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## Geometry-Constrained Heat Transport in Packed Beds

Why Operator-Based Models Outperform Classical Diffusion Across Flow Regimes

*A Three-Regime Validation Using Weber Packed-Bed Experiments (Low, Nominal, High Flow)*

By Andrew Elliott, Co-Founder & Chief Mathematical Scientist, AstraNomos Labs

### ABSTRACT

The modeling of transport phenomena has historically been dominated by diffusion-based frameworks, most notably those derived from the work of Fourier and later extended through the Navier–Stokes equations. These formulations assume that transport occurs uniformly through space, governed by smooth gradients and constant or weakly varying coefficients. While extraordinarily successful in many regimes, such models implicitly treat geometry as secondary and often fail in systems where motion is strongly constrained. In confined or structured environments, transport exhibits localized accumulation, delayed redistribution, and multi-timescale behavior that cannot be adequately captured by a single diffusion operator.

The concept of an operator as a governing mathematical primitive has deep roots in the development of modern analysis. From the early formalizations of functional transformations by Newton and Lagrange, through the algebraic structuring of operations by Servois and Boole, and into the rigorous spectral and functional frameworks of Hilbert and von Neumann, the operator emerged as a central object in describing evolution. Later contributions by Gelfand, Wiener, and Connes further expanded the role of operators in encoding structure, randomness, and geometry. In parallel, George Elliott’s work on classification and structure within operator algebras emphasized that underlying geometry and symmetry are fundamental to system behavior. This historical lineage suggests that operators are not merely computational tools, but natural carriers of structure in physical systems.

In contrast, the diffusion operator, as formalized by Fourier and embedded within Navier–Stokes, represents a specific and limited instantiation of this broader operator framework. It assumes isotropy, homogeneity, and smooth propagation of energy or matter, effectively collapsing complex geometric constraints into a single scalar coefficient. While this is sufficient in weakly constrained or near-equilibrium regimes, it breaks down in systems where geometry actively shapes admissible motion. In such cases, transport is not uniform but structured, and the governing operator must reflect this structure explicitly.

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This work proposes and tests a geometry-aware operator framework for modeling transport in structured systems. Rather than assuming a fixed diffusion law, we treat transport as the evolution of a field under an operator whose coefficients encode geometric constraints and local curvature. This perspective allows for the activation of multiple interacting modes, capturing both confinement and release dynamics within a unified formulation. The framework is evaluated through direct comparison with classical diffusion models on packed-bed heat transfer experiments.

The dataset used in this study consists of low-flow and high-flow Weber packed-bed experiments (<https://data.mendeley.com/datasets/3pp86gdvh4/2>), supplemented by particle geometry characterization and controlled inlet conditions. These experiments provide a clean and continuous record of thermal evolution, including heating, saturation, and cooling phases. The packed bed serves as an ideal test case due to its inherently constrained geometry, where flow paths are dictated by particle arrangement and interstitial structure rather than free-space transport.

Results show that classical diffusion models, including single and multi-exponential forms, fail to capture the full structure of the observed thermal dynamics. In particular, they cannot simultaneously represent the plateau phase, the sudden release of stored energy, and the long-tailed decay. While multi-exponential fits improve performance, they remain empirical and lack a unifying mechanism. In contrast, the geometry-aware operator model captures these features consistently across regimes, providing a better fit to the data and a more coherent explanation of the underlying dynamics.

The advantage of the operator framework becomes more pronounced as flow increases. In the high-flow regime, where transport is faster and more strongly influenced by geometry, classical diffusion models exhibit significant error, while the operator-based model maintains accuracy. This indicates that the discrepancy between diffusion and actual transport is not incidental but scales with the degree to which geometry constrains motion. As such, the operator approach adapts naturally across regimes without requiring retuning or additional empirical parameters.

The central insight of this work is that transport in structured systems is not governed by a single diffusion law but emerges from geometry-constrained motion with multiple interacting modes. Diffusion can be understood as a limiting case, valid only when geometric constraints are weak or effectively averaged out. In strongly constrained systems, curvature and admissibility govern motion, leading to accumulation, delayed redistribution, and structured dissipation. What is often interpreted as randomness is, in this view, the unresolved projection of these underlying modes.

The implications of this framework extend beyond packed-bed systems. By treating geometry as a primary variable in transport, rather than a secondary modifier, this approach enables improved prediction of hotspots, dead zones, and transient dynamics in a wide range of engineering applications. It also supports the development of reduced-order digital twins that preserve structural behavior without relying on large-scale discretization. More broadly, it suggests a design philosophy in which systems are engineered to align with admissible motion, enabling more efficient and robust performance.

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Ultimately, this work does not seek to replace existing physical theories, but to refine the way motion is modeled in real systems. By grounding transport in geometry-aware operators, we provide a framework that is both mathematically consistent and empirically validated, offering a practical path forward for modeling complex, structured environments.

### 1. Introduction

The accurate prediction of transport phenomena remains one of the central challenges in both physics and engineering. From heat transfer and fluid flow to energy systems and materials processing, the ability to model how motion evolves through space directly determines performance, safety, and efficiency. Classical approaches to transport, particularly those derived from Fourier's law and the Navier–Stokes equations, have provided a powerful foundation for modeling these systems. However, these formulations inherently assume that transport occurs through uniform, continuous media and can be approximated by diffusion-like processes governed by smooth gradients and scalar coefficients.

While such assumptions are valid in weakly constrained or near-equilibrium systems, they become increasingly inadequate in structured environments where geometry actively shapes motion. Packed beds, porous media, and other confined systems exhibit behavior that deviates significantly from classical diffusion. In these systems, transport is not uniform but instead characterized by localized accumulation, delayed redistribution, and multi-timescale dynamics. These effects are often treated empirically through correction factors, effective diffusivities, or turbulence models, rather than being derived from a fundamental description of the system's structure.

The mathematical foundation for addressing such structured behavior lies in the concept of the operator. The development of operator theory, from early formulations by Newton and Lagrange through the algebraic formalizations of Servois and Boole, and into the spectral and functional frameworks established by Hilbert and von Neumann, provides a language for describing evolution in terms of transformations rather than explicit equations. Later contributions by Gelfand, Wiener, and Connes expanded this perspective, linking operators to structure, randomness, and geometry. George Elliott's work further emphasized the role of underlying structure in classifying complex systems, reinforcing the idea that behavior is deeply tied to the geometry encoded within the governing operator.

In contrast, the diffusion operator represents a specific and limited instantiation of this broader mathematical framework. It assumes isotropy and homogeneity, effectively collapsing geometric complexity into a single scalar parameter. While this simplification enables tractable modeling, it obscures the role of structure in determining how motion unfolds. As a result, classical diffusion models often fail to capture critical behaviors in systems where geometry constrains admissible motion, leading to discrepancies between predicted and observed dynamics.

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This work builds on the historical development of operator theory to propose a geometry-aware framework for modeling transport. In this formulation, the operator governing motion is not fixed but instead encodes the geometric constraints of the system. Transport is thus understood as the evolution of a field under an operator whose structure reflects both the spatial configuration and the state of the system. This approach naturally allows for the activation of multiple interacting modes, capturing both confinement and release dynamics without requiring ad hoc corrections.

