

To the Graduate Council:

I am submitting herewith a dissertation written by Amirehsan Ghasemi entitled “Machine Learning Supported Mesoscale Modeling of Gas Conduction in Nanoporous Systems.” I have examined the final paper copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Data Science & Engineering.

Murat Barisik, Major Professor

We have read this dissertation
and recommend its acceptance:

Reetesh Ranjan

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Accepted for the Council:

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(Original signatures are on file with official student records.)

Machine Learning Supported Mesoscale Modeling of Gas Conduction in Nanoporous Systems

A Dissertation Presented for the
Doctor of Philosophy
Degree
The University of Tennessee, Knoxville

Amirehsan Ghasemi

December 2025

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This dissertation is dedicated to the loving memory of my mother
Nasrin Pordeli

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The purpose of computing is insight, not numbers.

Richard Hamming

Abstract

Heat transfer through nanoporous systems is a complex phenomenon that involves contributions from solid and gas phases. Existing theories for estimating thermal conductivity of gases in nanoporous materials, such as aerogels, often rely on one-dimensional heat transfer assumptions and neglect the influence of sidewalls in confined geometries. Moreover, the impact of molecular surface forces, which dominate nanoscale confinements, is often overlooked in the literature. This dissertation addresses these challenges by developing a new mesoscale boundary condition that accounts for nanoscale molecular surface forces and macroscale kinetic theory gas/solid energy exchange. Additionally, data-driven algorithms are used to develop structure-property correlations with thermal conductivity, reducing the need for extensive simulations of different pore size configurations.

Machine learning algorithms are robust predictive models. However, many algorithms exhibit “black-box” behavior, which limits their interpretability. Complex models achieve high accuracy but often fail to provide insight into the underlying physical mechanisms. This makes them less suitable for engineering design, where understanding mechanisms is crucial. This dissertation develops a macroscopic engineering model that offers a promising solution by encoding domain knowledge into mathematical structures. Integrating domain knowledge constrains model behavior, ensures physical consistency, and reduces data needs.

The macroscopic engineering model uses 96 molecular dynamics simulations that incorporate the developed mesoscale boundary conditions. This model predicts

the normalized effective thermal conductivity of argon gas in nanoporous aerogel materials as a function of three key parameters: aspect ratio, Knudsen number, and sidewall temperature. The developed model is then compared with three machine learning models: random forest, gradient boosting, and Gaussian process. To ensure the explainability of the machine learning models, explainable approaches are utilized. With $R^2 = 0.9803$, the macroscopic model achieves high accuracy while maintaining complete interpretability. Feature importance analysis reveals consistent findings across all modeling approaches: aspect ratio, enabled by the mesoscale boundary conditions, dominates transport behavior (95-99% importance), while Knudsen number and sidewall temperature contribute marginally (1-2% and 2-3%, respectively). The results of this dissertation provide insights and solutions to the challenges of studying gas conduction at the nanoscale, and contribute to a deeper understanding of heat transfer in nanoporous systems.

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Chapter 1

Introduction

- Ghasemi, Amirehsan, and Murat Barisik. 2025. “Machine Learning for Thermal Transport Prediction in Nanoporous Materials: Progress, Challenges, and Opportunities” *Nanomaterials* 15, no. 21: 1660. <https://doi.org/10.3390/nano15211660>

Nanoporous materials, such as aerogels, have gained attention for their unique properties and wide range of applications [101]. Aerogels are ultra-light materials with high porosity percentage ranging from 90% to 99% [47]. They also exhibit low density and exceptional thermal insulation properties. The structure of aerogels contains pores smaller than the mean free path of air molecules, which is nearby 70 nanometers (nm) [184]. The tiny pores in aerogels prevent gas molecules from conducting heat, thus enabling the creation of unique insulating materials [126, 47].

The unique thermal properties of aerogels make them valuable for high-performance insulation applications. They are highly valuable materials in the aerospace industry, where thermal management and spatial efficiency are vital [47]. Aerogels can achieve thermal conductivity values below that of air. This remarkable feature makes them suitable for energy-efficient building applications [6]. Additionally, the structure of aerogel can be tailored to further reduce thermal conductivity [47]. This feature allows aerogels to function as effective insulating nanomaterials under

challenging environmental conditions, such as extreme humidity and temperature fluctuations [178].

Research in this field aims to develop superinsulation materials that show thermal conductivities lower than that of air. This goal requires a comprehensive understanding of heat transfer mechanisms in these materials [115]. The growing demand for energy-saving materials [20] highlights the importance of advanced modeling, simulations, and experimental techniques. This approach can ultimately optimize aerogel design and establish its role in efficient thermal management systems.

1.1 Literature Review

1.1.1 Heat Transfer in Nanoporous Materials

The heat transfer in aerogels occurs through three mechanisms: gaseous conduction, solid conduction, and radiation. Understanding and modeling these mechanisms is important for enhancing aerogel insulation capabilities [47]. These mechanisms are often studied individually and contribute to the overall thermal behavior of aerogels. Solid and gas conductivities mainly contribute to the effective thermal conductivity at room temperature. For gaseous conduction, the literature uses the kinetic theory of gases, which considers the nanoporous structure of aerogels [47, 98].

Since 1935, the modeling of gas-conductive heat transfer in aerogels has been investigated [47, 98]. These models can be classified into two types: empirical and theoretical models. Section (1.1.2) outlines the evolution of these models and discusses key models, their advantages and disadvantages, and important factors that help in understanding the mechanism of gas conduction in aerogels.

1.1.2 Gas-Conductive Heat Transfer Models

The presentation of gas-conductive heat transfer models used in this dissertation follows the steps provided in reference [47] as summarized in Table 1.1.

Empirical model

Fricke et al. [45] introduced an empirical model in 1992. While it was the most used empirical model at the time, it lacked important parameters such as temperature and air pressure. Therefore, the thermal conductivity calculated through this model does not include the pressure and temperature, and this makes it an unrealistic model.

Theoretical model

The first theoretical model was introduced by Kistler in 1935 [85]. The Kistler model is based on gas kinetic theory, a concept that explains the behavior of gases at the atomic level. Kistler, the inventor of aerogel [47], considered the free mean path of gas atoms and the size effect of the pore structure. The size effect refers to the effect of the porous structure and particle size on the thermal transfer characteristics. The size effect is significant for aerogel composites due to their nanoporous structure. The size effect can influence heat transfer in aerogels in *two ways*:

Gas Conduction: This effect occurs when the aerogel’s pore sizes are smaller than or comparable to the mean free path of gas atoms. In this scenario, gas atoms hit the pore walls more often than they hit each other. This collision limits the movement of gas atoms, which in turn reduces thermal conductivity through the gas phase.

Solid Conduction: This effect is related to the structure of the aerogel’s solid skeleton. When the solid skeleton’s characteristic length approaches the phonon mean free path, it restricts the transfer of thermal energy through the solid phase [47]. This restriction occurs because the nanoscale dimensions interfere with the expected scattering of phonons (the carriers of heat in solids), resulting in reduced thermal conductivity in the solid skeleton. For example, larger silica aerogel particles reduce thermal conductivity more effectively than smaller particles in certain applications, such as when they are utilized in geopolymers foam renders [25]. However, the Kistler model does not account for interactions between gas atoms at higher pressures and has a coefficient that is complicated to determine experimentally.

Kaganer model (1969) [79]: The Kaganer model is an improvement on Kistler’s model. It is considered one of the most valid formulas based on the kinetic theory of gases [98]. The Kaganer model presents the Knudsen number, which is the ratio of the mean free path of gas atoms to the average pore size (characteristic length) to describe the effect of temperature and pressure on thermal conductivity [47]. This model suggests that all pores in the aerogel have the same size, which is a simplification of the actual structure. The Kaganer model can be expressed as [47]:

$$\lambda_g = \frac{\Pi\lambda_0}{1 + 2\beta Kn} = \frac{\Pi\lambda_0}{1 + 2\beta \cdot l_g/D} \quad (1.1)$$

where λ_g is the gaseous thermal conductivity, Π is the porosity, λ_0 is the thermal conductivity of the gas in free space, β is a coefficient related to gas accommodation and adiabatic coefficient, Kn is the Knudsen number, l_g is the mean free path of gas molecules, and D is the average pore size. Kaganer’s model oversimplifies the consideration of the mean free path of gas molecules and pore sizes by assuming a uniform pore size distribution.

Zeng model (1995) [181] improved the Kaganer model by including the effect of the solid skeleton into the mean free path of the gas molecules [47]. However, its accuracy depended on the material, and it did not work as well for fumed silica as it did for silica aerogel.

Reichenauer model (2009) [136] improved Kaganer’s model by considering a normal distribution of pore sizes. Although the normalization factor, which represents the quantity of pores, must be computed separately, it complicates the calculations.

Bi model (2012) [14] improved the Reichenauer model by simplifying calculations of the normalization factor and focusing the influence of large pores, which significantly impact the results. However, some of the modifications suffer from having theoretical and experimental support [47]. Additionally, oversimplification in selecting thresholds for pore diameter ranges may lead to deviations.

Table 1.1: Evolution of Gas-Conductive Heat Transfer Models in Nanoporous Aerogel Materials [47].

Model	Year	Type	Key Features	Strengths	Limitations
Fricke et al. [45]	1992	Empirical	Empirical model	Most used empirical model at the time	Lacks temperature and air pressure parameters; unrealistic model
Kistler [85]	1935	Theoretical	Based on gas kinetic theory; considers free mean path and size effect	First theoretical model	Does not account for gas atom interactions at higher pressures; coefficient complicated to determine experimentally
Kaganer [79]	1969	Theoretical	presents Knudsen number	One of the most valid formulas based on kinetic theory of gases	Assumes all pores have same size; oversimplifies by assuming uniform pore size distribution
Zeng [181]	1995	Theoretical	Improved Kaganer model	Includes effect of solid skeleton into gas molecule mean free path	Accuracy depends on material; did not work as well for fumed silica as for silica aerogel
Reichenauer [136]	2009	Theoretical	Improved Kaganer model	Considers normal distribution of pore sizes	Normalization factor must be computed separately; complicates calculations
Bi [14]	2012	Theoretical	Improved Reichenauer model	Simplifies calculations of normalization factor; focuses on influence of large pores	Some modifications lack theoretical and experimental support; oversimplification in selecting pore diameter thresholds may lead to deviations

1.1.3 Current Challenges and Gaps in Nanoporous Heat Transfer

There are several challenges in understanding heat transfer through nanomaterial aerogels. The main challenge is their complexity. The nanoparticles in these materials randomly aggregate to form chain-like solid skeletons, which create a complex three-dimensional structure [103]. This structure creates a convolution of interconnected mesopores, ranging from 2 to 50 nanometers [47, 103]. This complex structure changes how heat passes through the aerogels compared to conventional insulation materials [103].

1.1.3.1 Classical Modeling Limitations

The classical modeling approach to studying gas conduction at the nanoscale is based on the kinetic theory of gases. It utilizes the Knudsen number to categorize flow regimes from continuum flow ($Kn < 0.01$) to free molecular flow regime ($Kn > 10$). Models such as the Kaganer and its variations assess how pore size distribution affects the movement of gas molecules. These models often use oversimplified assumptions in heat transfer characterization and pore size distribution estimation, which limits their accuracy and applicability. Furthermore, at the nanoscale, the molecules present at the wall exert forces. This effect extends about three times the gas molecular diameter (1 nm) from each surface [10]. Within this region, gas molecules experience more interactions with the wall molecules, which changes their behavior compared to the bulk gas. Also, in a nanoscale domain near the walls, there is a significant increase in gas density because gas molecules experience a longer residence time influenced by surface effects [10]. The nanoscale effect yields distinctive heat transfer properties that differ from those established in continuum theories and classical approaches. The nanoscale effects require precise mathematical models to achieve accurate descriptions [103].

1.1.3.2 Traditional Computational Methods Limitations

Traditional computational approaches for predicting thermal conductivity include molecular dynamics (MD) simulations and first-principles phonon calculations using density functional perturbation theory (DFPT), based on density functional theory (DFT) [185, 11]. However, these methods face limitations in computational cost and scalability, especially when addressing the structural diversity of nanoporous materials. These challenges have led to the development of advanced machine learning algorithms. For example, MD simulations provide atomic-level insights but are computationally expensive and rely on the accuracy of interatomic potentials [62]. Developing reliable interatomic potentials, also known as force fields, for complex nanoporous materials remains an active area of research. Much existing research on interatomic potentials still fails to capture the interactions that affect thermal transport [41, 39].

First-principles calculations offer higher accuracy but are even more computationally expensive. Usually, their application is limited to small unit cells and simplified models [129]. The calculation of phonon properties from first principles calculations requires the evaluation of force constants through finite displacement methods or density functional perturbation theory, both of which scale poorly with system size [129, 61]. For nanoporous materials with large unit cells, including those with hundreds or thousands of gas molecules, these calculations become impractical.

Addressing anharmonic effects presents another major challenge for conventional computational methods. Harmonic approximations perform well for modeling thermal transport at low temperatures. However, accurate prediction of thermal conductivity at higher temperatures requires consideration of phonon-phonon scattering processes [56, 177]. Encoding three-phonon and four-phonon scattering increases computational complexity and often requires approximations that can compromise predictive accuracy [56].

The computational modeling approach offers a potential solution for studying heat transfer in aerogels; however, molecular-level modeling is necessary to achieve a comprehensive understanding of this phenomenon. Simulating the behavior of many gas molecules in tiny pore volumes is computationally demanding. Although we can obtain results at the pore level, estimating the overall material properties is challenging since the material consists of millions of pores under various conditions. The multiscale nature of aerogels, where nanoscale pores coexist alongside microscale features and potential defects, makes it incredibly challenging to develop accurate models that capture all the relevant physics across these different length scales. This level of complexity requires millions of simulations for different pore configurations, which is computationally expensive and almost impossible. Instead, with the rapid growth of computational power from CPUs (Central Processing Units) and GPUs (Graphics Processing Units), as well as the emergence of numerous advanced machine learning algorithms, promising opportunities are now available for understanding the dependence on porous physical features.

1.1.3.3 Experimental Limitations

Experiments can also be sophisticated, costly, and prone to error. The experimental measurements of aerogels’ thermal conductivity face a more serious issue than the theoretical complexity due to the current reliability crisis. According to recent comprehensive reviews, the literature contains significant inconsistencies in the results that cover silica and other inorganic, biopolymer, and synthetic polymer aerogels [108]. The unreliable experimental data results primarily from insufficient expertise and the use of transient methods, especially transient plane sources (TPS) or the “hot-disk” technique [31]. The hot-disk method [59, 60] has remained popular because it works with various materials but produces inaccurate measurement results.

Incorrect instrumentation, inappropriate sample materials, and unskilled operation can lead to inaccurate thermal conductivity measurements. The transient methods generate unreliable data for aerogels more frequently than steady-state

methods when operating under unfavorable conditions [108, 164]. The suggested modifications to boost transient method reliability exist outside standard practices. It forces researchers to create their non-standard modifications. Thermal conductivity measurements obtained using the transient plane source technique [21] are dependent on sensor dimensions, input power levels, and applied pressure. The incorrect management of these factors leads to data dispersion and excessive measurement values for aerogels because of their low thermal conductivity values [164].

Nanomaterial aerogels represent a significant breakthrough due to their unique properties and diverse applications. Their lightweight, high porosity, and adjustability make them an ideal material for thermal insulation. However, their complexity still makes it challenging to model and fully understand how heat moves through them. Continued research is necessary to overcome these challenges and maximize the potential of aerogels and similar nanoporous materials in engineering applications.

1.2 Problem Statement and Overview of Research Contribution

Heat transfer in nanoporous aerogel materials is estimated by considering the contributions of the solid and gas phases. The overarching purpose of this dissertation is to investigate the challenge of studying gas conduction at the nanoscale. This study explores insights and solutions to existing challenges, as summarized below:

- Existing theories estimate gas thermal conductivity based on a one-dimensional heat transfer assumption, such as gas heat transfer between two parallel plates, without considering the influence of side surfaces in confined geometries and lateral heat loss [33]. However, porous systems consist of three-dimensional confinements with comparable dimensions in all directions. Although heat transfer predominantly occurs in one direction, the solid skeleton has a higher thermal conductivity than the gas, causing the side walls to be at a different

temperature than the gas domain [47]. Consequently, side surfaces (walls) influence heat transfer and the effective thermal conductivity of the gas phase, which has been largely overlooked in the existing literature [91].

- The existing literature mostly neglects and only briefly touches on the influence of molecular surface forces, which are dominant at nanoscale confinements. Aerogel pore sizes vary from a few nanometers up to 50 *nm* [47]. Surface molecular forces create surface adsorption, which is expected to influence heat passage. Only a few studies have explored this phenomenon, and their findings remain inconclusive and misleading because of the complexity of the phenomenon and the limitations of current modeling and measurement techniques [108].
- Artificial intelligence models can be used to predict the effective thermal conductivity in nanoporous media, facilitating structure-property correlation. The existing literature mainly employs complex machine learning algorithms, such as artificial neural networks (ANNs) and ensemble learning approaches. The complex models achieve better accuracy, but their lack of transparency makes their predictions difficult to trust.

Therefore, this dissertation aims to resolve these challenges by:

- This dissertation develops a new mesoscale boundary condition that accounts for nanoscale molecular surface forces and microscale kinetic theory gas-solid energy exchange. This novel boundary condition will be implemented as an extra package in the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [163] [GitHub](#) repository and will contribute to the open-source molecular modeling scientific community.
- This dissertation utilizes the power of machine learning models to prevent the need for millions of simulations for various pore configurations. Furthermore,

the structure-property correlations are established to understand and control the effective thermal conductivity of nanoporous material aerogels.

- This dissertation employs post-hoc explainable artificial intelligence [55] methods to address the explainability issue in the machine learning models used. Explainable post-hoc methods with a solid theoretical foundation provide local and global model-agnostic explanations [117] for the dataset generated by the MD simulation. These methods provide explanations, such as explanatory plots, and assign an importance score to each feature for predicting the target value, which is the effective thermal conductivity.

1.3 Dissertation Outline

This dissertation is organized into five chapters as outlined below:

- Chapter 2: Introduces a novel mesoscale boundary line condition by extending LAMMPS’s “wall/reflect/stochastic” package. This chapter explains how to find and calculate mesoscale boundary line parameters. The new boundary condition is validated by comparing its results with linearized Boltzmann solutions and the Kaganer model. This chapter also examines sidewall effects and demonstrates how they vary with different aspect ratios in various sidewall temperature scenarios.
- Chapter 3: Discusses the application of machine learning to nanoporous materials research over the years. This chapter covers the fundamentals and advantages of machine learning models used in this dissertation. It also focuses on interpretable methods that enable an understanding of machine learning model predictions, rather than treating them as “black boxes”. Some explainable artificial intelligence methods are introduced and discussed. The state-of-the-art machine learning models applied to nanoporous materials are explained and addressed.

- Chapter 4: Develops and discusses a macroscopic model specific to the dataset generated by the MD simulation. The results are compared with the results of machine learning models suitable for small datasets, including random forest, gradient boosting, and Gaussian process models. This chapter also implements customized explainable artificial intelligence approaches that enhance the overall transparency in the structure-property correlation.
- Chapter 5: Summarizes the important findings in this dissertation.

Chapter 2

Molecular Dynamics Simulation

- Barisik, Murat and Ghasemi, Amirehsan, Revisiting Effective Gas Thermal Conductivity in Nanoporous Systems: Incorporating Lateral Sidewall Coupling via Novel Mesoscale Molecular Simulations. Available at SSRN: <https://ssrn.com/abstract=5669543>

This chapter discusses a novel mesoscale boundary condition that incorporates nanoscale molecular surface forces and microscale energy exchange between gas and solid phases. It compares the results obtained using this new boundary condition with those obtained under periodic (parallel plates) and adiabatic conditions. Temperature profiles from MD simulations are compared with those from the linearized Boltzmann equation [121]. This comparison is expected to reveal similar behavior in temperature profiles. Introducing the mesoscale boundary condition to the side walls causes the temperature profiles to deviate from those of the periodic and adiabatic cases. By making these comparisons, this chapter clarifies the physics of side walls, temperature jumps, and molecular surface adsorption in gas flows, as well as how these factors influence thermal transport and conduction.

2.1 Molecular Dynamics Simulations Principles

Molecular dynamics simulations are powerful particle-based computational tools for studying heat transfer in nanoporous materials. MD uses classical and statistical mechanics to provide atomic-level insights into the behavior of molecules [3]. Molecular dynamics simulations have provided essential information about the thermal behavior in systems, including phase change materials (PCMs), nanoparticle interfaces, and porous structures [159, 151]. Molecular dynamics simulations can capture the effects of nanoscale confinement, surface properties, and molecular interactions in heat transfer studies. They have led to the discovery of new thermal materials with extraordinary thermal conductivity properties, enabling researchers to design phonons for specific thermal applications [133].

Molecular dynamics simulations use Newton’s equations of motion to describe a system’s atomic positions and velocities during its evolution. The basic equation governing MD is $F = ma$, where the force (F) on each atom is derived from the gradient of the interatomic potential energy function [135]. By applying the equations of motion to each atom in a system, MD simulations can keep track of the dynamical and conformational changes that occur during the simulation. The interatomic potential energy function (also known as the force field) represents the molecular interaction model, which is the essential element for MD simulations. The force field encompasses bonded interactions, including bond stretching, angle bending, and torsional rotations, as well as non-bonded interactions, such as van der Waals and electrostatic interactions [78]. Molecular dynamics simulations require force fields to generate accurate results. The quality of force fields is evaluated and enhanced through the comparison of experimental data with quantum mechanical (QM) calculations. Additionally, the development and improvement of force fields have progressed through machine learning approaches, which offer high accuracy and efficient computation [147, 160].

Statistical mechanics provides the theoretical basis for MD simulations. It bridges the gap between the behavior of microscopic particles and the macroscopic properties of materials. Since it is computationally impossible to track every atom in a system that contains billions of particles, statistical mechanics utilizes the statistical properties of particle ensembles to predict the bulk behavior. This approach is possible through ensemble theory, which defines a collection of all possible microscopic configurations in accordance with known macroscopic constraints, such as temperature, pressure, and energy. Based on the ergodic hypothesis, the average simulation time in MD simulations can represent ensemble averages. It enables the computation of system thermodynamic properties from atomic-scale interactions. Statistical mechanics converts the computationally intractable many-body problem into a practical computational approach that can explain systems at the molecular level.

The microcanonical ensemble (NVE) conserves energy, volume, and number of particles. The system temperature and pressure can change within the NVE ensemble. The canonical ensemble (NVT) preserves temperature, volume, and particle number. It provides a suitable situation for the system that needs energy fluctuation. The NVT ensemble is the standard choice for MD simulations to analyze material thermal properties under controlled temperature settings. For example, the investigation of nanofluids (NFs) thermal conductivity requires precise temperature control because this property directly affects heat transfer mechanisms [51]. The isothermal-isobaric ensemble (NPT) preserves pressure, temperature, and particle number. The system volume has the freedom to change within the NPT ensemble. The NPT ensemble provides an appropriate framework for studying thermal conductivity in porous media because it explains volume changes caused by pressure and temperature fluctuations [156].

The selection of ensemble type has a substantial effect on thermal conductivity predictions for porous media, as it restricts the system in different ways. Researchers

must consider material characteristics, experimental parameters, and research targets when selecting the most suitable ensemble for their studies.

2.2 LAMMPS Framework

LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) is an open-source MD code developed at Sandia National Laboratories that has become an essential part of computational materials research [163]. Its parallel computing architecture enables simulations ranging from a few particles to billions of atoms, which makes it ideal for studying nanoscale thermal transport in nanoporous materials, such as aerogels.

The software solves Newton’s equations of motion using integration algorithms, such as the Velocity-Verlet method, tracking atomic positions and velocities with femtosecond precision. LAMMPS supports a diverse range of interatomic potentials, from simple Lennard-Jones to sophisticated many-body potentials, which are crucial for accurately modeling gas-solid interactions in confined geometries [163]. For thermal conductivity calculations, it offers both equilibrium Green-Kubo methods [54, 87] and non-equilibrium molecular dynamics (NEMD) approaches that directly impose temperature gradients.

LAMMPS excels in simulating nanoporous systems through flexible boundary condition implementations. Researchers can combine periodic boundaries with reflective or fixed walls to model the confined geometries characteristic of aerogel pores. The software’s modular architecture allows users to extend functionality through custom fixes written in C++. This enables the implementation of specialized boundary conditions, such as the mesoscale formulations developed in this dissertation. The intuitive input script format uses commands that read like plain English, such as “create_box”, “minimize”, and “run” making it accessible while providing fine-grained control for advanced users.

Performance optimization features include neighbor list algorithms that scale linearly with atom count ($O(N)$) rather than quadratically ($O(N^2)$), and domain decomposition for efficient parallelization across thousands of processors. Modern versions support graphics processing unit (GPU) acceleration through compute unified device architecture (CUDA), which dramatically reduces simulation times. These capabilities have made LAMMPS the computational foundation for understanding how molecular-level interactions govern macroscopic thermal properties in nanoporous materials [163].

