

Machine Learning Assessment of Fiber Morphology Descriptors in Solution Blow Spinning

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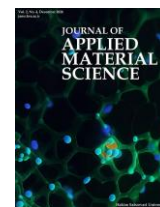
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Editor's note: This study by Rivera Vera and coworkers uses machine learning to reanalyze Box-Behnken datasets for solution-blow-spun polystyrene (PS) and polysulfone (PSf) mats, focusing on fiber diameter (DoF) and relative fiber amount (RoF). PS showed strong predictive performance for DoF ($R^2 = 0.8142$), while PSf showed much lower performance ($R^2 = 0.0043$). Results indicate that descriptor suitability depends on morphology, highlighting the need for machine learning to identify effective characterization parameters in fibrous materials.

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Original Research

Machine Learning Assessment of Fiber Morphology Descriptors in Solution Blow Spinning

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Abstract

Machine-learning-assisted reanalysis of two previously published Box–Behnken datasets for solution-blow-spun (SBS) polystyrene (PS) and polysulfone (PSf) mats is presented. The analysis focused on fiber diameter (DoF) and the relative amount of fibers (RoF). Regression models were trained using coded processing variables and evaluated by 5-fold cross-validation. For PS, whose morphology was predominantly fibrous, DoF showed the strongest predictive performance; linear regression achieved a coefficient of determination (R^2) of 0.8142, a root mean square error (RMSE) of 142.45 nm, and a mean absolute error (MAE) of 91.32 nm. In contrast, PSf mats, characterized by bead-on-string morphology, showed substantially lower predictive performance for DoF and RoF, with mean DoF reaching an R^2 of only 0.0043. These findings indicate that descriptor suitability depends on the structural regime of SBS materials. Fiber diameter is an informative characterization parameter when continuous fibers dominate the architecture but becomes insufficient when bead-related features contribute substantially to the morphology. Machine learning can therefore complement conventional morphological characterization by helping identify which descriptors most effectively represent processing–structure relationships in solution-blow-spun fibrous materials.

Keywords: Fiber diameter; Machine learning; Morphology prediction; Solution blow spinning.

1. Introduction

Polymeric materials composed of micro- and submicrometric fibers have attracted considerable attention because their morphology provides a high surface area, interconnected porosity, and surface

roughness, all of which are important for surface-dependent applications. These fibrous materials have been explored for oil absorption, wettability control, filtration, separation processes, biomedical devices, tissue engineering, wound dressings, drug delivery, and functional coatings [1-4]. Accordingly, controlling fibrous morphology is important when tailoring

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polymeric materials for specific or enhanced performance.

Among the morphological features used to describe fibrous mats, the diameter of fibers (DoF) is one of the most commonly reported parameters. In many cases, DoF provides a direct way to relate processing conditions to the final material morphology. However, morphologies produced by solution-based spinning processes are not always exclusively fibrous. Depending on the polymer-solvent system and processing conditions, fibers may coexist with beads, pearls, corpuscular structures, fiber aggregates, or fused domains [1, 2, 4, 5]. In such cases, mean fiber diameter alone may not adequately describe the overall material architecture. Additional morphological descriptors, such as the relative amount of fibers (RoF) or the fiber/bead ratio, may therefore be required to represent complex bead-fiber morphologies more comprehensively [1, 4].

Solution blow spinning (SBS) has emerged as a versatile and low-cost technique for producing polymeric micro- and nanofibers from solution [6]. The method is based on the interaction of two fluid streams in a concentric nozzle: a polymer solution flows through the inner channel, while a pressurized gas flows through the outer channel [2, 3, 5, 7]. At the nozzle exit, the gas stream stretches the polymer solution, promotes solvent evaporation during flight, and ultimately deposits the fibers on a collector positioned at a defined working distance. Compared with electrospinning, SBS does not require high electric fields or conductive collectors and has been reported as suitable for faster and more direct fiber deposition on different substrates [2, 3, 5, 7]. Nevertheless, the apparent simplicity of the technique does not imply simple morphology control.

