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Solubility-Driven Prediction of Electrospun Nanofibers' Diameters via Generalized Linear Models

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INTRODUCTION

Electrospinning is a technique used to generate nanofibers by applying a high-voltage electric field. The fiber diameter is influenced by both operating and solution parameters and represents a critical property in numerous applications [1]. Solution parameters, such as viscosity, dielectric constant, among others are determined by the molecular compatibility of the solvent–solute system.

In this work, a model is developed to quantify the relative contribution of each parameter and to predict nanofiber diameter as a function of operating parameters and solution parameters. The latter are characterized by Flory–Huggins (χ), Hildebrand (δ), and Hansen solubility parameters, which describe solute–polymer affinity [2].

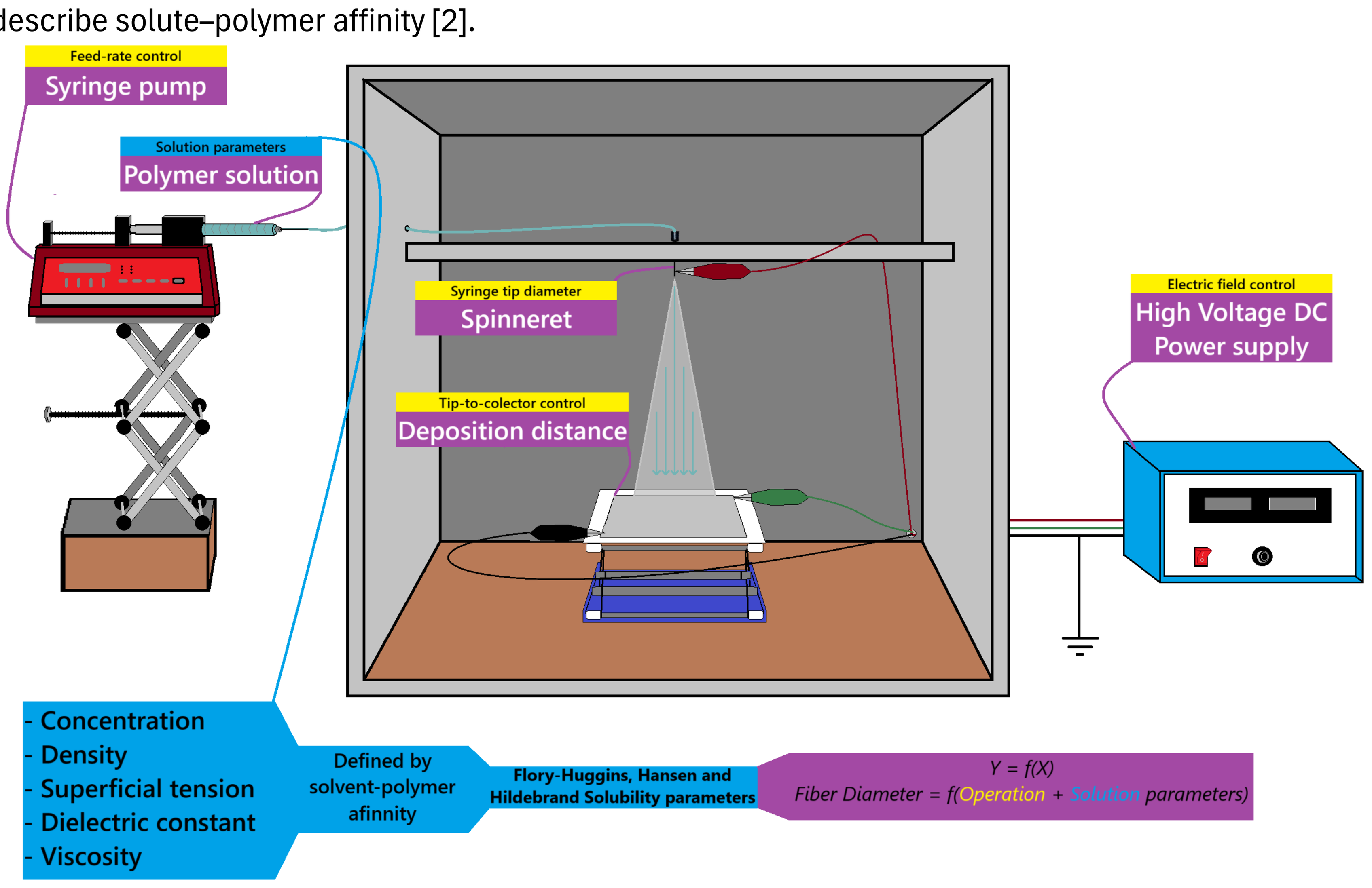

Figure 1. Experimental Setup and Parameters Governing Fiber Diameter in Electrospinning

METHODOLOGY

Define best fit in terms of distribution and link function and then train prediction GLM model with best configuration and then test prediction model.