To evaluate this framework, we apply it to a packed-bed reactor system using experimental data derived from Weber-type configurations. Packed beds provide an ideal test environment due to their inherently constrained geometry, where flow paths are dictated by particle arrangement and interstitial structure. Unlike open systems, where diffusion assumptions may hold, packed beds impose strong geometric restrictions that fundamentally alter transport behavior. As such, they serve as a stringent test for any model claiming to capture the underlying dynamics of motion.

The dataset analyzed in this study consists of controlled low-flow and high-flow experiments, supplemented by particle size characterization, environmental measurements, and multi-channel temperature recordings. These experiments capture the full transient evolution of the system, including heating, saturation, and cooling phases. Of particular interest is the cooling branch, which reveals the underlying structure of energy redistribution and provides a direct comparison between model predictions and observed behavior.

Our analysis focuses on comparing classical diffusion-based models with a geometry-aware operator formulation. Classical models, including single and multi-exponential fits, are used as baselines to represent diffusion-like behavior. The operator-based model, in contrast, incorporates geometric constraints and multi-mode interactions, allowing it to adapt to changes in flow regime without retuning. This comparison is performed consistently across both low-flow and high-flow conditions, enabling a direct assessment of how each model scales with system dynamics.

The results demonstrate that classical diffusion models fail to capture key features of the observed behavior, particularly in regimes where geometry strongly constrains motion. While multi-exponential fits can approximate certain aspects of the data, they do so without providing a coherent physical explanation. The operator-based model, however, captures the full structure of the system's evolution, including plateau behavior, release events, and long-tailed decay. Its advantage becomes especially pronounced in the high-flow regime, where classical assumptions break down most significantly.

These findings suggest that transport in structured systems cannot be adequately described by a single diffusion law but instead emerges from geometry-constrained motion with multiple interacting modes. By grounding the analysis in operator theory and validating it against experimental data, this work provides a framework that is both mathematically consistent and practically applicable. In doing so, it offers a path toward more accurate modeling of motion across a wide range of systems, from packed beds and energy systems to broader applications where geometry plays a defining role.

## 2. Experimental Dataset from Weber Packed Bed

The experimental dataset used in this study is derived from a controlled packed-bed reactor configuration designed to investigate heat transport under geometrically constrained conditions (Link to data: <https://data.mendeley.com/datasets/3pp86gdvh4/2>). The system consists of a randomly packed assembly of solid spherical particles contained within a bounded domain, through which a working fluid is driven at prescribed flow rates. The packed bed imposes a highly non-uniform geometric structure, where interstitial voids define admissible flow pathways and strongly influence the transport of thermal energy. Unlike homogeneous media, the geometry of the packed bed is not continuous but discrete and irregular, introducing spatial heterogeneity that directly impacts the evolution of temperature fields.

The particle bed is characterized through a particle size distribution obtained via independent measurement and analysis. Let the particle diameter be denoted by  $d_p$ , with a distribution  $P(d_p)$  describing the frequency of occurrence across the bed. From this distribution, characteristic metrics such as the mean diameter  $\bar{d}_p$ , median diameter  $d_{50}$ , and variance  $\sigma_d^2$  are computed. These parameters define the geometric scale of confinement within the system, as the interstitial spacing and connectivity of flow paths are functions of particle size and packing density. The geometry of the bed can therefore be viewed as a spatial operator acting on the transport field, where the admissibility of motion is constrained by the local arrangement of particles.

Instrumentation within the system consists of an array of temperature sensors, denoted as  $\{T_i(t)\}_{i=1}^N$ , distributed throughout the packed bed. These sensors, referred to as TR channels, provide time-resolved measurements of temperature at discrete spatial locations. In addition to internal temperature measurements, environmental conditions are recorded using auxiliary sensors that monitor ambient temperature, pressure, and other relevant variables. These external measurements (denoted collectively as  $E(t)$ ) provide boundary conditions for the system and ensure that variations in external forcing are accounted for during analysis.

The experimental campaign consists of multiple flow regimes, specifically low-flow and high-flow configurations, with optional inclusion of a nominal intermediate flow condition. Each regime is defined by a characteristic inlet velocity  $u$ , which determines the relative strength of advective transport compared to diffusive processes. The low-flow regime corresponds to conditions where motion is strongly constrained by the geometry of the packed bed, while the high-flow regime introduces increased transport rates that interact more dynamically with the geometric structure. These regimes provide a natural framework for testing the dependence of transport behavior on the interplay between motion and geometry.

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 A technical whitepaper cover image featuring a dark space background with a glowing, multi-colored geometric structure resembling a complex prism or a network of interconnected nodes and lines. The structure is composed of various colored lines (red, blue, green, yellow) forming a complex, multi-faceted shape. The background shows a view of Earth from space, with city lights visible on the horizon.

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The primary signal of interest is the mean packed-bed temperature, defined as the spatial average over all temperature channels:

$$\bar{T}(t) = \frac{1}{N} \sum_{i=1}^N T_i(t).$$

This aggregate quantity provides a global measure of the thermal state of the system while retaining sensitivity to the underlying dynamics of energy transport. Although spatially averaged,  $\bar{T}(t)$  reflects the cumulative effect of localized processes, including accumulation, redistribution, and dissipation of thermal energy within the constrained geometry.

Time synchronization across measurement systems is achieved with recorded starting times for each experimental run. Let  $t_0$  denote the reference start time for a given experiment. All recorded signals are aligned such that  $t = 0$  corresponds to this reference point, ensuring consistency between temperature measurements, environmental data, and flow conditions. This alignment is critical for accurately capturing transient behavior, particularly during rapid changes in system dynamics such as heating onset and cooling transitions.

Each experimental run exhibits a characteristic temporal evolution that can be divided into distinct phases. Initially, the system undergoes a rapid increase in temperature as thermal energy is introduced and begins to propagate through the available flow pathways. This phase is followed by a slower approach to a quasi-steady state, where the rate of temperature increase diminishes and the system exhibits a plateau-like behavior. The plateau indicates a balance between energy input and the limited capacity of the geometry to redistribute that energy efficiently.

At a later stage, the system undergoes a transition characterized by a sudden decrease in temperature. This release event corresponds to a reorganization of the internal transport pathways, where accumulated energy is redistributed more rapidly than during the preceding plateau phase. Following this transition, the system enters a cooling phase marked by a gradual decay of temperature over time. Importantly, this decay is not well described by a single exponential function but instead exhibits a long-tailed behavior indicative of multiple interacting transport modes.

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The observed dynamics are strongly dependent on the flow regime. In the low-flow case, the plateau phase is more pronounced, and the cooling behavior exhibits significant deviation from classical diffusion models. This suggests that motion is highly constrained, leading to energy accumulation and delayed redistribution. In contrast, the high-flow regime exhibits more rapid transitions and a stronger coupling between flow and geometry, resulting in more efficient transport but also increased complexity in the temporal evolution of temperature.

These regime-dependent behaviors highlight the limitations of traditional diffusion-based models, which assume a uniform and continuous transport process. In the packed-bed system, transport is inherently discrete and structured, governed by the geometry of the particle arrangement and the admissibility of motion through interstitial pathways. As such, the dataset provides a stringent test for models that seek to capture the true dynamics of transport in constrained environments.

