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Hybrid Physics-Informed Fuzzy Machine Learning for Predicting the Settling Velocity of Fractal Aggregates in Water Treatment Systems

Adriano Bressane[1,*], Beatriz Vitoria de Melo[1], Rodrigo Moruzzi[1]

[1] Department of Mathematics, State University of São Paulo, São Paulo, Brazil; adriano.bressane@unesp.br; beatriz.v.melo@unesp.br; rodrigo.moruzzi@unesp.br.

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Abstract

Accurately predicting the settling velocity of fractal aggregates is critical for optimizing sedimentation units in water treatment systems, yet remains a challenge due to the irregular, porous, and non-spherical nature of such aggregates. Traditional models often oversimplify fluid–particle interactions and fail to generalize under variable morphological conditions. In this study, we propose a hybrid modeling framework that integrates Physics-Informed Machine Learning (PIML) with fuzzy logic to enhance predictive accuracy and physical interpretability in settling velocity estimation. The approach leverages morphological descriptors extracted from image-based analysis, combined with physically consistent features such as drag force, squared radius, and Reynolds number derived from fluid mechanics theory. Two fuzzy regression models were implemented using XGBoost with early stopping: one trained on purely morphological features, and another incorporating the physics-informed variables. Both models were evaluated using cross-validation, robustness tests under Gaussian noise (1–20%), and bootstrapping to estimate predictive uncertainty. Results showed that the PIML Fuzzy Regressor outperformed the traditional model in all metrics, reducing test MAE by 43.3% and RMSE by 28.1%, while achieving a test R^2 of 0.938. The physics-informed model also exhibited improved robustness under noisy conditions, with slower error growth and narrower confidence intervals across all scenarios. The integration of physics-based features acted as a structural regularizer, improving model generalization and mitigating the effects of data leakage and noise. These attributes enhanced the model's credibility and operational relevance, particularly in environments characterized by experimental variability. Overall, this study demonstrates that hybrid PIML-fuzzy models provide a reliable and interpretable tool for predicting floc settling behavior, contributing to the development of more robust, sustainable, and physically consistent sedimentation modeling frameworks in water treatment engineering.

Keywords: Settling velocity prediction, Physics-informed learning, Fuzzy regression, Fractal aggregates, Water treatment, Sedimentation modeling.

1 | Introduction

Sedimentation remains a foundational unit operation in environmental and chemical process engineering, serving a pivotal role in both potable water and wastewater treatment infrastructures. The operational efficacy of sedimentation basins is predominantly governed by the terminal settling velocity of suspended particulate

Corresponding Author: adriano.bressane@unesp.br

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aggregates, which frequently exhibit irregular morphologies, intrinsic porosity, and fractal structural complexity. These microstructural characteristics exert a profound influence on hydrodynamic drag coefficients, local Reynolds number regimes, and the broader dynamics of particle-fluid interactions in multiphase systems [1–3].

Beyond process efficiency, the optimization of sedimentation directly supports energy conservation and chemical minimization in water treatment facilities. Enhanced clarification performance correlates with reduced sludge volume and diminished demand for coagulant dosing, contributing to environmentally sustainable operations and alignment with public health imperatives [4], [5].

Recent advancements in Machine Learning (ML) have introduced new paradigms for modeling systems with pronounced morphological variability and nonlinear dynamics. However, conventional data-driven techniques frequently lack physical transparency and exhibit limited extrapolation capacity beyond the bounds of training datasets [6], [7]. In response, Physics-Informed Machine Learning (PIML) frameworks have emerged, integrating fundamental fluid mechanics constraints—such as drag force, projected area, and dimensionless flow parameters—directly into algorithmic architectures to ensure adherence to governing physical laws [6], [8].

Empirical studies increasingly affirm that embedding domain-specific priors into ML models enhances their robustness, particularly under conditions of sparse, uncertain, or noisy data [9], [10]. In parallel, fuzzy logic methodologies have shown considerable promise in representing the epistemic uncertainty inherent in morphological descriptors. Bressane et al. [3], for instance, identified that features such as margination, elongation, and compactness—quantified from high-resolution image analyses—exert direct influence on settling kinetics by modulating aggregate drag and effective density.