The final morphology of solution-blow-spun materials depends on a combination of solution and processing variables. Polymer concentration, molecular weight, viscosity, surface tension, solvent volatility, solution feed rate, gas pressure, nozzle geometry, working distance, and environmental conditions can affect jet stability, solvent evaporation, fiber stretching, bead formation, fiber diameter, and mat homogeneity [2, 3, 5, 7, 8]. In particular, polymer concentration and molecular weight are directly related to chain entanglement, which is commonly described through the overlap concentration, c^* . When polymer concentration is below the required entanglement level,

corpuscular or bead-on-string morphologies may form instead of continuous fibers [2, 3, 5]. Conversely, increasing concentration and viscosity generally favors fiber formation, although it may also increase fiber diameter or broaden the diameter distribution. Thus, SBS morphology should be understood as the result of coupled effects rather than the consequence of a single isolated factor.

Because of this multivariable nature, response surface methodology (RSM) and design-of-experiments approaches have been used to optimize SBS processing conditions. In particular, Box-Behnken designs have reduced the number of experiments required while enabling empirical relationships to be established between SBS variables and morphological responses. Previous studies on polystyrene (PS) and polysulfone (PSf) demonstrated that combining Box-Behnken designs with desirability functions can be useful for obtaining polymeric materials with tailored morphologies [1, 4]. For PS, optimization focused on maximizing the amount of fibers while minimizing fiber diameter, leading to superhydrophobic materials with improved oil absorption [1]. For PSf, optimization considered RoF and DoF to obtain materials with specific wettability behavior, although the resulting morphology was characterized mainly by the coexistence of beads and fibers [4].

Although RSM is useful for optimization within a defined experimental domain, it does not necessarily establish whether a given morphological descriptor is equally predictable or representative across different morphological regimes. This distinction is important because DoF and RoF contain different types of morphological information. DoF describes the size of the fibrous fraction, whereas RoF captures broader aspects of the material architecture. Therefore, when fibers coexist with beads, pearls, or material accumulations, the predictive behavior of each descriptor may reflect not only model performance but also the ability of the descriptor to represent the actual morphology of the system.

In recent years, machine learning (ML) has emerged as a complementary tool for analyzing complex processing-structure relationships in materials systems. In nanofiber research, ML has increasingly been used to relate processing parameters to morphological responses, particularly fiber diameter, and to compare the predictive performance of different algorithms [9].

Its application to SBS, however, remains limited. A recent study comparing RSM and ML algorithms for poly(methyl methacrylate) (PMMA) nanofiber production by SBS demonstrated that fiber diameter can be predicted from concentration, flow rate, and air pressure [10]. Such approaches primarily treat the selected morphological response as a predefined prediction target.

An unresolved issue is whether a morphological descriptor that is informative in one structural regime remains equally representative when the material architecture changes. This distinction is particularly relevant to SBS because processing conditions may produce predominantly fibrous mats or more complex bead-fiber structures. In the former case, fiber diameter may describe a dominant structural feature, whereas in bead-containing morphologies it represents only the fibrous fraction and does not account for bead size, bead density, bead spacing, bead shape, or fiber-bead connectivity. Consequently, limited model performance may reflect not only the regression algorithm or available predictors but also the ability of the selected response variable to represent the morphology being modeled.

The novelty of the present study therefore lies in using ML performance as a diagnostic approach to evaluate

the morphology-dependent suitability of conventional SBS descriptors rather than solely as a tool for predicting a predefined morphological response. To examine this concept, two previously reported Box-Behnken datasets representing contrasting SBS morphologies were independently reanalyzed: predominantly fibrous PS mats and bead-fiber PSf mats. The predictive behavior of DoF and RoF was evaluated within each material-specific experimental domain using the same ML validation framework. The objective was to determine whether these descriptors retain predictive consistency and structural representativeness as the morphology changes from predominantly fibrous to bead-containing architectures.

2. Experimental

2.1. Source datasets and original experimental workflow

Experimental data previously reported for solution-blow-spun polymer mats were used to evaluate the predictive behavior of morphology descriptors using ML. Two source datasets were considered: PS [1] and PSf [4]. No additional material-synthesis experiments were conducted. The original data were reorganized and analyzed to compare the relationships between SBS