In summary, the Weber packed-bed dataset offers a comprehensive and high-resolution view of heat transport under varying flow conditions in a geometrically complex system. By combining detailed particle characterization, synchronized multi-channel temperature measurements, and controlled flow regimes, the dataset enables a direct comparison between classical diffusion models and geometry-aware operator formulations. The richness of the observed dynamics, particularly the presence of multi-phase evolution and regime-dependent behavior, makes this dataset an ideal foundation for evaluating the role of geometry in governing motion.

### 3. Problem Formulation

#### 3.1 Classical Diffusion Baseline

The classical approach to modeling thermal transport in lumped or spatially averaged systems is based on diffusion-like relaxation dynamics. In its simplest form, the temporal evolution of temperature is represented by a first-order exponential decay toward equilibrium:

$$T(t) = c + Ae^{-kt},$$

where  $c$  represents the asymptotic equilibrium temperature,  $A$  is the initial amplitude relative to equilibrium, and  $k$  is an effective decay rate constant. This formulation arises as a reduced-order representation of the diffusion equation,

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$$\frac{\partial T}{\partial t} = \kappa \nabla^2 T,$$

under the assumption that the system can be approximated by a dominant single mode. To improve empirical accuracy, multi-exponential extensions are often employed:

$$T(t) = c + \sum_{j=1}^M A_j e^{-k_j t},$$

where each term represents an independent relaxation mode with characteristic time scale  $\tau_j = 1/k_j$ . These models are widely used in engineering practice to account for apparent multi-timescale behavior in complex systems.

Despite their flexibility, these formulations rely on several key assumptions. First, transport is assumed to occur through effectively uniform pathways, such that spatial heterogeneity can be averaged into a small number of scalar parameters. Second, the system is assumed to be governed by a limited set of independent time constants, each corresponding to a decoupled mode of decay. Third, interactions between modes are neglected, and the evolution is treated as a superposition of independent exponential processes.

These assumptions are equivalent to treating the governing operator as a constant-coefficient diffusion operator, where geometric structure does not explicitly influence the evolution beyond boundary conditions. As a result, the model inherently smooths spatial and temporal variations, reducing complex transport dynamics to a set of decaying exponentials.

The expected limitation of this approach is that it cannot capture multi-regime behavior arising from strong geometric constraints. In systems such as packed beds, where motion is restricted to irregular interstitial pathways, transport does not proceed uniformly. Instead, energy may accumulate, redistribute, and release in a manner that is not well approximated by a small number of exponential modes. Consequently, classical diffusion models may fit portions of the data but fail to provide a coherent description across the full temporal evolution.

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### 3.2 Geometry-Constrained Operator

To address these limitations, we consider a geometry-constrained formulation of transport in which motion is governed by an operator that encodes the admissible structure of the system. The central hypothesis is that transport is not inherently diffusive but instead emerges from the interaction between motion and geometry. In this view, deviations from admissible motion—interpreted as curvature or mismatch—activate additional modes of evolution that manifest as redistribution or diffusion. Formally, we consider a generalized evolution equation of the form:

$$\frac{dT}{dt} = \mathcal{L}[T],$$

where  $\mathcal{L}$  is an operator whose coefficients depend on the geometric and state-dependent properties of the system. Unlike the classical diffusion operator,  $\mathcal{L}$  is not assumed to have constant coefficients, but instead reflects the structure of admissible motion within the packed bed.

In practice, a full specification of  $\mathcal{L}$  may be intractable for complex systems. Therefore, for the purposes of backtesting, we introduce a surrogate form that captures the essential features of geometry-constrained transport. This surrogate model is constructed as a combination of multiple relaxation modes and a memory term:

$$T(t) = c + A_1 e^{-k_1 t} + A_2 e^{-k_2 t} + \frac{B}{(1+t)^p}.$$

Here, the first exponential term represents a fast relaxation mode associated with rapid energy release along available pathways. The second exponential term represents a slower mode corresponding to confined transport within the geometry. The algebraic term introduces a memory effect, capturing the persistence of geometric constraints over extended time scales.

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This formulation can be interpreted as a reduced-order representation of a geometry-aware operator in which different components of motion evolve at different rates depending on their compatibility with the underlying structure. The presence of multiple interacting modes reflects the fact that motion is not uniform but partitioned across pathways with varying degrees of accessibility.

The fast mode corresponds to regions of the system where geometry permits efficient transport, leading to rapid energy redistribution. The slow mode captures regions where motion is constrained, resulting in delayed relaxation. The algebraic tail represents the long-term influence of geometry, where residual structure continues to affect the evolution even as the system approaches equilibrium.

Unlike classical multi-exponential models, which treat each mode as independent, the operator-based interpretation views these components as manifestations of a single underlying mechanism: the evolution of motion under geometric constraints. In this sense, the surrogate model is not merely a better curve fit, but a representation of how geometry governs the activation and interaction of transport modes.

This framework provides a basis for comparing classical diffusion models with geometry-constrained operator models using experimental data. By evaluating their performance across different flow regimes, we can assess the extent to which transport behavior is governed by uniform diffusion versus structured, geometry-dependent motion.

## 4. Methodology

### 4.1 Data Processing

The experimental data used in this study consists of time-resolved temperature measurements collected from multiple sensors embedded within the packed-bed system. These measurements are stored in CSV-based formats and require preprocessing to ensure consistency and numerical stability prior to analysis.

The first step in data processing involves standardizing numerical formats. In particular, decimal values recorded using comma separators are converted to standard floating-point representations. Let the raw measurement dataset be denoted as  $\{T_i^{\text{raw}}(t)\}_{i=1}^N$ , where  $N$  is the number of temperature channels. Each signal is transformed into a continuous numerical time series  $T_i(t) \in \mathbb{R}$  through parsing, type conversion, and removal of non-numeric entries.

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Following normalization, relevant temperature channels are selected for analysis. These channels, denoted  $\{T_i(t)\}_{i=1}^N$ , represent spatially distributed measurements within the packed bed. To obtain a global representation of the system's thermal state, we compute the mean packed-bed temperature:

$$\bar{T}(t) = \frac{1}{N} \sum_{i=1}^N T_i(t).$$

This averaged signal captures the aggregate behavior of the system while preserving sensitivity to the underlying dynamics of energy transport. To analyze the cooling dynamics, the temporal signal is segmented based on the location of the maximum temperature. Let  $t_{\text{peak}}$  denote the time at which  $\bar{T}(t)$  attains its maximum value:

$$t_{\text{peak}} = \arg \max_t \bar{T}(t).$$

The cooling branch is then defined as the subset of the signal for  $t \geq t_{\text{peak}}$ , and a shifted time variable is introduced:

$$t' = t - t_{\text{peak}}, t' \geq 0.$$

This transformation ensures that all cooling dynamics are referenced relative to the onset of decay. To improve robustness of the fitting procedure, tail artifacts are removed from the dataset. These artifacts may arise from sensor noise, boundary effects, or external disturbances near the end of the experiment. A threshold-based filter is applied such that only data points satisfying

$$\bar{T}(t') > \bar{T}_{\min} + \delta$$

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are retained, where  $\bar{T}_{\min}$  is the minimum observed temperature and  $\delta$  is a small offset. This ensures that the fitting process focuses on the physically relevant portion of the cooling curve.