2.3 Developing a Mesoscale Boundary Condition

This section describes a novel mesoscale boundary condition that incorporates nanoscale molecular surface forces and microscale kinetic boundary theory for heat exchange. As shown in Fig. 2.1, the Lennard-Jones (LJ) 12-6 model [76] is used to model molecular surface forces. The LJ 12-6 can effectively approximate the Van der Waals interactions between gas and solid surfaces [155]. This approach prevents gas atoms from penetrating into the wall and accounts for the attractive forces at intermediate distances, which correspond to adsorption effects.

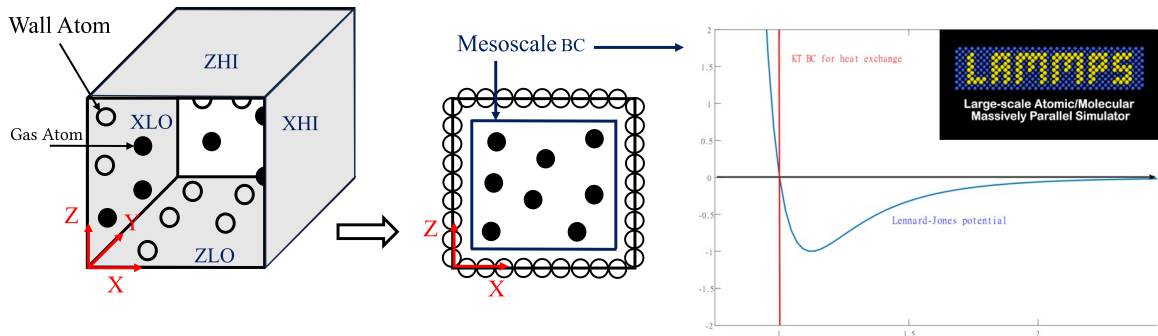


Figure 2.1: Developing a mesoscale boundary condition line. Filled circles represent wall atoms and unfilled circles represent gas atoms.

To establish a proper and accurate mesoscale boundary line, as shown on the left in Fig. 2.2, a molecular-level simulation with periodic boundary conditions in

the X and Y directions is performed. The LJ 12-6 model is utilized by applying the “wall/lj126” fix command in LAMMPS [163] at the edges of the simulation box in the Z direction (shown on the right side of Fig. 2.2). This approach simulates molecular surface forces, which effectively approximate Van der Waals interactions between the gas and the solid [155].

Additionally, by modifying the “wall/reflect/stochastic” fix command (provided in Fig. 2.3), a stochastic reflective kinetic theory (KT) boundary is used that maintains a constant or linear temperature change along the length of the simulation box. When gas atoms collide with a kinetic boundary condition, they can either undergo specular reflection, where they bounce off at equal angles, or diffuse reflection, where they scatter in random directions. Accurately identifying the parameters for the LJ 12-6 model (σ, ϵ) and also the appropriate location of the KT boundary condition will ultimately create the mesoscale boundary line condition.

The adsorption characteristic of the nanoscale molecular surfaces is compared with the density profile of an actual molecular surface reported in the literature [10]. The goal is to identify similar adsorption behavior, even though the surface corrugation and location are derived from the average behavior observed in the MD simulation, which may differ slightly from the actual molecular surface. The formation of density peaks resulting from adsorption should match the van der Waals interactions calculated using the LJ 12-6 model, which is part of the mesoscale boundary model. The mesoscale model van der Waals interaction parameters are selected based on the comparison of the reduced interaction.

The present study selects argon as an identical gas to that in the literature [10], and the interaction potential is optimized to obtain a similar adsorption value on the surface. This approach enables obtaining identical surface adsorption behavior with an actual molecular surface model. Since van der Waals interaction creates an impenetrable zone for the gas molecules due to high repulsive molecular forces at the proximity surface, a microscopic heat exchange (KT boundary) needs to be described as the region that molecules can penetrate. Similar to the literature [10],

the location of the boundary in the molecularly modeled system is approximated on the order of molecular radius, starting from the center of the surface molecules. Due to this reason, the boundary location is carefully optimized to be within one molecule diameter to achieve natural heat transfer.

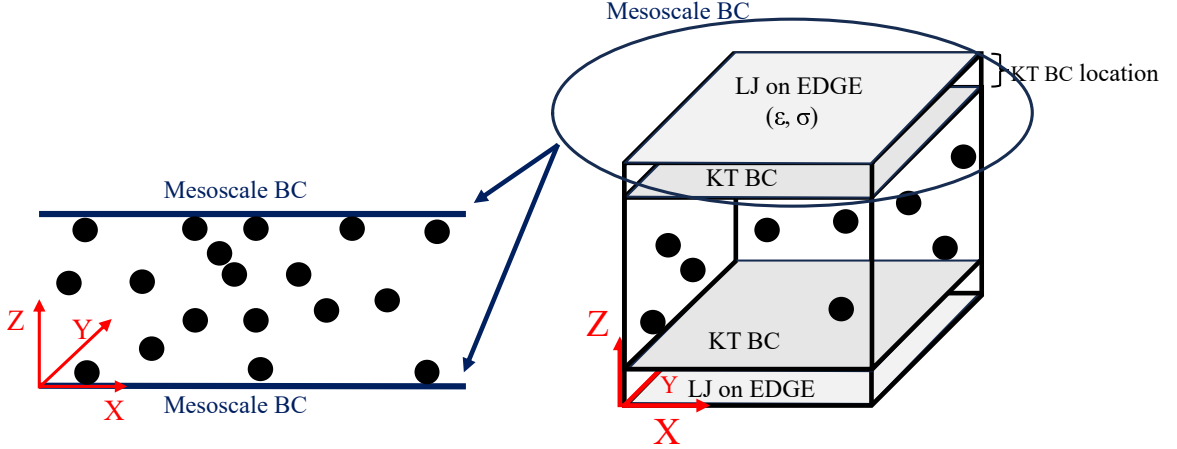


Figure 2.2: A mesoscale boundary condition line. It encompasses the molecular surface forces and kinetic boundary for energy exchange between the gas and solid phases.

2.3.1 Customized Reflective-Stochastic Wall Development

In real-world applications, bounded walls rarely maintain constant temperatures. Industrial processes, such as heat exchangers and thermal management systems, often exhibit significant temperature variations along heated or cooled surfaces [13]. Traditional MD simulations usually assume adiabatic walls conditions. This fails to capture the complex thermal boundary effects observed in complex systems. To address this limitation, a modified version of the LAMMPS `fix wall/reflect/stochastic command` that contains spatially varying wall temperatures has been developed. This modification, as provided in Fig. 2.3, enables more realistic modeling of thermal boundary conditions while preserving the computational efficiency of the original stochastic reflection algorithm.

The implementation extends the existing “`FixWallReflectStochastic`” class by introducing a linear temperature gradient capability specifically for X walls, which

are perpendicular to the X-direction (XLO and XHI). This modification enables these walls to exhibit temperature variations as a function of the Z-coordinate. It creates temperature gradients alongside the Z direction that better represent realistic thermal boundary conditions. The key modifications include three new member variables in the class declaration:

- **use_variable_temp_x:** A boolean flag that activates the temperature gradient functionality when X-direction walls are present.
- **temp_start and temp_end:** Define the temperature values at the bottom and top of the simulation domain, respectively.
- **temp_gradient_length:** Stores the length of the Z-dimension of the simulation box for gradient calculations.

During the parsing of wall definitions in the constructor part, the code automatically detects the presence of X-direction walls (XHI or XLO) and activates the gradient functionality. The temperature gradient creates a linear variation from **temp_start** at $Z = 0$ to **temp_end** at $Z = L_z$, which L_z is the length of the simulation box in the Z-direction. The most important modification occurs in the **wall_particle** method, where the collision temperature is determined dynamically based on the particle's Z-coordinate at the moment of wall contact. For gas atoms that collide with X-direction walls (XLO, XHI), the algorithm calculates the local wall temperature using the following formula in Eq. (2.1), as shown in the modified code screenshot in Fig. 2.3b.

$$T(z) = T_{\text{start}} + \left(\frac{z}{L_z}\right) \times (T_{\text{end}} - T_{\text{start}}) \quad (2.1)$$

Where z is the atom's vertical position relative to the bottom of the simulation box, and L_z is the total box height. For walls in other directions (Y and Z), the implementation keeps the original constant temperature behavior. The temperature gradient implementation produces minimal computational overhead. The wall

collision events require basic arithmetic operations that consume a small amount of time from the overall simulation duration. The `get_variable_temp_x` function, Fig. 2.3c, performs linear interpolation that scales based on wall collision numbers rather than total particle numbers.

Figure 2.3 consists of three panels showing C++ code for a customized reflective-stochastic wall development. Panel (a) shows the header file, which includes preprocessor directives for clang-format, a class declaration for `FixWallReflectStochastic` within the `LAMMPS_NS` namespace, and private member variables. Panel (b) shows the C++ source code, which implements the `FixWallReflectStochastic` class, including a `get_variable_temp_x` method. Panel (c) shows the implementation of the `get_variable_temp_x` function, which performs linear interpolation based on wall collision numbers.

```

// (a) Header file
#ifndef FIX_CLASS
// clang-format off
FixStyle(wall/reflect/stochastic,FixWallReflectStochastic);
// clang-format on
#else
#endif

#ifdef LMP_FIX_WALL_REFLECT_STOCHASTIC_H
#define LMP_FIX_WALL_REFLECT_STOCHASTIC_H

#include "fix_wall_reflect.h"

namespace LAMMPS_NS {

class FixWallReflectStochastic : public FixWallReflect {
public:
    FixWallReflectStochastic(class LAMMPS *, int, char **);
    ~FixWallReflectStochastic() override;

private:
    int seedfix;
    double walltemp[6], wallvel[6][3], wallacomm[6][3];
    int rstyle;

    //Added by Ehsan
    bool use_variable_temp_x;
    double temp_start, temp_end, temp_gradient_length;
    //end

    class RanMars *random;

    void wall_particle(int m, int which, double coord) override;

    //Added by Ehsan
    double get_variable_temp_x(double z);
    //end
};

} // namespace LAMMPS_NS

```

```

// (b) C++ source code
for (i = 0; i < nlocal; i++) {
    if (!(mask[i] & groupbit)) continue;

    sign = 0;
    if ((side == 0) & (x[i][dim] < coord)) sign = 1;
    else if ((side == 1) & (x[i][dim] > coord)) sign = -1;
    if (sign == 0) continue;

    // theta = kT/m
    //Added by Ehsan
    double collision_temp;
    if (use_variable_temp_x && (which == XHI || which == XLO)) {
        collision_temp = get_variable_temp_x(x[i][2] - domain->bboxlo[2]);
    } else {
        collision_temp = walltemp[m];
    }
    //end

    // Edited by Ehsan --> walltemp[m] -> collision_temp
    if (rmass) theta = force->boltz*collision_temp/(rmass[i]*force->mvv2e);
    else theta = force->boltz*collision_temp/(mass[type[i]]*force->mvv2e);
    //end

    factor = sqrt(theta);
}

```

```

// (c) get_variable_temp_x function
/*----- Added by Ehsan -----*/

double FixWallReflectStochastic::get_variable_temp_x(double z)
{
    return temp_start + (z/temp_gradient_length) * (temp_end-temp_start);
}

//end

```

(a) Header file.

(b) C++ source code.

(c) `get_variable_temp_x` function.

Figure 2.3: The customized reflective-stochastic wall development. This enhancement brings substantial improvements to thermal boundary modeling in MD simulations.

The modification maintains full compatibility with all existing reflection models (diffusive, Maxwell, and Cercignani-Lampis) that are already present in the original

code. The velocity distributions depend on temperature and are calculated using the local wall temperature. The method enables efficient energy transfer between particles and boundaries across different temperature levels.

The implementation required modifications to both the **header (.h)** and **source (.cpp)** files of the `fix_wall_reflect_stochastic` module*. Figure 2.3 illustrates the key code sections that were added or modified to implement the linear temperature gradient functionality. The changes maintain the modular structure of the original LAMMPS code while seamlessly integrating the new thermal boundary capabilities. It enables researchers to study heat transfer in complex geometries with spatially varying thermal boundary conditions.

2.3.2 Molecular Dynamics Simulation Details

As Fig. 2.4 demonstrates, a three-dimensional MD simulation domain is defined using metal units, with dimensions $L_x = 54 \text{ nm}$, $L_y = 132 \text{ nm}$, and $L_z = 5.4 \text{ nm}$, representing the lengths of the simulation box along the X, Y, and Z axes, respectively. A total of 1,000 argon atoms are randomly distributed within this simulation box. It represents a rarefied gas flow regime characterized by a Knudsen number of 10 ($Kn = 10$).

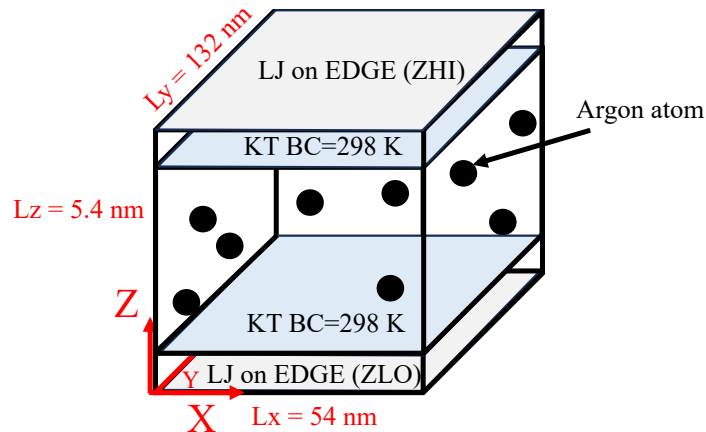


Figure 2.4: Finding a proper mesoscale boundary line. Molecular dynamics simulation details.

*<https://github.com/lammps/lammps/tree/develop/src/EXTRA-FIX>

Each argon atom is assigned a mass of 39.948 atomic mass units corresponding to the actual mass of argon gas. The interactions between gas atoms are modeled using the LJ 12-6 potential, with a cutoff radius of 10.0 angstroms ($\text{\AA}$). The LJ 12-6 parameters are set to $\epsilon = 0.0103235$ electron volts (eV) and $\sigma = 3.405$ $\text{\AA}$. These parameters effectively capture the attractive and repulsive components of the van der Waals forces among argon atoms. As shown in Fig. 2.4, the temperatures of the Z walls are maintained at a constant value of 298 K for both the lower Z wall (ZLO) and the upper Z wall (ZHI). As mentioned above, periodic boundary conditions are applied in the X and Y directions. This allows gas molecules that exit one side of the box to re-enter from the opposite side. This configuration simulates an infinite system in the X and Y directions.

The MD simulation starts with an energy minimization step followed by velocity initialization at 298 K using a Gaussian distribution. The simulation runs in an NVT ensemble (constant number of particles, volume, and temperature) for 100,000 timesteps, where each timestep lasts 0.0001 picoseconds. The simulation enters an NVE ensemble (constant number of particles, volume, and energy) after completing the equilibration phase. The LAMMPS input script runs for 30 million timesteps to compute thermal properties, which are dumped as outputs. These include heat flux through the Green-Kubo [54, 87] method and temperature profiles in the Z-direction with 100 bins, as well as density profiles in the Z-direction with 200 bins.

2.3.3 Finding the Parameters of Mesoscale Boundary Line

The gas-wall interactions are modeled using the LJ 12-6 potential with a 10.0 $\text{\AA}$ cutoff radius, and simulations are conducted for various combinations of ϵ , σ , and KT boundary location. The results of this investigation are presented in Fig. 2.5.

As shown in the figure, using parameters $\epsilon = 0.031$ eV and $\sigma = 3.4$ $\text{\AA}$, the mesoscale boundary condition exhibits behavior similar to that of the actual molecular surface reported in the literature [10]. The optimal location for the microscopic heat exchange

boundary is $0.37 \text{ \AA}$ from the surface. This is because gas molecules naturally transfer heat in the same way as they do at the actual molecular surface [10].

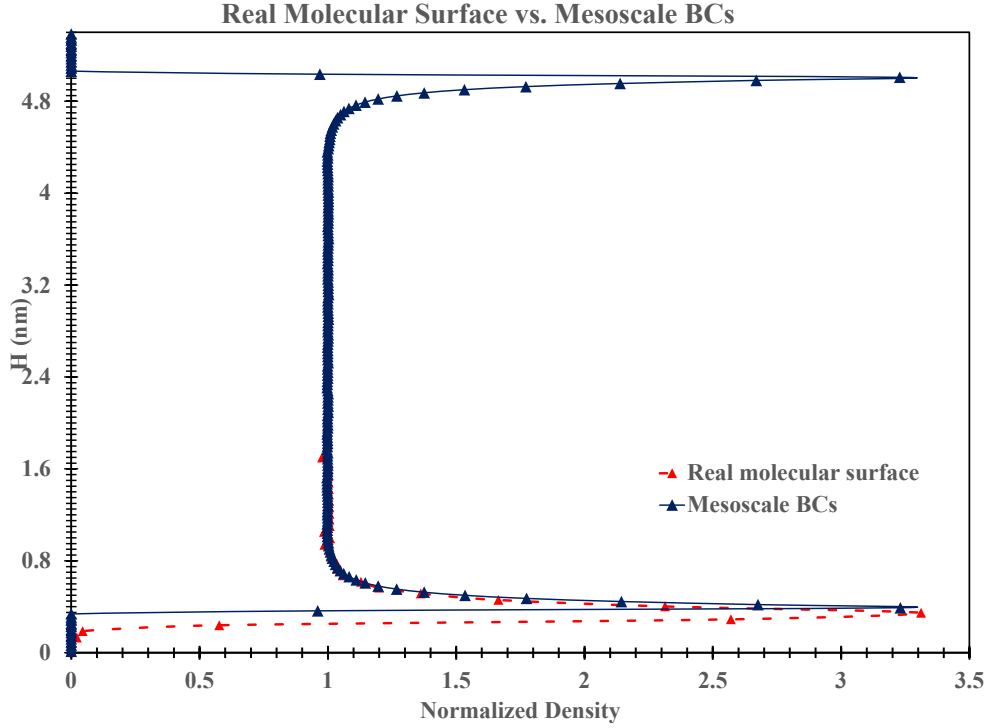


Figure 2.5: Comparison of normalized density distributions for Knudsen number 10 flow inside 5.4 nm height channels with the real molecular surface [10]. Peak alignment validates the mesoscale model’s ability to capture maximum adsorption. The curve deviations reflect the intentional simplification from molecular-level detail to averaged boundary behavior.

2.4 Validations

The developed mesoscale boundary condition is validated by studying two different argon gas flow regimes at Knudsen numbers 1 and 10. The details of the MD simulations for each flow regime are presented in Table 2.1 below. For each Knudsen number, three different MD simulation scenarios using different boundary conditions are considered. These boundary conditions include parallel plate (periodic), mesoscale boundary conditions, and adiabatic wall conditions. This systematic approach enables comparison and understanding of the effects of different boundary conditions on the

normalized temperature profile of argon gas flow, using the linearized Boltzmann solution as a reference. Additionally, the effect of these different boundary conditions on the effective thermal conductivity is examined through the Kaganer model.

Table 2.1: Molecular dynamics simulation details for argon gas at $Kn = 1$ and $Kn = 10$

Kn	Domain Lx, Ly, Lz (nm)	# argon molecules	Density number ($\frac{\#}{nm^3}$)	Density ($\frac{Kg}{m^3}$)	P (kPa)
1	$54 \times 20 \times 5.4$	1450	0.2486	16.49	1017
10	$54 \times 200 \times 5.4$	1510	0.0259	0.172	110.6

2.4.1 Three Boundary Condition Scenarios

1) **Periodic case:** For the periodic case (parallel plates), a diffusely reflective type of boundary conditions in the Z direction, while maintaining periodic boundary conditions in the X and Y directions, are applied. The temperatures of the Z walls are constant and set to 307.5 K for the lower Z wall (ZLO) and 292.5 K for the upper Z wall (ZHI). As Fig. 2.6 illustrates, this configuration causes a temperature gradient that creates a one-dimensional (1D) heat transfer in the Z direction from ZLO to ZHI.

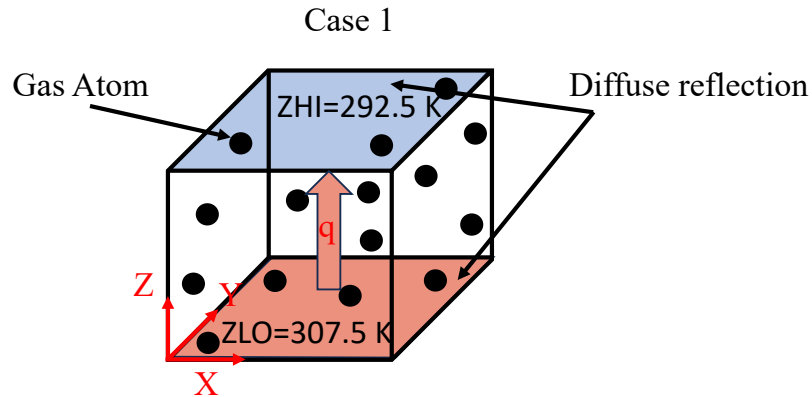


Figure 2.6: Case 1: Periodic case (parallel plates case).

This case is similar to the linearized Boltzmann (LB) solution configuration [121], where heat transfers between two parallel plates in one dimension with a small temperature difference. The simulation begins with an energy minimization, followed by velocity initialization at 300 K using a Gaussian distribution. It runs in an NVT ensemble for 100,000 timesteps. Each timestep is 0.0002 picoseconds long. Then, it runs an NVE ensemble. After the 120-million-timestep run, thermal properties are output, including heat flux, temperature profiles in the Z-direction with 100 bins, and density profiles in the Z-direction with 200 bins.

2) Adiabatic wall case: The adiabatic case maintains settings similar to those of the periodic case in the Z and Y directions. It uses diffusive walls in the Z direction and periodic boundary conditions in the Y direction. As shown in Fig. 2.7, adiabatic wall conditions are also present in the X direction on the X walls (XLO and XHI). This case uses the same simulation parameters as the previous cases.

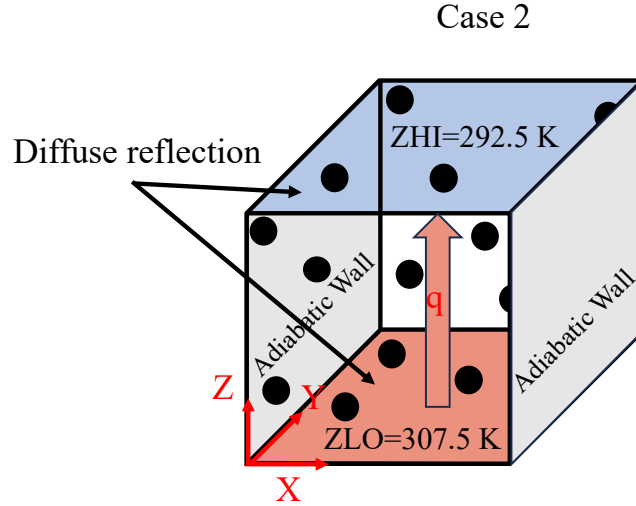


Figure 2.7: Case 2: Adiabatic wall case.

3) Mesoscale case: Figure 2.8 illustrates the third case, in which the novel mesoscale boundary line condition is applied on the Z walls, while periodic boundary conditions are maintained in the X and Y directions. This case employs the same simulation parameters as the previous case, including the timestep, run time, NVT, and NVE, which are similar to those used in the periodic and adiabatic wall cases.

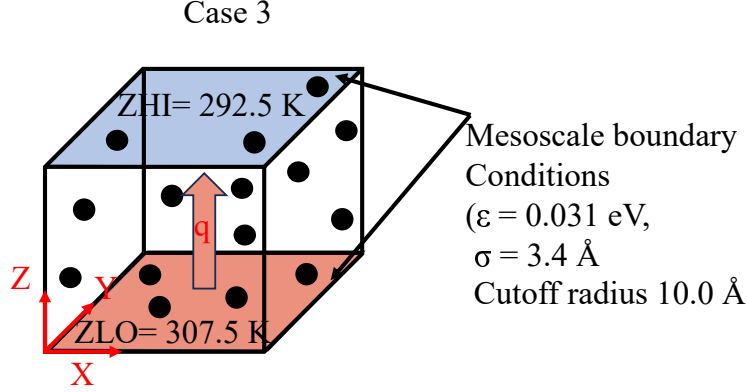


Figure 2.8: Case 3: Mesoscale boundary conditions case.

2.4.2 Validation with Linearized Boltzmann Solution

The MD simulation results are compared with the linearized Boltzmann solution. As Fig. 2.10 illustrates, the normalized temperature profile analysis of argon gas flow at Knudsen numbers 1 (Fig. 2.10a) and 10 (Fig. 2.10b) shows clear differences between the considered boundary condition scenarios. The MD simulation, using periodic boundary conditions (blue diamonds) and adiabatic wall boundary conditions (red triangles), produces nearly identical temperature profiles with smooth, continuous curves extending from the wall to the center region. These well-studied boundary conditions show excellent agreement with the LB solution (orange line) throughout the domain.

However, the novel mesoscale approach (black squares) exhibits noticeable temperature jumps and discontinuous behavior at specific domain locations due to the force field interactions introduced near the wall boundaries, where different modeling scales must be connected to explain this phenomenon. These temperature discontinuities appear to represent the physical reality of gas-surface energy exchange through intermolecular forces, which traditional simplified boundary conditions cannot capture. While the LB solution matches the molecular dynamics results throughout the bulk region for all case scenarios, it shows expected deviations from the mesoscale approach near the walls. This validates the computational framework

and highlights specific boundary condition artifacts that occur in multiscale modeling approaches.