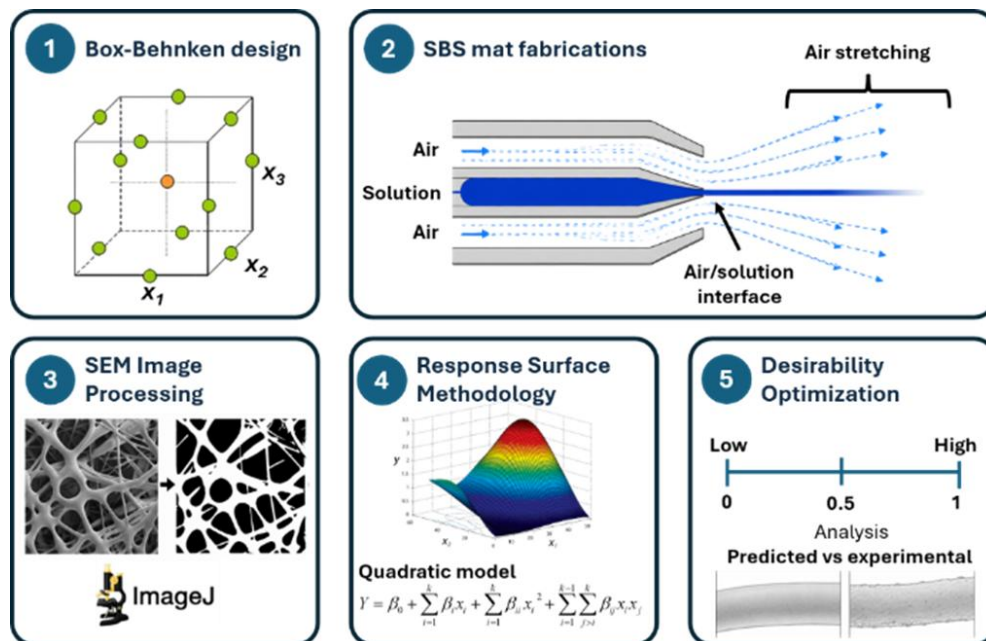


Figure 1. Conventional experimental-statistical workflow used in the original SBS studies. SBS, solution blow spinning; SEM, scanning electron microscopy.

Table 1. Source datasets used for the machine-learning-assisted reanalysis

Polymer system	SBS variables considered	Morphological responses	Main purpose of the original study
Polystyrene (PS)	Polymer concentration; air pressure; solution feed rate	Mean DoF; RoF	Preparation of PS materials with tailored morphology, superhydrophobic behavior, and enhanced oil absorption ability
Polysulfone (PSf)	Working distance; solution feed rate; air pressure	Mean DoF; median DoF; RoF	Preparation of PSf materials with controlled bead-fiber morphology and tailored wettability behavior

Notes: SBS, solution blow spinning; DoF, diameter of fibers; RoF, relative amount of fibers.

processing conditions and morphological responses within each polymer system.

Both datasets originated from studies in which polymer mats were prepared by SBS and analyzed using a similar experimental-statistical workflow. As shown in Figure 1, the original studies first defined the SBS processing conditions using a three-factor Box-Behnken design. The materials were then produced by varying the corresponding processing variables. Mat morphology was examined by scanning electron microscopy (SEM), and the images were analyzed with ImageJ to determine DoF and RoF. Finally, RSM and desirability functions were used to identify processing conditions that produced tailored morphologies [1, 4].

The PS dataset was originally designed to obtain materials with a high RoF and reduced DoF, aiming to produce superhydrophobic mats with improved oil absorption [1]. The PSf dataset focused on controlling bead-fiber morphology to obtain materials with specific wettability behavior [4]. The datasets were therefore selected because they represent contrasting morphological regimes obtained by SBS: a predominantly fibrous morphology for PS and a mixed bead-fiber morphology for PSf.

Table 1 summarizes the datasets used in this work. Although both studies used Box-Behnken designs with fifteen experimental runs, including three center points, the physical meaning of the processing variables differed between the two polymer systems. In the PS dataset, the variables were polymer concentration, air pressure, and solution feed rate; in the PSf dataset, they were working distance, solution feed rate, and air pressure. For this reason, the datasets were analyzed independently. The objective was not to generate a universal model of SBS morphology but to evaluate whether DoF and RoF remained predictable descriptors within each material-specific experimental domain.

2.2. Dataset coding and morphology descriptor selection

The PS and PSf datasets were organized independently because the processing variables in their respective Box-Behnken designs represented different physical factors. To provide a common input structure for ML analysis, the experimental variables in each dataset were expressed as three coded predictors, x_1 , x_2 , and x_3 . This allowed the models to use normalized design variables rather than predictors expressed in different units. The coded variables were interpreted only within each polymer system.