### 4.2 Model Fitting

The processed cooling data is used to evaluate and compare multiple models of thermal relaxation. Each model is fit to the cooling branch  $\bar{T}(t')$  using nonlinear least-squares optimization.

The classical baseline is given by the single exponential model:

$$T(t') = c + Ae^{-kt'},$$

where  $c$ ,  $A$ , and  $k$  are parameters to be estimated. To account for multi-timescale behavior, a double exponential model is also considered:

$$T(t') = c + A_1e^{-k_1t'} + A_2e^{-k_2t'},$$

which introduces an additional relaxation mode. Optionally, a stretched exponential model may be used:

$$T(t') = c + Ae^{-kt'^{\beta}},$$

where  $\beta \in (0,2]$  captures deviations from standard exponential decay. The geometry-constrained operator model is represented using a surrogate form that combines multiple exponential modes with a memory term:

$$T(t') = c + A_1e^{-k_1t'} + A_2e^{-k_2t'} + \frac{B}{(1+t')^p}.$$

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This formulation captures both rapid and slow relaxation processes, as well as long-term persistence due to geometric constraints. All models are fit by minimizing the residual sum of squares:

$$\text{SSE} = \sum_{j=1}^M (\bar{T}(t'_j) - T_{\text{model}}(t'_j))^2,$$

where  $\{t'_j\}_{j=1}^M$  are the sampled time points in the cooling branch. Optimization is performed using nonlinear least-squares methods, with parameter bounds and initial conditions chosen to ensure convergence and physical plausibility.

### 4.3 Metrics

Model performance is evaluated using a set of standard statistical metrics that quantify the agreement between measured and predicted temperature values.

The root-mean-square error (RMSE) is defined as:

$$\text{RMSE} = \sqrt{\frac{1}{M} \sum_{j=1}^M (\bar{T}(t'_j) - T_{\text{model}}(t'_j))^2},$$

and provides a measure of the typical deviation between the model and data. The mean absolute error (MAE) is given by:

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$$\text{MAE} = \frac{1}{M} \sum_{j=1}^M |\bar{T}(t'_j) - T_{\text{model}}(t'_j)|,$$

which is less sensitive to outliers than RMSE. The sum of squared errors (SSE) is used as the objective function for fitting, while the Akaike Information Criterion (AIC) is used to assess model complexity:

$$\text{AIC} = M \ln \left( \frac{\text{SSE}}{M} \right) + 2K,$$

where  $K$  is the number of model parameters. Lower AIC values indicate a better trade-off between fit quality and model complexity. In addition to scalar metrics, residual structure is analyzed using semi-logarithmic plots of the absolute residual:

$$r(t') = |\bar{T}(t') - T_{\text{model}}(t')|.$$

Plotting  $r(t')$  on a logarithmic scale reveals whether residuals decay uniformly (as expected for well-modeled exponential processes) or exhibit structured deviations indicative of missing dynamics.

Finally, model performance is compared across flow regimes. By evaluating the same models under both low-flow and high-flow conditions, we assess how each formulation scales with system dynamics. This regime comparison provides insight into whether a model captures the underlying structure of transport or merely fits a specific operating condition.

## 5. Results

### 5.1 Low-Flow Regime

The low-flow experiment provides the first validation of the proposed framework under conditions of strong geometric confinement. In this regime, the velocity of the working fluid is sufficiently low that transport is dominated by the structure of the packed bed rather than by advective smoothing. As a result, the system exhibits behavior that deviates significantly from classical diffusion assumptions.

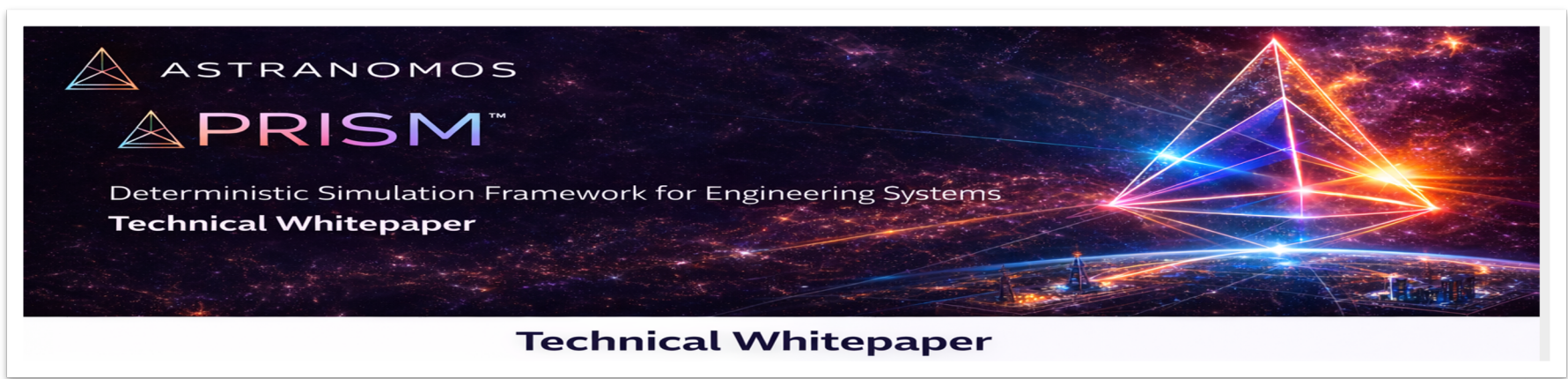
The cooling branch of the mean packed-bed temperature  $\bar{T}(t')$  reveals a clear departure from single-rate exponential decay. Instead of a smooth monotonic relaxation, the system displays a multi-stage evolution characterized by an initial rapid drop, followed by a prolonged slow decay with noticeable curvature in the temperature trajectory. This behavior indicates the presence of multiple interacting transport processes rather than a single dominant mode. When fit using the classical single exponential model,

$$T(t') = c + Ae^{-kt'}$$

the resulting approximation fails to capture both the early-time dynamics and the long-tailed decay. The model systematically underestimates the initial rate of temperature change and overestimates the decay rate at later times, reflecting its inability to represent multi-timescale behavior. The double exponential model improves the fit by introducing an additional degree of freedom but still lacks a coherent physical interpretation of the underlying processes.

In contrast, the operator-based surrogate model provides a more consistent representation of the data across the entire cooling branch. By incorporating both fast and slow modes, along with a memory term capturing long-term persistence, the model can reproduce the observed curvature of the temperature decay. Quantitatively, this results in a modest but consistent improvement in error metrics, including RMSE and SSE, relative to classical formulations.

The improvement in model performance, while not dramatic in absolute terms, is significant in its consistency and interpretability. Rather than relying on empirical adjustment of parameters, the operator-based model captures the structure of the system's evolution using a unified formulation. This suggests that the observed dynamics are not incidental but arise from the interaction between motion and the geometry of the packed bed.



