Deep Learning-Based Surrogate Modeling of PDE Governed Systems Using Fourier Neural Operators (FNOs): Application to Clarifier Dynamics in Wastewater Treatment

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Abstract

Clarifiers are critical to wastewater treatment, where accurate prediction of sludge settling dynamics is essential for maintaining effluent quality and enabling real-time process control. Mechanistic modelling of clarifiers typically requires solving nonlinear advection–diffusion–settling PDEs, which, while accurate, impose heavy computational costs that limit their use in digital twins, optimization, and rapid scenario analysis. This work develops a fast surrogate based on the Fourier Neural Operator (FNO) to learn the solution operator of a validated one-dimensional clarifier model. A comprehensive synthetic dataset is generated using a finite-difference solver across varying initial concentration profiles, hydraulic loads, and feed conditions. Trained to map initial and boundary conditions to final solids concentration fields, the FNO achieves sub-percent relative L_2 errors, generalizes robustly to unseen operating regimes, and delivers inference speedups exceeding $10^3\times$ compared to the numerical solver. Spatial error analysis shows that the surrogate accurately captures key settling phenomena, including stratification, hindered settling, and compression-zone behavior. Limitations include minor boundary inaccuracies and a fixed prediction horizon, which motivate future hybrid extensions incorporating physics-informed constraints. Overall, the proposed framework demonstrates that neural operator learning provides an accurate, mesh-independent, and computationally efficient surrogate for clarifier dynamics, supporting real-time simulation and decision-making in process engineering.

1 Introduction

Clarifiers are fundamental components of wastewater treatment systems, where they enable the gravitational settling of suspended solids and directly influence effluent quality, sludge recirculation, and the stability of downstream biological processes. Their importance has been widely recognized in both operational practice and modeling studies Ekama (1997); Alex et al. (2006). As treatment plants increasingly rely on advanced automation and real-time decision support, the need for accurate and computationally efficient clarifier models has grown significantly.

A variety of one-dimensional models have been developed to describe clarifier dynamics. Empirical approaches, such as the Takács model (Takács et al. (1991)), provide a simplified representation of settling behavior through layer-based flux relationships. Although these models are computationally efficient, they often struggle to capture key transitions such as compression settling or sludge blanket movement under transient hydraulic conditions. To address these limitations, more detailed mechanistic formulations have been introduced. Notably, the Bürger–Diehl family of models Bürger & Hvistendahl Karlsen (2001); Bürger et al. (2011) describes solids transport using nonlinear convection–diffusion PDEs with degenerate diffusion and compression effects, offering a physically grounded description of sedimentation processes. However, solving these PDEs typically requires high-resolution numerical schemes, which can make repeated or real-time simulations computationally prohibitive Bürger et al. (2013).

Machine learning has emerged as a promising avenue for accelerating complex environmental and process simulations. Yet conventional neural network architectures are generally constrained to fixed spatial discretizations and are not inherently equipped to learn operator-level behavior or generalize across varying boundary and initial conditions capabilities that are essential for modeling clarifier dynamics. While Physics-Informed Neural Networks (PINNs) Raissi et al. (2019) incorporate PDE constraints directly into the training process, they often face convergence challenges and may perform poorly in regions with sharp concentration gradients or discontinuities, such as those occurring in compression zones.

Neural operator learning offers a fundamentally different perspective. Rather than predicting pointwise values, neural operators aim to approximate mappings between entire function spaces, enabling grid-independent generalization and improved handling of nonlinear spatial interactions. Among these approaches, the Fourier Neural Operator (FNO) Li et al. (2020) has shown strong performance across a range of physical systems involving complex PDEs, due in large part to its spectral convolution framework and ability to capture long-range spatial dependencies efficiently. Despite these advantages, neural operator methods have not yet been applied to clarifier modeling, leaving an important gap in both wastewater treatment research and scientific machine learning.

To address this gap, the present work develops a Fourier Neural Operator–based surrogate model trained on high-fidelity mechanistic clarifier simulations. By learning the nonlinear operator that governs solids transport, the proposed surrogate provides fast and accurate predictions of clarifier settling behavior while drastically reducing computational cost. This enables new capabilities for real-time scenario evaluation, digital twin integration, and process monitoring. The remainder of this paper details the underlying clarifier model, data generation pipeline, FNO architecture, and a comprehensive evaluation demonstrating prediction accuracy, generalization, robustness, and computational efficiency.

