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ENHANCING THERMAL CONDUCTIVITY MODELING OF POLYURETHANE WITH PHASE CHANGE MATERIALS VIA PHYSICS-INFORMED NEURAL NETWORKS AT MULTIPLE SCALES

Bokai Liu[1,2], Yizheng Wang[2,3], Thomas Olofsson[1] and Weizhuo Lu[1]

[1] Intelligent Human-Buildings Interactions Lab, Department of Applied Physics and Electronics,Umeå University, 901 87 Umeå, Sweden

[2] Institute of Structural Mechanics, Bauhaus-Universität Weimar, Marienstr. 15, D-99423 Weimar, Germany

[3] Department of Engineering Mechanics, Tsinghua University, Beijing, 100084, China

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Summary. Polyurethane (PU) is an excellent thermal insulator, and incorporating Phase Change Material (PCM) capsules into PU significantly enhances building envelope performance by improving indoor thermal stability and reducing temperature fluctuations. We propose a hierarchical multi-scale model using Physics-Informed Neural Networks (PINNs) to accurately predict and analyze the thermal conductivity of PU-PCM composites at both micro and macro scales. This approach effectively addresses complex inverse problems and multi-scale phenomena, offering insights that optimize material design. A case study further demonstrates the model's potential in improving thermal comfort and reducing energy consumption in buildings. The successful development of this PINNs-based model holds great promise for advancing PU-PCM applications in thermal energy storage and innovative building insulation design.

1 INTRODUCTION

The increasing global energy consumption has raised concerns about potential supply shortages, depletion of resources, and significant environmental impacts, including ozone layer depletion, global warming, and climate change[1]. The International Energy Agency warns that greenhouse gas emissions will continue to rise, exacerbating extreme weather patterns worldwide. In response, the European Union (EU) aims to reduce greenhouse gas emissions by at least 55% by 2030 compared to 1990 levels, with a key strategy focused on improving energy performance in buildings, which contribute 36% of total CO2 emissions[2]. Heating, ventilation, and air conditioning (HVAC) systems alone account for 50% of the EU's final energy consumption, making energy efficiency in this sector a critical area of research [3, 4, 5].

Recent decades have seen growing interest in using phase change materials (PCMs) for thermal energy storage to enhance building energy efficiency. PCMs, when integrated into building materials or envelopes, can improve latent heat storage capacity, thereby enhancing indoor

thermal comfort and overall energy efficiency[6]. However, PCMs face challenges such as suboptimal thermal conductivity and leakage during phase transitions. These issues can be mitigated by developing shape-stable polymer composites with PCM inclusions, particularly through microencapsulation techniques that confine PCMs within polymeric shells [7]. Among polymers, polyurethane (PU) rigid foams are highly regarded for thermal insulation due to their low thermal conductivity, mechanical stability, and ability to form sandwich structures with various facer materials.

While most research has focused on the synthesis and experimental evaluation of PU-PCM foams' thermal energy storage capacity, there has been limited exploration of their thermal properties across multiple scales, leaving a gap in the comprehensive understanding of these materials [8, 9, 10]. To address this, our study employs a multi-scale modeling approach using Physics-Informed Neural Networks (PINNs). PINNs integrate physics-based knowledge with data-driven learning, making them ideal for predicting the thermal conductivity of PU-PCM materials while handling complex multi-scale phenomena and reducing computational costs.

The primary goal of this study is to develop a PINNs-based multi-scale model to accurately predict the thermal behavior of PU-PCM materials. By incorporating fundamental physics and governing heat transfer equations, this model aims to capture the intricate relationship between microstructure and thermal properties. Leveraging experimental data and simulations, the model will learn the connection between microstructural features and resulting thermal conductivity, providing reliable predictions even with noisy or limited data. This research has the potential to advance the design and optimization of materials for thermal energy storage, building insulation, and electronic cooling applications.