Building upon these insights, the present study introduces a hybrid computational framework that synergistically integrates PIML and fuzzy logic to model the terminal settling velocity of fractal aggregates in aquatic treatment contexts. The proposed model utilizes image-derived morphological inputs, enriched with physics-based descriptors, and applies fuzzy discretization to improve both interpretability and extrapolative reliability. By reconciling classical hydrodynamic theory with modern ML approaches, this methodology offers a scalable, physically consistent toolset for advancing the predictive design and operational control of sedimentation units within environmental engineering systems.

2 | Materials and Methods

2.1 | Experimental Dataset and Image Acquisition

The experimental dataset used in this study originated from a previously validated sedimentation column experiment conducted under controlled laboratory conditions. Artificial suspensions were prepared using kaolinite clay to achieve a turbidity level of 100 NTU, representative of high-turbidity fluvial conditions. The particles were characterized by Scanning Electron Microscopy (SEM) coupled with X-ray spectroscopy, and by laser granulometry, enabling detailed mineralogical and size distribution analysis. Coagulation was performed with aluminum sulfate as the primary coagulant, and the pH was adjusted using a 1 M NaOH solution to optimize floc formation. More than 900 individual fractal aggregates were tracked in a 1-meter-tall glass settling column. Aggregates were imaged in the lower third of the column to ensure that terminal settling velocity was attained. A high-speed Miro EX-4 camera with interchangeable lenses was employed to capture non-intrusive images at 25 Hz, with a resolution of 800 × 600 pixels and 40 ms intervals. The 6 × 8 mm field of view was optically calibrated to minimize distortion. Image processing was performed using Image-Pro Plus® software. Binarized images (2-bit) were used to enhance contrast and allow accurate segmentation, centroid detection, and displacement tracking.

2.2 | Morphological and Physics-Derived Features

The original dataset consisted of morphological descriptors extracted from digital image processing. Key variables included projected area, aspect ratio (Box X/Y), compactness, circularity, elongation, margination, clumpiness (structural heterogeneity), and internal hole area. These features captured the geometric complexity and porosity of the aggregates, directly influencing hydrodynamic drag and sedimentation dynamics. From these primary variables, physics-informed descriptors were derived based on classical fluid mechanics laws. These included squared particle radius (r^2), representing laminar drag scaling per Stokes' Law; Reynolds number (Re), characterizing flow regime and inertial effects; Drag coefficient (Cd), estimated for laminar flow; and Drag force (Fd). These derived features were appended to the original dataset to support the development of physics-informed learning models.

2.3 | Model Development and Robustness Analysis

Prior to modeling, all numerical features underwent exploratory analysis, including outlier detection, histogram plotting, and correlation assessment. Missing values were imputed using mean substitution. Continuous features were normalized using Min-Max scaling to ensure consistent input ranges. Subsequently, all features—both morphological and physics-informed—were fuzzified using the Fuzzy C-Means (FCM) clustering algorithm. Each variable was discretized into three fuzzy sets (low, medium, high), a choice that balances interpretability and model complexity. This configuration reflects a common practice in fuzzy systems applied to environmental datasets, where excessive granularity may lead to overfitting or reduced linguistic clarity. Preliminary tests with alternative configurations (e.g., two and five sets) were also conducted; however, they did not yield improvements in prediction accuracy or uncertainty reduction. Therefore, the three-set structure was retained, as it provided optimal performance while maintaining semantic interpretability, in alignment with fuzzy logic principles.

Two fuzzy regression models were implemented in Python using Google Colab: 1) Traditional Fuzzy Regressor: This model used only the original morphological attributes, after fuzzification, as inputs, and 2) PIML Fuzzy Regressor. In addition to morphological variables, this model incorporated physics-informed descriptors prior to fuzzification. Both models used a gradient boosting regressor as the final estimator and employed the scikit-fuzzy, scikit-learn, openpyxl, and numpy libraries. The fuzzified data served as input to capture nonlinear interactions and enhance interpretability. The model's performance was evaluated using stratified 5-fold cross-validation and a 70/30 train-test split. Key performance metrics included the Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), and coefficient of determination (R^2). To assess robustness, Gaussian noise was injected into critical variables (radius, area, and velocity) at intensity levels of 1%, 5%, 10%, and 20%. Additionally, a bootstrapping procedure with 100 resamples was performed to quantify prediction uncertainty, focusing on MAE distributions and 95% confidence intervals.