2 Background

Modeling clarifier behavior has been an active research area for several decades, with approaches ranging from empirical settling formulations to detailed mechanistic and numerical models. This section summarizes the foundational developments in clarifier modeling, numerical solution strategies, and machine learning–based surrogate modeling, culminating in neural operator learning frameworks that motivate this work.

2.1 Classical and Mechanistic Clarifier Models

Early clarifier models aimed to represent zone settling and hindered settling using flux theory. A widely used formulation is the Takács model (Takács et al. (1991)), which divides the clarifier into discrete layers and employs empirical settling velocity expressions to capture solids behavior across varying concentration regimes. Although computationally efficient, these flux-based models may oversimplify key transitions such as compression settling and often struggle to capture sludge blanket movement under dynamic hydraulic conditions.

To overcome these limitations, more advanced mechanistic models were developed, most notably the Bürger–Diehl family of one-dimensional PDE-based formulations. Bürger and

Hvistendahl Karlsen Bürger & Hvistendahl Karlsen (2001) introduced a conservation-law framework for sedimentation in which solids concentration evolves according to a nonlinear convection–diffusion equation with degenerate diffusion. Subsequent work by Bürger, Diehl, and collaborators Bürger et al. (2011) incorporated compression settling, sludge rheology, and variable clarifier geometry, establishing a consistent and physically grounded methodology that has become a benchmark for secondary settling tank modeling.

2.1.1 Numerical Solution Methods for Clarifier PDEs

Mechanistic clarifier models rely on robust numerical solvers due to the nonlinear and often stiff nature of the underlying PDEs. Standard finite-difference (FDM) and finite-volume (FVM) approaches can encounter challenges when resolving steep concentration gradients, discontinuities, and degenerate diffusion terms inherent to clarifier dynamics. To address these difficulties, Bürger et al. (2013) proposed high-resolution numerical schemes, including variants of the Yee–Roe–Davis (YRD) method, which provide improved mass conservation and sharp resolution of settling fronts without introducing spurious oscillations.

Despite these advances, high-resolution solvers remain computationally intensive, particularly when simulating long time horizons, performing sensitivity analyses, or executing repeated simulations for real-time control or optimization. As wastewater treatment facilities increasingly adopt digital twins and model-based decision-support systems, the computational burden associated with mechanistic PDE solvers presents a significant practical limitation.

2.1.2 Machine Learning Approaches in Environmental and Process Modeling

Machine learning has been explored as a means to accelerate environmental and process simulations, including applications in hydrodynamics, water-quality modeling, and fluid flow. Conventional neural networks and convolution-based architectures typically operate on fixed grids and are not designed to learn nonlinear operator mappings or generalize across varying boundary and initial conditions. This limits their applicability for clarifier systems, where complex nonlinear interactions, sharp interfaces, and regime transitions are common.

Physics-Informed Neural Networks (PINNs) Raissi et al. (2019) mitigate some of these issues by embedding PDE residuals directly into the training loss. While effective for smooth or moderately complex problems, PINNs often converge slowly and struggle with the steep gradients and discontinuities characteristic of compression settling and sludge blanket formation. These limitations have prevented PINNs from replacing traditional mechanistic solvers for clarifier modeling.

2.2 Neural Operator Learning: A New Paradigm for PDE-Based Surrogates

Neural operator learning has emerged as a powerful framework for learning mappings between infinite-dimensional function spaces, enabling models to approximate full PDE solution operators rather than pointwise responses. This capability allows neural operators to generalize across grid resolutions, parameter regimes, and boundary conditions, making them well suited for complex physical processes.

Among neural operator architectures, the Fourier Neural Operator (FNO) proposed by Li et al. (2020) has demonstrated strong performance across diverse PDE systems, including Navier–Stokes, Darcy flow, and reaction–diffusion equations. By leveraging Fourier transforms for spectral convolution, FNOs efficiently capture long-range spatial dependencies and nonlinear interactions while exhibiting mesh-independent generalization and superior scalability compared with PINNs and conventional neural networks. These properties make FNOs particularly promising for environmental systems characterized by nonlinear, spatially heterogeneous dynamics such as clarifiers.