2 Methodology of research

This study proposes a multi-scale modeling approach to analyze the behavior of building envelopes, integrating Physics-Informed Neural Networks (PINNs) with the Representative Volume Element - Finite Element Method (RVE-FEM). The approach bridges three length scales, from micro to macro, using a hierarchical bottom-up method where detailed information at finer scales informs coarser scales [11, 12, 13, 14, 15]. The process begins with micro-scale modeling using PINNs to capture system physics, followed by meso and macro-scale modeling with RVE-FEM to understand larger system behavior. The multi-scale model is then applied to evaluate the building envelope's thermal properties and optimize its design. Additionally, the study explores composite material design by incorporating polyurethane (PU) as the matrix and microencapsulated paraffin phase change materials (PCMs) to enhance energy storage stability and reduce thermal conductivity.

The framework for using Physics-Informed Neural Networks (PINNs) in micro-scale modeling is presented through a detailed schematic that outlines the structure and process of the model. The Multi-scale modeling scheme is shown in Figure 1

Neural Network Structure

Feed-Forward Neural Network: The network is designed as a feed-forward model, which involves multiple layers of neurons that process input data through a series of linear transformations followed by non-linear activation functions. The mathematical representation of the network's operations at each layer is provided, where the activation function used is typically a

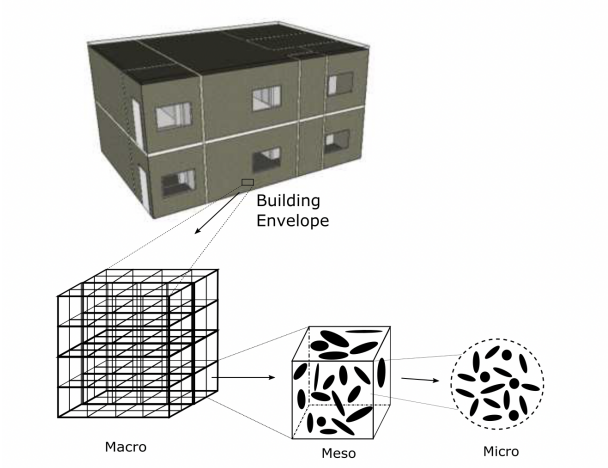

Figure 1: Multi-scale modeling scheme

non-linear function such as tanh or sigmoid.

Components of the Model

1. **Data Net:**

   - **Purpose:** This neural network approximates the temperature distribution $T(x)$ at specific spatial coordinates x_i.
   - **Parameters:** The network parameters are denoted as θ_D.
   - **Loss Function (Loss_D):** The discrepancy between the predicted temperature $\hat{T}(x_i;\theta_D)$ and the observed temperature $T(x_i)$ is calculated using the Mean Square Error (MSE):
   $$\text{Loss}_D = \sum_{i=1}^{n} \left| \hat{T}(x_i;\theta_D) - T(x_i) \right|^2$$
   - **Training:** The data net is trained using observed temperature data to minimize this loss function.

2. **PDEs Net:**

   - **Purpose:** This network models the unknown thermal conductivity field $\kappa(x)$ by solving the heat conduction partial differential equation (PDE) over a given domain.
   - **Parameters:** The parameters of this network are denoted as θ_k.
   - **Loss Function (Loss_PDE):** The loss function incorporates the difference between the predicted temperature and the solution to the PDE, with additional terms for

boundary conditions:

$$\begin{aligned}\text{Loss}_{PDE} = \lambda_1 \sum_{i=1}^{n} \left| \hat{T}(x_i;\theta_D) - T(x_i) \right|^2 \\ + \lambda_2 \sum_{i=1}^{l} \left| \frac{d\hat{T}(x)}{dx} - q_1 \right|^2 \\ + \lambda_3 \left| \kappa(x;\theta_k) \frac{d\hat{T}(x)}{dx} - f(x) \right|^2 \\ + \lambda_4 \left| \hat{T}(b) - q_2 \right|^2\end{aligned}$$

- **Training:** The PDEs Net is optimized by minimizing this loss function, ensuring that the neural network adheres to the underlying physical laws and boundary conditions.