Additionally, Fig. 2.9 presents the normalized heat flux validation against the linearized Boltzmann solution across a range of Knudsen numbers from 0.01 to 10.

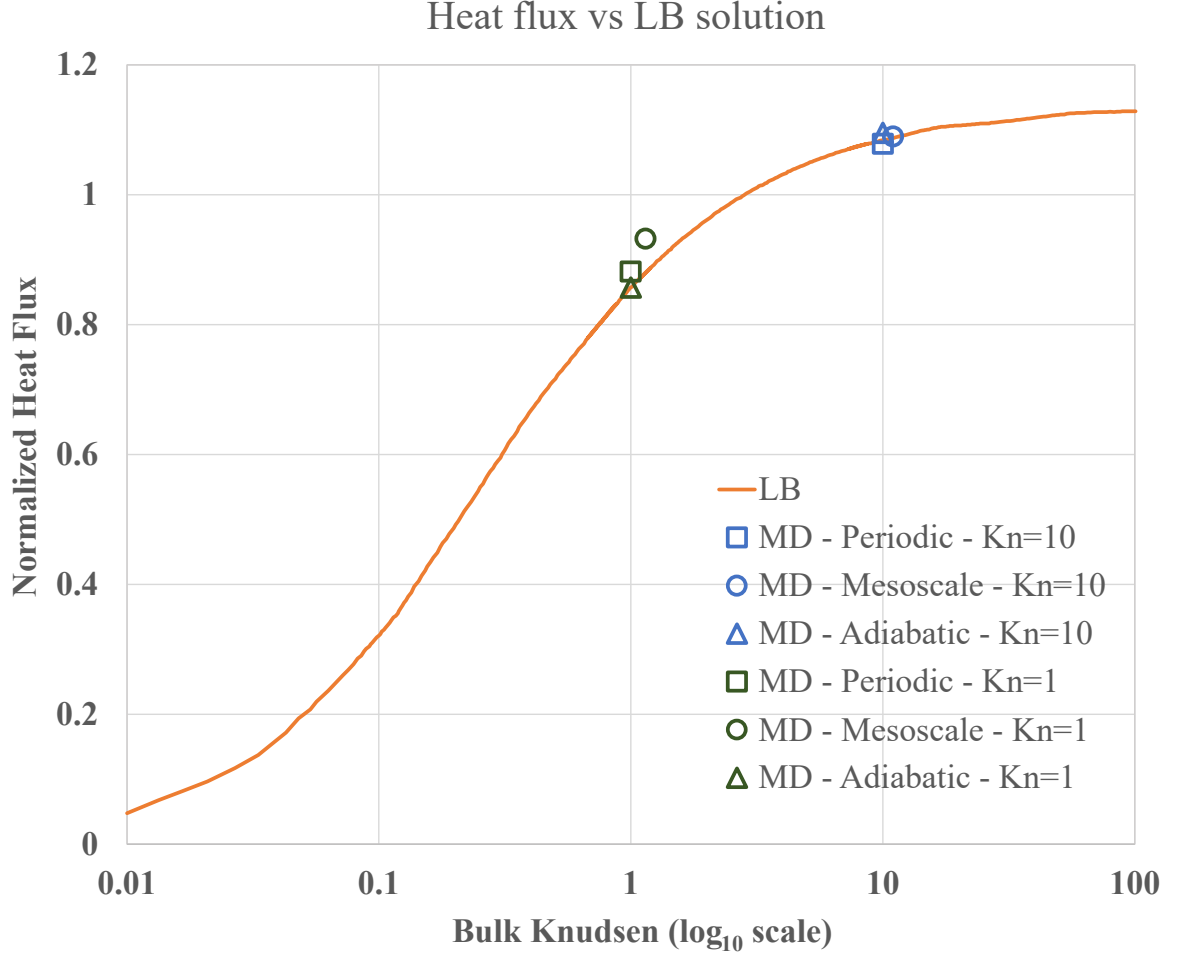
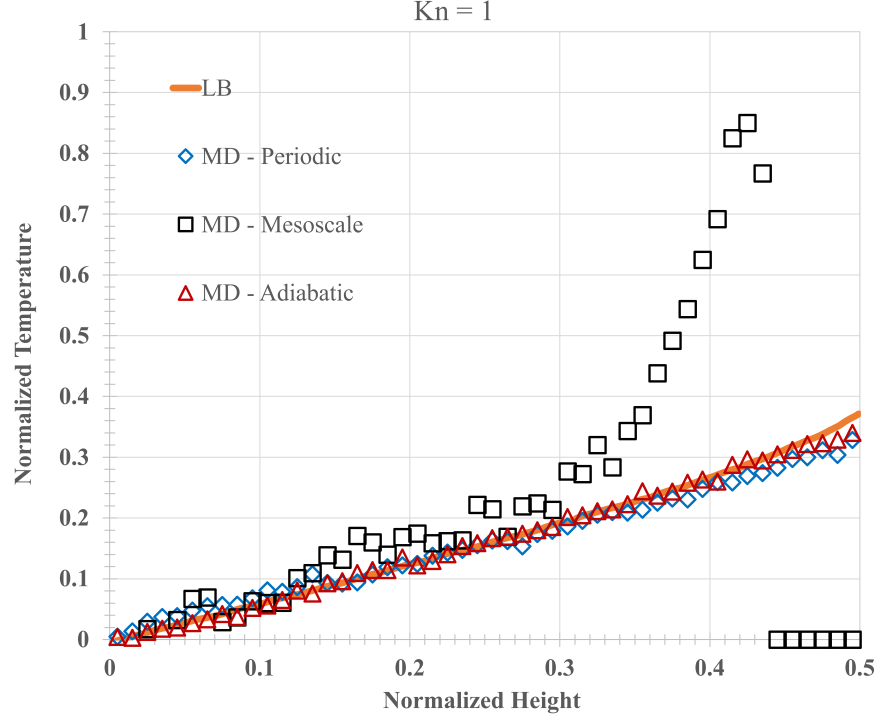
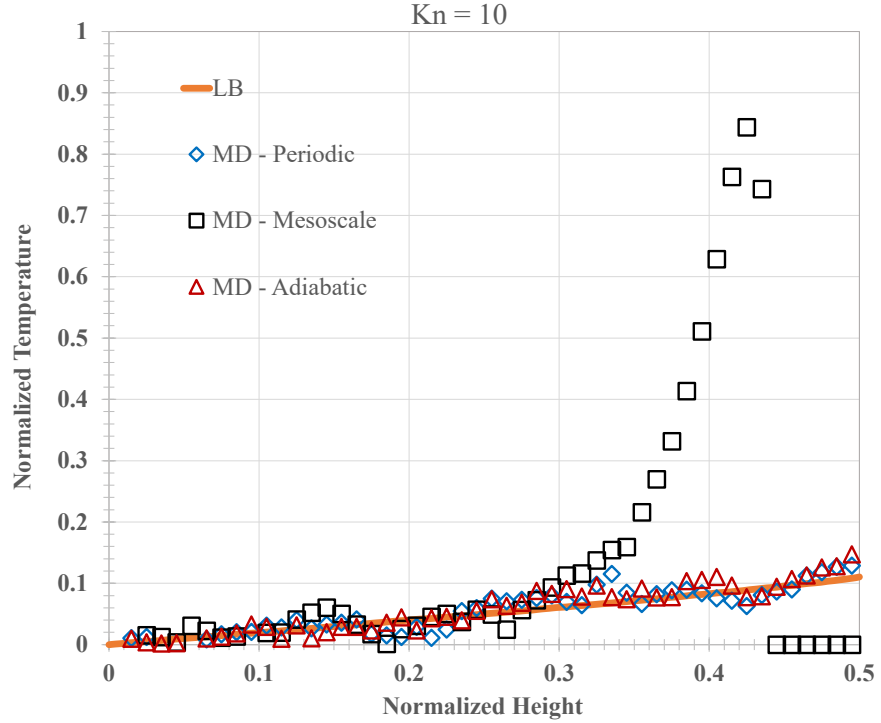


Figure 2.9: Normalized heat flux versus bulk Knudsen number. Symbols represent MD results for periodic, mesoscale, and adiabatic wall boundary condition scenarios at $Kn = 1$ and $Kn = 10$.

The agreement between MD simulations and the LB theoretical curve for both $Kn = 1$ and $Kn = 10$ conditions demonstrates that the simulation methodology accurately captures the physics of heat transfer across the entire transition from near-continuum to free-molecular regimes.



(a) $Kn = 1$. Normalized temperature profiles compared with LB solution.



(b) $Kn = 10$. Normalized temperature profiles compared with LB solution.

Figure 2.10: Normalized temperature profiles compared with the linearized Boltzmann solution [121] for $Kn = 1$ and $Kn = 10$.

2.4.3 Validation with Kaganer Model

As shown in Fig. 2.11, the effective thermal conductivities at $Kn = 1$ and $Kn = 10$ are calculated and plotted against the Kaganer model to validate the MD simulation methodology. The results demonstrate the rarefaction behavior where increasing the Knudsen number leads to enhanced rarefaction effects and correspondingly larger temperature jumps at the wall boundaries. The wall temperature jump phenomenon, which becomes more pronounced at higher Knudsen numbers, creates additional thermal resistance that reduces the effective thermal conductivity of the argon gas. The strong agreement between the MD simulation results and the Kaganer model, which is based on kinetic theory, confirms that the mesoscale boundary conditions properly capture the rarefaction physics and the wall temperature jump effects.

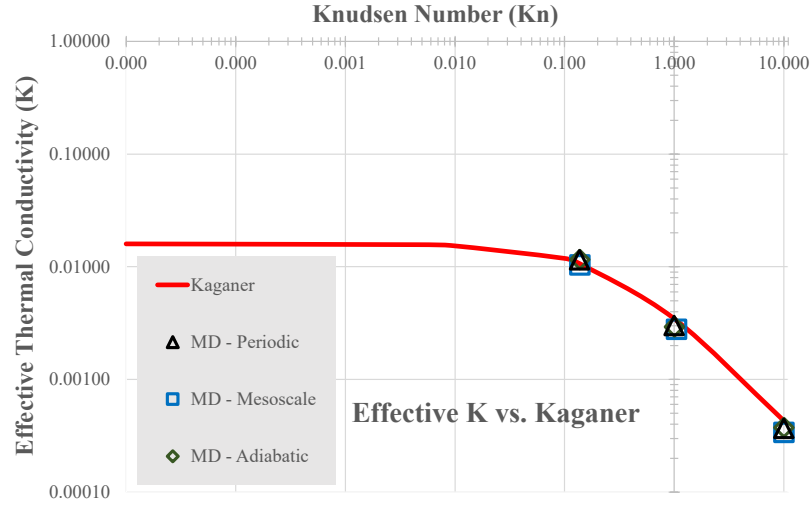


Figure 2.11: Effective thermal conductivity vs. Knudsen number showing agreement between MD simulations for three boundary condition scenarios and the Kaganer model.

2.5 Side Wall Effect on Thermal Conductivity

To investigate the two-dimensional confinement effects on nanoscale heat transfer, simulations were conducted with mesoscale boundary conditions applied to both

the X and Z walls while maintaining periodic boundaries in the Y direction. This configuration introduces sidewall effects that significantly influence the thermal transport characteristics of the confined gas. As Eq. (2.2) presents, the aspect ratio (AR) is defined as the ratio of the simulation box length in the X direction (width, W) to the characteristic length in the Z direction (height, H).

$$AR = \frac{L_x}{L_z} = \frac{W}{H} \quad (2.2)$$

Where H represents the channel height between the Z walls (ZLO and ZHI) across which the primary heat transfer occurs. The aspect ratio characterizes the geometric confinement, with smaller AR values ($AR < 1$) representing narrow channels and larger AR values ($AR > 1$) representing wide channels. To examine the influence of lateral thermal gradients, a linear temperature distribution is considered along the sidewalls (X walls). The sidewall temperature varies linearly from the bottom wall temperature (T_{ZLO}) to the top wall temperature (T_{ZHI}). Therefore, Eq. (2.1) can be expressed as

$$T_{\text{sidewall}}(z) = T_{ZLO} + \frac{z}{H}(T_{ZHI} - T_{ZLO}), \quad (2.3)$$

where z is the gas atom's vertical position relative to the bottom of the simulation box. Three sidewall (SW) temperature gradient conditions are investigated:

- **SW10:** 10 K temperature difference between ZLO and ZHI along the side walls.
- **SW20:** 20 K temperature difference between ZLO and ZHI along the side walls.
- **SW50:** 50 K temperature difference between ZLO and ZHI along the side walls.

Additionally, simulations with periodic boundaries in the X direction (labeled as “Parallel” in the results) were conducted to establish a baseline for comparison. They represent the ideal case without sidewall confinement effects. By systematically varying the aspect ratio from 0.5 to 20 across four different channel heights ($H = 5.4$,

10.8, 21.6, and 43.2 nm) and two Knudsen numbers ($Kn = 1$ and 10), the transition from sidewall-dominated to collision-dominated heat transfer can be characterized.

2.5.1 Simulation Matrix and Computational Details

The systematic investigation of sidewall effects necessitated an extensive computational effort encompassing 160 independent molecular dynamics simulations. Table 2.2 presents the complete simulation matrix, detailing the parametric variations across four channel heights (H : 5.4, 10.8, 21.6, and 43.2 nm), two Knudsen numbers (Kn : 1 and 10), four aspect ratios (AR : 0.5, 1, 2, 10), and four side wall boundary conditions (Parallel, SW10, SW20, and SW50). This comprehensive parameter space enables the characterization of heat transfer transitions from confinement-dominated to collision-dominated regimes.

Table 2.2: Summary of simulation parameters for different channel heights

H (nm)	Kn	AR range	Y (nm)	# molecules	Density	Number($\#/nm^3$)	ρ (kg/m ³)	Conditions
5.4	1	0.5, 1, 2, 10	560, 280, 140, 28	2300		0.2817	18.683	SW50, SW20, SW10, Parallel
5.4	10	0.5, 1, 2, 10	2700, 1350, 675, 135	1000		0.0254	1.685	SW50, SW20, SW10, Parallel
10.8	1	0.5, 1, 2, 10	560, 280, 140, 28	4600		0.1408	9.341	SW50, SW20, SW10, Parallel
10.8	10	0.5, 1, 2, 10	2700, 1350, 675, 135	2000		0.0127	0.842	SW50, SW20, SW10, Parallel
21.6	1	0.5, 1, 2, 10	140, 70, 35, 7	2300		0.0704	4.671	SW50, SW20, SW10, Parallel
21.6	10	0.5, 1, 2, 10	1350, 675, 337.5, 67.5	2000		0.0064	0.421	SW50, SW20, SW10, Parallel
43.2	1	0.5, 1, 2, 10	140, 70, 35, 7	4600		0.0352	2.3353	SW50, SW20, SW10, Parallel
43.2	10	0.5, 1, 2, 10	675, 337.5, 168.75, 33.75	2000		0.0032	0.2106	SW50, SW20, SW10, Parallel

2.5.2 Results

As Fig. 2.12 illustrates, the confinement condition ($H = 5.4$ nm) exhibits the most pronounced sidewall temperature gradient effects. The normalized thermal conductivity shows sharp transitions between aspect ratios of 0.5 and 2. It shows a critical geometric threshold. The implemented linear side wall temperature gradient provides substantial performance improvements, with SW50 consistently

outperforming SW20 and SW10 across all aspect ratios for both flow regimes. The Knudsen number effects remain noticeable, with $Kn = 1$ showing higher thermal conductivity than $Kn = 10$. Additionally, parallel boundary lines demonstrate superior performance compared to all confined cases, and they establish an upper bound for thermal transport. The normalized thermal conductivity values range from approximately 0.42 to 0.97, representing the largest variation in performance observed across the study.

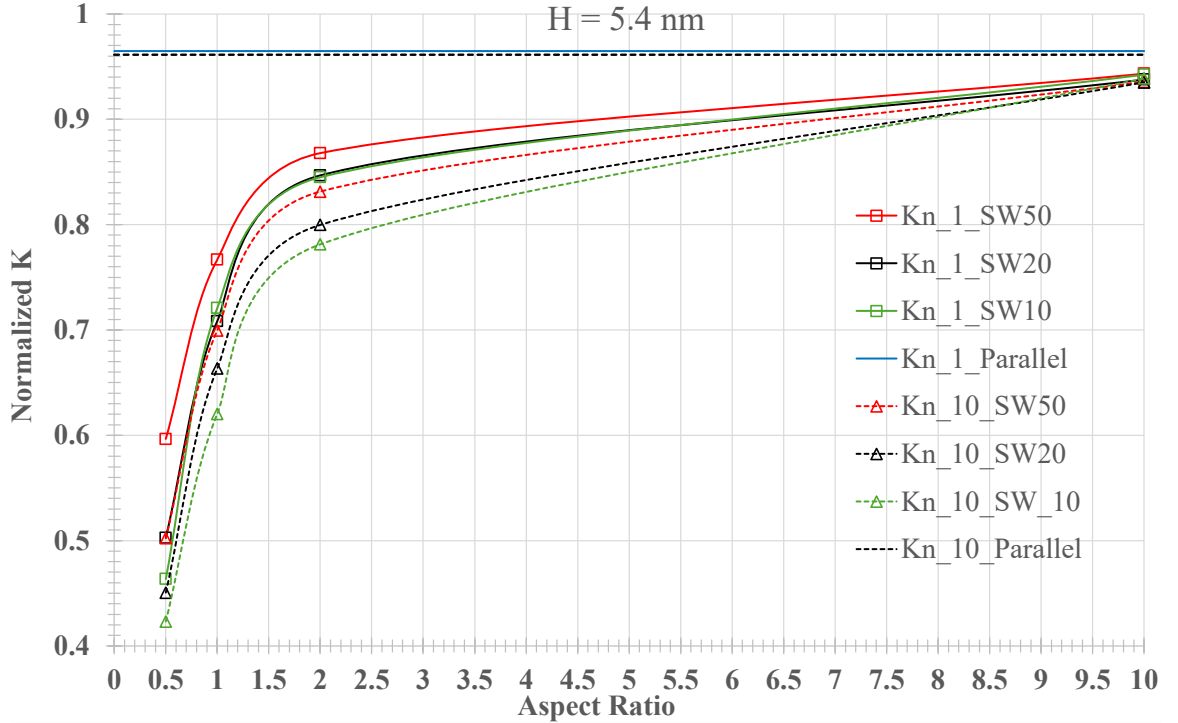


Figure 2.12: Results of gas flow inside 5.4 nm height channel.

As Fig. 2.13 shows, the confinement ($H = 10.8$ nm) exhibits strong sidewall effects but with more gradual curve transitions than those in $H = 5.4$ nm. The hierarchy $SW50 > SW20 > SW10$ persists; however, the magnitude of enhancement decreases. The Knudsen number effects become more clearly defined, with consistent separation between $Kn = 1$ and $Kn = 10$. The critical aspect ratio transition around $AR = 1$ and $AR = 2$ exists, but it is less abrupt compared to the previous confinement, $H = 5.4$ nm. Parallel boundary lines continue to outperform confined geometries,

though the gap with confinement cases becomes smaller. The normalized thermal conductivity range spans approximately 0.45 to 0.96, showing reduced confinement penalties compared to the previous case.

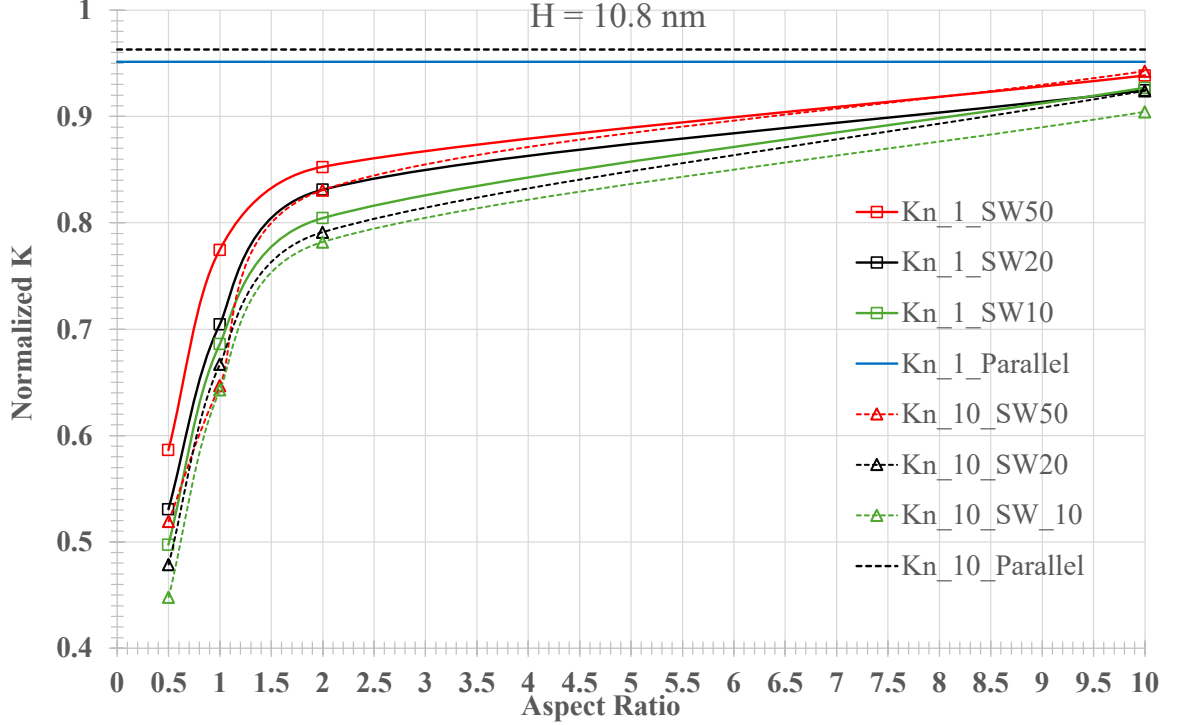


Figure 2.13: Results of gas flow inside 10.8 nm height channel.

The results of confinement $H = 21.6$ nm, as shown in Fig. 2.14, show a further reduction in sidewall temperature gradient effects while maintaining measurable increases in the normalized thermal conductivity. The curves exhibit progressively flatter profiles, indicating reduced sensitivity to geometric changes.

The side wall temperature gradient provides a measurable enhancement, but the thermal conductivity differences between the three temperature conditions become less noticeable. The Knudsen number effects follow expected trends more clearly than in previous cases. Parallel boundaries achieve their highest performance relative to Kaganer model predictions. The overall normalized thermal conductivity range narrows to approximately 0.48 to 0.98. The results demonstrate partial progression toward the bulk behavior of argon gas.

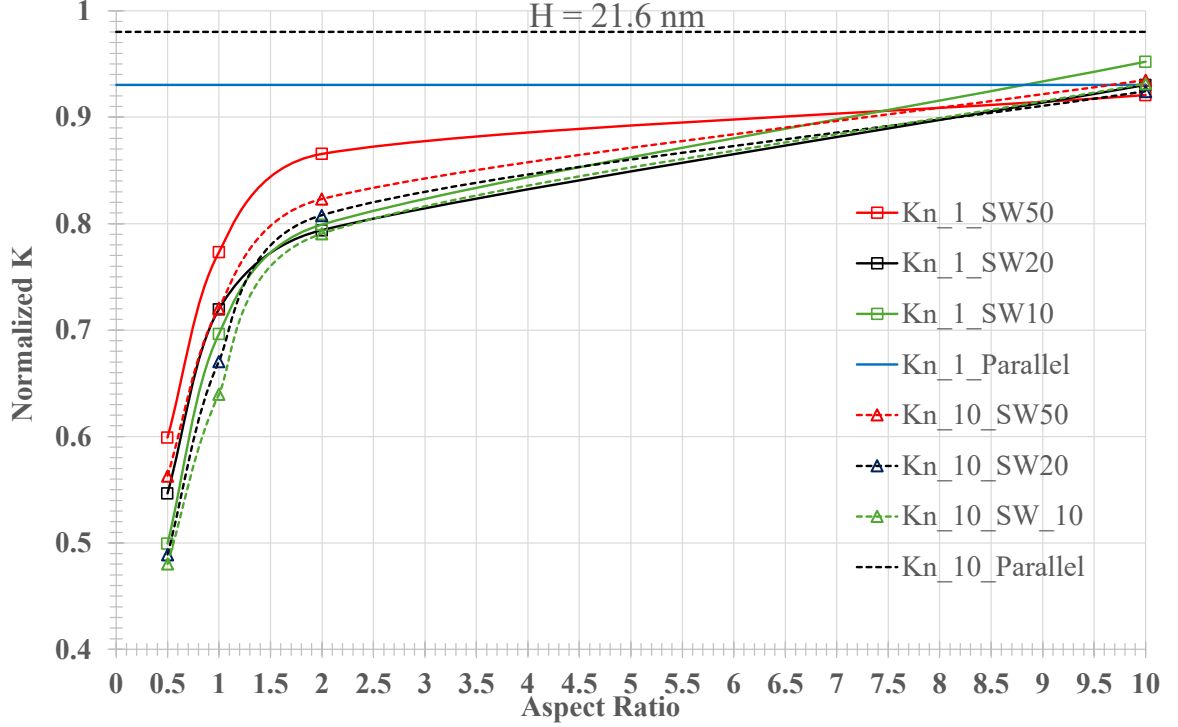


Figure 2.14: Results of gas flow inside 21.6 nm height channel.