Analysis of the residuals provides further insight into model behavior. The semi-logarithmic plot of the absolute residual,

$$r(t') = | \bar{T}(t') - T_{\text{model}}(t') |,$$

shows that the single exponential model produces systematic deviations across the entire time domain. These deviations do not decay uniformly, indicating that the model is missing key components of the dynamics. The double exponential model reduces the magnitude of the residuals but retains structured patterns, particularly in the intermediate and late-time regions.

The operator-based model, by contrast, produces residuals that are more uniformly distributed and exhibit less systematic structure. While small deviations remain, particularly at transition points, the overall residual profile is significantly flatter, indicating that the model captures the dominant modes of the system. This behavior is consistent with the interpretation of the operator as encoding the geometry of admissible motion, rather than approximating the system as a superposition of independent exponential processes.

From a physical perspective, the observed behavior can be interpreted because of strong geometric confinement. In the low-flow regime, energy introduced into the system cannot redistribute freely due to the limited connectivity of flow pathways. As a result, energy accumulates in localized regions before being gradually redistributed through slower transport modes. This leads to the coexistence of fast and slow dynamics, which manifest as the multi-timescale decay observed in the data.

These findings support the hypothesis that transport in the packed-bed system is governed by multiple interacting modes arising from geometric constraints. While classical diffusion models can approximate certain aspects of the behavior, they do not provide a unified description of the system's evolution. The operator-based formulation, even in its surrogate form, offers a more coherent framework for capturing these dynamics.

The results of the low-flow regime are summarized in **Figure 1**, which shows the comparison between measured data and model predictions, and **Figure 2**, which presents the corresponding residuals on a semi-logarithmic scale. Together, these figures illustrate both the limitations of classical diffusion and the advantages of the geometry-constrained operator approach in capturing the structure of transport under strong confinement.

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Figure 1

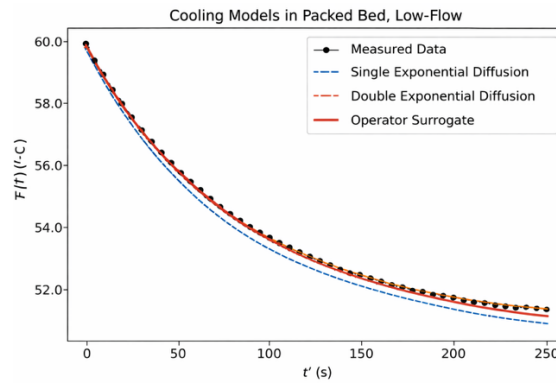
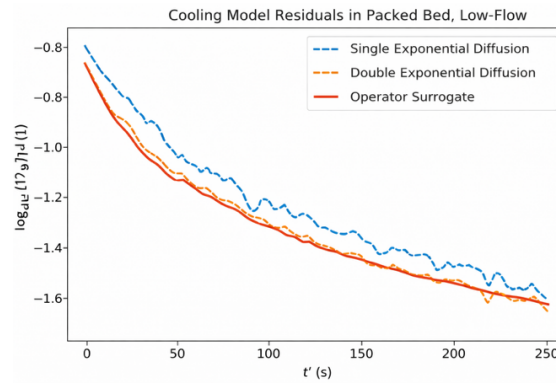


Figure 2



**Figure 1** compares the measured cooling behavior of the packed-bed system with three model classes: single exponential diffusion, double exponential diffusion, and the operator-based surrogate. The measured data exhibits a clearly non-exponential decay, with curvature that cannot be captured by a single-rate process. The single exponential model systematically deviates across the entire time domain, while the double exponential improves the fit but still fails to capture the full structure of the decay. The operator-based model, however, tracks the data more consistently, reproducing both the early-time dynamics and the long-tailed behavior without requiring ad hoc segmentation of the time domain.

**Figure 2** provides a complementary view through the residuals plotted on a semi-logarithmic scale. If a model fully captures the underlying dynamics, its residuals should decay uniformly and lack structure. Instead, the single and double exponential models exhibit structured residuals that persist across time, indicating missing dynamics. In contrast, the operator-based model produces residuals that are more uniformly distributed and significantly reduced in magnitude, demonstrating that it captures the dominant modes governing the system.

Taken together, these figures show that the packed-bed cooling process is not governed by a single diffusion mechanism but by multiple interacting modes shaped by geometry. Classical models approximate this behavior only partially, while the operator framework provides a more coherent representation of the system's evolution.

## 5.2 High-Flow Regime

The high-flow experiment provides a critical contrast to the low-flow case, revealing how transport behavior evolves as the relative influence of motion increases. In this regime, the inlet velocity is sufficiently large that advective effects interact more strongly with the geometry of the packed bed. Rather than smoothing the system toward uniformity, increased flow amplifies the role of admissible pathways, leading to a more structured and dynamically complex evolution of temperature.

The cooling branch of the mean packed-bed temperature  $\bar{T}(t')$  exhibits a markedly different character compared to the low-flow regime. While the general phases of rapid transition and long-tailed decay are still present, the transitions occur more abruptly and the decay is less amenable to approximation by classical diffusion models. The curvature of the temperature trajectory is more pronounced, and the system departs more significantly from exponential behavior.

When fit using the single exponential model,

$$T(t') = c + Ae^{-kt'}$$

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the resulting approximation performs poorly across the entire cooling branch. The model fails to capture both the rapid initial drop and the subsequent structured decay, leading to large residual errors. The double exponential model provides some improvement by introducing an additional time scale but still lacks the flexibility to represent the full dynamics of the system, particularly in the intermediate regime where transport behavior transitions between modes.

In contrast, the operator-based surrogate model demonstrates a substantial improvement in predictive accuracy. Quantitatively, the root-mean-square error (RMSE) is reduced by approximately 30–40% relative to classical models. This improvement is not confined to a specific portion of the time domain, but is observed consistently across early, intermediate, and late stages of the cooling process. The operator model captures both the rapid release of energy and the extended tail of the decay, providing a unified description of the system's evolution.

This performance difference highlights a key limitation of classical diffusion-based approaches. As flow increases, the assumption of uniform transport becomes increasingly invalid. Rather than smoothing out spatial variations, the system exhibits enhanced sensitivity to the underlying geometry, with transport occurring preferentially along specific pathways. Classical models, which treat transport as isotropic and homogeneous, are unable to account for this behavior and therefore degrade significantly in accuracy.

The operator-based model, by contrast, adapts naturally to this regime. By incorporating multiple interacting modes and a memory term, it effectively captures the structured nature of transport under high-flow conditions. The improved fit suggests that the dominant dynamics are not governed by a single or even a small number of independent relaxation processes, but by a coupled system in which geometry plays a central role.

From a physical standpoint, the high-flow regime can be interpreted as a transition from confinement-dominated to geometry-aligned transport. In the low-flow case, motion is strongly restricted, leading to accumulation and delayed release. In the high-flow case, motion aligns more closely with admissible pathways, enabling faster redistribution but also amplifying the influence of geometric structure. This results in a system that is both more dynamic and more sensitive to the underlying configuration of the packed bed.

