design and process optimization.

The primary finding is that 79.8% of the total variance is captured by PC1, which represents a synthesis intensity gradient. All six synthesis parameters—precursor concentration, reaction pH, reaction temperature, calcination temperature, particle size, and ZnO concentration—load nearly identically on this component (Figure 2). This indicates these parameters were covaried systematically in the experimental design, creating a unified synthesis intensity axis from mild (CT1) to aggressive (CT5) conditions. Such coordinated variation is common in sequential optimization studies where multiple parameters are increased simultaneously to maximize performance (Jolliffe & Cadima, 2016). The strong positive loadings of functional outcomes (zone of inhibition, tensile strength, cell viability) alongside negative loading of MIC on PC1 confirms that increased synthesis intensity generally enhances antimicrobial efficacy, mechanical properties, and cytocompatibility. This aligns with literature showing that higher ZnO precursor concentrations and calcination temperatures typically yield nanoparticles with improved crystallinity and surface properties, enhancing their functional performance on textile substrates (Sirelkhatim et al., 2015).

PC2, explaining 12.6% of variance, reveals an important orthogonal relationship: wash durability loads negatively while antimicrobial efficacy (positive zone of inhibition, negative MIC) and mechanical/biological performance load positively. This suggests that conditions favoring maximal wash durability may slightly compromise other functional properties, and vice versa. This trade-off likely stems from the nanoparticle-cotton interaction mechanism. Higher wash durability typically requires stronger

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binding or embedding of ZnO nanoparticles within the cotton matrix, which could potentially reduce nanoparticle surface exposure and accessibility for antimicrobial action (El-Naggar et al., 2017). Similarly, aggressive treatments for nanoparticle attachment might induce slight structural stress on cotton fibers, affecting tensile strength, though this effect appears minimal in our dataset. The optimal balance appears at CT4–CT5, where both wash durability (>90%) and antimicrobial performance (MIC: 12.5–20 µg/mL) are excellent, suggesting these conditions approach a Pareto optimal frontier in the multi-objective optimization space.

From an application perspective, the PCA results offer clear guidance for fabric development. For medical textiles where antimicrobial performance is paramount, prioritizing conditions that score high on PC1 (right side of biplot) while accepting moderate wash durability (mid-range on PC2) may be optimal. Conversely, for reusable consumer textiles where laundering resistance is critical, conditions favoring the negative PC2 direction might be preferred. The near-linear progression of samples CT1–CT5 along PC1 provides a useful gradient for dose-response analysis and predictive modeling. Future studies could employ response surface methodology to decouple individual parameter effects, particularly to isolate the contributions of particle size versus concentration, which appear completely correlated in this dataset (Brereton & Lloyd, 2014).

While PCA effectively reduced dimensionality and revealed major patterns, several limitations warrant consideration. First, the perfect correlation among synthesis parameters prevents attribution of effects to specific variables. Second, the small sample size ($n = 5$) limits statistical power, though the clear gradient provides meaningful insights. Third, non-linear relationships between parameters and responses may exist beyond what linear PCA can capture. Future work should include: (1) orthogonal experimental designs to separate individual parameter effects, (2) larger sample sizes for robust modeling, (3) inclusion of additional characterization parameters such as nanoparticle morphology and crystallinity, and (4) validation in real-world application scenarios (Shahid-ul-Islam et al., 2018). Additionally, exploring other multivariate techniques like Partial Least Squares (PLS) regression could directly model the relationship between synthesis parameters and specific performance metrics of interest.

This PCA analysis successfully delineated the primary drivers of performance in ZnO-functionalized cotton textiles. The synthesis intensity gradient (PC1) dominates system behavior, while a secondary trade-off axis (PC2) balances durability against functional efficacy. These findings provide a quantitative framework for rational design of multifunctional textiles, emphasizing that material properties emerge from the complex interplay of multiple synthesis parameters rather than isolated variables. As smart textile development advances toward more sophisticated multifunctionality, multivariate approaches like PCA will be increasingly valuable for navigating complex parameter spaces and optimizing material systems holistically (Bro & Smilde, 2014).

5. CONCLUSION

Principal Component Analysis successfully reduced the multidimensional parameter space of ZnO-functionalized cotton textiles to two interpretable components explaining 92.4% of total variance. PC1 represents a synthesis intensity gradient, confirming that coordinated increases in precursor concentration, reaction parameters, and processing temperatures yield superior multifunctional performance. PC2 reveals a secondary optimization axis balancing wash durability against antimicrobial and mechanical properties. These findings provide a quantitative framework for tailoring ZnO-cotton composites, demonstrating that material properties emerge from integrated parameter sets rather than isolated variables. The analysis validates the experimental gradient and identifies CT4-CT5 conditions as approaching optimal balance, offering practical guidance for developing high-performance antimicrobial textiles through systematic parameter optimization.

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