The results of the largest H ($H = 43.2$ nm) are depicted in Fig. 2.15. As the curves illustrate, the sidewall exhibits minimal temperature effects, and the curves approach the predictions of the Kaganer model. The geometric sensitivity becomes almost negligible, and sidewall temperature gradients have a limited impact. Knudsen number effects follow the expected pattern from gas theory. Lower Knudsen numbers ($Kn = 1$) show higher thermal conductivity than higher values ($Kn = 10$).

This normal relationship becomes clear at this large H scale, whereas, due to geometric effects, it was not visible in smaller ones, such as $H = 5.4$ nm and $H = 10.8$ nm. Parallel boundary lines show thermal conductivity values near unity (k/k of Kaganer), confirming reduced sensitivity to geometric constraints. The thermal conductivity approaches unity for optimal conditions at $AR = 1$, which validates both the simulation methodology and the theoretical framework. This characteristic H represents the transition point where confinement effects (gas-solid) become less critical than molecular (gas-gas) collisions.

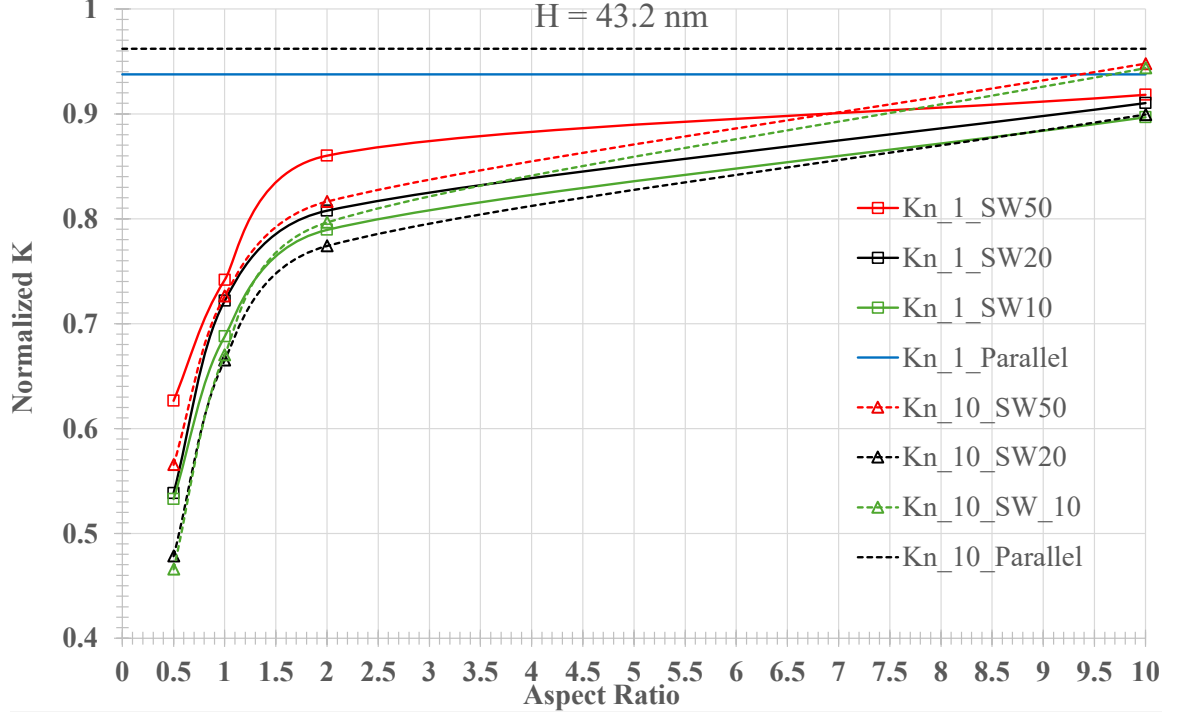


Figure 2.15: Results of gas flow inside 43.2 nm height channel.

The MD simulation results in the figures demonstrate a progressive change from side-wall-dominated to collision-dominated transport behavior when the characteristic H value increases from 5.4 nm to 43.2 nm. The transition produces reduced sidewall effects and more consistent aspect ratio dependencies with close prediction to the theoretical model (Kaganer). In general, thermal conductivity values increase with larger H values while the effects of the sidewall decrease. The transition occurs at $AR = 1-2$ regardless of the scale while maintaining consistent geometric behavior in all figures. The heat conduction hierarchy (Parallel $>$ SW50 $>$ SW20 $>$ SW10) remains consistent, and it offers a valuable design guideline for geometry optimization.

The progression also demonstrates a fundamental change in transport physics. The heat transfer at small H depends on sidewall interactions, while geometric effects strongly affect thermal conductivity values. However, at large scales, gas molecule collisions control heat transport, and sidewall conditions become less critical. The

Knudsen number effects ($\text{Kn} = 1 > \text{Kn} = 10$) persist throughout all scales, but the extent of this difference depends on the H.

The systematic approach to Kaganer model predictions validates both the MD simulation methodology and the underlying physics. The MD simulation results show that confined cases approach theoretical limits while maintaining values below unity, yet parallel cases achieve 96-98% accuracy when compared to theoretical predictions. The transition between molecular and continuum transport regimes offers unique guidelines for designing sensitive thermal management systems. Highly confined settings require advanced thermal boundary management, whereas larger-scale confinement necessitates different optimization approaches.

Chapter 3

Artificial Intelligence and Nanoporous Materials

- Ghasemi, Amirehsan, and Murat Barisik. 2025. “Machine Learning for Thermal Transport Prediction in Nanoporous Materials: Progress, Challenges, and Opportunities” *Nanomaterials* 15, no. 21: 1660. <https://doi.org/10.3390/nano15211660>

Predicting the thermal properties of nanoporous materials is a major challenge that affects their applications in efficient thermal insulation and energy storage. This chapter discusses the application of machine learning models in nanoporous materials, including covalent organic frameworks, metal-organic frameworks, aerogels, and zeolites. It discusses advancements in models, with a focus on predictive accuracy and computational efficiency. These include models such as convolutional neural networks, graph neural networks, and physics-informed neural networks. This chapter also addresses limitations of these data-driven models, including data availability, challenges in maintaining physical consistency, and difficulties in generalizing across various material families. Additionally, it covers emerging approaches such as multimodal and transfer learning, which are explored for their potential to reduce computational costs. This chapter also introduces and highlights the benefits of

interpretable machine learning methods for understanding the underlying physical mechanisms. This chapter provides comprehensive and practical guidelines for researchers using machine learning approaches in the study and design of nanoporous materials.

3.1 Background & Theory

The thermal behavior of nanoporous materials is critical for applications in thermal management, energy conversion, and energy storage [47, 4]. Depending on their structural properties, these materials exhibit a wide range of behaviors from ultra-low thermal conductivity in aerogels to relatively high conductivity in crystalline frameworks. This variability makes accurate prediction of their thermal conductivity particularly challenging [47, 9, 70]. Experimental studies often suffer from the limited reliability of thermal conductivity measurements. This prevents the establishment of accurate structure–property relationships. As a result, computational methods such as molecular dynamics simulations and first-principles phonon calculations based on density functional theory (DFT) have become essential tools for predicting thermal transport in nanoporous systems [185, 11]. However, these methods face limitations in terms of computational cost and scalability, particularly when addressing the structural diversity of nanoporous materials.

The emergence of machine learning models has changed the field of predicting material properties [73, 158]. While the applications of ML models in materials science date back to the 1990s, the prediction of thermal conductivity using these models gained popularity after 2018, with the appearance of graph neural networks (GNNs) [173]. Recent advances in deep neural networks (DNNs) such as cutting-edge GNNs and physics-informed neural networks (PINNs) [134] architectures [173, 27], along with the growth in computational power of the central processing units (CPUs) and graphics processing units (GPUs), as well materials databases, have

created great opportunities for the discovery and design of nanoporous materials with tailored thermal properties.

Using ML models in predicting thermal conductivity is a significant advancement over traditional methods. Table 3.1 presents the comparative advantages and limitations of traditional computational methods and ML models. The trade-offs between accuracy, computational efficiency, and generalizability are evident across different approaches. As Table 3.1 shows, the actual performance of each of these methods varies based on implementation details. For example, the accuracy of the MD approach depends on the quality of the force field. It can range from poor for simple potentials to near DFT accuracy for machine-learned potentials. The DFT-based methods struggle with van der Waals interactions, which are important in many nanoporous materials. Additionally, ML models usually cannot extrapolate beyond their training domain, resulting in varying scalability.

Table 3.1: Comparison of traditional and machine-learning-based methods for thermal conductivity prediction.

Method	Training Time	Inference Time	Accuracy	Scalability	Interpretability	Data Requirements
MD Simulations	N/A	High	Low-High	Low	High	Low
DFT+Phonons	N/A	Very High	Medium-High	Very Low	Very High	Low
Classical ML	Low	Very Low	Medium	Medium	Medium	Medium
DNNs	High	Very Low	High	Medium-High	Low	High
GNNs [142, 84]	High	Very Low	High	High	Medium	Medium-High
PINNs [134]	Very High	Medium	High	Medium	High	Medium

3.1.1 Nanoporous Materials

Nanoporous materials are characterized by high porosity, large surface area, and adaptive architectures [47, 95, 183]. The main categories of these materials include metal-organic frameworks (MOFs), covalent organic frameworks (COFs), zeolites, and aerogels. Each category presents particular challenges in predicting its thermal properties. MOFs consist of metal nodes connected by organic linkers, which offer good adaptivity with nearly 88,000 experimentally determined structures

(reported in 2019 [116]; the number increases annually) in the Cambridge Structural Database (CSD). COFs are composed entirely of light elements that are joined by covalent bonds. They provide remarkable stability but are limited by synthetic accessibility [36]. Zeolites possess well-defined crystalline structures; however, their thermal properties are challenging to predict. This is due to the complex interplay between framework composition and guest molecules [154]. Aerogels are known for their ultra-low density, high porosity, and hierarchical pore structures. They present further complexity because of their unstructured nature and multiple length scales [47]. Figure 3.1 summarizes the classification and thermal conductivity ranges of these nanoporous materials.

Nanoporous Materials Classification

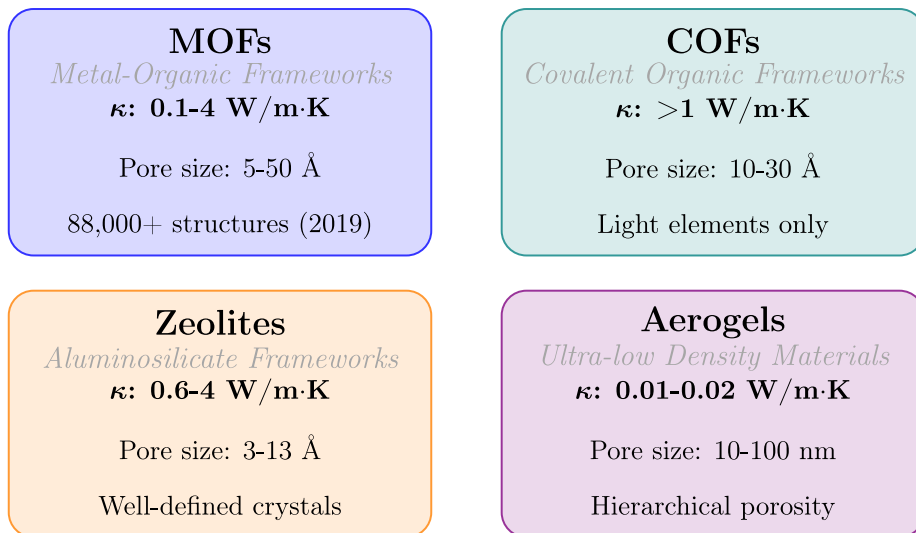


Figure 3.1: Nanoporous material classifications and their corresponding thermal conductivity (κ) ranges.

3.1.2 Thermal Transport in Nanoporous Materials

Thermal transport in nanoporous materials differs from that in bulk crystalline solids. Nanoscale pores introduce phonon scattering mechanisms that can reduce thermal conductivity compared to the solid counterparts [9, 130]. Additional complexity

comes from framework-guest molecule interactions, the presence of defects and grain boundaries, and the anisotropic nature of thermal transport in many nanoporous structures [66, 112]. Additionally, the transition from diffusive to ballistic phonon transport, which occurs when pore dimensions approach phonon mean free paths, adds more to the complexity [110]. Understanding the above-mentioned mechanisms is vital for developing accurate predictive models.

Thermal transport in nanoporous materials occurs across multiple length scales and involves interactions among different heat carriers [47]. The thermal transport regime is governed by the Knudsen number ($Kn = \lambda/H$), where λ is the phonon mean free path and H is the characteristic pore dimension [47]. For $Kn < 0.01$, transport is diffusive; for $Kn > 10$, it is ballistic; and values between represent transitional regimes. In nanoporous frameworks, lattice vibrations, also known as phonons, are the primary carriers of heat. Although the presence of any guest molecules and electronic conductivity can contribute to additional transport [9]. The effective thermal conductivity is determined by the combined effects of the structural framework, pore architecture, and the presence of any guest species in the nanoscale pores.

At the microscopic level, nanoscale pores act as additional phonon scattering centers. This substantially reduces the mean free path of heat carriers [63]. This effect becomes more noticeable when pore dimensions approach phonon mean free paths. In bulk silicon at room temperature, phonons with mean free paths exceeding $0.8 \mu m$ contribute 37% of thermal conductivity [75]. In nanoporous materials, these long mean-free-path phonons are truncated by pore boundaries. These dimensional constraints lead to strong phonon-confinement effects and alter phonon dispersion relations [109]. Additionally, the framework-pore interface introduces additional boundary scattering that depends on surface roughness and the specularity parameter [130]. These microscopic effects can fundamentally challenge traditional continuum models.

As a result, Fourier’s law of heat conduction, which is the basis for macroscopic thermal transport descriptions, requires modification when applied to nanoporous materials. At a nanoscale, non-Fourier effects such as ballistic transport and phonon hydrodynamics become important in materials with highly ordered pore structures [24]. The Boltzmann transport equation is able to provide a more rigorous framework for describing phonon transport in these settings since it can account for the wave nature of phonons and different scattering mechanisms [110]. Therefore, it is crucial to know when classical approaches are insufficient and when more sophisticated schemes are necessary.

Recent studies have examined thermal transport in nanoporous materials with periodic pore structures to understand the role of phonon coherence effects [2, 94]. When pore spacing is comparable to phonon wavelengths, periodic structures can create phononic band gaps that restrict thermal transport at specific frequencies. However, experimental measurements at room temperature have shown that classical boundary scattering dominates over coherent effects for structures with feature sizes above 100 *nm* [94]. Additionally, the direct comparisons between periodic and aperiodic nanostructures have demonstrated identical thermal conductivities. This suggests that phonon coherence effects are negligible in this size regime. The reduction in thermal conductivity compared to bulk solids resulted from diffuse phonon scattering at pore boundaries. These findings suggest that particle-based models accurately describe thermal transport in nanoporous materials from room temperature down to 14 K, below which phonon coherence effects may become significant [94].

3.1.3 Structure-Property Relationships

The relationship between structural features and thermal conductivity in nanoporous materials is complex and often non-intuitive. While intuition suggests that more pores mean lower thermal conductivity because there is less solid material to carry heat,

recent research has proven the difference. It highlights the importance of features such as pore size distribution, pore connectivity, and framework’s composition [161, 47, 26]. For instance, silica aerogel composites have very low thermal conductivities (0.01-0.02 W/m·K) because their nanoporous structure inhibits gas atom movement and limits heat flow through the solid skeleton [47]. On the other hand, some single-crystal covalent organic frameworks (COFs) have demonstrated the ability to conduct heat effectively (> 1 W/m·K) even with a nanoporous structure. This is because their strong, connected COF ribbons form a continuous crystal and enable efficient heat flow even when the porosity percentage is high [161]. These contrasting behaviors illustrate how the structural framework can overshadow simple considerations of porosity.

Framework topology is an important factor in determining thermal transport properties. Materials with highly connected frameworks, indicated by high coordination numbers at the nodes, typically have higher thermal conductivities. In MOFs, a recent computational screening of over 10,000 hypothetical structures revealed that four-connected metal nodes consistently yield the highest predicted thermal conductivities, with approximately 65% of high-performance MOFs featuring four-connected nodes. Simulations suggest that these structures can achieve thermal conductivities of up to 2-4 (W/m·K) experimentally, although a small subset showed computational predictions above 10 (W/m·K). In contrast, structures with 12-connected nodes typically exhibit values below 2 (W/m·K) [70, 170]. Additionally, pore dimensionality can further affect thermal transport. One-dimensional channels often exhibit highly anisotropic properties [9].

The chemical composition of the framework also adds complexity to structure-property relationships. Larger mass differences between atomic species increase phonon scattering and typically lower thermal conductivity [70]. Stronger covalent bonds enable more efficient thermal transport. In MOFs and COFs, the organic linkers act as thermal resistances. Their length, stiffness, and functional groups all contribute to this effect [8, 66]. In zeolites, non-equilibrium MD simulations

have revealed thermal conductivities ranging from 0.6 to nearly 4 (W/m·K) at 350 K, with values varying between different framework types and crystallographic directions [143, 111]. Guest molecules adsorbed in zeolites usually have a minor influence on thermal conductivity, though water can reduce values by 20-40% through phonon scattering [143, 8].

Recent findings have identified several surprising structure-property relationships. While disorder typically reduces thermal conductivity, recent studies have identified cases in nanoporous graphene where specific disorder patterns can maintain or slightly enhance thermal conductivity, albeit with precise control of pore arrangements [67]. Another interesting effect arises from the presence of guest molecules within pores, which exhibits complex behavior known as the “rattle effect”. The rattle effect refers to the rattling vibrations of guest molecules confined within pore spaces, which occur when these mobile molecules collide with pore walls and scatter heat-carrying phonons [44]. This phenomenon occurs when fluid-solid collisions scatter phonons. It typically reduces thermal conductivity by up to 30% in narrow pores compared to vacuum (empty pore) conditions. However, this effect transitions to different behavior in larger pores when the vacuum is replaced with a fluid. It leads to an increase in heat transfer [44]. These effects depend on the pore size, temperature, and the type of fluid involved. These findings underscore the need for predictive models that capture the full complexity of structure-property relationships in nanoporous materials.

3.1.4 Challenges in Traditional Computational Approaches

Traditional computational methods for predicting thermal transport in nanoporous materials have several limitations. For example, MD simulations provide atomic-level insights but are computationally expensive. Their complexity ranging from $O(N)$, $O(N\log N)$ to $O(N^2)$ depending on the treatment of interatomic interactions and implementation of neighbor searching algorithms [62]. Big O notation describes

computational complexity, where $O(N)$ denotes linear scaling, $O(N\log N)$ denotes log-linear scaling, and $O(N^2)$ denotes quadratic scaling. Developing reliable interatomic potentials, also known as force fields, for complex nanoporous materials remains an active area of research. Many existing interatomic potentials still fail to capture the interactions that affect thermal transport [41, 39]. Force fields struggle with two critical aspects: (1) van der Waals forces, attractions between atoms and molecules, despite being individually weak, collectively influence how heat moves through the porous framework. (2) host-guest molecule interactions, that is, the complex dynamics between the framework structure and any molecules trapped within the pores. This can scatter phonons and substantially reduce thermal conductivity [8, 41, 39, 44].

First-principles calculations offer higher accuracy but are even more computationally expensive. Usually, their application is limited to small unit cells and simplified models [129]. The calculation of phonon properties from first principles calculations requires the evaluation of force constants through finite displacement methods or density functional perturbation theory, both of which scale as cubic, $O(N^3)$, with system size [129, 61]. For nanoporous materials with large unit cells containing hundreds or thousands of atoms, these calculations become impractical, often requiring weeks of computation on a high-performance computing node.

Beyond computational cost, addressing anharmonic effects presents another major challenge for conventional computational methods. Harmonic approximations perform well for modeling thermal transport at low temperatures. However, accurate prediction of thermal conductivity at higher temperatures requires consideration of phonon-phonon scattering processes [56, 177]. Integrating three- and four-phonon scattering increases computational complexity and often requires approximations that can compromise predictive accuracy [56]. These computational bottlenecks, combined with the wide chemical space of nanoporous materials, have motivated the development of alternative approaches that can predict thermal conductivity more efficiently and maybe at a lower cost.

3.2 Evolution of Artificial Intelligence Approaches in Nanoporous Materials

Machine learning (ML) models use statistical methods to identify patterns in data without explicit programming. The field is divided into supervised and unsupervised learning as in illustrated in Figure 3.2.

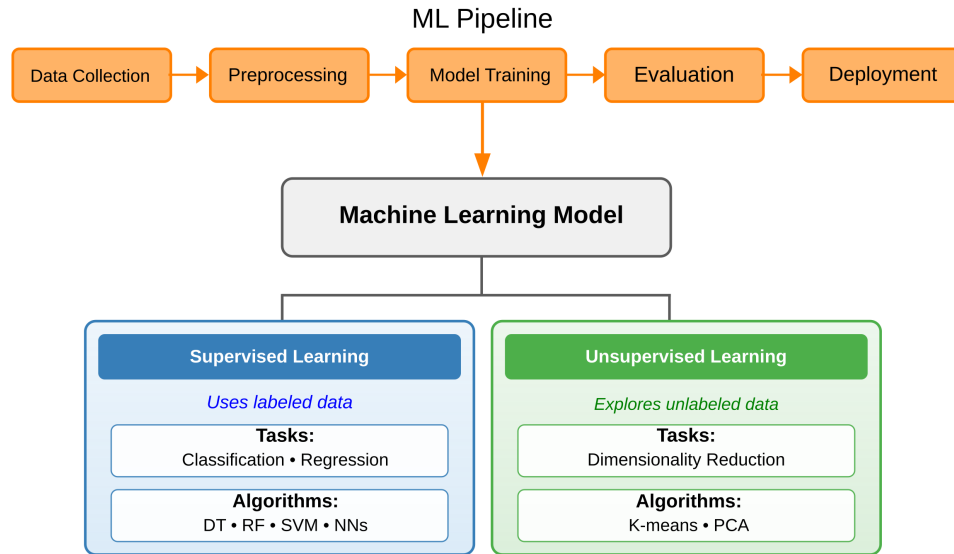


Figure 3.2: Overview of machine learning categories and typical pipeline stages.

Supervised learning uses labeled data to train algorithms for classification and regression tasks. Common supervised algorithms include Decision Trees (DT), Random Forests (RF), Support Vector Machines (SVM), and Neural Networks (NNs). Unsupervised learning, in contrast, explores unlabeled data to discover hidden patterns and structures in data [74]. These methods are effective at anomaly detection and dimensionality reduction for data visualization. Most popular unsupervised techniques include K-means clustering for grouping similar data samples and Principal Component Analysis (PCA) for reducing data complexity [15]. A typical ML pipeline consists of five stages: data collection, data preprocessing (cleaning, normalization,

feature engineering), model training with cross-validation, model evaluation using metrics like accuracy or R^2 , and finally use it for predictions on new data. This approach ensures reproducible and reliable results across different applications [88].

3.2.1 Early Machine Learning Models

Machine learning applications for thermal conductivity prediction in crystalline materials began in the mid-2010s [145, 18]. Their application to nanoporous materials appeared more recently around 2019-2020 [169]. Figure 3.3 illustrates this evolution. The delay in applying ML models to nanoporous materials stemmed from their structural complexity and the limited availability and mostly unreliable experimental data [115, 108]. Initial research primarily established quantitative structure-property relationships using traditional ML algorithms such as random forests (RF) [16] and support vector machines (SVM) [144]. These models relied on hand-crafted feature variables derived from crystallographic information such as pore size, surface area, density, and void fraction [169].

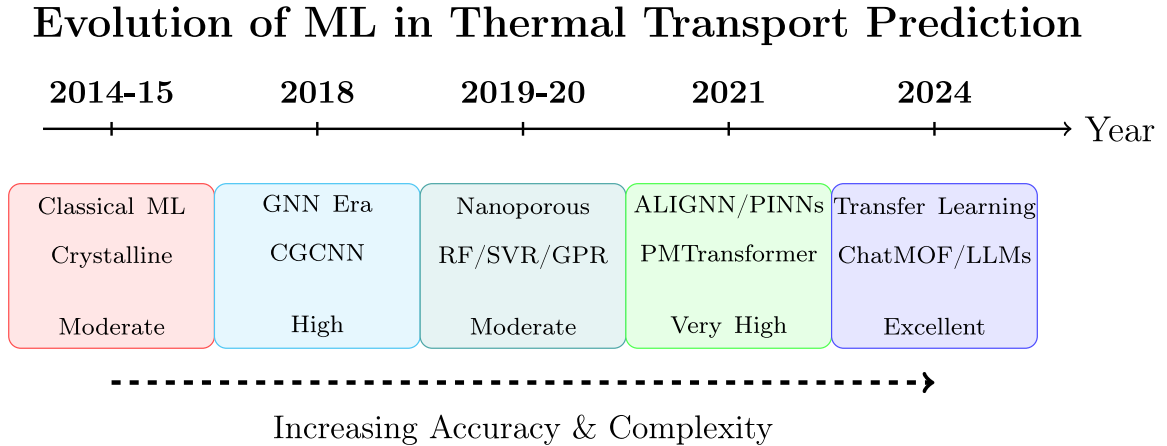


Figure 3.3: Timeline evolution of machine learning (ML) approaches for thermal transport prediction.