For the PS dataset, x_1 , x_2 , and x_3 corresponded to polymer concentration, air pressure, and solution feed rate, respectively [1]. For the PSf dataset, the same coded notation corresponded to working distance, solution feed rate, and air pressure, respectively [4]. Therefore, although both datasets shared the same Box-Behnken structure, they were not merged into a single model. Each dataset was analyzed separately to avoid assigning the same physical meaning to predictors that represented different SBS processing conditions.

The selected response variables were DoF and RoF. DoF was treated as the primary response because fiber diameter is one of the most widely used quantitative descriptors for comparing solution-blow-spun polymer systems [11]. RoF was analyzed as a complementary descriptor because it provides information about the relative contribution of fibers compared with beads, aggregates, or other morphological features observed in SEM images [1, 4].

In the PS dataset, DoF and RoF described a predominantly fibrous material system. In the PSf dataset, the same descriptors were evaluated in a mixed bead-fiber morphology. Mean and median DoF values were additionally considered for PSf to determine whether the statistical representation of fiber diameter affected predictive performance. This comparison was

used to assess whether DoF remained informative when the morphology shifted from predominantly fibrous mats to bead-containing structures.

2.3. Machine learning modeling, validation, and performance assessment

The ML analysis was performed independently for each polymer dataset and each morphology descriptor. As shown in Figure 2, the workflow comprised five main stages: data preprocessing, data splitting, regression model training and validation, performance evaluation, and descriptor predictability interpretation. This structure was used to compare the predictive behavior of DoF and RoF within each material-specific experimental domain.

The original experimental information was reorganized into a format suitable for analysis in MATLAB R2025b. The coded variables x_1 , x_2 , and x_3 were used as predictors, while DoF and RoF were used as response variables. Models were trained using the Regression Learner App and included regression algorithms spanning different levels of flexibility. Linear regression and stepwise linear regression were included as baseline models, whereas support vector machines, Gaussian process regression, regression trees, ensemble trees, kernel regression, and neural network models were evaluated to explore possible nonlinear

relationships between SBS processing variables and morphological descriptors [9, 10].

Given the small size of the Box–Behnken datasets, model validation was carried out using 5-fold cross-validation rather than a single train–test split. This strategy preserved more observations for model training while providing a more stable estimate of predictive performance. This consideration is particularly important in materials ML, where small experimental datasets require careful validation to reduce overfitting and avoid overinterpretation of model performance [12, 13]. Similar approaches have been reported in nanofiber-related ML studies using limited experimental datasets to predict fiber diameter or morphology under controlled validation strategies [9, 14, 15].

Model performance was evaluated using the root mean square error (RMSE), mean absolute error (MAE), and coefficient of determination (R^2). RMSE and MAE quantified the magnitude of prediction errors, whereas R^2 estimated the proportion of experimental variability explained by each model. For each material and response, the best-performing model was selected by considering the lowest RMSE together with the highest R^2 . MAE was used as a complementary criterion when models showed similar performance.

The objective of this analysis was not to develop a universal predictive model of SBS morphology but to evaluate whether each morphological descriptor could