Adaptive Weighting Strategy

Importance of Weights: The weights $\lambda_1, \lambda_2, \lambda_3, \lambda_4$ are crucial as they control the relative importance of different terms in the loss functions for both networks. Proper adjustment of these weights is necessary to ensure that the network balances the contributions of data fitting and adherence to physical laws.

Adaptive Weighting Method: An adaptive weight method based on the gradient is employed to dynamically adjust these weights during training. This method is designed to give more importance to the loss components that are more challenging to optimize, thereby ensuring a balanced and efficient learning process:

$$\lambda_i = \text{Factor} \times \frac{\sum_{j=1}^{l} \text{mean}\left(|\nabla_\theta \text{Loss}_i|\right)}{\text{mean}\left(|\nabla_\theta \text{Loss}_i|\right)}$$

Optimization Objective: The ultimate goal is to minimize both loss functions, Loss_D and Loss_{PDE}, to determine the optimal network parameters θ_D and θ_k.

Special Case Consideration

Constant Conductivity Field: If the thermal conductivity field $\kappa(x)$ is constant, it can be represented by a single parameter κ, simplifying the modeling process. In such cases, a neural network may not be required, and the optimization would focus on determining this constant value directly to minimize the PDE loss.

Meso and macro scales

In our multi-scale modeling approach, **Representative Volume Elements (RVEs)** are used at the meso-scale to represent material properties. RVEs are typically cubic and contain spherical PCM (Phase Change Material) fillers. The distribution of these fillers is determined by **probability density functions (PDFs)** to capture their statistical distribution [16, 17, 18, 19, 20].

We assess agglomeration and dispersion of fillers using two indices:

$$\xi = \frac{V_{\text{inclusion}}}{V_{RVE}}, \quad \zeta = \frac{V_{\text{inclusion\_Graphene}}}{V_{\text{Graphene}}}$$

where ξ represents the volume fraction of inclusions, and ζ indicates the dispersion within the composite.

The RVE size is determined by ensuring the homogenized **thermal conductivity** converges:

$$\langle R \rangle = \frac{1}{M} \sum_{k=1}^{M} R^{(k)}$$

where $R^{(k)}$ is the thermal conductivity in the k-th RVE.

The thermal behavior at this scale is governed by the heat equation:

$$\nabla \cdot (\kappa \nabla \theta) + Q = 0$$

with Fourier's law providing the relationship for homogenized thermal conductivity:

$$q = -\kappa \nabla T$$

This meso-scale model is essential for predicting the thermal properties of composites, informing larger-scale simulations and material design.

The **Mori-Tanaka method** is used to estimate the effective thermal conductivity of composite materials by considering the thermal conductivities of the matrix material and reinforcement, as well as their respective volume fractions. This method assumes that the composite's thermal conductivity is governed by the thermal conductivity of the matrix and the enhanced conduction pathways provided by the reinforcement.

The effective thermal conductivity (k_{eff}) of a composite with PU-PCMs is calculated using the following equation:

$$k_{\text{eff}} = k_m + \frac{4 k_p V_p}{(1 - V_p) + \frac{k_m}{k_p}}$$

where:

- k_{eff} is the effective thermal conductivity of the composite,
- k_m is the thermal conductivity of the polymer matrix,
- k_p is the thermal conductivity of paraffin,
- V_p is the volume fraction of PCMs in the composite.

This equation provides a means to predict the overall thermal performance of the composite material at the macroscopic scale.

This case study evaluates the energy consumption and thermal comfort of a typical single-family house in Umeå, Sweden, using Polyurethane Phase Change Materials (PU-PCMs) within the building envelope. Umeå, characterized by cold winters and mild summers, requires effective thermal management due to its subarctic climate. The study focuses on how PU-PCMs can

reduce energy consumption and improve indoor thermal comfort by storing and releasing thermal energy. The Building construction elements and window properties is shown in Table 1

The analysis is based on hourly temperature data from 2022 and simulates heating needs to maintain indoor temperatures at 21° C in winter and 25°C in summer. The effectiveness of PU-PCMs is measured through annual energy consumption and thermal comfort indicators such as Predicted Mean Vote (PMV) and Predicted Percentage of Dissatisfied (PPD).