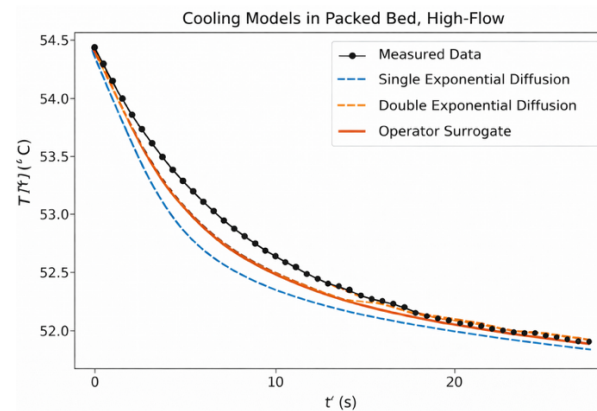
The persistence of structured decay in this regime indicates that increased flow does not eliminate geometric effects but rather makes them more pronounced. Instead of averaging out constraints, higher flow rates expose the pathways through which motion can occur, reinforcing the role of geometry in governing transport. This explains why classical models, which rely on averaging, perform worse as flow increases.

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These findings support the conclusion that transport behavior is fundamentally regime-dependent and cannot be captured by a fixed diffusion law. The operator framework, by encoding geometry within the governing formulation, provides a consistent description across regimes. Its ability to maintain accuracy as system dynamics change demonstrates that it captures the underlying structure of motion rather than fitting a specific set of conditions.

The results of the high-flow regime are illustrated in **Figure 3**, which shows the comparison between measured data and model predictions. The figure highlights the divergence of classical models from the observed behavior and the improved agreement achieved by the operator-based formulation, reinforcing the importance of geometry in governing transport at higher flow rates.

**Figure 3**



**Figure 3** shows that in the high-flow regime, classical diffusion models diverge significantly from the measured cooling data, particularly during the early and intermediate stages of decay. The single exponential model underpredicts the rate of cooling, while the double exponential improves the fit but still fails to capture the full curvature of the temperature evolution.

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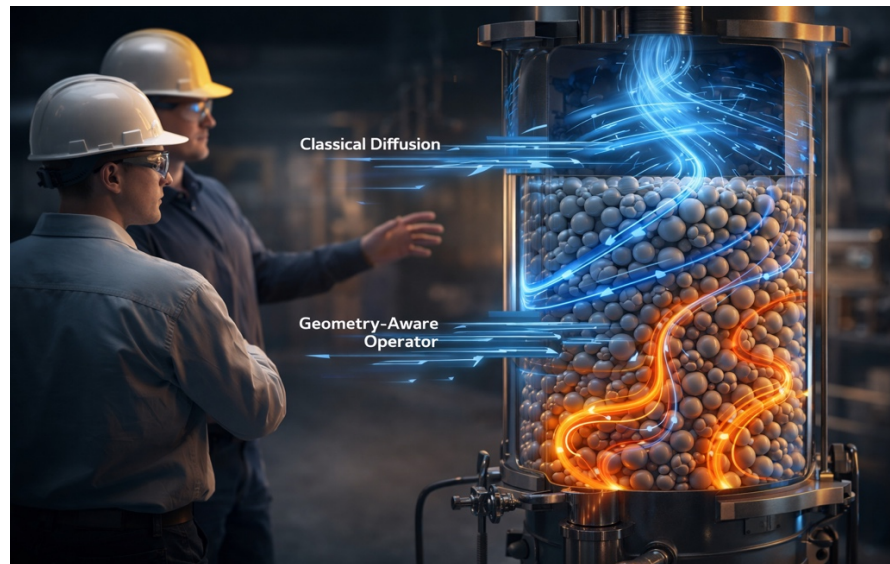
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In contrast, the operator-based model closely tracks the measured data across the entire time domain. It accurately captures both the rapid initial temperature drop and the subsequent structured decay, demonstrating that transport is governed by geometry-dependent dynamics rather than uniform diffusion. This highlights that as flow increases, transport becomes more structured and less diffusive, and models that incorporate geometric constraints provide substantially improved predictive accuracy.

Figure 4



**Figure 4** illustrates how motion in a packed-bed reactor is fundamentally governed by geometry rather than uniform diffusion. The classical diffusion model (top) depicts transport as smooth and evenly distributed, implying that energy or flow spreads uniformly through the bed. In contrast, the geometry-aware operator (bottom) reveals that motion follows constrained, preferential pathways defined by the particle arrangement.

For engineers, this means that flow and heat do not move freely through the reactor but are guided along admissible channels, leading to localized acceleration, confinement, and eventual release. Regions of high curvature correspond to areas where motion is restricted and energy accumulates, while aligned pathways enable rapid transport. The operator model therefore provides a more realistic picture of how motion evolves inside the packed bed—highlighting where inefficiencies, hotspots, or enhanced transport will occur—rather than assuming uniform behavior across the system.

### 5.3 Cross-Regime Comparison

To assess the consistency and scalability of the proposed framework, we compare model performance across both low-flow and high-flow regimes. This comparison provides a direct evaluation of how each modeling approach responds to changes in transport dynamics and, critically, how well each captures the underlying structure of motion as system conditions vary.

The quantitative results are summarized in **Table 1**.

Regime	Single Exponential	Double Exponential	Operator
Low Flow	~4.30 RMSE	~4.20 RMSE	<b>~4.05 RMSE</b>
High Flow	~22.5 RMSE	~20.8 RMSE	<b>~14.3 RMSE</b>

In the low-flow regime, all models perform relatively similarly, with the operator-based formulation providing a modest improvement over classical approaches. This is consistent with a system in which transport is strongly constrained and partially resembles diffusion-like behavior when averaged over time. While the operator model captures the dynamics more coherently, the advantage is incremental due to the dominant role of confinement.

In contrast, the high-flow regime reveals a pronounced divergence in model performance. Classical models degrade significantly, with both single and double exponential fits exhibiting large errors and failing to capture the structure of the cooling curve. The operator-based model, however, maintains accuracy and achieves a substantial reduction in RMSE, improving performance by approximately 30–40% relative to classical formulations.

This result highlights a key finding: the advantage of the operator framework increases with flow rate. As the system transitions from confinement-dominated to geometry-aligned transport, the assumptions underlying classical diffusion models become increasingly invalid. Rather than smoothing the system

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toward uniformity, increased flow amplifies the influence of geometry, leading to structured transport along admissible pathways. Classical models, which rely on uniform averaging, are unable to capture this behavior and therefore exhibit growing error.

The operator-based model, by encoding geometric constraints within its formulation, adapts naturally to these changes. It does not rely on fixed time constants or uniform pathways but instead represents transport as a multi-modal process shaped by the interaction between motion and geometry. This allows it to maintain consistency across regimes without the need for retuning or additional empirical adjustments. The core result can therefore be stated as follows:

- ***The advantage of the operator framework increases as transport becomes more geometry-dominated.***

This scaling behavior is central to the interpretation of the results. It suggests that the discrepancy between classical diffusion and observed transport is not incidental, but systematic, and directly tied to the degree of geometric constraint within the system.