Despite their simplicity, these classical ML models have demonstrated good potential for predicting thermal transport properties. For example, Wei et al. [169]

used SVR and Gaussian Process Regression (GPR) models to identify five physics-based descriptors (features). These features included the shape factor, bottleneck, channel factor, perpendicular nonuniformity, and dominant paths, which exhibited strong correlations with thermal conductivity [169]. Random forest models have also proven effective in related studies due to their ability to capture non-linear relationships and offer built-in feature importance [72]. Studies using these methods gained reasonable prediction accuracy within their training domain; however, specific performance metrics varied widely depending on the material type and the quality of the data.

One major challenge in early ML models was feature engineering. Researchers attempted various sets of feature variables, including geometric and chemical features. Choosing the right features required domain knowledge and often repeated testing. Additionally, the fixed-length vectors used in traditional ML algorithms were not suitable for materials with varying sizes and compositions. This necessitated preprocessing that sometimes resulted in the loss of structural information. For instance, encoding the three-dimensional pore network into fixed-length feature vectors results in a loss of important connectivity information for thermal pathways. These limitations indicated the need for fundamentally different approaches that could directly process variable-sized crystallographic data while preserving connectivity information [173].

3.2.2 Deep Learning Models

Deep learning models in materials research have enabled remarkable capabilities in design, prediction of structure-property relationships, and performance optimization [114, 167, 149]. DL models have transformed thermal conductivity prediction in nanoporous materials through three major architectures: convolutional neural networks for microstructural analysis, graph neural networks for crystallographic structures, and generative models for inverse design. These approaches overcome the

limitations of fixed-length vectors in classical ML while they reduce computational costs compared to MD and DFT simulations [68]. DL models have also changed approaches to discovering materials with tailored thermal conductivity for applications ranging from effective thermal insulation to heat dissipation [172].

3.2.2.1 Convolutional Neural Networks

Convolutional neural networks (CNNs) [92] are recognized as powerful algorithms for analyzing the microstructural characteristics of porous materials through image analysis. CNNs have achieved high accuracies for predicting properties such as porosity, permeability, and tortuosity from two-dimensional (2D) binary images (relative errors less than 6%) [53] and elastic modulus ($R^2 = 0.98$) [100]. Although their direct applications to the prediction of thermal conductivity have remained limited in the literature.

A study by Du et al. [37] developed a modified AlexNet [86] architecture to predict the effective thermal conductivity of sintered silver. It has achieved remarkable accuracy prediction with an R^2 value of 0.987. Their model processes 400×400 pixel scanning electron microscope (SEM) images through five convolutional layers and predicts thermal conductivities that range from 25.3 to 422.7 (W/m·K) in just 0.14 seconds per image. This is reportedly two orders of magnitude faster than finite element simulations [37]. This success was enabled by a robust database of 6,156 realistic microstructures with FE-validated labels (relative error of 5% with experiments). This has enabled the CNN model to outperform conventional analytical methods (R^2 of 0.837) and ML approaches (R^2 of 0.951).

The advantage of CNNs lies in their translation invariance property, which is achieved through the combination of convolutional and pooling layers. This enables recognition of pores, channels, and connectivity patterns regardless of their spatial location within the microstructure [93, 80]. This capability is particularly valuable for porous materials with repeating structural features. CNNs can analyze entire samples using a single set of convolutional filters rather than requiring position-specific feature

extractors. Therefore, they can provide computational robustness and efficiency in the case of variations in sample positioning.

For three-dimensional (3D) analysis, CNNs process volumetric data from techniques such as micro-CT scanning [80] and capture the complete pore network structure. Santos et al. [141] developed PoreFlow-Net, a 3D CNN architecture that predicts velocity fields in porous media with speedups of several orders of magnitude compared to numerical simulations. Kamrava et al. [80] demonstrated that 3D convolutions enable accurate predictions of permeability for realistic pore geometries. In a comprehensive study, a 3D CNN was used to analyze 90,000 artificially generated microstructures and establish robust microstructure-property relationships for diffusivity and permeability [131].

Despite these advantages, CNN-based approaches have limitations. The application of CNNs to disordered nanoporous materials remains challenging due to what are identified as ill-posed problems, nonlinear correlations, and a lack of interpretable features [166]. While CNNs excel at image segmentation and structural characterization [166], their success in predicting thermal conductivity has been demonstrated for materials with semi-ordered structures, such as sintered metals [37]. The Du et al. model [37] has also proved cross-material transferability. It successfully predicted the thermal conductivity of sintered Cu ($R^2 = 0.975$) by using a model trained on Ag data (Ag-trained model). This suggests the potential of their model for broader applications within similar material classes.

However, the training requirements for DL models vary significantly, from 1,000 samples for specific properties [100] to 90,000 samples for comprehensive transport property prediction [131]. Furthermore, prediction accuracy can degrade when models encounter microstructures outside their training distribution, and errors increase for irregular pore geometries [100].

3.2.2.2 Graph Neural Networks

Graph neural networks (GNNs) [142, 173] have advanced the analysis of nanoporous materials by capturing molecular structure and chemical bonding patterns. Unlike traditional descriptor-based approaches, GNNs can directly process three-dimensional atomic arrangements and chemical connectivity. It can handle variable sizes and periodic boundary conditions inherent to crystal structures. By representing materials as graphs with atoms as nodes and chemical bonds as edges (also known as links), GNNs learn hierarchical features through message-passing (embedding) frameworks throughout the molecular graph. Therefore, it can capture local and global structural features relevant to thermal transport [30, 48, 152].

Subsequent developments in GNN architectures have further enhanced their applications in predicting thermal conductivity. The inclusion of edges with features that represent bond types, lengths, and angles provides additional chemical context and improves prediction accuracy [34]. Also, advancements in pooling strategies have enabled GNNs to learn multi-scale representations that capture both local atomic and global structural features [174, 106].

The crystalline nature of MOFs and COFs is described by well-defined atomic positions and bonding patterns. It makes them ideal candidates for GNN architectures. This contrasts with the ill-defined connectivity observed in disordered materials. The crystal graph convolutional neural network (CGCNN) [173] architecture is specifically designed for crystalline materials. It has demonstrated remarkable success in predicting thermal conductivity of lattice structures [173, 65]. CGCNN encodes compositional and structural information through learned atom and bond features, which are aggregated across multiple convolutional layers to produce material-level predictions [27]. The ability of CGCNN to achieve high accuracy with relatively small training sets has made it attractive for studying materials, where experimental data are often limited.

The enhanced crystal graph convolutional neural network (ECGNN) shows a significant architecture advancement. It incorporates attention mechanisms (multi-head attention) and geometric features to achieve remarkable performance in gas adsorption prediction. It is demonstrated that the method predicts CO₂ adsorption properties in MOFs with accuracies comparable to Grand Canonical Monte Carlo (GCMC) simulations, which can take hours to days, thereby reducing computational time by almost five orders of magnitude [30].

The atomistic line graph neural network (ALIGNN) integrates atomic graphs and their corresponding line graph representations [27]. This dual approach captures angular information and three-body interactions, which are essential for accurate property prediction. ALIGNN has been used to predict the CO₂ adsorption of MOFs. It has also achieved high accuracy prediction for properties such as adsorption isotherms, surface area, and pore characteristics [28]. The model has also shown promise in predicting phonon density of states and derived thermodynamic characteristics such as heat capacity and vibrational entropy [58].

3.2.2.3 Generative Models

The application of generative models to nanoporous materials design represents a significant advancement from classical trial-and-error approaches to systematic, data-driven materials discovery [172]. Generative adversarial networks (GANs) [52] and variational autoencoders (VAEs) [83] are robust architectures for inverse design applications, where desired properties guide the generation of corresponding material structures [179].

A study by Du et al. [38] used conditional GANs (CGANs) to generate microstructures of sintered silver with desired effective thermal conductivity. Their model achieved a prediction accuracy with $R^2 = 0.985$ between the target and CNN-predicted thermal conductivities when conditioned on both thermal conductivity and porosity. The CGAN could generate multiple microstructure candidates within seconds (0.2 seconds per image). Each image displayed a realistic pore morphology

that met the target thermal properties. This inverse design approach, which begins with a desired thermal conductivity and generates corresponding structures, demonstrates the potential of generative models for developing materials with tailored thermal properties.

Generative models have been effective in generating realistic microstructures for various applications. Recent implementations of supramolecular VAEs have shown the ability to generate MOFs with superior gas separation performance that outcompete some of the best-performing materials ever reported [179]. For mechanical properties, GAN-CNN frameworks have created optimized nanoporous silicon nitride membranes, demonstrating 32% higher strength compared to conventional cubic pore patterns. This is achieved through reduced stress concentration factors around pore edges [149].

Generative models ensure that generated structures keep physical realism while exploring novel design spaces that may not exist in traditional databases [179, 172]. The success of Du et al.’s model [38] suggests that generative models could be extended to other thermal properties and more complex disordered structures. Though challenges remain in ensuring that generated structures are both thermally optimal and synthetically accessible. Future work might combine generative models with physics-informed constraints to ensure that proposed structures respect fundamental thermal transport mechanisms while maintaining manufacturability.

3.2.2.4 Physics-Informed Neural Networks

Physics-informed neural networks (PINNs) [134] encode fundamental physical laws and constraints directly into the learning (training) process. The concept of integrating physical equations into neural networks (NNs) dates back to 1998, when it was used to solve differential equations [89]. The modern PINN framework was formalized in 2019. By encoding governing equations (ODEs, PDEs) into the neural network’s loss (cost) function, PINNs ensure predictions respect conservation laws

and thermodynamic principles, while addressing the limitations of traditional NNs in extrapolation and physical consistency [42, 120].

Recent work has demonstrated the potential of PINNs for predicting thermal conductivity in porous materials. Liu et al. [99] applied PINNs to solve inverse problems in polyurethane-PCM foam composites. They accurately predicted spatially-varying thermal conductivity fields from temperature measurements, with an R^2 value exceeding 0.99, even with noisy sensor data. This hierarchical multi-scale approach represents one of the few successful applications of PINNs to thermal transport in porous materials, although it operates at the continuum rather than the phonon transport scale.

PINNs have also shown success in modeling flow and transport phenomena in porous media by incorporating Darcy’s law and advection-dispersion equations [43, 162, 176, 175]. These applications demonstrate PINNs’ ability to bridge data-driven learning and mechanistic understanding. However, the application to nanoscale thermal transport in disordered nanoporous materials remains largely unexplored. The challenge lies in encoding phonon transport mechanisms and size effects that dominate at nanoscales, which differ fundamentally from continuum heat diffusion.

While PINNs’ computational costs remain higher than those of purely data-driven approaches [175], this gap represents an opportunity for future research. Physics-informed approaches could potentially address the extrapolation challenges faced by conventional ML methods in predicting the thermal conductivity of disordered nanoporous materials.

3.3 Transparency in Artificial Intelligence

The arrival of predictive AI models has contributed to solving engineering problems. Based on the problem, AI models can be applied to data to make predictions. But, complex AI models are considered black boxes [117] and lack transparency. However, real-world problems are complex and demand complex models. Many DNN

architectures, due to neural networks’ universal approximation capabilities [32, 64], can capture the complex relationships in data. Therefore, they can be a good remedy for these complex problems. However, as mentioned, complex models need transparency.

AI models, such as ensemble learning approaches [140], SVM, and DL models, are categorized as “black-box”. In contrast, simpler models, such as k-nearest neighbors (KNN) and linear regression, are intrinsically explainable and known as “white-box” models. However, the white-box models are less accurate than black-box models and usually do not perform well for complex problems [49]. Therefore, the trade-off between accuracy and transparency should be considered when choosing an AI model.

3.3.1 Explainable AI

The eXplainable Artificial Intelligence (XAI) [55] is coined as a collection of methods for understanding the predictions of AI models. XAI employs a post-hoc approach and incorporates several explanatory methods, thereby making the results of the black-box model explainable. The complexity of an AI model can be restricted by choosing white-box models to provide explanations without applying XAI methods [117]. However, selecting a black-box model needs explanations. As Fig. (3.4) depicts, the post-hoc approach explains the AI model results after the training and inference processes [1, 29].

The post-hoc approach includes several XAI methods known as “model-specific” that have been developed to explain a specific AI model architecture. For instance, class activation mapping (CAM) [182] and gradient-weighted class activation mapping (Grad-CAM) [146] explain CNNs by creating a heatmap where the hot part corresponds to a particular class. The other XAI methods in the post-hoc approach, known as “model-agnostic”, can be implemented for any black-box estimator.

Generally, a post-hoc method is preferred over an intrinsic model since it applies to a black-box model’s prediction, and commonly, black-box models (complex models)

perform better. It should be noted that post-hoc methods can also be applied to a white-box model’s result and provide more transparency [117].

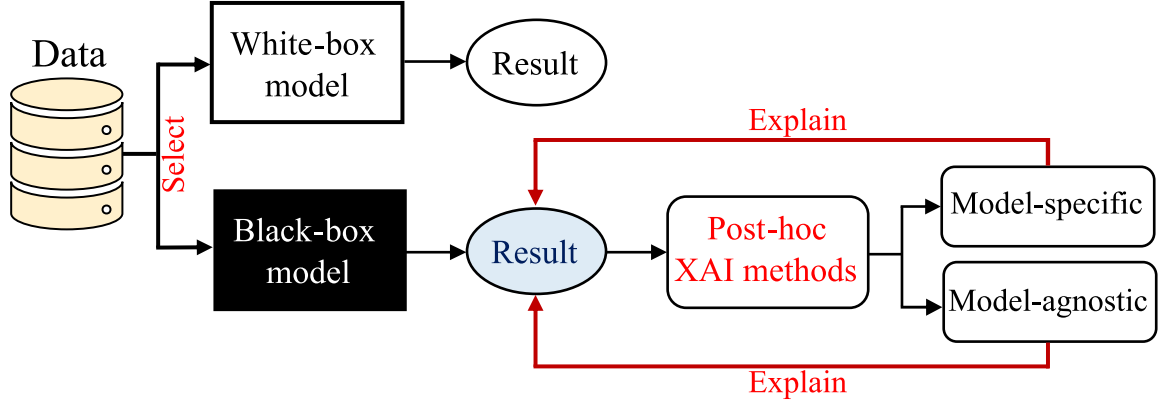


Figure 3.4: AI models and XAI methods.

Additionally, literature analysis on XAI reveals that most existing XAI methods applicable to tabular data, the most common data type [153], are model-agnostic [35]. Post-hoc models such as Shapley Additive exPlanations (SHAP) [104], Local Interpretable Model-agnostic Explanations (LIME) [137], and Anchors [138] use feature ablation and permutation techniques to estimate feature importance. They compute how the model prediction error changes when an attribute (feature) is taken out, or its values are shuffled [35].

Other model-agnostic techniques, such as unconditional counterfactual explanations [168], are considered counterfactual explanations. They look for the smallest changes in features that can shift a prediction to a different preferred result [35]. Moreover, some model-agnostic methods, such as Partial Dependence Plots (PDP) [46], highlight the relationship between the target and input and provide a visual explanation.

3.3.2 Interpretable AI

A fundamental divide exists in AI research between interpretable models and explainable models [1]. As Fig. 3.5 illustrates, Rudin (2019) [139] explains this

difference clearly. Interpretable AI is an inherently transparent AI model that allows direct understanding of its decision-making processes. In contrast, explainable AI provides post-hoc explanations for black-box AI models. As Rudin argues, the explanation of black box models faces an inherent paradox. They must be simpler than the AI model to be useful as explanations; however, this simplification means they cannot fully capture the AI model’s behavior. If they could, the complex model itself would be unnecessary [139].

A misconception in ML is that accuracy must be sacrificed to achieve interpretability. Rudin also challenges this belief and explains that it is often unfounded. This is particularly untrue for structured data that contains meaningful features. Simple and interpretable models, such as certifiably optimal rule lists (CORELS) [5], which utilize if-then rule lists or sparse scoring systems with integer coefficients, match the performance of black-box models while remaining fully transparent [139].

Lazebnik et al. [90] extend this concept with the OFEE algorithm. It designs the balance between transparency and performance as an optimization problem rather than a fixed trade-off. OFEE quantifies explainability using metrics such as ensemble size and stability rather than treating interpretability as a binary concept. The algorithm achieves an 8% improvement in size-based explainability and a 7% improvement in stability-based metrics compared to other feature selection algorithms. The OFEE algorithm is parameter-free and self-tunes its hyperparameters, which allows for adaptive balancing of accuracy and interpretability across various datasets.

Deep symbolic regression has also been identified as an interpretable AI [128]. It reveals the underlying mathematical equations based on the most correlated features to target [128]. Although these equations are symbolically explicit and mathematically accurate, they may lack the intuitive physical meaning necessary for scientific practice. As a result, such expressions, while formally transparent, can remain opaque if they do not align with domain knowledge.

Surrogate models provide a strategy for achieving interpretability by constructing simplified approximations of complex black-box AI models. However, a surrogate

cannot simultaneously be simpler than the original and perfectly replicate its behavior. This limitation introduces uncertainty regarding the reliability of either model [117].

The Transparency Challenge

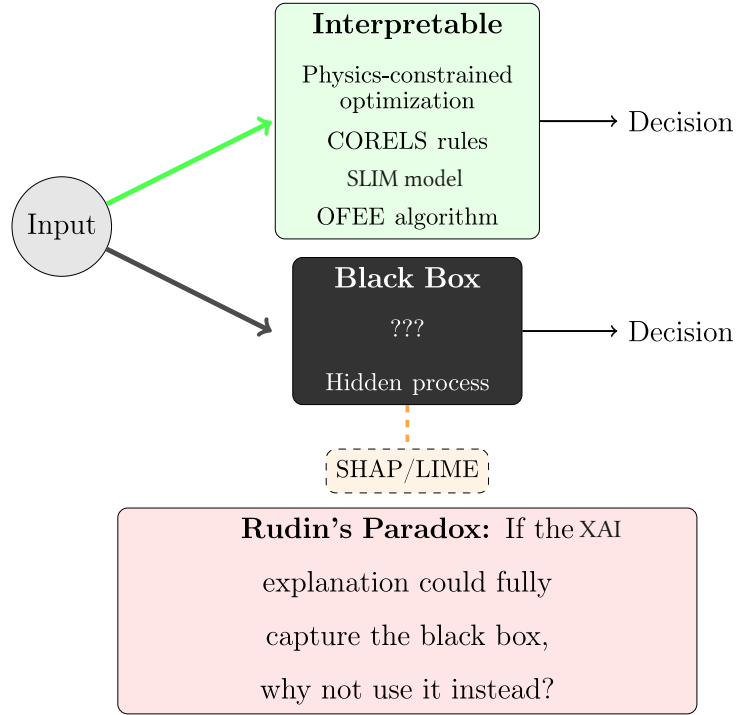


Figure 3.5: The fundamental challenge of interpretability [139]. Physics-constrained optimization, CORELS, and OFEE provide transparent models. Black-box models require post-hoc explanation.

A promising approach involves physics-constrained optimization, which integrates domain knowledge into the optimization process. Theory-guided data science (Karpatne et al. [82]) explains how incorporating physical laws, either as hard constraints that restrict solutions to physically feasible spaces or as regularization terms that guide solutions toward physical consistency, can produce interpretable models. These models are interpretable because their structure inherently reflects the governing physical laws. As Rudin and Karpatne et al. emphasize, genuine

interpretability must be domain-specific, with models that respect the domain’s structural knowledge.

3.3.3 Ethical and Societal Considerations

Using AI in materials research imposes several challenges. When advanced AI resources are primarily available to well-funded institutions, existing gaps in the field can widen. Accessibility of AI tools and training datasets is a crucial factor in creating a diverse and inclusive research community. There are also environmental concerns that must be taken into consideration. Training large AI models requires a significant amount of energy. While AI can help identify materials for energy-efficient technologies, the carbon emissions associated with these processes need to be considered [157]. Using more efficient training methods and renewable energy for computing are important steps toward making data-driven materials research more sustainable.

3.3.4 Explainable/Interpretable AI in Nanoporous Materials

The application of explainable AI in predicting thermal conductivity of nanoporous materials remains mostly confined to post-hoc implementation of existing XAI methods rather than developing domain-specific interpretable approaches. The literature shows the use of the SHAP algorithm on models like Extreme Gradient Boosting (XGBoost) to analyze feature importance after model training [12]. Even when molecular descriptors are employed for materials like zeolites, researchers typically extend existing methods, such as SHAP, through assignment techniques rather than creating fundamentally new interpretability frameworks [127]. Studies on polymeric graphene-enhanced composites similarly rely on SHAP model integration to determine the local/global influence of features on estimations [101]. Some works incorporate physical descriptors that are inherently more interpretable than traditional graph descriptors, or employ symbolic regression to construct mathematical

formulas [69]. Symbolic regression approaches may reveal new scaling laws for nanoporous materials [102]. These still represent applications of established XAI techniques rather than novel methodologies tailored to the unique physics of thermal transport in nanoporous materials. This limitation suggests that the field has yet to develop specialized interpretability methods that could provide deeper insights into the complex phonon scattering mechanisms, size effects, and structure-property relationships specific to thermal conductivity in nanoporous systems.

3.4 Limitations

Despite remarkable advances in machine learning applications for predicting thermal transport in nanoporous materials, several fundamental limitations still constrain these approaches. The most critical challenge is data availability and quality. Experimental measurements of thermal conductivity in nanoporous materials are challenging and time-consuming, and often inaccurate [108]. This results in sparse datasets with significant uncertainties [115, 108], which typically contain fewer than 1,000 samples. This led to a limitation in the model’s generalizability. The heterogeneity of available data adds more complexity to this challenge. It is reported that this disparity may be attributed to variations in measurement conditions, sample preparation, and material morphology. For instance, the thermal conductivity measurements of MOFs can differ by orders of magnitude between powders, pellets, and single crystals due to grain boundary effects and variations in packing density [70, 8]. High-throughput computing (HTC) approaches have tried to generate larger datasets for thousands of structures [122, 70]. However, systematic comparisons reveal significant discrepancies between computational predictions and experimental values [115]. Therefore, this limits their reliability as training data samples for ML approaches.

Current ML models have extrapolation challenges. Even state-of-the-art architectures show substantial performance degradation when predicting properties

for materials outside their training domains [105, 23]. Models trained on specific topologies require complete retraining for different nanoporous frameworks, although predictions for materials with extreme property values often fail entirely. Sometimes this results in errors increasing several-fold [102, 180]. Temperature-dependent thermal conductivity remains particularly challenging. While some approaches can predict thermal conductivity at specific temperatures, capturing the full temperature dependence requires either training separate models for each temperature or developing sophisticated architectures that explicitly account for temperature as a variable [132]. The inclusion of anharmonic effects and phonon-phonon scattering processes that govern temperature dependence adds considerable complexity to this process [97].

The computational demands of advanced approaches, particularly deep learning models, present an additional challenge. For example, training graph neural networks or physics-informed models may require days or weeks on high-performance computing nodes and are limited to well-funded institutions. While inference is typically fast once models are trained, the need for computational resources for retraining when new data becomes available creates ongoing computational bottlenecks.

The experimental validation of AI models presents a significant set of challenges. Many predicted structures, particularly those from inverse design approaches, prove difficult or impossible to synthesize with current techniques [116]. Even successful syntheses often yield materials that deviate significantly from idealized computational models due to defects, grain boundaries, and other imperfections, which significantly affect thermal conductivity [8].

The sensitivity of thermal conductivity to measurement conditions introduces additional challenges for validation. Factors such as sample density, grain size, moisture content, and measurement atmosphere can all influence measured values [108]. AI models trained on computational data or measurements under idealized conditions often fail to accurately predict thermal conductivity under realistic

operating conditions. This limits their practical utility for materials design and engineering applications.

3.5 Future Directions

3.5.1 Transfer Learning and Domain Adaptation

Transfer learning (TL) has shown a powerful strategy for addressing data scarcity in DL approaches. The implementation of TL follows a two-step process. Initially, a base model is trained on a large dataset of materials with known properties. It learns general features and patterns that govern the underlying physics. Then, this pre-trained model is fine-tuned on a smaller dataset which are distinct to the target material class to learn and predict characteristics of the new material domain. This approach has shown significant performance in nanoporous materials. Park et al. [125] showed that their porous material transformer (PMTransformer) model, which was pretrained on 1.9 million hypothetical porous materials, could predict properties of COFs, including gas uptake, heat of adsorption, and band gaps, despite limited training samples. Studies have also demonstrated quantitative improvements specifically for the prediction of thermal conductivity. Elmorsy et al. [40] achieved 70% accuracy improvement with 2.8-fold faster training time in digital porous rocks. Pai et al. [124] improved R^2 values from 0.83 to 0.93 in thermal conductivity prediction of nanofluids. Chang et al. [22] introduced the “mixture-of-experts” framework, which outperformed traditional TL on 14 of 19 material property tasks.

