The 9th European Congress on Computational Methods in Applied Sciences and Engineering
ECCOMAS Congress 2024
3 – 7 June 2024, Lisbon, Portugal

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

Key Words: *Physics-Informed Neural Networks (PINNs), Phase Change Materials (PCMs), Thermal properties, Multi-scale modelling, RVE-FEM.*

Polyurethane (PU) boasts exceptional thermal properties, making it an attractive choice for thermal insulation. The incorporation of Phase Change Materials (PCMs) capsules into Polyurethane (PU) has emerged as a highly effective method for enhancing building envelope performance. This innovative configuration significantly enhances indoor thermal stability while reducing fluctuations in indoor air temperatures.

To investigate the thermal conductivity of the PU-PCM composite material, we propose the use of a hierarchical multi-scale model that employs Physics-Informed Neural Networks (PINNs). This model allows for precise prediction and analysis of the material's thermal conductivity at both micro and macro scales. By harnessing the synergy between physics-based knowledge and data-driven learning inherent in PINNs, we adeptly address complex inverse problems and multi-scale phenomena. Furthermore, the insights gained into thermal conductivity facilitate material design optimization.

To comprehensively consider occupants' thermal comfort within a building enclosure, we conduct a case study to evaluate the performance of this optimized material in a single-room setting. Simultaneously, we estimate the energy consumption associated with this scenario. All findings collectively highlight the promising potential of this design, enabling passive building energy management and significantly improving occupants' comfort.

The successful development of this multi-scale model based on PINNs holds immense promise for advancing our understanding of PU-PCM's thermal properties. It is positioned to make substantial contributions to the formulation and enhancement of materials for various practical applications, including thermal energy storage systems and the design of insulation for cutting-edge building envelopes.

REFERENCES

[1] E. Samaniego, C. Anitescu, S. Goswami, V. M. Nguyen-Thanh, H. Guo, K. Hamdia, X. Zhuang, T. Rabczuk, An energy approach to the solution of partial differential equations in computational mechanics via machine learning: Concepts, implementation and applications, Computer Methods in Applied Mechanics and Engineering 362 (2020) 112790.

[2] M. Raissi, P. Perdikaris, G. E. Karniadakis, Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, Journal of Computational Physics 378 (2019) 686-707.

[3] Y. Wang, J. Sun, W. Li, Z. Lu, Y. Liu, Cenn: Conservative energy method based on neural networks with subdomains for solving variational problems involving heterogeneous and complex geometries, Computer Methods in Applied Mechanics and Engineering 400 (2022) 115491.

[4] J. Sun, Y. Liu, Y. Wang, Z. Yao, X. Zheng, Binn: A deep learning approach for computational mechanics problems based on boundary integral equations, Computer Methods in Applied Mechanics and Engineering 410 (2023) 116012.

[5] L. Lu, R. Pestourie, W. Yao, Z. Wang, F. Verdugo, S. G. Johnson, Physics-informed neural networks with hard constraints for inverse design, SIAM Journal on Scientific Computing 43 (2021) B1105-B1132.

[6] B. Liu, N. Vu-Bac, X. Zhuang, X. Fu, T. Rabczuk, Stochastic full-range multiscale modeling of thermal conductivity of polymeric carbon nanotubes composites: A machine learning approach, Composite Structures 289 (2022) 115393.

[7] S. Wang, Y. Teng, P. J. S. J. o. S. C. Perdikaris, Understanding and mitigating gradient flow pathologies in physics-informed neural networks, SIAM Journal on Scientific Computing 43 (2021) A3055-A3081.

[8] B. Liu, N. Vu-Bac, X. Zhuang, T. Rabczuk, Stochastic multiscale modeling of heat conductivity of polymeric clay nanocomposites, Mechanics of Materials 142 (2020) 103280.

[9] B. Liu, N. Vu-Bac, T. Rabczuk, A stochastic multiscale method for the prediction of the thermal conductivity of polymer nanocomposites through hybrid machine learning algorithms, Composite Structures 273 (2021) 114269.

[10] B. Liu, N. Vu-Bac, X. Zhuang, X. Fu, T. Rabczuk, Stochastic integrated machine learning based multiscale approach for the prediction of the thermal conductivity in carbon nanotube reinforced polymeric composites, Composites Science and Technology 224 (2022) 109425.