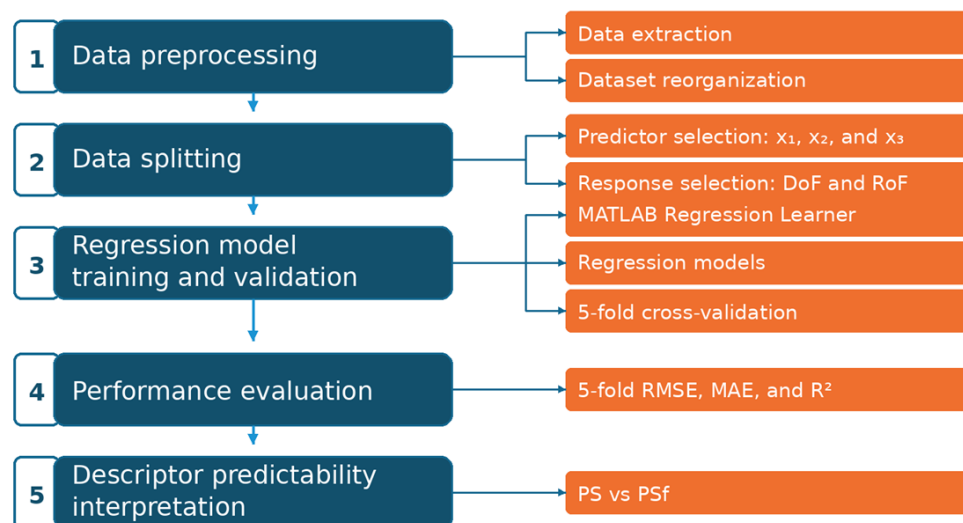


Figure 2. Machine-learning workflow used for the reanalysis of the SBS Box–Behnken datasets. SBS, solution blow spinning; DoF, diameter of fibers; RoF, relative amount of fibers; RMSE, root mean square error; MAE, mean absolute error; R^2 , coefficient of determination; PS, polystyrene; PSf, polysulfone.

be predicted reliably within the experimental limits of the original Box–Behnken designs. Accordingly, model performance was treated as a diagnostic indicator of descriptor predictability, while its relationship to morphological representativeness was interpreted in the context of the material regime and available predictors. The complete model comparison generated by MATLAB was retained as supplementary material, whereas the main manuscript reports only the best-performing model for each response.

3. Results and discussion

3.1. Predictive performance of morphology descriptors in PS and PSf datasets

The ML analysis was conducted independently for each polymer system and morphological descriptor. The best-performing models obtained under 5-fold cross-validation are summarized in Table 2. Model performance was compared using R^2 together with RMSE and MAE, rather than categorical performance labels, so that each response could be evaluated directly within its material-specific experimental domain.

For the PS dataset, mean DoF showed the highest predictive performance among the evaluated responses. The Linear Regression model yielded an R^2 of 0.8142, an RMSE of 142.45 nm, and an MAE of 91.32 nm. Within the analyzed Box–Behnken design space, these results indicate a clear relationship between the coded processing variables and fiber diameter. By comparison, RoF was substantially less predictable: the support vector machine model yielded an R^2 of 0.0934, an RMSE of 0.270, and an MAE of 0.210. Thus, although RoF was useful as an optimization response in the original study, its variation was not captured by the available predictors as consistently as DoF.

The PSf dataset showed a different pattern. Mean DoF yielded an R^2 of 0.0043, an RMSE of 23.60 nm, and an MAE of 20.14 nm. The numerically smaller absolute errors relative to PS should not be interpreted as better predictive performance because the response scales and variances differ between datasets. The near-zero R^2 indicates that the model captured little of the observed variation in mean DoF. Replacing the mean with the median did not materially change this behavior: the Tree model produced an R^2 of 0.0480, an RMSE of 24.86 nm, and an MAE of 20.63 nm. This finding suggests that the weak DoF prediction was not primarily attributable to the choice of central-tendency statistic.

For PSf, RoF produced the highest R^2 among the evaluated responses, with the Kernel model reaching an R^2 of 0.2158, an RMSE of 0.243, and an MAE of 0.179. Nevertheless, most of the response variability remained unexplained by the available processing variables. Overall, the two datasets exhibited a marked contrast in descriptor predictability, particularly for DoF. The morphological basis of this difference is examined in Section 3.2.

3.2. Morphology-dependent predictability of DoF

The contrast in DoF predictability between the PS and PSf datasets becomes clearer when the validation parity plots are examined (Figure 3). For PS, predicted DoF values generally followed the experimental trend and were distributed relatively close to the perfect-prediction line. This behavior is consistent with the quantitative performance reported in Table 2 and indicates that, within the PS experimental domain, changes in polymer concentration, air pressure, and solution feed rate produced variation in fiber diameter that could be captured by the regression model.

Table 2. Best-performing ML models and validation metrics for the PS and PSf datasets

Material	Morphology regime	Descriptor	Best model	RMSE	MAE	R^2
PS	Predominantly fibrous	Mean DoF	Linear Regression	142.45	91.32	0.8142
PS	Predominantly fibrous	RoF	SVM	0.270	0.210	0.0934
PSf	Bead–fiber	Mean DoF	Ensemble	23.60	20.14	0.0043
PSf	Bead–fiber	Median DoF	Tree	24.86	20.63	0.0480
PSf	Bead–fiber	RoF	Kernel	0.243	0.179	0.2158

Notes: ML, machine learning; DoF, diameter of fibers; RoF, relative amount of fibers; SVM, support vector machine; RMSE, root mean square error; MAE, mean absolute error; R^2 , coefficient of determination. RMSE and MAE are expressed in nanometers for DoF and in the original response units for RoF.