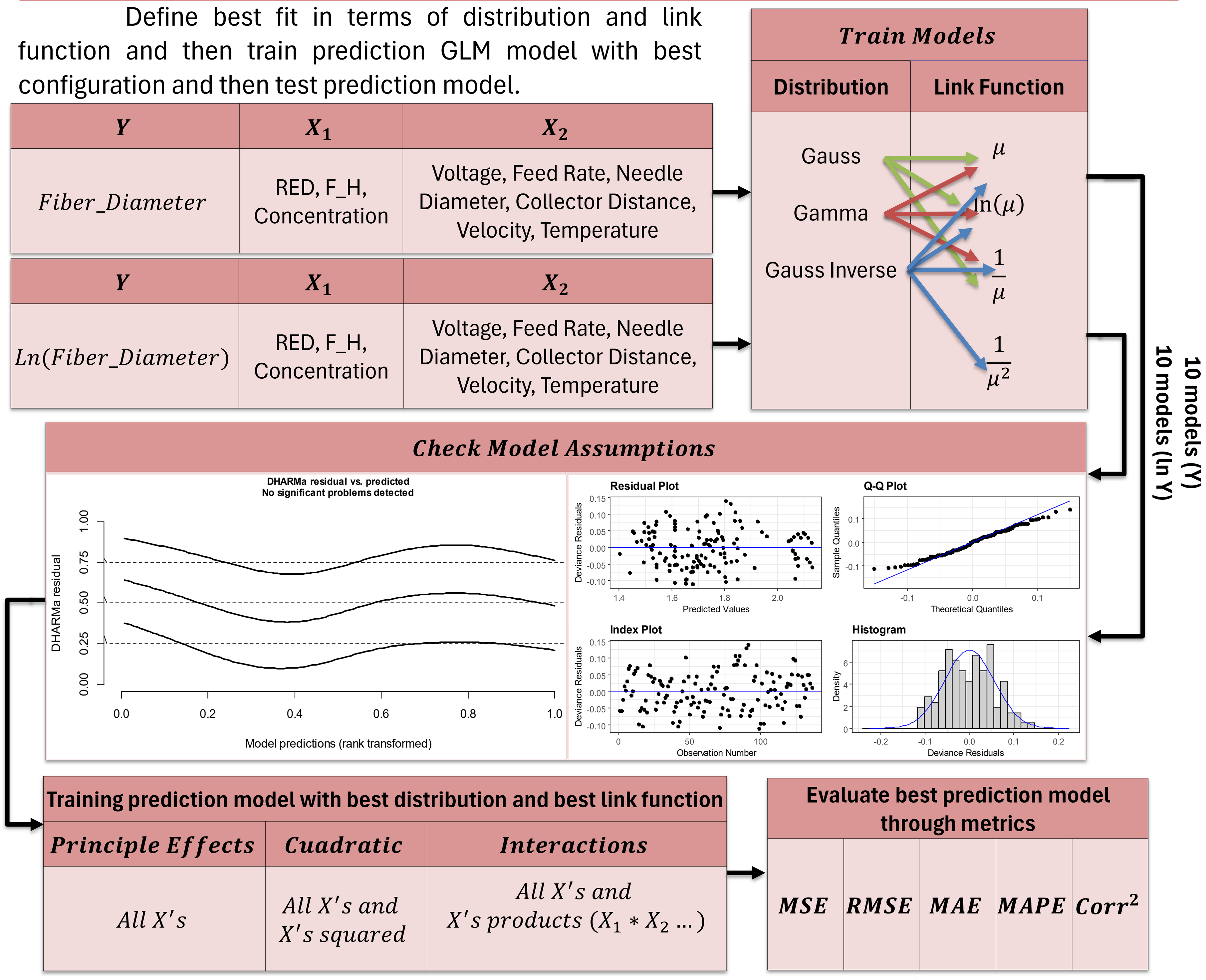

Figure 2. Methodology of Inference and Prediction across multiple GLM testing

RESULTS & DISCUSSION

INFERENCE & PREDICTION

Among the three tested distributions, Gamma showed lower AIC values denoting goodness-of-fit for both non transformed (Y) and transformed (ln Y) response variable. To maintain parsimony the model chosen was set to being Gamma distributed $\ln(Y) \sim Gamma(\alpha, \beta)$ with identity link $E[\mu] = X\beta$.