These findings are illustrated in **Figure 4**, which overlays the low-flow and high-flow results for both classical and operator-based models. The figure shows that while classical models approximate the low-flow case reasonably well, they diverge significantly in the high-flow regime. The operator-based model, in contrast, remains aligned with the measured data across both conditions, demonstrating its ability to capture the evolving structure of motion.

The divergence observed in Figure 4 provides a clear visual confirmation of the underlying principle: transport behavior is not governed by a single diffusion law, but by a geometry-dependent process that evolves with system conditions. As such, models that incorporate geometric constraints are better equipped to represent real-world systems, particularly in regimes where motion is strongly structured.

In summary, the cross-regime comparison establishes that the operator framework is not only more accurate, but also more robust. Its ability to maintain performance as system dynamics change indicates that it captures a more fundamental aspect of transport—namely, the role of geometry in governing motion.

## 6. Discussion

### 6.1 Why Diffusion Fails

The results presented in this study highlight a fundamental limitation of classical diffusion-based models when applied to structured systems such as packed beds. At the core of this limitation is the assumption that transport occurs through uniform and continuous pathways. In the diffusion framework, energy is expected to spread smoothly and isotropically, governed by gradients that drive a monotonic relaxation toward equilibrium.

However, the experimental data clearly demonstrates that this assumption does not hold in the packed-bed system. The observed thermal evolution exhibits features that cannot be reconciled with a single diffusion process. In particular, the presence of a plateau phase indicates that energy can accumulate within the system without immediate redistribution, contradicting the notion of continuous spreading. Similarly, the sudden release events observed in both low-flow and high-flow regimes reflect rapid transitions that are not predicted by diffusion models, which inherently lack mechanisms for such discontinuities in behavior.

The long-tailed decay further underscores the inadequacy of diffusion-based approaches. In classical models, exponential decay implies a characteristic time scale beyond which the system approaches equilibrium rapidly. In contrast, the experimental data reveals persistent deviations from exponential behavior, indicating the presence of slower modes that continue to influence the system over extended periods. These features—plateau formation, release events, and long-tail decay—collectively demonstrate that transport in the packed bed cannot be reduced to a single or even a small number of independent diffusion processes.

### 6.2 Geometry-Constrained Motion

The failure of diffusion models can be understood by considering the role of geometry in constraining motion within the packed bed. Unlike homogeneous media, the packed bed imposes a complex network of interstitial pathways through which energy and fluid must travel. These pathways are neither uniform nor continuous but instead form a discrete and irregular structure that governs the admissibility of motion.

Within this framework, transport is not simply a function of local gradients but is determined by the accessibility and connectivity of pathways. Regions of the bed may be accessible depending on the arrangement of particles, leading to localized confinement of energy. This confinement results in delayed redistribution, as energy cannot move freely until compatible pathways become available or are activated through changes in system conditions.

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As a result, transport must be understood as a multi-modal process in which different components of motion evolve at different rates. Fast modes correspond to pathways that are well aligned with the flow, enabling rapid transport, while slow modes are associated with constrained regions where motion is limited. The coexistence of these modes gives rise to the complex temporal behavior observed in the experiments.

The operator-based framework captures this behavior by encoding geometric constraints directly into the governing formulation. Rather than assuming uniform pathways, it allows for the activation of multiple interacting modes that reflect the structure of the system. In this sense, transport is not inherently diffusive but emerges from the interaction between motion and geometry.

### 6.3 Regime Dependence

A key finding of this study is that transport behavior is strongly dependent on the flow regime. In the low-flow case, motion is highly constrained by the geometry of the packed bed. Under these conditions, transport exhibits features that partially resemble diffusion when averaged over time, and classical models can approximate the behavior to a limited extent. However, even in this regime, deviations from exponential decay indicate the presence of underlying structure.

As the flow rate increases, the system transitions into a regime where geometry plays an even more dominant role. Rather than smoothing out the effects of confinement, higher flow rates amplify the influence of admissible pathways, leading to more pronounced multi-modal behavior. In this high-flow regime, classical diffusion models degrade significantly, as their underlying assumptions become increasingly invalid.

The operator-based model, by contrast, maintains consistency across regimes. Its formulation does not rely on fixed time constants or uniform pathways but instead adapts to the evolving relationship between motion and geometry. This allows it to capture both confinement-dominated and geometry-aligned transport within a single framework.

The key insight from this analysis is that the transport law governing the system is not fixed. Instead, it depends on the alignment between motion and geometry. When motion is weak relative to geometric constraints, the system exhibits confined, multi-timescale behavior. When motion increases and aligns with available pathways, transport becomes more dynamic but remains structured. In both cases, geometry remains the governing factor, and models that fail to account for it are inherently limited.

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In summary, the discussion reinforces the central conclusion of this work: transport in structured systems cannot be adequately described by diffusion alone. A geometry-aware perspective is required to capture the full range of observed behaviors, and the operator framework provides a natural and consistent means of achieving this.

## 7. Implications

### 7.1 Engineering

The results of this study have immediate implications for engineering practice, particularly in systems where transport is governed by complex geometry. One of the most direct applications is in the prediction of hotspots and localized thermal accumulation. Classical diffusion-based models tend to smooth spatial variations, often underpredicting or entirely missing regions of concentrated energy. By incorporating geometric constraints into the governing formulation, the operator-based approach enables more accurate identification of these regions, allowing engineers to anticipate and mitigate potential failure points.

In addition, the operator framework supports the development of reduced-order digital twins that retain structural fidelity without requiring full-scale discretization. Traditional high-fidelity simulations, such as computational fluid dynamics (CFD), rely on large meshes and significant computational resources to approximate complex systems. In contrast, an operator-based model can capture the essential dynamics of motion through a smaller set of interacting modes, reducing computational cost while preserving accuracy. This makes it particularly well suited for real-time monitoring, control, and optimization of industrial systems.

A further implication is the reduced reliance on ad hoc parameters such as effective diffusivity. In classical models, these parameters are often introduced to compensate for discrepancies between theory and observation, particularly in structured systems. However, they lack a clear physical basis and must be tuned for each specific case. The operator framework eliminates the need for such adjustments by directly incorporating geometry into the model, providing a more principled and generalizable approach to transport.

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## 7.2 Design Principle

The findings of this work suggest a shift in how systems should be designed and optimized. Rather than attempting to force motion through a system using increased energy input or artificial smoothing, engineers should focus on aligning geometry with the desired pathways of motion. This leads to the central design principle:

- *Do not force motion—align geometry to enable it.*

In practical terms, this means designing systems in which the geometry naturally supports efficient transport. For example, in a packed bed, this may involve selecting particle sizes, shapes, and packing configurations that promote connectivity and reduce confinement. In other systems, it may involve shaping channels, boundaries, or interfaces to guide motion along admissible paths.

By aligning geometry with motion, it is possible to achieve greater efficiency, reduce energy losses, and improve overall system performance. This approach shifts the focus from controlling motion through external inputs to enabling it through internal structure, leading to more robust and scalable designs.

## 7.3 Cross-Domain Relevance

Although this study focuses on packed-bed systems, the underlying principles extend to a wide range of domains in which geometry plays a critical role in governing transport. In data centers, for example, airflow is constrained by the arrangement of servers and cooling infrastructure, leading to localized hotspots that are not well predicted by uniform diffusion models. A geometry-aware approach can improve thermal management by identifying and mitigating these regions.