Despite these advances, no prior studies have applied neural operators to clarifier sedimentation modeling, leaving a clear gap in both the wastewater treatment and machine learning literature. Clarifier dynamics are complex and transient, and resolving them with numerical solvers remains computationally expensive. Neural operator surrogates therefore present a compelling, unexplored opportunity for achieving real-time clarifier simulation.

2.3 Summary of Research Gap

The existing literature highlights three key limitations that motivate this work:

- **Computational cost:** Mechanistic PDE models, while accurate, are too slow for real-time applications.
- **Modeling capability:** Traditional machine learning models lack the ability to learn operator-level behavior required for PDE-governed clarifier dynamics.
- **Unexplored potential:** Neural operators have shown success in multiple physical domains but have not been applied to sedimentation or wastewater treatment processes.

Motivated by these gaps, this study develops a Fourier Neural Operator–based surrogate model that learns clarifier dynamics directly from high-fidelity mechanistic simulations, providing fast and accurate predictions suitable for real-time engineering applications.

3 Method

This section presents the clarifier PDE formulation and boundary conditions, the numerical pipeline used to generate training data, the Fourier Neural Operator (FNO) surrogate architecture and training setup, and the evaluation protocol. The goal is a fast, accurate surrogate that learns the nonlinear operator mapping from initial/boundary conditions to final solids concentration profiles.

3.1 Governing Equations and Boundary Conditions

We model a one-dimensional vertical clarifier with spatial coordinate $z \in [0, H]$, where $z = 0$ denotes the underflow and $z = H$ the effluent as shown in figure 1 .

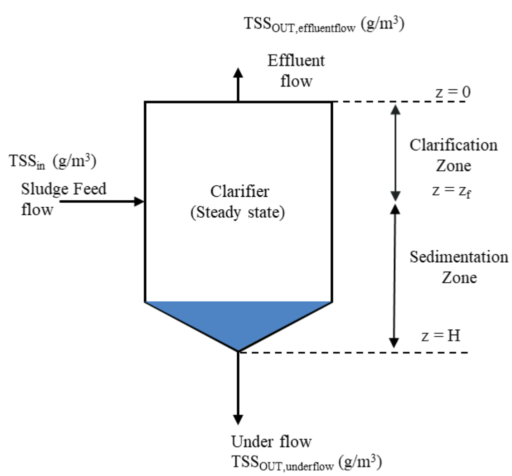


Figure 1: 1D Vertical Clarifier Layout with Boundary Zones and Settling Velocity Field.

Let $C(z, t)$ denote the suspended solids concentration. Following established clarifier formulations De Clercq et al. (2003); Bakiri et al. (2012), the dynamics are written as a nonlinear convection–diffusion balance:

$$\frac{\partial C}{\partial t} = -\frac{\partial F(C; z)}{\partial z} + \frac{\partial}{\partial z}\left(D(C)\,\frac{\partial C}{\partial z}\right) + R(C), \tag{1}$$

where $F(C; z)$ is a zone-dependent sedimentation flux, $D(C)$ is an effective (possibly concentration-dependent) diffusivity, and $R(C)$ can include compression or other source terms. A standard empirical form for the settling velocity is

$$v_s(C) = \max\Big(0,\, \min\big(v_0',\; v_0\,[e^{-r_h(C-C_{\min})} - e^{-r_p(C-C_{\min})}]\big)\Big), \tag{2}$$

with parameters $(v_0, v_0', r_h, r_p, C_{\min})$ is taken from Takács et al. (1991); David et al. (2009). The flux $F(C; z)$ incorporates effluent and underflow through zone-wise expressions consistent with clarifier hydraulics (clarification, feed interface, thickening). We consider multiple initial profiles $C(z, 0) = C_0(z)$ (symmetric/skewed) and enforce physically consistent boundary conditions at the underflow (solids withdrawal) and effluent (quality constraint), implemented in discrete form to ensure mass conservation.