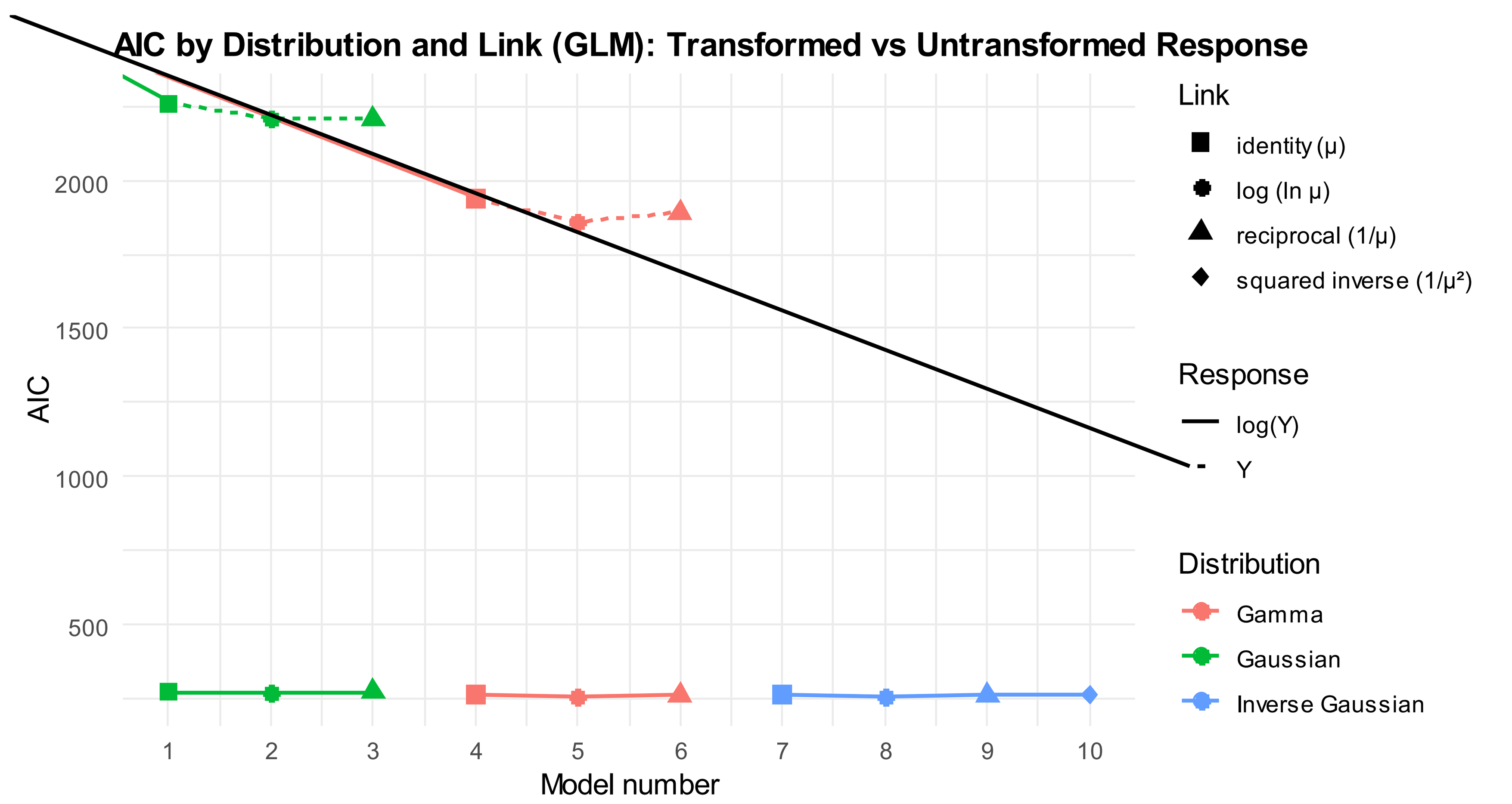

Figure 3. AIC Comparison of GLMs: Transformed vs. Untransformed Response

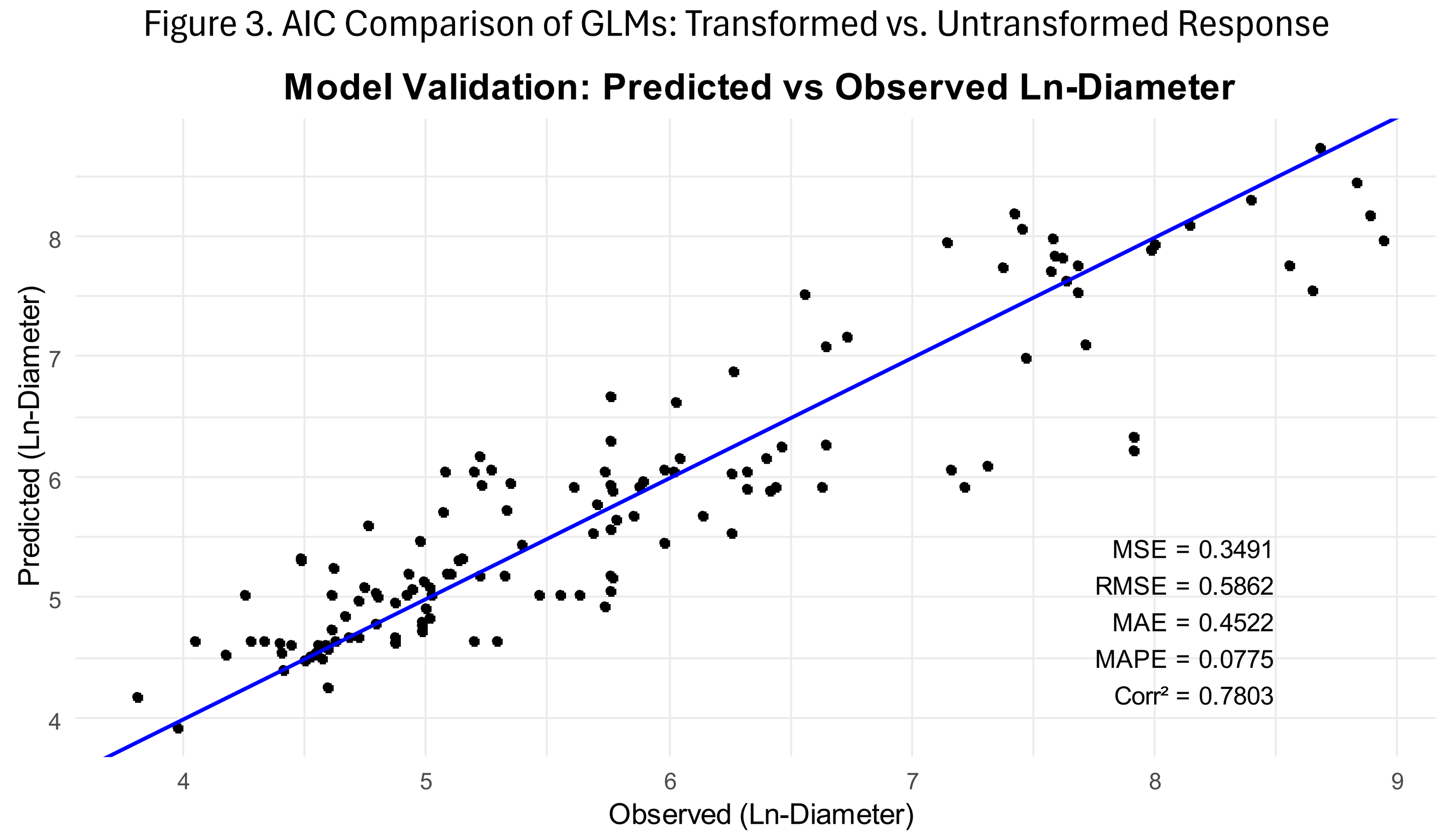

Figure 4. Model Validation: Predicted vs Observed Ln-Diameter

EXPERIMENTAL TESTING

Gamma(Identity) model (GLM 4) was used to predict PVA electrospun nanofibers. Electrospinning operation and solution parameters as well as theoretical and real nanofiber diameters are shown in table below. ImageJ software was used to measure SEM microscopies which are also displayed below.