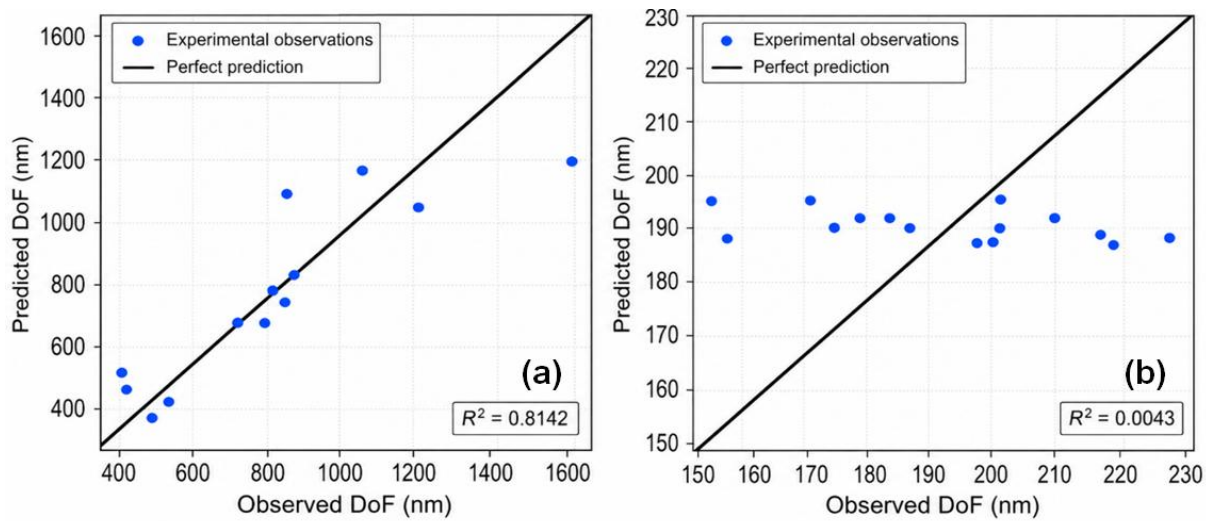


Figure 3. Validation parity plots for DoF prediction in predominantly fibrous PS (A) and bead-fiber PSf (B) mats. DoF, diameter of fibers; PS, polystyrene; PSf, polysulfone.

The PSf parity plot showed a markedly different pattern. Predicted DoF values were concentrated within a comparatively narrow range and did not reproduce the full variation in the experimental observations. This pattern is consistent with the near-zero R^2 obtained for mean DoF and the similarly weak performance obtained when median DoF was used. Thus, changing the central-tendency statistic did not resolve the limited relationship between the available PSf processing variables and measured fiber diameter.

The difference is consistent with the morphology of the two material systems. In the PS dataset, the mats were predominantly fibrous, and DoF therefore described one of the principal structural features of the material. Under this regime, changes in processing conditions were reflected directly in fiber diameter. In the PSf dataset, however, fibers coexisted with beads. Under these conditions, DoF characterizes only the fibrous fraction and does not describe bead size, bead density, bead spacing, bead shape, or fiber-bead connectivity. Consequently, samples with similar DoF values may still differ substantially in their overall architecture.

The processing context must also be considered when interpreting this contrast. Fiber formation in SBS is governed by coupled solution and operating variables, including polymer concentration, viscosity, chain entanglement, surface tension, air pressure, solution feed rate, and working distance [16-19]. Recent SBS results further show that changes in spraying distance, pressure,

feed rate, and polymer concentration can affect fiber diameter distributions, mat density, and fiber uniformity [19]. The PSf dataset did not include polymer concentration or direct solution-property descriptors among its predictors, even though these factors can influence the transition between droplets, beads, and continuous fibers. Therefore, the low predictive performance for PSf should not be interpreted as evidence that DoF alone caused the reduced model performance. Rather, with the available predictors, DoF did not provide a robust processing-morphology response for this bead-fiber regime.

Taken together, these observations indicate that the predictive usefulness of DoF depends on both the structural regime represented by the dataset and the information contained in the selected predictors. When fibers dominate the material architecture, DoF can provide a direct and informative process response. When beads and fibers coexist, additional structural descriptors are needed to characterize the morphology more comprehensively.