3.2 Numerical Data Generation

To create supervised training data, equation (1) is solved using a validated finite-difference solver. The implementation follows a forward-time, centered-space (FTCS) strategy with stabilizing practices typical of high-resolution clarifier solvers, providing reliable approximations under steep gradients and near interfaces. We systematically vary operating conditions effluent, underflow, and influent flow rates (Q_e, Q_u, Q_f), influent concentration C_f, and diverse $C_0(z)$ profiles to generate approximately 1000 samples at fixed horizons $T \in \{1, 2\}$ hours. Each sample comprises an input–output pair $(C_0,\, C(\cdot, T))$. Inputs are min–max normalized; the coordinate z is provided as a channel to preserve vertical structure. The dataset is split 70/15/15 into train/validation/test.

3.3 FNO Surrogate and Training Setup

The surrogate model learns the operator $G : C_0(z) \mapsto C_T(z)$ using a one-dimensional Fourier Neural Operator (FNO) Li et al. (2020). The input field is first projected into a latent representation through a linear lifting layer with 128 channels. This is followed by a stack of four to five Fourier layers, each performing spectral convolution by retaining 16–32 dominant Fourier modes and applying residual connections to enhance stability. A final projection layer maps the latent field back to the physical space, yielding the predicted concentration profile at time T. The spectral formulation enables the model to capture long-range spatial interactions efficiently while preserving mesh-independent generalization.

Training is performed using the Adam optimizer with a base learning rate of 10^{-3} and either cosine or step-wise learning rate scheduling. Batch sizes of 16–32 are chosen based on memory constraints and training stability. The model is trained in a supervised manner using mean squared error (MSE) between the predicted and reference final concentration profiles. Performance is evaluated using relative L_2 error on held-out test scenarios, along with qualitative comparisons between predicted and numerically simulated profiles. Although not used in this study, the framework can be extended with physics-regularized loss terms, such as PDE residual or boundary penalties, to further enhance physical consistency in future work.

3.4 Evaluation Protocol

The surrogate model is evaluated across several dimensions to assess its accuracy, robustness, and practical usefulness for clarifier simulation. First, prediction accuracy is quantified using the relative L_2 error between the FNO-predicted concentration profiles and the corresponding numerical solutions, complemented by visual comparisons to assess qualitative agreement. Second, spatial error characteristics are examined through pointwise error maps, which highlight deviations in regions with strong nonlinear behavior such as compression zones and sludge blanket interfaces. Third, the model's ability to generalize is tested under out-of-distribution operating conditions, including unseen influent concentrations, variations in initial blanket height, changes in hydraulic loading, and modified settling parameters. Fourth, computational performance is measured by comparing FNO inference time with the finite-difference solver used to generate the training data. Finally, an iterative rollout procedure is used to evaluate the surrogate's capacity to approximate steady-state behavior by repeatedly feeding its predictions back as initial conditions. Figures and tables summarize the results and illustrate the surrogate's performance across these evaluation dimensions.

4 Results

This section evaluates the performance of the Fourier Neural Operator (FNO) surrogate for one-dimensional clarifier dynamics, focusing on prediction accuracy, spatial–temporal error behavior, generalization, computational efficiency, robustness, interpretability, and practical applicability. All comparisons use the finite-difference (FDM) solver as reference.

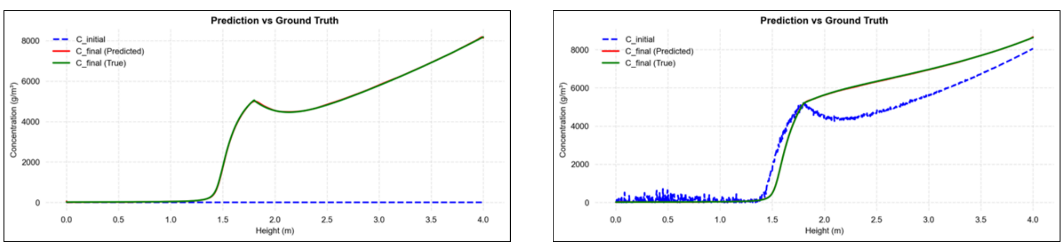
4.1 Accuracy of FNO Predictions and Physical Consistency

The FNO surrogate achieves high predictive accuracy, with average relative L_2 errors below 1% across the test set. As shown in Figure 2, predicted final concentration profiles closely overlap with numerical solutions after one hour, despite using only the initial solids profile as input. Quantitatively, Table 1 reports a mean relative L_2 of 0.0033 and MSE of 0.013 (Case-a), with further improvement for a variant (Case-b).