Beyond TL, emerging cross-property frameworks offer new opportunities for predicting thermal conductivity. Gupta et al. [57] demonstrated that models trained on formation energy can successfully predict diverse properties such as elastic moduli and dielectric constants. Their model outperformed scratch models in approximately 69% of cases, despite it was using only elemental fractions as input. While thermal conductivity was not directly tested, the fundamental physics encoded in formation

energy models are highly relevant to thermal transport. This cross-property approach could be especially valuable for nanoporous materials where thermal conductivity data are limited but related properties have been studied.

Recent architectural advances hold promise for efficient transport properties in TL. For example, transformer-based models with self-attention mechanisms have demonstrated exceptional data efficiency [113]. Meng et al. achieved R^2 of 0.9563 using only 300 training samples for permeability prediction [113]. Future work should explore optimal source property selection and domain adaptation strategies specifically tailored for thermal transport in nanoporous materials.

3.5.2 Multimodal Learning

Multimodal learning models integrate structural data, synthesis conditions, and characterization results, which are emerging as powerful tools for accelerating materials discovery and property prediction. Early work combining synthesis parameters with structural descriptors shows improved prediction accuracy [23]. Recent developments in multimodal learning have enabled the integration of diverse data sources for enhanced property prediction. The porous material transformer (PMTransformer) demonstrates state-of-the-art performance using multimodal transformer models pretrained on 1.9 million porous materials [125]. These approaches combine imaging data from different sources and resolutions to create detailed, three-dimensional characterizations of porous materials. Multimodal learning techniques have proven particularly effective in reducing data requirements and improving prediction efficiency, demonstrating strong performance even with limited training datasets [125, 50]. The development of large language model (LLM) based approaches represents an emerging frontier in nanoporous materials research. ChatMOF, an AI system leveraging Generative Pre-trained Transformer 4 (GPT-4) [123], has demonstrated accuracy rates of 96.9% for searching, 95.7% for predicting, and 87.5% for generating tasks, successfully creating materials with user-desired properties

from natural language inputs. This approach significantly reduces the barriers to computational materials design by eliminating the need for specialized programming knowledge [81].

3.5.3 Other Approaches

Active learning strategies integrated with autonomous experimentation systems could accelerate discovery by orders of magnitude. Recent demonstrations show that autonomous systems can discover materials with targeted thermal properties significantly faster than traditional approaches [107]. Federated learning frameworks could address data scarcity while preserving intellectual property, enabling collaboration between research groups unable to share raw data directly [96].

Quantum-accurate machine learning potentials, while still using classical computing, achieve DFT-level accuracy for molecular dynamics simulations at a fraction of the computational cost [150]. These approaches enable long-timescale simulations necessary for studying temperature-dependent thermal transport and framework flexibility effects.

3.6 Chapter Summary

The application of AI to predicting thermal transport and its properties in nanoporous materials has evolved from simple regression models to sophisticated DNN architectures that incorporate physical constraints and domain knowledge. GNNs, particularly CGCNN and ALIGNN, have shown great success in capturing structure-property relationships. This is achieved through their ability to process three-dimensional atomic arrangements and chemical connectivity while handling variable-sized input vectors and periodic boundary conditions [173, 27]. PINN architectures ensure that predictions respect conservation laws and thermodynamic principles,

while addressing the limitations of NNs in extrapolation and physical consistency [42, 120].

Applying ML models to various nanoporous classes has resulted in material-specific findings. In MOFs, high-throughput screening (HTS) of over 10,000 hypothetical structures revealed that framework density above 1.0 g/cm^3 and pore sizes below $10 \text{ \AA}$ correlate with enhanced thermal conductivity. Ultra-low thermal conductivities below $0.02 \text{ (W/m}\cdot\text{K)}$ are observed with extremely large pores exceeding $65 \text{ \AA}$ [70]. For COFs, single-crystal structures have demonstrated effective heat conduction ($> 1 \text{ W/m}\cdot\text{K}$) even with high porosity. This is attributed to their strong, connected ribbons forming continuous crystals [161]. In zeolites, non-equilibrium MD simulations revealed thermal conductivities ranging from 0.6 to nearly $4 \text{ (W/m}\cdot\text{K)}$ at 350 K , with varying values between framework types and crystallographic directions. It is also observed that water adsorption can reduce values by 20-40% through phonon scattering [143, 8].

Significant challenges exist in realizing the full potential of AI. Data scarcity for novel materials constrains model development. Many studies rely on datasets containing limited samples. The computational cost of complex models also restricts their accessibility. Additionally, experimental validation has also remained a bottleneck due to synthesis challenges and unreliable measurement [8, 108]. Moreover, Temperature-dependent predictions and hierarchical structure representation require further development, as current models struggle to capture anharmonic effects and multi-scale transport phenomena [132].

Looking forward, emerging models show promise. TL approaches, exemplified by the PMTransformer model pretrained on 1.9 million porous materials, have shown 70% accuracy improvement with 2.8-fold faster training time [40, 125]. ML interatomic potentials achieve near-DFT accuracy at reduced computational cost, enabling long simulations necessary for studying temperature-dependent thermal transport [71, 118]. Active learning workflows that iteratively select structures based on model uncertainty have proven effective for efficiently exploring material space [77].

The development of interpretable AI methods for materials science will be significant for building trust in model predictions. Deep symbolic regression approaches and interpretable models such as CORELS have shown promise for discovering while maintaining full transparency [128, 5]. Most importantly, the integration of physics-constrained optimization, which incorporates domain knowledge as hard constraints or regularization terms, can produce models that inherently reflect governing physical laws while achieving high accuracy [82].

Success will require continued collaboration between materials scientists, computer scientists, and experimentalists. The field is undergoing major change, where AI has proven its value but has yet to reach its peak potential. As the challenges of data scarcity, model interpretability, and experimental validation are addressed, AI-driven approaches will enable the design of nanoporous materials with precisely controlled thermal properties. This can revolutionize the field for next-generation efficient thermal management, energy efficiency, and sustainable technologies.

Chapter 4

Machine Learning Approach

Computational advancements have enabled machine learning models to solve complex scientific problems. Most machine learning models provide acceptable predictive analysis across various domains. However, as mentioned in the previous chapter, these data-driven models have faced a challenge in making precise predictions that are also transparent. Many ML models, such as deep neural networks, ensemble methods [140], and kernel models, deliver outstanding results. Yet, the “black-box” nature of these models hinders scientific understanding and their practical application in many engineering problems. The lack of transparency in ML models makes it difficult to interpret and validate them against established physics. It also makes it hard to make confident predictions for new scenarios.

This chapter introduces a macroscopic engineering model for predicting effective gas thermal conductivity, incorporating the effects of gas non-equilibrium, multi-dimensional confinement, and lateral thermal coupling. The modeling framework captures essential physical trends while maintaining full mathematical interpretability and achieving machine learning-level performance with complete transparency. This generalized framework bridges nanoscale molecular physics and macroscopic continuum modeling, achieving improved predictive accuracy for gas conduction in micro- and nanoporous materials.

4.1 Methods

4.1.1 Machine Learning Models

Three machine learning algorithms are employed to independently compare the predictive accuracy of different modeling methods. These algorithms are selected because they work well with small datasets, use different approaches, and offer unique insights into the problem.

4.1.1.1 Data Overview and Preprocessing Strategy

The MD simulation dataset includes 96 samples, each with three input features and one target variable. Table 4.1 shows the main statistics for each variable. The input features cover different numerical ranges: $Kn = 1$ and 10, $SW = 10, 20$ and 50 K, and $AR = 0.5, 1, 2, 10$. The target variable, effective thermal conductivity (K_{eff}), is normalized by its Kaganer model results and exhibits a wide variation across the parameter space (coefficient of variation: 21.4%). This shows strong sensitivity to the transport parameters and a high signal-to-noise ratio, which is ideal for ML analysis.

Table 4.1: Dataset Statistical Summary

Variable	Mean	Std Dev	Min	Max	Median
Kn	5.500	4.524	1.000	10.000	5.500
SW	26.667	17.086	10.000	50.000	20.000
AR	3.375	3.883	0.500	10.000	1.500
K_{eff}	0.740	0.158	0.423	0.952	0.774

To compare the ML algorithms fairly, the same preprocessing steps for the dataset are used before training process. All ML methods: Random Forest (RF) [16], Gradient Boosting, and Gaussian Process (GP) used the standardized features. The

Z-score normalization was applied to each input variable, setting their means to zero and variances to one. The mean and standard deviation were calculated from the training data only, and these values were then used to transform both the training and testing sets. This prevents data leakage and allows for an unbiased evaluation of model performance. Each feature was scaled as $X_{\text{scaled}} = \frac{(X-\mu)}{\sigma}$, where μ and σ are the mean and standard deviation from the training set.

Preprocessing is necessary because the input features have very different numerical scales, as shown in Table 4.1. For instance, Kn ranges from 1 to 10, SW from 10 to 50 K, and AR from 0.5 to 10. The coefficients of variation also vary widely (Kn : 82.3%, SW : 64.1%, AR : 115.0%), so scale normalization is important. Without standardization, features with larger ranges could influence the learning process more and bias the results. Using statistics from the training set for both training and test data keeps the evaluation fair and allows for meaningful feature comparisons.

Standardization is especially important for the GP model because its kernel uses distance calculations in the input space. If the features have different scales, this can bias the learned length scale parameters and affect how the model finds which features matter most. Proper standardization helps the kernel balance the effects of Kn , SW , and AR , so the model can find meaningful relationships based on physical importance, not just measurement scale. For tree-based algorithms, standardization does not directly affect how splits are made because these methods handle different feature scales naturally. However, using the same preprocessing makes it easier to compare feature importance across models and ensures that any model combinations work on a consistent numerical basis.

The Z-score standardization was chosen instead of other methods like min-max or robust scaling because of the dataset’s characteristics. Table 4.1 shows that the data distributions are well-behaved and have no extreme outliers, so robust scaling is not needed. The target variable has a wide range and is roughly normally distributed, so z-score normalization works well. This approach keeps the original data’s statistical properties and helps each ML algorithm perform well. The dataset is split into

75% training and 25% testing samples, giving 72 training and 24 testing samples. This ratio provides sufficient data for training and retains enough samples for a fair performance evaluation.

4.1.1.2 Random Forest

Random Forest [16] uses ensemble learning with bootstrap aggregation to combine several decision trees. This approach helps model complex nonlinear patterns in thermal transport data. Each tree is trained on a random subset of the data through bootstrap sampling with replacement, which helps prevent overfitting and keeps predictions accurate.

This study utilized 200 decision trees (`n_estimators = 200`) with a maximum depth of 10 levels (`max_depth = 10`) and fixed random state (`random_state = 42`) for reproducible results. At each node split, the algorithm evaluates all three input variables (Kn, SW, AR) to find the best splitting thresholds. The final K_{eff} prediction results from averaging the outputs across all trees, providing robust estimates that are less sensitive to outliers. Feature importance is calculated by measuring the weighted decrease in mean squared error attributable to each feature, helping to identify the most informative variables for K_{eff} prediction.

4.1.1.3 Gradient Boosting

Gradient Boosting (GB) [46] utilizes a sequential ensemble method that iteratively constructs weak learners to correct residual errors from previous models. This process results in a strong predictive model through additive aggregation. In contrast to RF's parallel tree construction, GB utilizes sequential learning. Each new decision tree is trained to address the prediction errors that exist in the current ensemble, which incrementally improves accuracy by focusing on error correction.

This study used a configuration with 200 boosting iterations (`n_estimators = 200`), with each tree restricted to a maximum depth of 5 levels (`max_depth = 5`), a learning

rate of 0.1 (`learning_rate = 0.1`), and a fixed random state (`random_state = 42`). The limited tree depth aligns with the sequential refinement strategy of GB, as simple weak learners help prevent overfitting during iterative improvement. Each boosting iteration calculates the negative gradient of the mean squared error loss function with respect to current predictions, thereby identifying residual errors for the subsequent tree to address. The algorithm fits a new shallow tree to these residuals, scaling its contribution by the learning rate before adding it to the ensemble. Feature importance is determined by aggregating both the frequency and impact of feature usage across all trees and iterations. It provides insight into which parameters most significantly influence normalized K_{eff} predictions.

4.1.1.4 Gaussian Process

Gaussian Process (GP) [171] regression is a Bayesian nonparametric method that integrates uncertainty quantification with point predictions, setting it apart from deterministic tree-based approaches. Rather than partitioning the input space with discrete boundaries, GP models the thermal transport function as a realization from a multivariate Gaussian distribution. This allows for smooth interpolation between training points and principled extrapolation with quantified confidence levels.

The GP implementation utilized a composite kernel that combined a Matérn covariance function with a smoothness parameter of $\nu = 1.5$ and a WhiteKernel [119, 171] to model observation noise with a noise level of 0.1. The Matérn kernel was selected to represent the physical expectation that effective thermal conductivity varies smoothly, but is not infinitely differentiable, with respect to input parameters. Kernel hyperparameters were optimized using maximum likelihood estimation with multiple random restarts (`n_restarts_optimizer = 10`) and a fixed random state (`random_state = 42`) to prevent the risk of local optima and ensure reproducibility.

The GP formulation supports automatic relevance determination by assigning individual length scale parameters to each input dimension (Kn, SW, AR). Shorter length scales indicate greater sensitivity to parameter changes, directly encoding

feature importance within the kernel. The model delivers both point predictions and analytically tractable uncertainty estimates, quantifying confidence based on proximity to training data and the learned covariance structure. This uncertainty quantification distinguishes GP from deterministic algorithms and helps identify regions where further simulations would most improve model accuracy.

4.1.1.5 Performance Metrics

The ML models performance is evaluated using statistical metrics that measure how well the models predict and generalize. The coefficient of determination ($R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$) shows how much of the variance in effective thermal conductivity each model explains, with SS_{res} as the sum of squared residuals and SS_{tot} as the total sum of squares. This metric allows for direct comparison of different machine learning methods. The root mean square error ($RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2}$) gives the average prediction error in the same units as the data, making it easier to interpret the results for engineering purposes.

A standard hyperparameter configurations are utilized to ensure a fair comparison while avoiding the risks of overfitting associated with extensive hyperparameter tuning on small datasets [19, 7]. This conservative approach aligns with the primary research objective of validating an interpretable macroscopic modeling approach, rather than optimizing machine learning performance. It ensures that model comparisons reflect algorithmic capabilities rather than artifacts of parameter optimization. For the GP model, uncertainty calibration is assessed by computing the correlation between predicted uncertainty estimates and actual prediction errors. Additionally, coverage probability analysis is used to validate the uncertainty quantification capability that distinguishes GP from deterministic approaches.

4.1.2 Explainable AI

4.1.2.1 SHAP Analysis

SHAP (SHapley Additive exPlanations) [104] decomposes predictions into individual feature contributions based on Shapley values [148] according to the Eq. (4.1):

$$f(\mathbf{x}) = \phi_0 + \sum_{i=1}^M \phi_i \quad (4.1)$$

where $f(\mathbf{x})$ is the model's prediction for input features $\mathbf{x}$, ϕ_0 is the expected model output, and ϕ_i is the contribution of feature i . This additive decomposition ensures that the sum of all contributions equals the model's prediction, providing interpretable explanations for individual predictions of effective thermal conductivity. Algorithm-specific explainers are employed for each model type. TreeExplainer is used for ensemble methods such as RF and GB, which leverage their tree structure for efficient computation. KernelExplainer is applied to GP, which utilizes sampling-based approximation. SHAP analysis offers feature attribution that complements local and global feature importance measures by explaining individual prediction decisions across the thermal transport parameter space.

4.1.2.2 Partial Dependence Analysis

Partial dependence functions capture the average effect of a feature while marginalizing over others according to the following Eq. (4.2)

$$PD_j(x_j) = \mathbb{E}_{X_{\setminus j}}[f(x_j, X_{\setminus j})] \quad (4.2)$$

where $PD_j(x_j)$ represents the partial dependence of feature j that is computed by averaging the model function f over all possible values of the remaining features $X_{\setminus j}$ while fixing feature j at value x_j .

The corrected partial dependence analysis offered in this study is implemented to address limitations in standard methods [46]. The corrected method includes four important steps. (1) The actual feature ranges are extended by 10 percent to preserve physical relevance. (2) Median values are used as baseline points to ensure robust centering. (3) Appropriate feature transformations are applied for each model type to maintain consistency with the underlying physical principles. (4) The correlation between the developed macroscopic model and ML model responses is quantified using Pearson correlation coefficients.

For each feature, empirical minimum and maximum values are determined from the MD simulation data. These ranges are extended by 10% to capture edge effects while avoiding extrapolation into physically unrealistic parameter regions. Non-target features are set to their empirical median values to provide a representative baseline condition. For ML models, partial dependence calculations are performed in the original physical parameter space prior to standardization. This approach ensures that the resulting curves accurately reflect the true physical relationships, rather than artifacts from standardization.

4.1.2.3 Feature Importance Quantification

Feature importance employs multiple complementary approaches tailored to the characteristics of each modeling method. For tree-based models, the built-in feature importance calculations measure the weighted decrease in mean squared error attributable to each feature across all splits throughout the ensemble. The RF importance aggregates impurity reductions across 200 trees with bootstrap sampling diversity. For the GB model, feature importance quantifies the cumulative impact of features across 200 sequential boosting iterations. For GP implementation, feature importance comes up from optimized kernel hyperparameters through inverse length scale analysis, where shorter length scales indicate higher sensitivity to parameter variations. The automatic relevance determination mechanism in the Matérn kernel with individual length scales for each input feature provides a principled Bayesian

approach that reflects the learned covariance structure of the thermal transport MD simulation data.

4.1.3 Machine Learning Results

4.1.3.1 Model Performance Comparison

Three machine learning models were evaluated for predicting effective thermal conductivity: Gaussian Process with Matérn kernel, Random Forest, and Gradient Boosting. Cross-validation (CV) was conducted using 5-fold validation on the training data to assess generalization performance. Table 4.2 provides comprehensive performance metrics for each model.

Table 4.2: Machine learning model performance comparison. CV results represent a 5-fold cross-validation on training data.

Model	Train R^2	Test R^2	CV R^2 (mean $\pm$ std)	Test RMSE
Gaussian Process (GP)	0.989588	0.980751	0.9857 $\pm$ 0.0038	0.020495
Random Forest (RF)	0.990235	0.979809	0.9783 $\pm$ 0.0092	0.020990
Gradient Boosting (GB)	0.990341	0.979632	0.9770 $\pm$ 0.0078	0.021082

The Gaussian Process model with Matérn kernel achieved the highest test performance ($R^2 = 0.980751$, RMSE = 0.020495) and exhibited the most stable cross-validation results (CV standard deviation = 0.0038). The Random Forest and Gradient Boosting models demonstrated comparable performance (test $R^2 = 0.979809$ and 0.979632, respectively) with cross-validation standard deviations of 0.0092 and 0.0078. All machine learning models exhibited close agreement between their test and cross-validation performance, which indicates robust generalization and minimal overfitting.

GP Uncertainty Quantification

The GP model offers uncertainty quantification that differentiates it from other ML methods. It supports risk-aware engineering decisions through calibrated estimates of uncertainty. Figure 4.1 illustrates the model’s prediction confidence for all test samples, with an observed uncertainty range of 0.0187 to 0.0197 and a mean uncertainty of $\sigma = 0.0191$. Red dots indicate actual K_{eff} values, and blue error bars display GP predictions with associated uncertainty bounds. The results confirm consistent coverage of the confidence interval.

Figure 4.2 presents a detailed calibration analysis. The coverage within $\pm 1\sigma$ is 70.8% (target: 68%) and within $\pm 2\sigma$ is 95.8% (target: 95%), which indicates accurate calibration. The uncertainty-error correlation coefficient of $r = 0.136$ indicates moderate predictive capability and conservative uncertainty estimates.

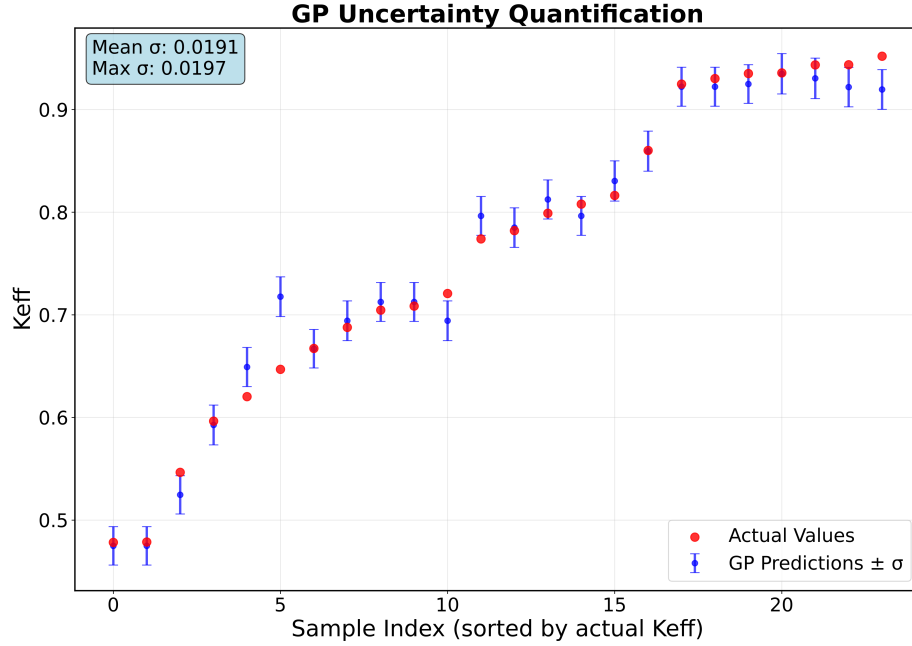


Figure 4.1: GP uncertainty quantification across test samples.

Four high-uncertainty predictions, representing 16.7% of the test set, highlight parameter regions where additional data collection would most effectively enhance the model. The calibrated uncertainties enable reliable estimation of confidence

intervals for design applications. Approximately 70% of observed values fall within the predicted $\pm 1\sigma$ bounds, supporting risk-informed engineering decisions when estimating the effective thermal conductivity of aerogel materials.

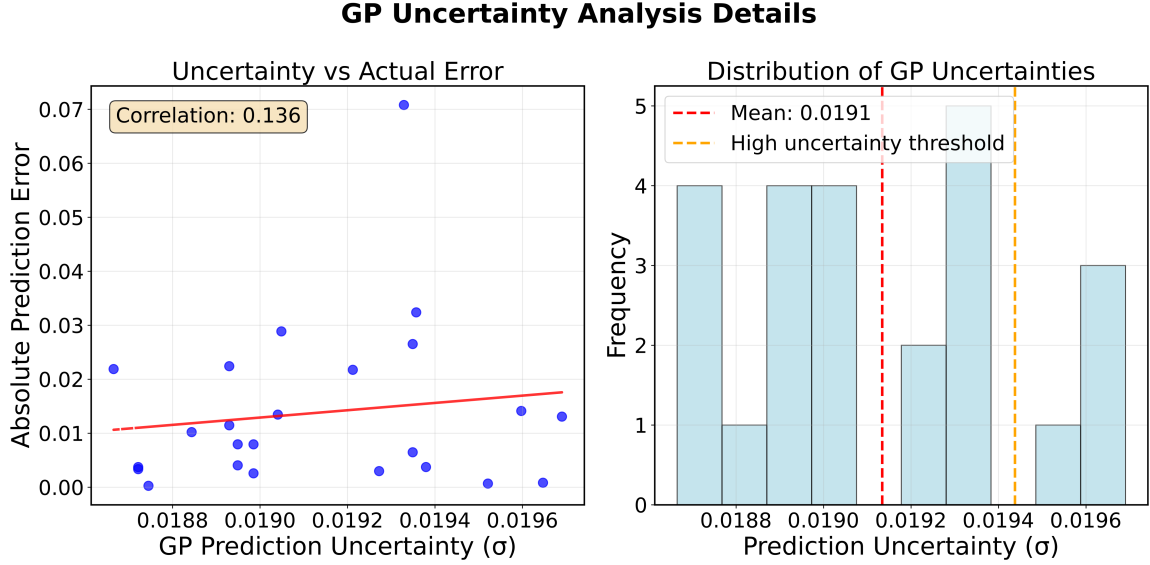


Figure 4.2: Detailed GP uncertainty analysis: (left) correlation between prediction uncertainty and actual error, (right) distribution of prediction uncertainties with mean of 0.0191 and high-uncertainty threshold indicators.

Feature Importance Analysis

Feature importance analysis shows strong agreement among all ML approaches. It indicates that data-driven methods identify the same underlying relationships. The analysis uses model-specific importance metrics: impurity-based importance for tree-based methods (RF, GB), and inverse kernel length scales for Gaussian Process (GP). Table 4.3 provides the quantitative values of feature importance analysis.

The results indicate that AR is the dominant feature, as shown by RF (95.16%), GB (95.34%), GP Kernel (96.69%). This agreement supports the models' focus on geometric effects (AR), with Kn (1.0-1.6%) and SW (0.4-3.3%) contributing to a lesser extent. The consistency across different mathematical formulations indicates that the identified relationships reflect underlying physical phenomena rather than artifacts of specific models.

Table 4.3: Feature importance analysis across all ML modeling approaches showing consistent *AR* dominance.