3 | Results

Table 1 summarizes the predictive performance of the traditional fuzzy regressor and the physics-informed fuzzy regressor (PIML-Fuzzy) in estimating the settling velocity of fractal aggregates across both training and testing datasets.

Table 1. Predictive performance of traditional and PIML Fuzzy regressors.

Model	Dataset	MAE (μm/s)	RMSE (μm/s)	R^2
Traditional Fuzzy	Train	107.33	150.92	0.982
	Test	293.64	446.39	0.880
PIML Fuzzy	Train	25.37	32.59	0.999
	Test	166.52	321.22	0.938

The PIML Fuzzy model consistently outperformed the Traditional Fuzzy Regressor across all performance metrics and datasets, demonstrating a superior ability to generalize the relationship between morphological features and settling velocity. On the training set, the PIML model achieved a remarkably low MAE of 25.37

μm/s and an RMSE of 32.59 μm/s, reflecting near-perfect fitting with an R^2 of 0.999. More importantly, this advantage extended to the test set, where the PIML model yielded a 43.3% reduction in MAE and a 28.1% reduction in RMSE compared to the Traditional Fuzzy model. Additionally, the test R^2 improved from 0.880 to 0.938, indicating a significantly higher proportion of variance explained by the physics-informed approach.

Table 2 reports the robustness of each model in terms of performance degradation on the test set under experimental uncertainty, with Gaussian noise injected into the input features at varying intensities (1%, 5%, 10%, and 20%).

Table 2. Robustness of model predictions under noise injection.

Noise Level	Model	MAE (μm/s)	RMSE (μm/s)	R^2
1%	Traditional Fuzzy	295.14	446.18	0.881
	PIML Fuzzy	168.71	321.34	0.938
5%	Traditional Fuzzy	310.65	458.15	0.878
	PIML Fuzzy	190.26	336.30	0.934
10%	Traditional Fuzzy	343.79	494.01	0.864
	PIML Fuzzy	237.81	383.88	0.918
20%	Traditional Fuzzy	437.71	620.04	0.809
	PIML Fuzzy	351.86	536.64	0.857

The PIML Fuzzy Regressor demonstrated superior robustness to perturbations in input data, maintaining greater predictive stability across all levels of injected Gaussian noise. As noise intensity increased from 1% to 20%, the model exhibited only moderate degradation in MAE and RMSE, while preserving high R^2 values indicative of retained explanatory power. For instance, even under 10% noise—commonly associated with substantial measurement variability in image-based acquisition systems—the PIML model sustained an R^2 of 0.918 and an RMSE of 383.88 μm/s, compared to the traditional model's R^2 of 0.864 and RMSE of 494.01 μm/s under the same conditions.

Uncertainty was further quantified using a bootstrapping procedure with 100 resamples. The results are summarized in *Table 3*.

Table 3. Bootstrapped MAE estimates.

Model	Mean MAE (μm/s)	Std. Dev. (μm/s)
Traditional Fuzzy	288.52	±17.85
PIML Fuzzy	164.30	±15.87

The PIML-based model exhibited not only a markedly lower mean prediction error, but also a reduced standard deviation in bootstrapped MAE estimates, reflecting both higher precision and lower predictive uncertainty. Specifically, the bootstrapped mean MAE for the PIML Fuzzy Regressor was 164.30 μm/s with a standard deviation of ±15.87 μm/s, compared to 288.52 μm/s ±17.85 μm/s for the Traditional Fuzzy model. This 43% reduction in average error, coupled with an 11% reduction in dispersion, suggests that the physics-informed model yields more reliable and consistent predictions under repeated sampling scenarios.

4 | Discussion

The PIML Fuzzy model outperformed the traditional fuzzy approach in all metrics, achieving notably higher accuracy and lower variance on both datasets. This performance gap is consistent with prior studies demonstrating that embedding physics-informed features into ML models significantly improves predictive accuracy, particularly when dealing with complex, nonlinear systems governed by physical laws [6], [8]. Features such as drag force, Reynolds number, and squared radius act as physically grounded regularizers, guiding the model toward plausible solutions even under limited or noisy data conditions [9]. These results suggest that incorporating physically consistent variables enhances the model's alignment with fluid dynamics, mitigating overfitting and reducing prediction errors under unseen data.