Metric	**PDE**	**Case A**	**Case B**
Relative L_2 error	0	0.0033	0.0021
MSE	–	0.013	0.009

Table 1: Quantitative comparison of FNO predictions and numerical solver results.

These low errors indicate that the FNO learns the underlying sedimentation operator and reproduces key clarifier phenomena, including clear-water zone formation, transitions through the hindered-settling regime, and compression behavior near the sludge blanket.



(a) (b)

Figure 2: Comparison of predicted profiles (FNO surrogate) and numerical solutions after 1 hour for two representative cases a and b .

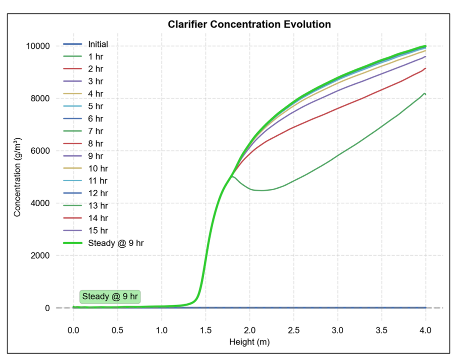


Figure 3: Iterative FNO surrogate predictions converging to a steady state by feeding the predicted profile back as the next initial condition.

Across all test cases, the predicted final profiles (Figure 2a, Figure 2b) nearly overlap with the numerical curves, supporting physical consistency and stability. As illustrated in Figure 3, iteratively reusing the FNO output as the next initial condition enables rapid steady-state estimation within seconds, avoiding hours of high-fidelity simulation.

4.2 Spatial–Temporal Error Characteristics and Their Implications

To better understand where prediction deviations occur, pointwise error maps were computed (Figure 4). Across most of the clarifier height, absolute errors remain very small relative to the operating concentration range. The FNO maintains high accuracy in regions characterized by strong nonlinear behavior, including compression zones and interfaces near the sludge blanket, where steep gradients typically challenge both numerical solvers and data-driven models.

A notable portion of the error occurs near the domain boundaries. These boundary deviations range approximately from -40 to $+40\,\mathrm{g/m^3}$, which is minor compared to the clarifier's typical solids concentration range of 1000–$8000\,\mathrm{g/m^3}$. The errors are therefore localized and amplitude-wise insignificant in practical terms. This behavior is likely influenced by limited boundary exemplars in the training data and the effects of reflective padding during spectral convolution.

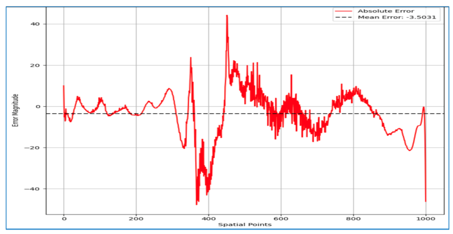


Figure 4: Heatmap of absolute error across space and time for FNO predictions relative to numerical solutions.

Overall, the analysis shows that the surrogate not only matches global concentration profiles but also preserves fine spatial details that are operationally critical. These include accurate representation of sludge blanket height, clear-water layer formation, and effluent solids levels key indicators for clarifier performance and process decision-making.

4.3 Computational Efficiency and Real-Time Potential

A key motivation for FNO surrogates is real-time simulation. Table 2 summarizes representative runtime comparisons: the numerical solver requires on the order of hours per simulation, while the surrogate produces predictions in seconds, yielding speedups of approximately 10^3–$10^4\times$ depending on grid resolution and stiffness.

Model	**Simulation time**	**Speedup**
PDE solver	3 h	$1\times$
FNO surrogate	5 s	$2160\times$

Table 2: Computational runtime analysis: FNO surrogate vs. high-fidelity PDE solver.

Beyond single-step predictions, the iterative rollout in Figure 3 converges rapidly to steady state, enabling near real-time estimation for scenario analysis, digital twin integration, and optimization workflows.

4.4 Robustness and Stability Analysis

We further probed reliability under three stressors:

- **Noise in initial conditions:** Small Gaussian perturbations to $C_0(z)$ produced negligible changes in predictions.
- **Grid variation:** Coarser/finer grids than those used in training retained stable, accurate performance, consistent with mesh-independent behavior.

- **Parameter sensitivity:** Moderate changes in settling parameters did not destabilize the surrogate.

These outcomes support stable generalization across function spaces and operating regimes, which is crucial for decision support.