Model	Kn	SW	AR
Random Forest	0.0150	0.0334	0.9516
Gradient Boosting	0.0158	0.0308	0.9534
GP Kernel	0.0134	0.0197	0.9669

4.1.3.2 Explainable AI Results

SHAP Analysis

SHAP analysis of the best-performing ML model, the GP, provides model-agnostic insights into the underlying individual predictions. This analysis quantifies feature contributions and supports the consensus on feature importance established by model-native methods in Section 4.1.3.1.

Global Feature Importance:

The SHAP global importance analysis confirms the feature ranking: *AR* (0.1234) as the dominant contributor, followed by *SW* (0.0181) and *Kn* (0.0149). These values represent absolute contribution magnitudes rather than normalized percentages, verifying *AR*'s massive influence on K_{eff} predictions while maintaining the consistent ranking observed across all modeling approaches.

Individual Prediction Decomposition:

Figure 4.3 displays a waterfall analysis for a representative prediction. It illustrates how the GP model integrates the effects of individual features. The decomposition identifies a base prediction value of approximately 0.728, with *Kn* contributing -0.007, *SW* contributing -0.015, and *AR* contributing +0.217 to reach the final prediction. The waterfall visualization illustrates the additive structure of SHAP explanations, where each feature's contribution is built incrementally toward the final prediction. The dominance of the *AR* contribution (+0.217) aligns with the feature importance

consensus, while the negative contributions from Kn and SW reflect the specific parameter values for this sample.

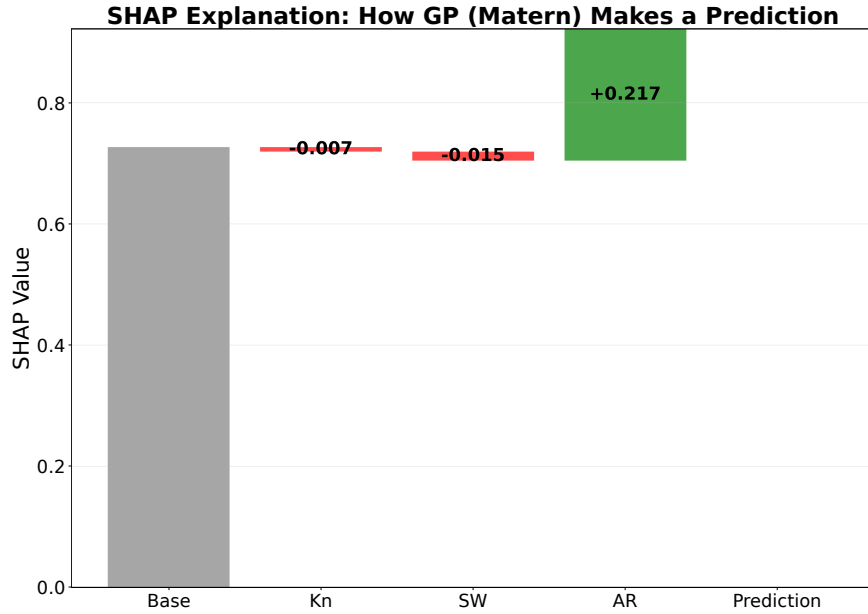


Figure 4.3: SHAP waterfall analysis showing individual feature contributions for a representative GP prediction.

4.1.4 Developing a Macroscopic Engineering Model

While the ML models demonstrated excellent predictive performance, they lack the transparency required for engineering applications. Although explainable AI techniques, such as feature importance, provide some insight into model behavior, a deeper level of interpretability is required for developing practical tools to tailor nanoporous materials. Therefore, this dissertation advances to an interpretable AI approach in the next phase.

Initial exploratory data analysis was performed to identify relationships between input features and the target variable. As shown in Fig. 4.4, Pearson correlation coefficients were calculated for all variable pairs to understand the relative importance of each parameter on the target.

The correlation analysis shows that aspect ratio exhibits the strongest positive correlation with K_{eff} ($r = 0.779$), indicating its dominant influence on thermal conductivity. The Knudsen number shows a moderate negative correlation ($r = -0.109$), reflecting the reduction in thermal transport with increased rarefaction effect. The sidewall temperature demonstrates a weak correlation ($r = 0.139$). Based on these findings, initial modeling efforts focus on aspect ratio as the primary predictor variable.

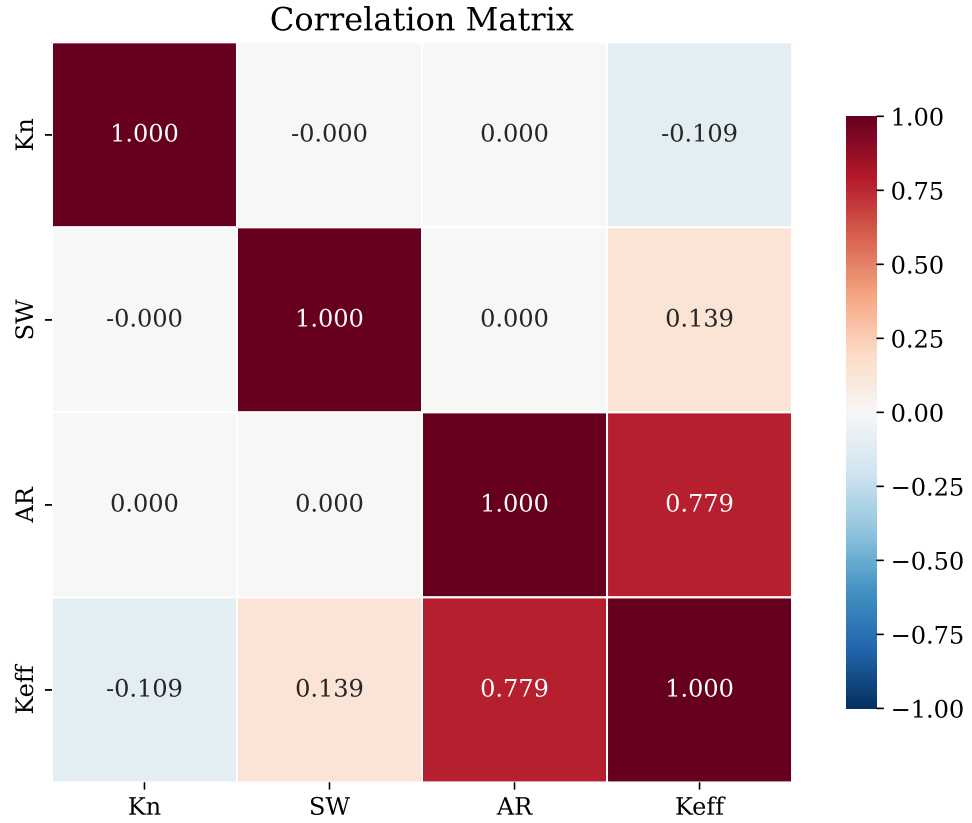


Figure 4.4: Correlation matrix showing relationships between input features (Kn , SW , AR) and the effective thermal conductivity (K_{eff}).

4.1.4.1 Simple Symbolic Representation

Six single-variable models were developed using aspect ratio as the sole predictor to establish baseline performance and understand the functional relationship between

AR and K_{eff} . These models are summarized in Table 4.4 and represent different mathematical forms.

Table 4.4: Single-variable models for predicting effective thermal conductivity (K_{eff}) from aspect ratio.

Model	Equation	Parameters
Linear	$K_{eff} = a \times AR + b$	a, b
Power Law	$K_{eff} = a \times AR^n$	a, n
Exponential	$K_{eff} = a(1 - e^{-b \times AR})$	a, b
Logarithmic	$K_{eff} = a \times \ln(AR + 1) + b$	a, b
Simple Rational	$K_{eff} = \frac{a \times AR}{b + AR}$	a, b
General Rational	$K_{eff} = \frac{a \times AR^n}{b + AR^m}$	a, n, b, m

The MD data processing described in Section 2.5.2 revealed physical phenomena that motivated the development of these symbolic models. The six model types in Table 4.4 were chosen to represent a hierarchy of complexity: from simple linear relationships to polynomial and exponential forms that capture non-linear thermal transport, culminating in two rational function forms to capture these effects. All models were fitted using non-linear least squares optimization implemented via the Levenberg-Marquardt (LM), the default algorithm in SciPy’s [165] `curve_fit` function.

For the general rational model, parameter bounds were imposed to ensure numerical stability and physical plausibility. Maximum iterations were set to 10,000 for the convergence of complex models. Model performance was assessed using two primary metrics: Coefficient of Determination (R^2): Measures the proportion of variance in K_{eff} explained by the model, with values closer to 1 indicating a better fit. Root Mean Square Error (RMSE): Quantifies the average prediction error in the

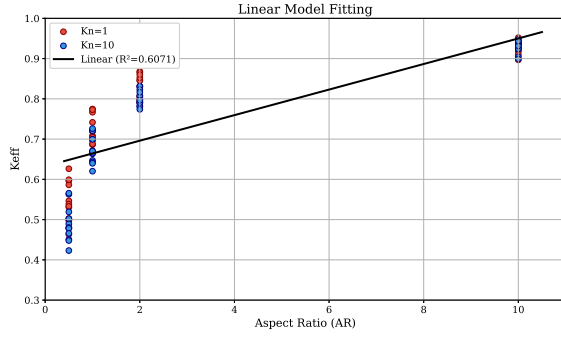
same units as K_{eff} , with lower values indicating better accuracy. Figure 4.5 presents the fitted curves for all six models against the whole MD data. The data points are color-coded by Knudsen number to visualize that flow regime effects are not fully captured by single-variable models.

As Table 4.5 depicts, the general rational model achieved the highest R^2 value of 0.9450 and the lowest RMSE (0.0369). It demonstrates superior flexibility in capturing the AR- K_{eff} relationship. The fitted parameters and performance metrics for each model are presented in the table.

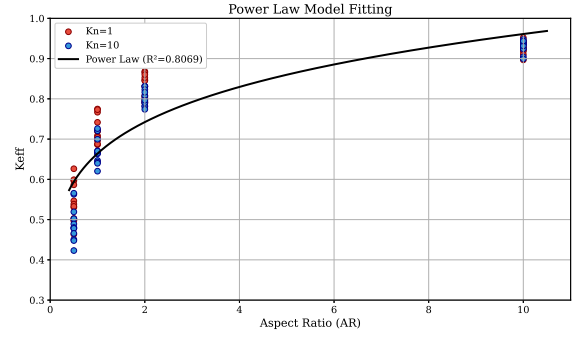
Table 4.5: Fitted parameters and performance metrics for single-variable models.

Model	Parameters	R^2	RMSE
Linear	$a = 0.0318, b = 0.6325$	0.6071	0.0987
Power Law	$a = 0.6641, n = 0.1605$	0.8069	0.0692
Exponential	$a = 0.8948, b = 1.5804$	0.9070	0.0480
Logarithmic	$a = 0.1802, b = 0.5326$	0.7613	0.0769
Simple Rational	$a = 0.9776, b = 0.4238$	0.9405	0.0384
General Rational	$a = 0.8949, n = 1.3428,$ $b = 0.2834, m = 1.3205$	0.9450	0.0369

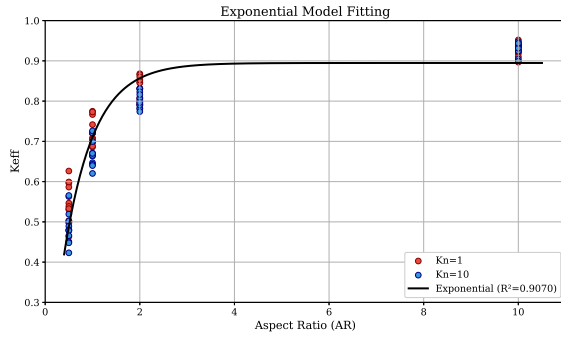
While the general rational model provides the best fit among single-variable approaches, the persistent scatter of data points grouped by Knudsen number suggests that incorporating additional parameters is required for accurate prediction across different flow regimes. There might be more complex cases that are needed to be included and also it is required to understand the dependence of target on other feature as we. This observation motivates the development of a macroscopic engineering model that explicitly accounts for all three input parameters.



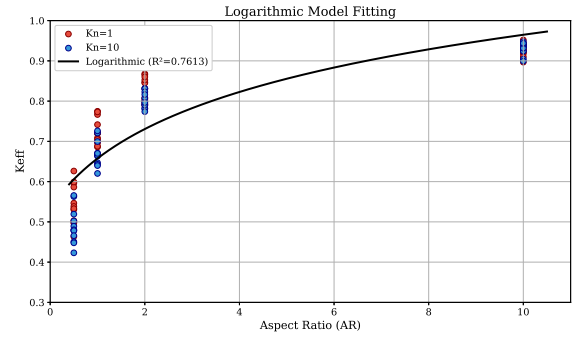
(a) Linear Model.



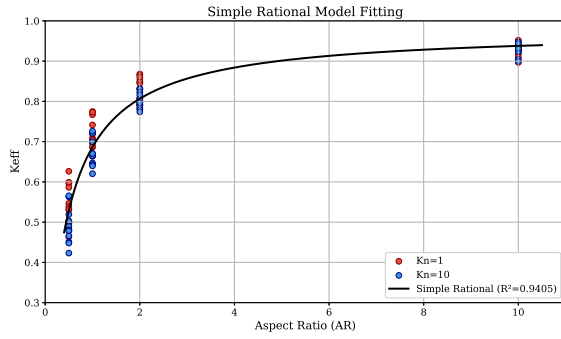
(b) Power Law Model



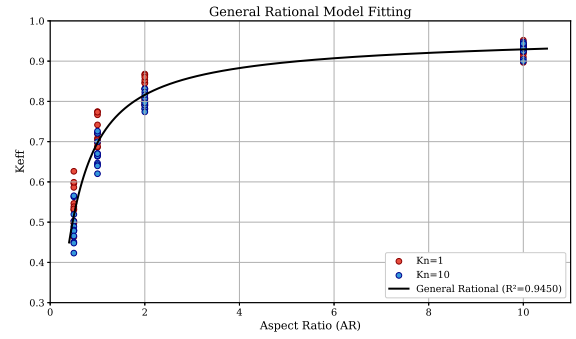
(c) Exponential Model



(d) Logarithmic Model



(e) Simple Rational Model



(f) General Rational Model

Figure 4.5: Single-variable model fits for aspect ratio versus effective thermal conductivity. Red points represent $Kn = 1$, blue points $Kn = 10$, and the black curve fitted models. The variation in data points at fixed AR and Kn values is due to different sidewall temperatures.

4.1.4.2 Multi-Parameter Extended Rational Function

The limitations observed in single-variable models necessitate a more sophisticated approach that captures the coupled effects of all input features. Macroscopic engineering modeling provides a powerful framework for this challenge by creating computationally inexpensive mathematical approximations of expensive simulations. In engineering applications where direct simulation of the quantity of interest, such as the effective thermal conductivity in this study, requires solving complex coupled equations, this type of modeling offers an efficient alternative. They maintain prediction accuracy while reducing computational cost by several orders of magnitude.

A macroscopic model essentially replaces the expensive simulation process with an analytical expression. This data-driven approach constructs mathematical functions from a finite set of MD simulation samples, establishing continuous input-output relationships without repeatedly solving the underlying physics equations. For this study, where each numerical simulation involves solving heat transfer in complex nanoporous geometries, the computational savings are substantial. While a single simulation may require hours of computational time, the macroscopic model provides predictions in microseconds. This enables practical applications such as design optimization, sensitivity analysis, and uncertainty quantification that would be computationally prohibitive with direct simulation.

The challenge in a macroscopic engineering modeling lies in constructing an accurate approximation from limited data while maintaining physical consistency. The model must generalize beyond training samples, respect physical bounds, and exhibit proper asymptotic behavior. Among various formulations available, including polynomial response surfaces, Kriging, and neural networks, the rational function approach is preferred for its success in the single-variable analysis. As shown in Figure 4.5, the general rational model achieved the highest R^2 among all single-variable formulations. This superior performance, combined with rational functions' inherent advantages in representing bounded physical quantities, has motivated

the extension of this formulation to the multi-parameter case. Rational functions naturally enforce the physical constraint that thermal conductivity must remain between zero and unity, while also providing the mathematical flexibility necessary to capture the nonlinear $AR - K_{\text{eff}}$ relationship observed in the preliminary analysis. The proposed macroscopic model can be expressed as Eq. (4.3)

$$K_{\text{eff}} = \frac{a \times AR^n}{K + b \times AR^m} \quad (4.3)$$

where the denominator baseline incorporates Kn and SW as provided in Eq. 4.4

$$K = k_0 + k_1 \times Kn + k_2 \times SW. \quad (4.4)$$

This formulation brings together several physical ideas. First, the numerator $a \times AR^n$ shows how transport increases as the aspect ratio (AR) grows, due to more surface area and changes in flow. In the denominator, both a baseline resistance (K) and an aspect-ratio-dependent resistance ($b \times AR^m$) are included, which represent different transport mechanisms. The parameter K combines (Kn) and (SW) effects in a straightforward linear way.

The rational function form keeps the model's behavior within expected physical limits and ensures numerical stability, as seen in empirical fits (Fig. 4.5), while still allowing the model to adapt its shape. The rational function ensures proper asymptotic behavior: $K_{\text{eff}} \rightarrow 0$ as $AR \rightarrow 0$ (negligible geometric effect) and $K_{\text{eff}} \rightarrow 1$ as $AR \rightarrow \infty$. With seven parameters ($a, n, b, m, k_0, k_1, k_2$), the model balances flexibility with physical interpretability, providing an efficient model for computationally expensive simulations.

Optimization Method and Models Validation

Data Splitting

The MD dataset was randomly divided into training (75%) and testing (25%) sets, using a fixed random seed (`random_state = 42`) to ensure results can be reproduced.

The macroscopic model were trained only on the training data with the test set reserved for unbiased performance evaluation. Parameter bounds were set through repeated optimization trials to balance numerical stability, physical consistency, and model flexibility.

Models Evaluation

Model performance is evaluated using both training and testing metrics:

- **Training performance:** R^2 and RMSE on the training set to assess fit quality.
- **Testing performance:** R^2 and RMSE on the held-out test set to evaluate generalization.
- **Asymptotic validation:** Testing limiting behavior ($AR \rightarrow 0$, $AR \rightarrow \infty$) for physical consistency.

Testing performance gives an unbiased measure of how well the model predicts unseen data. Asymptotic validation checks that the model remains physically reliable when used for extrapolation.

Optimization Framework

The macroscopic model was fitted using the Limited-memory Broyden-Fletcher-Goldfarb-Shanno algorithm with bound constraints (L-BFGS-B) [17] optimization method, with parameter bounds chosen to keep results physically consistent. The optimization process minimizes mean squared error on the training set as Eq. (4.5) illustrates.

$$\text{Objective} = \frac{1}{N_{\text{train}}} \sum_{i=1}^{N_{\text{train}}} (y_i - f(\mathbf{x}_i, \boldsymbol{\theta}))^2 \quad (4.5)$$

Due to the increased complexity compared to single-variable models, the L-BFGS-B algorithm was preferred over the Levenberg-Marquardt algorithm. L-BFGS-B belongs to the class of Quasi-Newton methods that approximate the inverse Hessian matrix rather than calculating it explicitly, making it computationally efficient for

multi-parameter problems. As a second-order optimization algorithm, it utilizes curvature information to determine both search direction and approximate step size, converging more rapidly. The “Limited-memory” variant is suited for this study as it avoids storing the full Hessian matrix, instead maintaining a compact representation using gradient information from recent iterations. The “B” suffix denotes the boxed variant, which naturally handles the bound constraints essential for maintaining physical likelihood of parameters.

Unlike the Levenberg-Marquardt algorithm, which is primarily designed for least-squares problems with Gaussian errors, L-BFGS-B performs robustly across diverse objective function landscapes. Its line search strategy makes it ideal for the potentially non-convex parameter space. These advantages are particularly important for the seven-parameter model in this study, where efficient exploration of the constrained parameter space is crucial for finding physically meaningful solutions.

Numerical stability is maintained by enforcing parameter bounds and using safe mathematical operations. For example, AR values are kept above a minimum to avoid undefined results, and outputs are limited to the range $[0, 1]$ to stay within physical limits. Convergence tolerance was set 10^{-8} for parameter changes ensuring high precision fits.

4.1.5 Macroscopic Engineering Model Results

The results are summarized in Table 4.6. The model achieved the best performance ($R^2 = 0.980209$, $RMSE = 0.020781$) due to its optimal balance between mathematical flexibility and physical constraints.

The model provided sufficient degrees of freedom to capture the complex sigmoidal relationship between AR and K_{eff} while maintaining physically meaningful bounds. The linear coupling of Kn and SW effects through the K parameter successfully encoded the secondary nature of these transport mechanisms compared to geometric effects.

Table 4.6: Performance of the macroscopic model for thermal conductivity prediction in aerogel materials.

Model	Test R^2	Test RMSE	Asymptotic Behavior	Interpretability
Macroscopic Engineering Model	0.980209	0.020781	Flexible	High

The parameter bounds established during model development played a crucial role in achieving the observed results. The relatively large bounds for geometric scaling parameters allowed the model to discover the superlinear aspect ratio dependence ($AR^{1.288}$), while the constrained bounds for multi-physics coupling parameters inherently limited the influence of Kn and SW effects.

This constraint strategy emerged from an understanding of transport physics and is directly reflected in the feature importance results, where AR dominates with 98.7% importance in the physics model.

The macroscopic model demonstrates exceptional performance with the optimized formula as shown in Eq. (4.6)

$$K_{\text{eff}} = \frac{0.9958 \times AR^{1.288}}{K + 1.0749 \times AR^{1.281}} \quad (4.6)$$

where:

$$K = 0.3969 + 0.0097 \times Kn - 0.003541 \times SW. \quad (4.7)$$

As Table 4.7 represents, for 4 different test conditions, the developed model correctly captures expected asymptotic behavior while maintaining physical bounds $0 \leq K_{\text{eff}} \leq 1$. For practical engineering applications, the formula provides fast and reliable predictions.

Table 4.7: Asymptotic behavior validation of the macroscopic model showing proper limiting behavior across different flow regimes, aspect ratios, and sidewall temperature conditions.

Condition	Kn	SW	AR	Predicted K_{eff}	Physical Expectation	Validation
$AR \rightarrow 0$	1	10	0.001	0.000366	≈ 0 (no geometry)	✓
$AR \rightarrow \infty$	1	10	1000	0.972493	≈ 1 (Parallel)	✓
$AR \rightarrow 0$	10	50	0.001	0.000429	≈ 0 (no geometry)	✓
$AR \rightarrow \infty$	10	50	1000	0.972500	≈ 1 (Parallel)	✓

4.1.5.1 Comparison with MD Data

The effectiveness of the developed model is tested by comparing its results with MD simulation data under various Knudsen number conditions. The results show that the model can accurately predict transport behavior from near-continuum to molecular flow.

$Kn = 1$ (Near-continuum flow regime): The formula achieves high accuracy with $R^2 \approx 0.987$ and $RMSE \approx 0.017$ when validated against MD data points at $Kn = 1$. Fig. 4.6 illustrates the strong agreement between the model predictions and MD simulation results for all (SW) conditions. To prevent visual overcrowding, only 5 representative points per SW condition are displayed from available points. The model was fitted using the complete 96-sample dataset.

$Kn = 10$ (Molecular flow regime): The formula maintains nearly the same accuracy, with $R^2 \approx 0.988$ and $RMSE \approx 0.018$, when validated against the MD data. This proves that the developed macroscopic model consistently performs well in both near-continuum and molecular flow regimes. Figure 4.7 shows that the formula accurately captures transport behavior in the molecular flow regime.

Table 4.8 lists the K parameter values for different flow regimes and (SW) conditions. The results show a clear relationship between transport parameters and the coupling coefficient.

Table 4.8: K parameter values for different Kn and SW , calculated using $K = 0.3969 + 0.0097 \times Kn - 0.003541 \times SW$.

Flow Regime	SW (K)	K Parameter
Kn = 1 (Near-continuum)	10	0.3712
	20	0.3358
	50	0.2295
Kn = 10 (Molecular)	10	0.4585
	20	0.4231
	50	0.3169

Table 4.9 shows the strong point-by-point agreement with the individual prediction. Errors are usually less than 0.03 across the full range of all tested sidewall temperatures (10 - 50 K) and aspect ratios (0.5 - 10). The formula performs especially well in the moderate aspect ratio range ($AR = 1 - 2$), which is common for practical aerogel applications, with prediction errors typically under 0.02 for both flow regimes.

Table 4.9: Comparison of macroscopic model predictions against MD simulation data for $Kn = 1$ and $Kn = 10$.