Key equations include:

- **PMV Calculation**:

$$\text{PMV} = \left(0.303 \cdot e^{-0.036 \cdot M} + 0.028\right) \cdot (T_a + 0.99 \cdot T_r) - 4.356 \times 10^{-8} \cdot (T_a + 273)^4 + \ldots$$

- **PPD Calculation**:

$$\text{PPD} = 100 - 95 \times \exp\left(-0.03353 \cdot \text{PMV}^4 - 0.2179 \cdot \text{PMV}^2\right)$$

The study concludes that PU-PCMs effectively reduce energy consumption and enhance thermal comfort, with a target of keeping PPD below 20% and maintaining PMV close to 0 for comfort.

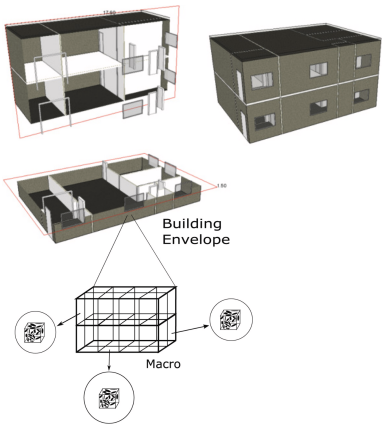

Figure 2: The application of PU-PCMs in building envelope

Table 1: Building construction elements and window properties.

Elements	Layer 1 (Inside)	Layer 2	Layer 3	Layer 4 (Outside)	Thickness (m)	U-value W/(m² K)	Width (m)	Height (m)
External walls	Concrete (0.15 m)	Light insulation (0.15 m)	Concrete (0.08 m)	Light insulation (0.1 m)	0.73 m	0.125	-	-
Internal walls	Gypsum (0.026 m)	Light insulation (0.03 m)	Gypsum (0.026 m)	/	0.296 m	0.2853	-	-
Roof	Render (0.013 m)	Light insulation (0.02 m)	Lightweight Concrete (0.25 m)	Light insulation (0.16 m)	0.463 m	0.1438	-	-
Type1: 90/90 Window	-	-	-	-	-	1.055	1.8	1.2
Type2: 90/90 Window	-	-	-	-	-	1.055	1.8	1.2

3 Numerical results and discussion

Micro scale results based on PINNs

This study evaluates the effectiveness of Physics-Informed Neural Networks (PINNs) in solving inverse problems related to thermal conductivity in PU-PCMs, focusing on both uniform and non-uniform conductivity scenarios.

Uniform Thermal Conductivity

The uniform thermal conductivity scenario is governed by:

$$k\frac{d^2T}{dx^2} = f(x) = -(15\pi)^2\cos(15\pi x), \quad x \in \left[-\frac{1}{2}, \frac{1}{2}\right]$$

$$\left.\frac{\partial T}{\partial x}\right|_{x=-\frac{1}{2}} = q_1 = -\frac{15\pi}{k}, \quad \left.\frac{\partial T}{\partial x}\right|_{x=\frac{1}{2}} = q_2 = \frac{15\pi}{k}$$

The analytical solution is:

$$T = \frac{\cos(15\pi x)}{k}$$

PINNs successfully predict the thermal conductivity k with high accuracy, achieving an R^2 value close to 0.99. The results are presented in Table 2.

Table 2: The L_1^{rel} error of uniform thermal conductivity with noisy data. σ_s denotes the variance of Gaussian distribution of noisy data. HL denotes the different number of hidden layers.