4.5 Interpretability and Physical Consistency

Although trained without explicit physics constraints, the FNO yields physically plausible fields: coherent settling fronts, stratification, and compression behavior are reproduced, and predicted gradients remain smooth and consistent with clarifier dynamics. In typical cases, the model qualitatively preserves mass trends, reinforcing its utility as a surrogate for process engineering tasks.

5 Limitations

Although the Fourier Neural Operator (FNO) surrogate demonstrates strong predictive performance across a wide range of scenarios, several limitations remain. The most prominent deviations occur near the domain boundaries, where the model exhibits localized overshoot or undershoot. These boundary-region errors typically lie within approximately -40 to $+40\,\mathrm{g/m^3}$, which is small relative to the operational solids concentration range of 1000–$8000\,\mathrm{g/m^3}$, but still indicate areas where predictive fidelity can be improved. This behavior is likely influenced by the lower density of training samples near boundary locations and the use of reflective padding in spectral convolutions, which can amplify discontinuities in regions with sharp concentration transitions.

Another limitation arises from the model's fixed prediction horizon. The surrogate predicts the concentration profile at a single final time T, rather than supporting arbitrary or continuous-time queries. Applications requiring intermediate-time predictions or fully time-continuous trajectories would benefit from adding time as an explicit input or integrating recurrent or Neural-ODE–style extensions.

While the FNO generalizes well within and beyond the training distribution, it does not explicitly enforce physical constraints such as strict mass conservation or non-negativity. Under extreme extrapolation or highly unusual operating conditions, the model can produce slight violations of these physical requirements. Such issues could be mitigated in future work through physics-regularized loss terms, including PDE residual penalties, boundary-condition constraints, or hybrid architectures that combine operator learning with physics-informed components.

6 Conclusion

This work presented a Fourier Neural Operator (FNO) based surrogate model for predicting one-dimensional clarifier dynamics, marking the first application of neural operator learning to sedimentation processes in wastewater treatment. By generating a comprehensive dataset through a high-fidelity finite-difference solver, the surrogate was trained to learn the nonlinear operator governing solids transport, hindered settling, and compression behavior. The resulting model demonstrated excellent predictive accuracy, achieving sub-percent relative L_2 errors while reproducing key physical features such as sludge blanket evolution, stratification, and clear-water layer formation.

A major advantage of the proposed framework is the substantial reduction in computational cost: the FNO produces high-quality predictions in seconds, compared with the hours required by mechanistic solvers. This improvement enables real-time scenario analysis, rapid sensitivity studies, and practical integration with digital twins, where fast simulation is essential for operational decision-making. The model also generalizes robustly to unseen operating conditions, preserving accuracy even when influent characteristics or hydraulic loads differ significantly from the training data.

Beyond its immediate predictive capabilities, this study demonstrates the broader potential of neural operator learning as a bridge between physics-based modeling and data-driven intelligence in process engineering. While the current implementation focuses on fixed-horizon predictions and remains sensitive near domain boundaries, these limitations highlight promising directions for future work. Incorporating physics-informed regularization, enabling time-continuous prediction, and extending the surrogate to higher-dimensional clarifier configurations represent natural next steps.

Overall, the findings show that FNO-based surrogate modeling is both scientifically sound and operationally impactful, offering a scalable and efficient pathway for real-time clarifier simulation, monitoring, and optimization in modern wastewater treatment systems.

7 Future Work

Future work will focus on improving boundary behavior, particularly reducing the localized overshoot observed near sharp transitions, by exploring boundary-aware sampling strategies or enhanced padding techniques. Extending the surrogate to support variable or continuous-time prediction is another important direction, which may be achieved by introducing time as an explicit input or by incorporating recurrent or Neural-ODE–style architectures. Incorporating physics-informed regularization such as PDE residual penalties, mass-conservation constraints, or non-negativity enforcement could further improve stability and reliability under extreme or out-of-distribution conditions. Finally, scaling the approach to higher-dimensional clarifier configurations and validating the surrogate with full-scale plant data would strengthen its applicability for digital twins and real-time operational control in wastewater treatment systems.

8 ethics

This paper contains AI-assisted writing, limited to editing and language refinement. All scientific ideas, experiments, code, and data generation are authored and verified by the human authors.

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