Table 1. Operating and solution parameters for PVA electrospun nanofibers

Solution parameters					Operation parameters					
Concentration			RED	Flory-Huggins solubility parameter	Voltage (kV)	Feed Rate (cm^3/h)	Needle Diameter (cm)	Collector distance (cm)	Velocity (cm/h)	Temperature (K)
Polyvinyl Alcohol (%)	Deionized water (%)	Acetic Acid (%)								
10.000	85.000	5.000	0.559	0.128	30.000	2.000	0.300	18.000	63.662	291.150

Table 2. Theoretical vs. Observed Diameter for PVA electrospun nanofibers

Average diameter comparison		
Theoretical Gamma, Identity (nm)	Observed via SEM (nm)	Percentual Error (%)
334.68	298.12	12.26%

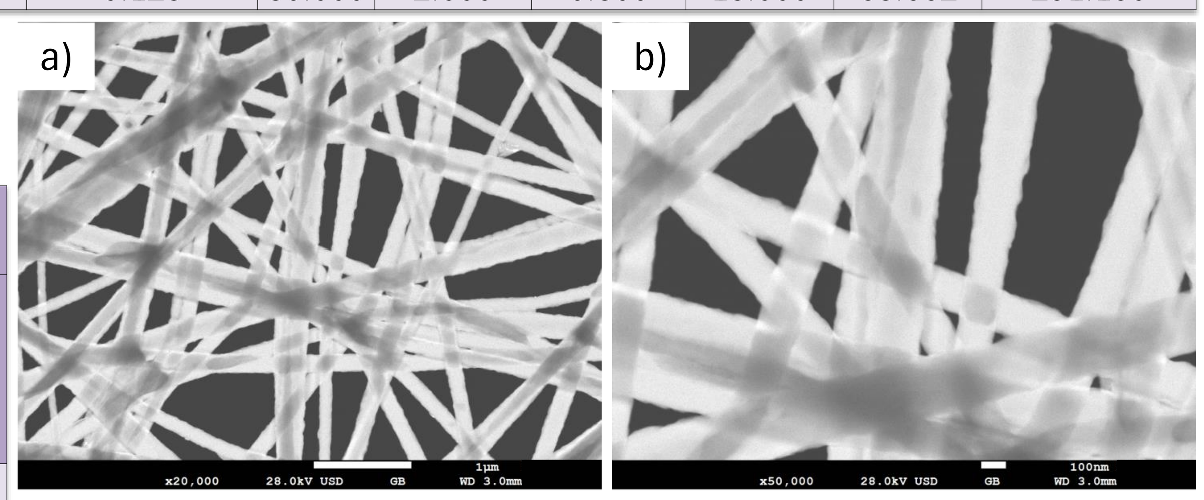

Figure 5. SEM micrographies (28.0 kV, WD 3.0 mm, GB detector) a) 20,000x, b) 50,000 for PVA electrospun nanofibers

CONCLUSION

- Electrospinning of synthetic and natural polymers nanofibers follow a Gamma distribution when transformed to logarithmic response. Goodness-of-fit enhances when transforming the variable.
- Inverse Gaussian distribution models cannot be fitted to untransformed response variable.
- Concentration and Flory-Huggins are the most important solution parameters to determine nanofiber diameter.
- Voltage and Flow Rate are among the most important operating parameters to determine nanofiber diameter.

FUTURE WORK / REFERENCES

For future work experimental samples will be tested considering additional parameter matrixes to confirm the influence of every operation and solution parameters.

[1] Bhardwaj, N., & Kundu, S. C. (2010, May-June). Electrospinning: A fascinating fiber fabrication technique. Biotechnology Advances, 28(3). https://doi.org/10.1016/j.biotechadv.2010.01.004
[2] Hansen, C. M. (1967). The Three Dimensional Solubility Parameter and Solvent Difusion Coefficient. Journal of Paint Technology, 39(505), 103.