σ_s	0 (no noise)	0.01	0.02	0.03	0.04	0.05	0.06	0.07	0.08	0.09	0.10
3HL	0.0288	0.0264	0.0402	0.0407	0.0523	0.0690	0.0543	0.0471	0.0512	0.0588	0.0614
4HL	0.0175	0.0353	0.0501	0.0378	0.0421	0.0527	0.0544	0.0324	0.0296	0.0494	0.0661
5HL	0.0297	0.0695	0.0345	0.0421	0.0531	0.0396	0.0579	0.0402	0.0747	0.0540	0.0683

Non-Uniform Thermal Conductivity

For the non-uniform scenario:

$$k(x)\frac{d^2T}{dx^2} = -(15\pi)^2\cos(15\pi x)k(x), \quad x \in \left[-\frac{1}{2}, \frac{1}{2}\right]$$

$$\left.\frac{\partial T}{\partial x}\right|_{x=-\frac{1}{2}} = q_1 = -15\pi, \quad \left.\frac{\partial T}{\partial x}\right|_{x=\frac{1}{2}} = q_2 = 15\pi$$

The solution is:

$$T = -\cos(15\pi x)$$

PINNs accurately predict the non-uniform thermal conductivity, maintaining an L^2 relative error around 10^{-3}, even with noisy data. Table 3 indicates the results

Table 3: The L_1^{rel} error of non-uniform thermal conductivity with noisy data. σ_s represents the variance of the Gaussian distribution of the noisy data, and HL denotes the different number of hidden layers.

σ_s	0 (no noise)	0.01	0.02	0.03	0.04	0.05	0.06	0.07	0.08	0.09	0.10
3HL	0.0129	0.0166	0.0115	0.0155	0.0139	0.0114	0.0181	0.0176	0.0132	0.0108	0.0140
4HL	0.0193	0.0121	0.0116	0.0172	0.0187	0.0151	0.0130	0.0153	0.0155	0.0107	0.0250
5HL	0.0163	0.0135	0.00593	0.00943	0.00656	0.00716	0.0162	0.0291	0.00819	0.00821	0.0120

2D Extension and Real Material Simulation

The 2D problem is modeled as:

$$k(x,y)\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right)=-\left[(15\pi x)^2+(15\pi y)^2\right]\cos(15\pi xy)k(x)$$

The analytical solution is:

$$T=-\cos(15\pi xy)$$

To simulate real PU-PCMs:

$$k(x)=0.24\exp\left(-\frac{x^2+y^2}{0.18}\right)$$

The highest thermal conductivity value in the center is 0.24, gradually decreasing towards the surrounding, with the boundary approaching an average thermal conductivity of 0.03.

Meso and Macro Scale Results

This section summarizes the temperature distribution at the meso and macro scales, obtained through FEM-RVE analysis. By analyzing different volume fractions within material regions, the study calculates a final thermal conductivity of 0.2474 W/mK for a 9% overall volume fraction. The numerical results are validated against existing experimental data, showing good accuracy, which supports their application in further engineering studies. Table 4 presents those results.

Table 4: The distribution of properties in material region.

Numbers	V_f (%)	**Thermal conductivity (W/m K)**	**Numbers**	V_f (%)	**Thermal conductivity (W/m K)**
1	0.043	1.8005	9	0.071	0.6038
2	0.025	0.2914	10	0.045	1.3574
3	0.096	2.3121	11	0.019	1.2374
4	0.075	0.3314	12	0.041	1.6799
5	0.049	1.6132	13	0.048	1.2015
6	0.082	0.6339	14	0.089	1.2315
7	0.037	0.2111	15	0.088	0.8957
8	0.057	1.1216	16	0.016	1.1912

Thermal conductivity in Mori–Tanaka method: 0.2473926 (W/m K) (Volume fraction: 9%).

Case study results

In this case study, we assess the performance of PU-PCMs (Phase Change Materials) in single-family houses by incorporating their properties into our models to evaluate their impact on energy consumption and thermal comfort. Using engineering parameters from a multi-scale modeling approach, we conduct a comprehensive physical simulation of a house with PINNs and FEM-RVE. We analyze annual energy usage for 2022 and hourly indoor temperature fluctuations using IDA-ICE, comparing scenarios with and without PU-PCMs in the building envelope. The results demonstrate the effectiveness of PU-PCMs in reducing energy consumption, as detailed in Table 5.