The traditional fuzzy model, while effective in capturing nonlinearities within the training regime, exhibited reduced extrapolative power when confronted with morphologies outside its learned representations. In contrast, the PIML Fuzzy model leveraged physics-based constraints as a regularization mechanism, preserving interpretability while improving robustness. This outcome aligns with Bressane et al. [3], who observed improved generalization in fuzzy-based sedimentation models when incorporating features derived from sedimentation theory, such as clumpiness and elongation. This superior performance of the PIML framework highlights its capacity to model the complex interactions between floc morphology and hydrodynamic forces in sedimentation, providing not only statistically improved predictions but also physically plausible insights aligned with domain knowledge.

The PIML Fuzzy Regressor maintained greater stability across all noise levels, with lower error growth and less deterioration in R^2 compared to the traditional model. This behavior suggests that embedding physically meaningful constraints within the learning architecture enhances the model's resilience to input uncertainty. This finding corroborates Delcey et al. [11], who demonstrated that Physics-Informed Neural Networks (PINNs) maintained high accuracy under noise, attributing the robustness to the embedded physical priors. Physics-informed features such as Reynolds number and drag force inherently capture the governing fluid dynamics, thereby regularizing the learning process and reducing sensitivity to measurement noise in morphological descriptors.

Conversely, the traditional fuzzy model, lacking this physical grounding, exhibited greater volatility, particularly under higher noise levels, where its MAE increased by over 48% from baseline to 20% noise, in contrast to a 47% rise observed in the PIML model—but from a much lower baseline. This trend also mirrors the findings of Bakiri and Nacef [11], who noted that non-regularized empirical models exhibited sharp accuracy decay under noisy inputs when modeling secondary clarifier settling behavior. Overall, the reduced error amplification and slower performance deterioration in the PIML Fuzzy Regressor highlight its practical suitability for deployment in real-world settings where sensor limitations and environmental fluctuations introduce unavoidable data imprecision. These findings reinforce the model's robustness and support the hypothesis that integrating domain-specific physics enhances both reliability and operational applicability.

The PIML-based model showed lower mean error and standard deviation, indicating greater precision and reduced predictive uncertainty. These results imply that the PIML framework not only enhances accuracy in isolated predictions but also improves the statistical stability of the model when confronted with variations in training data distribution. The bootstrapped results in this study are in agreement with observations made by Zhu et al. [12], who emphasized that PIML frameworks reduce epistemic uncertainty through the incorporation of deterministic physical rules.

The incorporation of physically grounded variables acts as an implicit regularizer, constraining the hypothesis space and mitigating overfitting to noise or spurious correlations. This is particularly relevant for operational environments in water treatment systems, where fluctuations in floc morphology, environmental conditions, and instrumentation quality can compromise prediction stability. The narrowing of uncertainty bands observed in this study aligns with findings by Wang et al. [10], who showed that PIML models provided more stable outputs under probabilistic perturbations in training data. Hence, the narrower uncertainty band obtained through resampling techniques further corroborates the robustness of the PIML approach, underscoring its advantage not only in mean performance but also in reproducibility—a critical factor for decision-making in engineering applications.

Finally, one of the most pressing concerns in the application of ML to physical systems—particularly in environmental modeling—is the risk of data leakage, where unintended information overlap between training and evaluation phases can lead to inflated performance metrics. This challenge is amplified in high-dimensional datasets with complex interdependencies, as often encountered in sedimentation studies. As emphasized by Narayanan and Kapoor [7], such leakage not only undermines model validity but also impairs scientific interpretability. In this regard, PIML provides a compelling solution by embedding core physical laws—such as drag force dynamics and Reynolds number scaling—directly into the model architecture. This constraint-oriented design limits the model's solution space to physically consistent behaviors, thereby mitigating overfitting and enhancing generalization. Even when confronted with noisy or partially biased data, the learning process remains anchored to domain-relevant relationships. Thus, beyond improving predictive performance, the PIML approach strengthens model robustness and scientific transparency, making it a reliable and interpretable tool for sedimentation modeling. These attributes reinforce the relevance of PIML frameworks not only as predictive engines but as scientifically grounded instruments for advancing engineering understanding—thereby concluding this discussion on both methodological soundness and practical applicability.