3.3. ML-assisted descriptor evaluation for SBS morphology analysis

Beyond predicting individual morphological responses, the present results suggest that ML performance can provide a complementary diagnostic criterion for evaluating descriptor suitability within a defined SBS experimental domain. In conventional

design-of-experiments and RSM approaches, response variables are selected before modeling and are subsequently related to processing factors and optimized. However, an optimizable response is not necessarily a complete representation of the resulting material morphology. Recent blow-spinning studies continue to use DOE, RSM, and quality-by-design frameworks to relate processing factors to selected material responses and optimize fabrication conditions [20–22].

This interpretation requires caution. Predictive performance alone does not establish the structural representativeness of a descriptor because model behavior also depends on dataset size, predictor selection, response variability, measurement uncertainty, and the validation procedure. In the present study, the contrasting PS and PSf results should therefore be regarded as a descriptor-level diagnostic within two material-specific Box–Behnken datasets rather than as evidence of universal predictive generalization. Nevertheless, the comparison highlights an important practical point: descriptors commonly used for morphological characterization should not automatically be assumed to be equally informative across different structural regimes.

For predominantly fibrous SBS mats, DoF may be an appropriate ML target because it describes a dominant structural feature. For bead–fiber systems, a more complete representation may require descriptors such as bead size, bead density, bead spacing, bead shape, fiber continuity, fiber–bead connectivity, and parameters describing the fiber-diameter distribution. Incorporating these features would allow future models to represent both fibrous and bead-related components of complex SBS morphologies rather than reducing the material architecture to a single size descriptor.

The small size of the datasets analyzed here is an additional limitation. Small experimental datasets require careful validation, transparent reporting of performance metrics, and restrained interpretation to reduce overfitting and avoid unsupported claims of generalization [12, 13]. Future SBS–ML studies should therefore combine larger and more diverse datasets with independent validation points, physicochemical solution properties, and image-derived morphology descriptors. Recent work has shown that deep features extracted directly from SEM images can be coupled with ML to estimate nanofiber diameter across smooth and beaded morphologies, supporting the potential of image-based

representations for morphology-aware modeling [23]. In parallel, the recent availability of curated public SBS datasets provides a useful basis for broader cross-system analyses by integrating processing conditions, solution-related variables, and fiber-morphology information from multiple polymer systems and published studies [24]. Such aggregated resources may facilitate model development and external validation, although differences in experimental protocols, variable definitions, and reporting practices should be carefully considered when combining data from independent studies. Within this framework, ML can serve not only as a predictive tool but also as a means of identifying which response variables provide the most informative links between SBS processing conditions and the resulting material structure.

4. Conclusions

A machine-learning-assisted reanalysis of two previously reported SBS datasets revealed a marked morphology-dependent difference in the predictive behavior of conventional morphological descriptors. Within the predominantly fibrous PS system, fiber diameter showed a strong relationship with the available processing variables, whereas its predictability was markedly reduced in the bead–fiber PSf system. These results indicate that the usefulness of a morphological descriptor depends not only on its conventional use in fiber characterization but also on the structural regime of the material and the information represented by the selected process variables.

More broadly, the results support the use of ML performance as a complementary diagnostic tool for evaluating descriptor suitability within a defined experimental domain. Predictive performance should not, however, be interpreted as direct evidence of structural representativeness, particularly when datasets are small or relevant physicochemical predictors are unavailable. Future SBS–ML studies should therefore integrate larger datasets, independent validation, solution-property information, and image-derived descriptors capable of representing both fibrous and bead-related features. Such an approach may improve the selection of response variables and strengthen the interpretation of processing–structure relationships in complex SBS morphologies.

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Conflict of Interest

The authors declare no conflict of interest.

Author Contributions

- **Claudia Ivette Rivera Vera** was responsible for Investigation, Resources, Writing – original draft, Project administration, and Supervision.
- **Jonathan Josué Cid Galiot** was responsible for Methodology, Software, Data curation, Formal analysis, and Visualization.
- **José Roberto Grande Ramírez** was responsible for Methodology, Resources, Software, Data curation, Formal analysis, and Visualization.
- **José Ernesto Domínguez Herrera** was responsible for Conceptualization, Funding acquisition, Resources, Validation, Writing – review & editing, and Project administration.

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Graphical Abstract