The assessment of the Fanger comfort index in Table 6, including PPD and PMV, reveals that PU-PCMs significantly enhance occupant satisfaction and thermal comfort, particularly in the

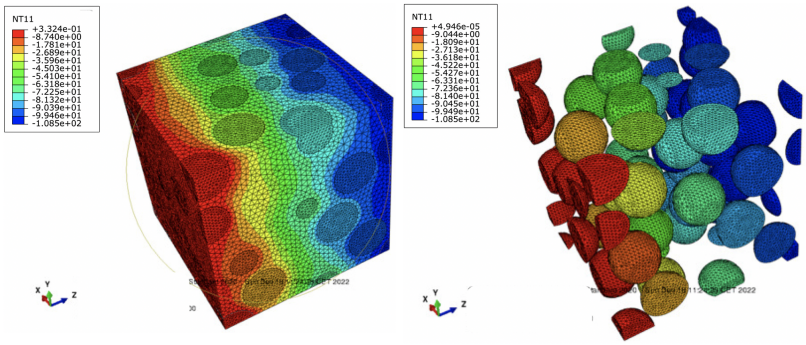

Figure 3: Temperature distribution of composites

Table 5: Annual energy usage without/with PU-PCMs.

Components	Without PU-PCMs		With PU-PCMs enhanced		Improvement (%)
	Purchased energy (kWh)	Energy Usage Intensity (kWh/m^2)	Purchased energy (kWh)	Energy Usage Intensity (kWh/m^2)	
Lighting, facility	32,199	126.1	32,199	126.1	0%
Electric cooling	16,062	62.9	16,322	64	1.74%
HVAC aux	7,258	28.4	7,258	28.4	0%
Fuel heating	15,369	60.2	14,973	58.6	2.64%
Total, Facility electric	55,519	217.4	55,809	218.5	0.52%
Total, Facility fuel	15,369	60.2	14,973	58.6	2.64%
Total	70,888	277.5	70,782	277.1	0.14%
Equipment, tenant	24,149	94.5	24,149	94.5	0%
Total, Tenant electric	24,149	94.5	24,149	94.5	0%
Grand total	95,037	372.1	94,931	371.7	0.11%

living room and 1st bedroom, by reducing dissatisfaction and improving thermal perception. The 2nd bedroom and Toilet show minor improvements, likely due to their smaller exterior wall areas, which limits the effectiveness of the PCM phase change. The PCM phase change, activated by significant temperature fluctuations, primarily in the summer, plays a crucial role in stabilizing indoor temperatures, with larger exterior wall areas contributing more to overall comfort improvement.

Table 6: Fanger's comfort indices without/with PU-PCMs.

Components	Without PU-PCMs		With PU-PCMs enhanced		Improvement (PMV) (%)
	Predicted Percentage of Dissatisfied (PPD)	Predicted Mean Vote (PMV)	Predicted Percentage of Dissatisfied (PPD)	Predicted Mean Vote (PMV)	
Living room	9.082%	-3.739	5.523%	-1.529	59.10%
Toilet	7.931%	3.615	7.829%	3.507	3.07%
2nd Bedroom	6.365%	2.405	6.354%	2.334	3.04%
1st Bedroom	6.034%	1.912	5.960%	1.634	17.01%

4 Conclusions

This study introduces a hierarchical multi-scale model for PU-PCM foam composites using Physics-Informed Neural Networks (PINNs) to predict and analyze thermal conductivity at both micro and macro scales. By integrating physics-based knowledge with data-driven learning, the model effectively addresses complex multi-scale phenomena and solves inverse problems. The RVE-finite element method is used to compute effective engineering parameters, capturing the relationship between microstructure and thermal properties. The model's accuracy in predicting thermal behavior, even with noisy or limited data, is crucial for real-world applications. A case study on building thermal comfort and energy consumption demonstrates the model's potential

in passive energy design and improving occupant comfort. This PINNs-based approach holds promise for advancing PU-PCM material design and optimizing thermal energy storage systems and building insulation.

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