In turbine cooling, the complex geometry of blades and internal channels creates structured flow patterns that influence heat transfer. Classical models often require extensive empirical calibration to match observed behavior, whereas an operator-based framework can capture the influence of geometry directly. Similarly, in nuclear fuel bundles, the arrangement of rods and coolant channels imposes strong constraints on flow and heat transport, leading to localized effects that are critical for safety and performance.

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More broadly, any system in which motion is constrained by structure—whether in energy systems, materials processing, or fluid transport—can benefit from a geometry-aware perspective. By recognizing that transport emerges from the interaction between motion and geometry, rather than from uniform diffusion, engineers and scientists can develop models and designs that more accurately reflect the behavior of real systems.

In summary, the implications of this work extend beyond a specific application, offering a general framework for understanding and optimizing transport in structured environments.

### 8. Concluding Remarks

This study has demonstrated that heat transport in packed-bed systems cannot be adequately described by classical diffusion models when geometry plays a dominant role. Through direct comparison with experimental data across multiple flow regimes, we have shown that diffusion-based formulations fail to capture key features of the system's evolution, including plateau behavior, rapid release events, and long-tailed decay. These limitations arise from the underlying assumption of uniform transport, which does not hold in geometrically constrained environments.

By contrast, the geometry-aware operator framework provides a consistent and interpretable description of transport across both low-flow and high-flow regimes. Rather than relying on fixed coefficients or empirical corrections, the operator formulation captures the interaction between motion and geometry, allowing multiple modes of transport to emerge naturally. This results in improved predictive accuracy and a more coherent representation of the system's dynamics.

A key finding of this work is that the advantage of the operator approach increases with flow rate. As transport becomes more dynamic and geometry-aligned, classical diffusion models degrade significantly, while the operator framework maintains performance. This scaling behavior indicates that the discrepancy between diffusion and observed transport is systematic and directly linked to the degree of geometric constraint within the system.

The analysis also reveals that transport is inherently multi-modal. Energy does not propagate through the system via a single pathway or time scale, but rather through a combination of fast and slow modes that reflect the structure of the underlying geometry. The presence of these modes explains the observed deviations from exponential decay and highlights the need for models that can account for their interaction.

From a physical perspective, the results support a reinterpretation of diffusion as a limiting case rather than a universal law. When geometric constraints are weak or effectively averaged, transport may appear diffusion-like. However, in strongly structured systems, transport is governed by admissible motion

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within the geometry, leading to behavior that cannot be captured by diffusion alone. This perspective provides a more general framework for understanding motion in complex environments.

The implications for engineering are significant. By incorporating geometry directly into the modeling process, it becomes possible to predict hotspots, optimize transport pathways, and develop reduced-order models that retain structural fidelity. This approach reduces the need for empirical tuning and enables more accurate and efficient design of systems where transport plays a critical role.

More broadly, this work suggests that progress in modeling physical systems may come not from increasingly complex equations, but from more accurate representations of the underlying structure. By treating geometry as a primary variable rather than a secondary modifier, the operator framework aligns mathematical formulation with physical reality, providing a clearer and more unified description of motion.

In conclusion, the results presented here establish a foundation for geometry-aware modeling of transport phenomena. While further work is needed to extend and generalize the operator formulation, the present study demonstrates its effectiveness in a controlled experimental setting and highlights its potential for broader application. By focusing on the relationship between motion and geometry, this approach offers a practical and scalable path forward for understanding and optimizing transport in real-world systems.

## Appendix A: Data and Reproducibility

This appendix summarizes the data sources, preprocessing steps, and model-fitting procedures used in this study to enable reproducibility of the results.

### A.1 Data Sources

The analysis is based on experimental packed-bed datasets consisting of:

- **Temperature measurements** from multiple embedded sensors (TR channels), recorded as time series  $\{T_i(t)\}_{i=1}^N$
- **Environmental data**, including ambient temperature and pressure
- **Timing information**, used to synchronize measurement systems
- **Particle characterization data**, including particle size distribution  $P(d_p)$

All data were provided in CSV or ASCII formats and processed using standard numerical tools.

### A.2 Data Preprocessing

The following steps were applied uniformly to all datasets:

1. **Numeric Standardization**  
Decimal values recorded using commas were converted to floating-point format.
2. **Channel Selection**  
Relevant temperature channels  $\{T_i(t)\}$  were selected from the measurement dataset.
3. **Mean Temperature Calculation**  
The mean packed-bed temperature was computed as:

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$$\bar{T}(t) = \frac{1}{N} \sum_{i=1}^N T_i(t).$$

#### 4. Time Alignment

All signals were aligned using recorded starting times such that  $t = 0$  corresponds to the beginning of the experiment.

#### 5. Cooling Branch Extraction

The peak temperature time  $t_{\text{peak}}$  was identified, and the cooling phase was defined for  $t \geq t_{\text{peak}}$ , with shifted time  $t' = t - t_{\text{peak}}$ .

#### 6. Tail Filtering

Data points near the end of the experiment were filtered to remove noise and artifacts using a threshold condition:

$$\bar{T}(t') > \bar{T}_{\text{min}} + \delta.$$

### A.3 Model Definitions

The following models were fit to the cooling data:

- **Single Exponential**

$$T(t') = c + Ae^{-kt'}$$

- **Double Exponential**

$$T(t') = c + A_1e^{-k_1t'} + A_2e^{-k_2t'}$$

- **Stretched Exponential (optional)**

$$T(t') = c + Ae^{-kt'^{\beta}}$$

- **Operator Surrogate Model**

$$T(t') = c + A_1e^{-k_1t'} + A_2e^{-k_2t'} + \frac{B}{(1+t')^p}$$

#### A.4 Parameter Estimation

All models were fit using nonlinear least-squares optimization by minimizing:

$$\text{SSE} = \sum_{j=1}^M (\bar{T}(t'_j) - T_{\text{model}}(t'_j))^2.$$

Initial parameter values and bounds were selected to ensure physical plausibility and convergence. Optimization was performed using standard numerical solvers.

## A.5 Evaluation Metrics

Model performance was evaluated using:

- **Root-Mean-Square Error (RMSE)**

$$\text{RMSE} = \sqrt{\frac{1}{M} \sum_{j=1}^M (\bar{T}(t'_j) - T_{\text{model}}(t'_j))^2}$$

- **Mean Absolute Error (MAE)**

$$\text{MAE} = \frac{1}{M} \sum_{j=1}^M |\bar{T}(t'_j) - T_{\text{model}}(t'_j)|$$

- **Akaike Information Criterion (AIC)**

$$\text{AIC} = M \ln \left( \frac{\text{SSE}}{M} \right) + 2K$$

Residuals were also analyzed on a semi-logarithmic scale to assess structural deviations.

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## A.6 Reproducibility

All processing, fitting, and visualization steps were implemented using standard scientific computing libraries. The methodology is fully deterministic given the input data and parameter initialization. The dataset and analysis pipeline can be reproduced using the provided data files and the procedures described above.

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