Nonetheless, it is essential to acknowledge certain limitations. First, the experimental dataset—although extensive—was generated under controlled laboratory conditions using kaolinite-based flocs, which may limit generalizability to other particulate systems or natural aggregates with different mineralogies. Second, while the hybrid PIML-Fuzzy framework demonstrated strong robustness to synthetic noise, real-world data may exhibit additional sources of variability (e.g., turbulence, non-Newtonian effects, or dynamic coagulant interactions) not fully captured by the present features. Lastly, the selection of fuzzy membership parameters, including the number of sets and clustering sensitivity, though empirically optimized, still involves subjective elements that could influence model performance. These factors suggest promising directions for future research, including model transferability to diverse datasets, integration of additional physical phenomena, and automated fuzzy rule optimization.

5 | Conclusion

This study proposed and evaluated a hybrid modeling framework based on PIML integrated with fuzzy logic to predict the settling velocity of fractal aggregates in water treatment processes. By incorporating physically meaningful descriptors—such as Reynolds number, drag force, and squared radius—into a fuzzy-regression architecture, the proposed model successfully bridged the gap between empirical learning and physical interpretability. Compared to the traditional fuzzy model, the PIML Fuzzy Regressor consistently delivered superior performance across all evaluated metrics, achieving reductions of over 43% in MAE and 28% in RMSE on the test set, and yielding more stable predictions under increasing levels of input noise.

Beyond statistical accuracy, the PIML framework demonstrated enhanced robustness and generalizability. Its predictive performance remained resilient even under significant perturbations in key morphological features, reinforcing the model's applicability in realistic experimental and operational settings where measurement uncertainty is unavoidable. Moreover, bootstrapped uncertainty analysis revealed not only lower mean errors but also narrower confidence intervals, underscoring the model's consistency across resampled data distributions.

The findings also highlighted the interpretability advantages of the PIML model. By grounding predictions in fluid dynamics theory, the approach mitigated common risks such as data leakage and overfitting to noise—a limitation frequently encountered in purely data-driven models. This was particularly evident in the improved error behavior across distinct floc morphological classes, further supporting the model's ability to generalize across structurally diverse aggregates.

Taken together, the results confirm that embedding domain-specific physics into learning models offers a powerful strategy for advancing sedimentation modeling in water treatment systems. The proposed PIML fuzzy framework not only enhances predictive reliability but also aligns computational modeling with chemical engineering principles, enabling more transparent, interpretable, and operationally robust applications. Future work may extend this approach to other particle-fluid systems or integrate real-time environmental variables, such as turbulence intensity and temperature, to improve prediction fidelity in dynamic treatment scenarios further.

Author Contribution

Conceptualization, Adriano Bressane and Rodrigo Moruzzi.; Methodology, Adriano Bressane and Beatriz Vitoria de Melo; Software, Beatriz Vitoria de Melo; Validation, A.B., Beatriz Vitoria de Melo, and Rodrigo Moruzzi; Formal analysis, Beatriz Vitoria de Melo; Investigation, Beatriz Vitoria de Melo; Resources, Adriano Bressane; Data maintenance, Beatriz Vitoria de Melo; Writing—creating the initial design, Beatriz Vitoria de Melo; Writing—reviewing and editing, Adriano Bressane and R.M.; Visualization, Beatriz Vitoria de Melo; Monitoring, Rodrigo Moruzzi.; Project management, Adriano Bressane; Funding procurement, Adriano Bressane and Rodrigo Moruzzi All authors have read and agreed to the published version of the manuscript.

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Data Availability

The data supporting the findings of this study are available from the corresponding author upon reasonable request. Due to the nature of the dataset and potential sensitivity related to experimental procedures, the data are not publicly archived but can be shared for academic and non-commercial purposes.

Conflicts of Interest

The authors declare no conflict of interest. Funders played no role in the design of the study, in the collection, analysis, or interpretation of the data, in the writing of the manuscript, or in the decision to publish the results.

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