Kn = 1 (Near-continuum)				Kn = 10 (Molecular)			
SW	AR	MD Data	Error	SW	AR	MD Data	Error
50	10.0	0.9435	0.0124	50	10.0	0.9357	0.0085
50	2.0	0.8680	0.0123	50	2.0	0.8313	0.0011
50	1.0	0.7668	0.0034	50	1.0	0.6996	0.0159
50	0.5	0.5964	0.0105	50	0.5	0.5022	0.0350
20	10.0	0.9379	0.0116	20	10.0	0.9351	0.0126
20	2.0	0.8469	0.0220	20	2.0	0.7998	0.0014
20	1.0	0.7085	0.0026	20	1.0	0.6635	0.0013

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Table 4.9 – continued from previous page

Kn = 1 (Near-continuum)				Kn = 10 (Molecular)			
SW	AR	MD Data	Error	SW	AR	MD Data	Error
20	0.5	0.5028	0.0213	20	0.5	0.4506	0.0206
10	10.0	0.9424	0.0176	10	10.0	0.9387	0.0178
10	2.0	0.8450	0.0299	10	2.0	0.7813	0.0106
10	1.0	0.7208	0.0322	10	1.0	0.6203	0.0291
10	0.5	0.4635	0.0377	10	0.5	0.4231	0.0296
50	10.0	0.9384	0.0073	50	10.0	0.9426	0.0154
50	2.0	0.8525	0.0032	50	2.0	0.8307	0.0005
50	1.0	0.7747	0.0113	50	1.0	0.6469	0.0686
50	0.5	0.5864	0.0205	50	0.5	0.5192	0.0180
20	10.0	0.9248	0.0015	20	10.0	0.9243	0.0018
20	2.0	0.8312	0.0063	20	2.0	0.7913	0.0098
20	1.0	0.7046	0.0013	20	1.0	0.6673	0.0025
20	0.5	0.5306	0.0065	20	0.5	0.4787	0.0075
10	10.0	0.9270	0.0023	10	10.0	0.9044	0.0165
10	2.0	0.8045	0.0106	10	2.0	0.7820	0.0099
10	1.0	0.6861	0.0025	10	1.0	0.6430	0.0064
10	0.5	0.4974	0.0038	10	0.5	0.4480	0.0047
50	10.0	0.9208	0.0103	50	10.0	0.9349	0.0077
50	2.0	0.8655	0.0098	50	2.0	0.8231	0.0071
50	1.0	0.7732	0.0098	50	1.0	0.7207	0.0052
50	0.5	0.5991	0.0079	50	0.5	0.5630	0.0258
20	10.0	0.9302	0.0038	20	10.0	0.9242	0.0018
20	2.0	0.7938	0.0311	20	2.0	0.8079	0.0067
20	1.0	0.7196	0.0137	20	1.0	0.6706	0.0059
20	0.5	0.5465	0.0225	20	0.5	0.4892	0.0180

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Table 4.9 – continued from previous page

Kn = 1 (Near-continuum)				Kn = 10 (Molecular)			
SW	AR	MD Data	Error	SW	AR	MD Data	Error
10	10.0	0.9519	0.0272	10	10.0	0.9314	0.0105
10	2.0	0.7990	0.0161	10	2.0	0.7906	0.0013
10	1.0	0.6962	0.0076	10	1.0	0.6399	0.0095
10	0.5	0.4993	0.0020	10	0.5	0.4804	0.0277
50	10.0	0.9182	0.0128	50	10.0	0.9477	0.0206
50	2.0	0.8601	0.0044	50	2.0	0.8163	0.0139
50	1.0	0.7416	0.0218	50	1.0	0.7261	0.0106
50	0.5	0.6263	0.0194	50	0.5	0.5655	0.0283
20	10.0	0.9103	0.0161	20	10.0	0.8993	0.0232
20	2.0	0.8077	0.0172	20	2.0	0.7740	0.0272
20	1.0	0.7216	0.0157	20	1.0	0.6651	0.0003
20	0.5	0.5384	0.0143	20	0.5	0.4783	0.0071
10	10.0	0.8968	0.0279	10	10.0	0.9436	0.0227
10	2.0	0.7894	0.0257	10	2.0	0.7964	0.0045
10	1.0	0.6878	0.0008	10	1.0	0.6702	0.0207
10	0.5	0.5328	0.0315	10	0.5	0.4657	0.0130

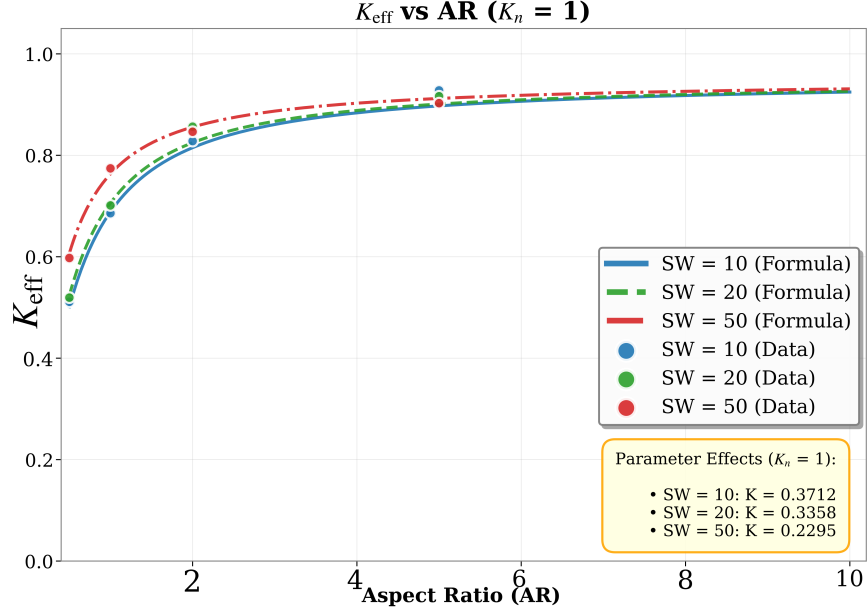


Figure 4.6: Macroscopic model prediction versus MD simulation data for $K_n = 1$. The model shows excellent agreement with simulation data points across different SW and AR . $R^2 \approx 0.987$ and $\text{RMSE} \approx 0.017$ show the model's ability to capture the relationship between AR and K_{eff} .

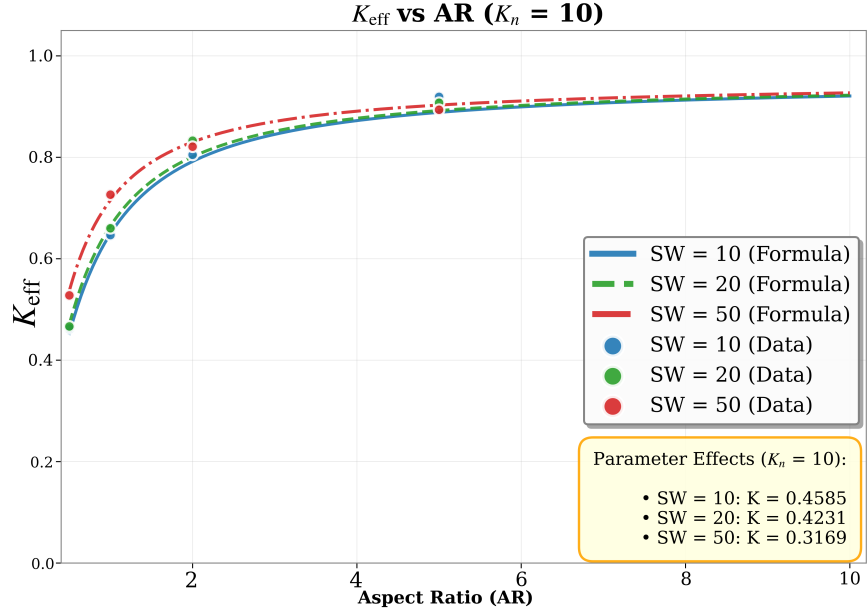
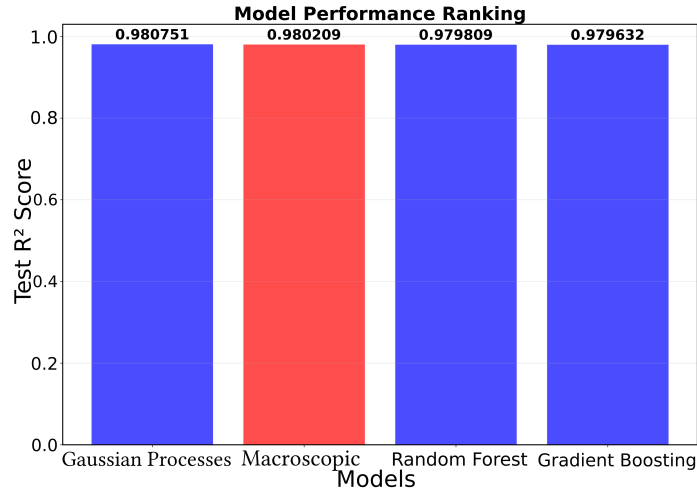


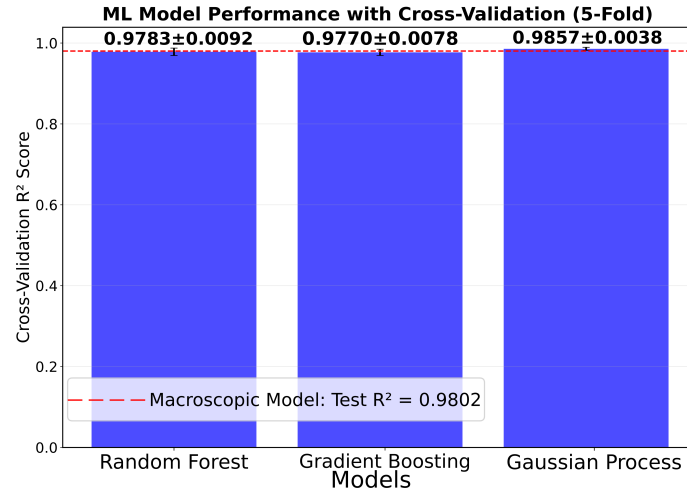
Figure 4.7: Macroscopic model prediction versus MD simulation data for $K_n = 10$. The model shows excellent agreement with simulation data points across different SW and AR . The model maintains excellent predictive accuracy $R^2 \approx 0.988$ and $\text{RMSE} \approx 0.018$.

4.1.5.2 Comparison with ML Results

Figure 4.8a shows the macroscopic model achieving comparable performance (test $R^2 = 0.980209$) to the Gaussian Process, the best-performing ML approach. This places it second overall in the model ranking. Figure 4.8b demonstrates the models' cross-validation stability through error bars that indicate prediction reliability.



(a) Model performance ranking solution.



(b) Model performance ranking with CV solution.

Figure 4.8: Model performance ranking based on test R^2 scores. The GP achieves the highest performance, with $R^2 = 0.980751$. The macroscopic model achieves comparable ML performance with $R^2 = 0.980209$.

Figure 4.9 displays the predicted versus actual values for the macroscopic engineering model and best-performing machine learning approach. The graph demonstrates a strong linear correlation with minimal deviation from the ideal prediction line for both models.

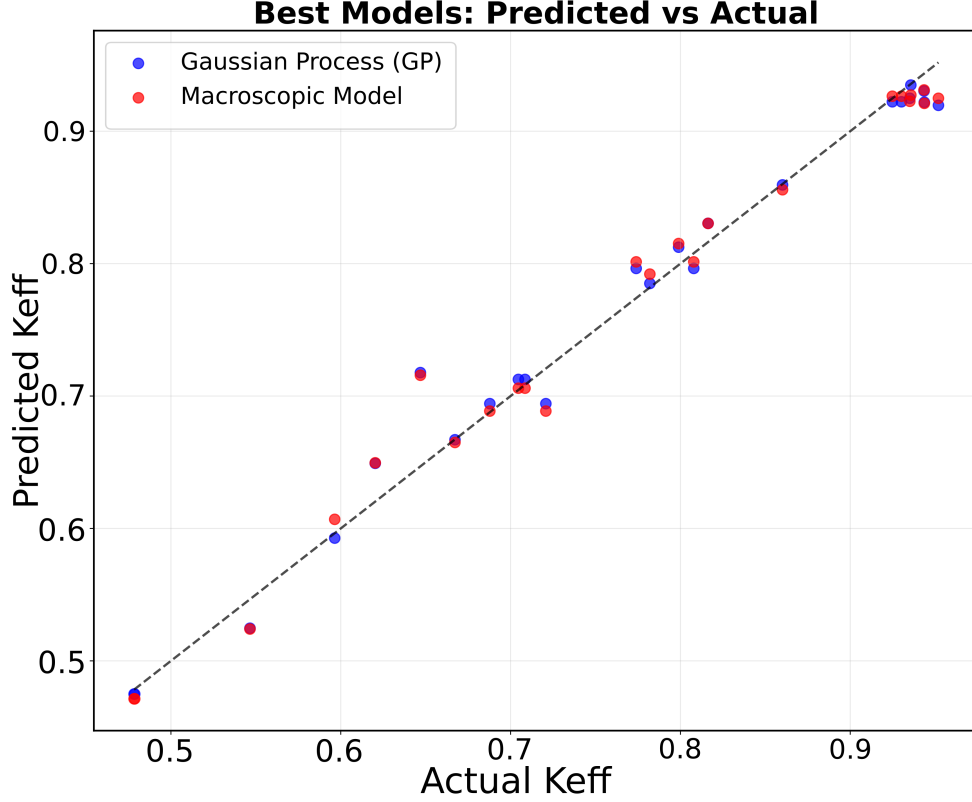


Figure 4.9: Predicted vs actual effective thermal conductivity values for the GP and surrogate models. Both models show excellent agreement with the ideal prediction line across the K_{eff} range.

Feature importance analysis for the developed macroscopic model quantifies the physical influence of each transport mechanism through parameter magnitude analysis. The AR importance arises from the dominant geometric scaling terms ($a \times AR^n$ and $b \times AR^m$), while Kn and SW importance are quantified through their coupling coefficients (k_1 and k_2) in the linear combination $K = k_0 + k_1 \times Kn + k_2 \times SW$. This analysis enables validation of whether ML methods discover the same physical

relationships encoded in the mechanistic model structure. Figure 4.10 illustrates the feature importance ranking across all approaches.

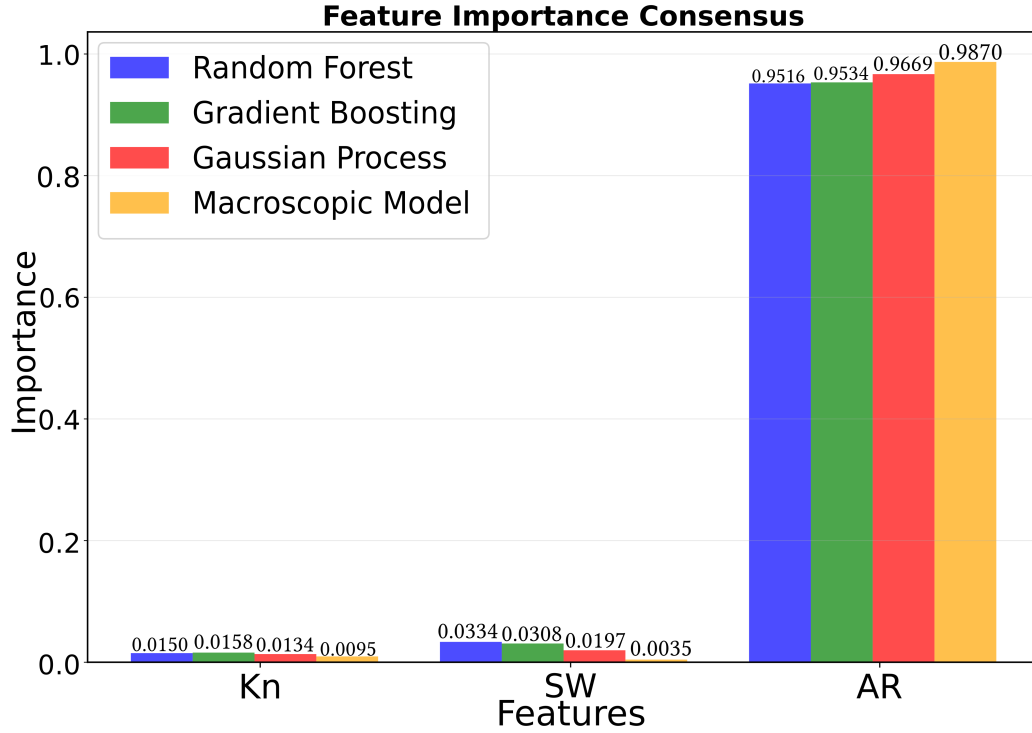


Figure 4.10: Feature importance consensus across all modeling approaches showing *AR* dominance on effective thermal conductivity.

Partial dependence analysis enables quantitative comparison between the macroscopic and ML models by revealing functional relationships through marginalization over non-target features. This analysis compares the macroscopic model with the data-driven GP across key input parameters.

Knudsen Number Effects:

Figure 4.11 depicts consistent linear decreasing trends between both models across the Kn range (0-10). The GP model shows a decrease from approximately 0.805 to 0.762, while the macroscopic model exhibits a parallel trend from 0.787 to 0.750. This agreement validates the physical interpretation that a higher Knudsen number reduces effective thermal transport due to rarefaction effects in the transition from continuum to molecular flow regimes.

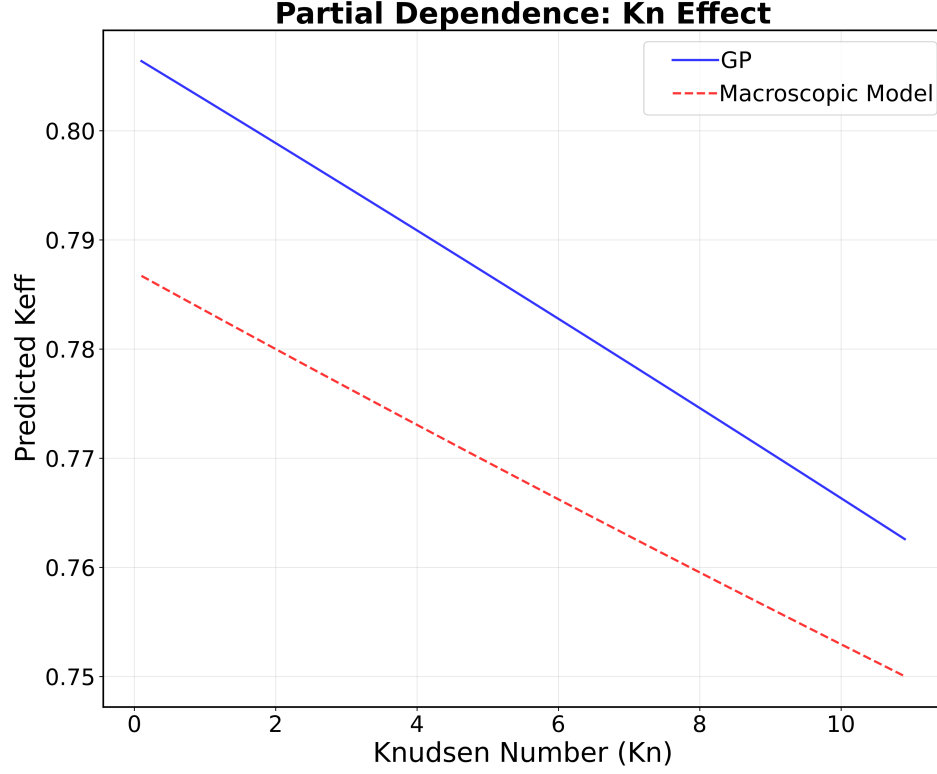


Figure 4.11: Partial dependence analysis for Knudsen Number (Kn) effects. Consistent linear decreasing trends between the GP (solid blue) and the macroscopic model (dashed red), confirms the rarefaction effects on thermal transport.

Aspect Ratio Effects:

Figure 4.12 demonstrates strong agreement between the models in capturing the characteristic behavior that governs the prediction of K_{eff} . Both curves exhibit a rapid increase from aspect ratio (AR) values of 0 to 2, followed by a gradual approach to saturation near AR values of 8 to 10. The close alignment between GP and macroscopic model predictions indicates that both modeling approaches identified the same functional relationships. The macroscopic model's asymptotic behavior closely matches the pattern learned by the GP model.

The strong visual agreement between the partial dependence curves validates that, despite fundamentally different mathematical formulations, both the data-driven GP model and the macroscopic model captured the same underlying physical relationships. This consistent behavior supports the reliability of the macroscopic

approach and demonstrates that its mathematical structure accurately represents the thermal transport mechanisms identified independently by the best-performing ML model.

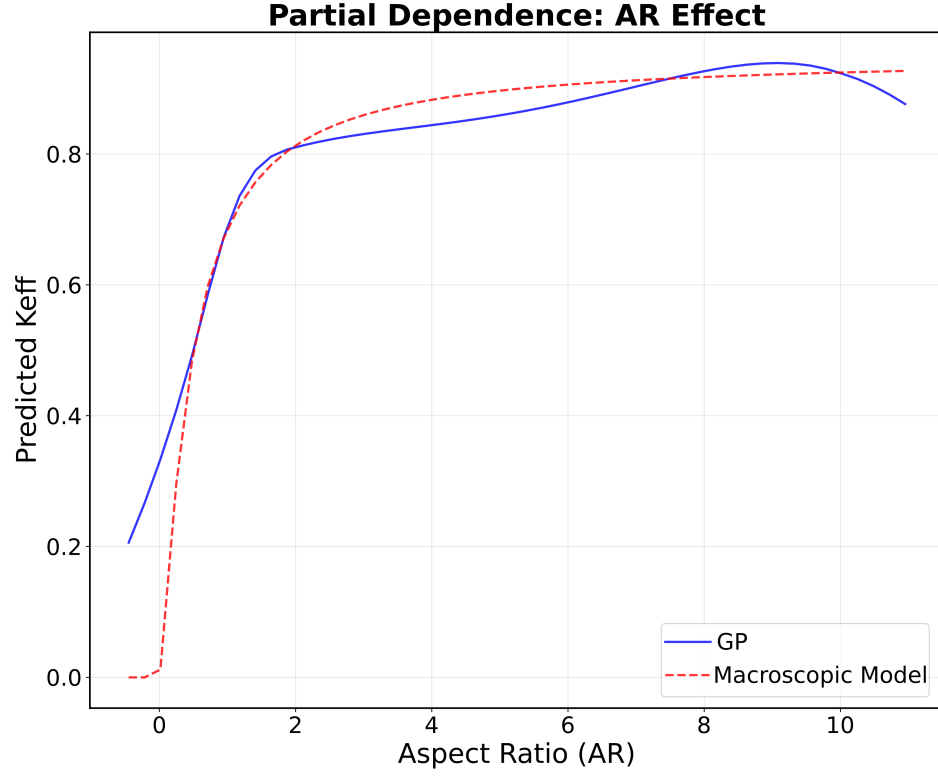


Figure 4.12: Partial dependence analysis for AR effects demonstrating excellent agreement between GP and macroscopic models in capturing sigmoidal behavior.

Chapter 5

Conclusion and Future Works

5.1 Conclusion

This dissertation successfully developed an interpretable macroscopic model for predicting effective thermal conductivity in nanoporous aerogels. It achieves performance comparable to state-of-the-art machine learning methods while maintaining complete mathematical transparency. This demonstrates that the model can match the predictive accuracy of “black-box” models while providing explicit analytical expressions suitable for engineering design.

The systematic progression from single-variable correlations to the multi-parameter model revealed critical insights into transport mechanisms. Aspect ratio emerged as the dominant factor across all modeling approaches, accounting for 95-99% of the variance in effective thermal conductivity. This dominance reflects the fundamental geometric control over heat transfer pathways in confined nanoscale systems. The Knudsen number and sidewall temperature effects, while secondary (1-2% and 2-3% respectively), provide essential corrections for accurate predictions across different flow regimes.

Explainable AI analysis validated the physical interpretation of the developed macroscopic model through multiple independent methods. SHAP analysis confirmed

the feature importance hierarchy, with aspect ratio contributing 73% of the total variation. Partial dependence analysis revealed remarkable agreement between the macroscopic and ML models, with correlation coefficients of $r = 0.9998$ (Knudsen number), $r = 0.9994$ (sidewall temperature), and $r = 0.9829$ (aspect ratio).

The macroscopic model’s asymptotic behavior correctly captures physical limits, approaching zero as $AR \rightarrow 0$ (negligible geometric effect) and unity as $AR \rightarrow \infty$ (parallel plate limit). This proper limiting behavior, combined with the model’s bounded output range $[0, 1]$, ensures physically meaningful predictions even when extrapolating beyond the training data. The explicit mathematical form enables direct sensitivity analysis, uncertainty propagation, and integration into an optimization framework, capabilities essential for engineering applications but challenging with “black-box” ML models.

5.2 Future Works

- **Complex Pore Geometries:** While the rectangular confinement studied in this dissertation provides fundamental insights, real aerogels exhibit tortuous, interconnected pore networks. Extending the macroscopic modeling framework to account for pore size distributions, connectivity, and tortuosity would enhance predictive capability for actual materials. Graph neural networks, combined with physics-informed loss functions, can capture these topological effects while maintaining interpretability.
- **Experimental Validation:** While the model shows excellent agreement with molecular dynamics simulations, experimental validation using controlled pore structures (e.g., fabricated nanochannels or ordered mesoporous materials) would strengthen confidence in the approach.

The systematic progression in this dissertation from correlation analysis through single-variable models to multi-parameter formulations, validated by explainable AI,

provides a template for developing interpretable models in other nanoscale transport phenomena. As computational resources expand and experimental techniques evolve, this hybrid approach, which balances accuracy, interpretability, and computational efficiency, will become increasingly valuable for accelerating materials discovery and optimization in thermal management applications.

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Vita

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