Title: Optimization of Polymeric Hollow Fiber Heat Exchangers Using Lattice Boltzmann Method
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The report was prepared based on a request from prof. prof. Ing. Ondřej Šikula, Ph.D., chairman of the dissertation committee, dated 09. 06. 2025.

This thesis investigates the numerical modeling, parametric optimization and experimental validation of Polymeric Hollow Fiber Heat Exchangers (PHFHEs). The work is well-motivated by the industrial need for advanced thermal management solutions and correctly identifies the limitations of existing design methodologies. The core of the thesis is the development and validation of a numerical optimization tool based entirely on open-source software. The candidate systematically navigates the process, beginning with a thorough theoretical introduction, followed by a critical comparison of two distinct CFD methodologies—the Lattice Boltzmann Method (LBM) and the Finite Volume Method (FVM). Based on this assessment, the candidate develops a parametric study workflow using OpenFOAM (FVM) and the Dakota optimization toolkit. The research concludes with the fabrication of physical prototypes of PHFHEs, which are then verified experimentally in a calorimetric tunnel and validated against simulation assumptions.

Relevance of the dissertation topic.

The topic of this dissertation is highly relevant. Heat exchangers are part of many systems and equipment and there is a growing demand across various industries, particularly in the automotive sector, for lightweight, cost-effective, increase in heat transfer efficiency, reduction of pressure losses, ect. PHFHEs represent a promising technology for meeting these requirements, but their widespread deployment is hampered by a lack of technological understanding. This thesis directly addresses this gap. Furthermore, the candidate's exclusive use of open-source software (OpenFOAM, Palabos, Dakota) aligns perfectly with current trends in both academia and industry. This research therefore lies at the intersection of modern materials science, heat transfer, and computational fluid dynamics.

Fulfillment of the Set Goals.

The thesis sets out to achieve two primary goals (defined based on State Doctoral Exam), both of which have been successfully fulfilled.

1. **Adaptation of the LBM for the design of PHFHEs:** This goal was fully met. The candidate adapted and tested the LBM for the specific application. Crucially, the work went beyond simple adaptation to include a critical assessment of the method's suitability. The well-justified conclusion that LBM was less practical than FVM for this specific task, due to stability and implementation challenges, demonstrates a deep and mature understanding of the numerical methods involved.
2. **Creation of an optimization tool usable in the design phase of PHFHEs:** This objective has also been achieved. The candidate successfully integrated the OpenFOAM CFD solver with the Dakota optimization toolkit to create a fully automated workflow for performing parametric studies in the design of PHFHEs. The usefulness of this tool has been demonstrated by extensive simulations and its accuracy has been confirmed by rigorous experimental validation, demonstrating its readiness for practical use.

Problem-Solving Procedure.

Initially, the study explored the suitability of the LBM using the Palabos C++ framework for simulating fluid flow and heat transfer in PHFHEs. While LBM showcased efficiency potential for complex 3D geometries, direct comparisons with OpenFOAM (FVM) revealed its limitations for this specific application. A crucial finding was that LBM did not offer convincing benefits for PHFHE simulation, primarily due to challenges with local mesh refinement.

A significant part of the research involved a parametric study utilizing the Pareto front concept for design optimization. This approach was chosen over a single cost function due to the inherent trade-offs between conflicting objectives, such as maximizing heat transfer rate while minimizing air pressure drop. The study effectively demonstrated how varying transversal and longitudinal pitches influences performance, offering practical guidelines for design.

Finally, experimental validation formed the foundation of this study. Three PHFHE prototypes fabricated in-house from steel and polymer materials were tested in a calorimetric tunnel. The experimental setup and methodology were thoroughly described, including an explicit discussion of data correction due to discrepancies in the measurements. Validation yielded an acceptable level of agreement between the CFD and experimental results for the graded arrangement. This positive outcome largely confirmed the accuracy of the numerical model for these arrangements.

Specific Contributions of the Doctoral Student.

- **Systematic Method Comparison:** The candidate conducted a detailed comparative study of LBM and FVM for simulating flow in complex micro-geometries. This provides valuable, application-specific insights for the wider CFD community.
- **Robust Numerical Model Development:** A key contribution is the development, verification and validation of the CFD model in OpenFOAM. The candidate has addressed critical details such as parametric mesh generation, appropriate boundary conditions and selection of a suitable turbulence model.
- **Implementation of an Advanced Optimization Workflow:** The candidate successfully implemented an automated optimization process in the open-source software Dakota, based on the concept of Pareto queuing. This enables the intuitive analysis of trade-offs between conflicting design objectives.
- **Experimental Validation:** A crucial contribution was the experimental validation, for which the candidate prepared the production of prototypes and carried out a series of experiments to verify the accuracy of the numerical model.

Significance of the Results for Practice or the Development of the Scientific Field.

The results of this thesis have clear significance for both industrial practice and scientific advancement.

- **For Practice:** The developed and validated optimization tool is directly applicable in an industrial R&D setting. It can significantly accelerate the design cycle for new PHFHEs, reduce the reliance on costly physical prototyping, and enable a systematic search for optimal designs. The open-source nature of the tool makes it accessible to a broad range of users, including small and medium-sized enterprises.
- **For the Development of the Scientific Field:** The thesis provides a valuable dataset and benchmark case for flow and heat transfer in micro-structured tube channels, which can be used by other researchers to validate their own numerical models.

Formal and Linguistic Level of the Work.

The thesis is written in English at a professional and academic standard. There are only a few stylistic errors and typos in the work. The language used is clear, precise and scientifically rigorous. The terminology is used correctly and consistently throughout the document. The overall structure is logical, and the presentation of data through figures, graphs, and tables is of good quality. The work meets all the formal requirements of a doctoral dissertation.

Unfortunately, the title “Optimization of Polymeric Hollow Fiber Heat Exchangers Using the Lattice Boltzmann Method” does not fully reflect the scope of the work, as the LBM method is ultimately not used for parametric optimization.

Conclusion and Recommendation

In summary, this dissertation makes an original and fundamental contribution to the field of PHFHEs. The candidate has demonstrated proficiency in the application of advanced numerical methods, an in-depth grasp of the physics underlying heat transfer, and proficiency in experimental verification.

I would like to suggest changing the title of the thesis to make it more representative of its scope.

In terms of its scope, originality and scientific quality, the thesis fully meets the requirements for a PhD. I **recommend this thesis for public defense**, and, following a successful defence, for the award of the Ph.D. degree.

Supplementary Questions for the Doctoral Thesis

Your doctoral thesis is of high quality and offers valuable insights. To further expand and deepen the topic, here are five supplementary questions, focusing on areas where more detail could be gained or future possibilities explored.

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1. Extending Turbulence Modeling in LBM and OpenFOAM.

The candidate mentioned that turbulence modeling wasn't considered for LBM because it would require a 3D domain, which was deemed inefficient. Meanwhile, RANS models were used in OpenFOAM.

- How would the conclusions regarding the competitiveness of LBM vs. FVM (OpenFOAM) change if LBM implemented a suitable 2D turbulence model (if one exists or is under development for Palabos) or if 3D simulations with turbulence models were optimized for more efficient runs? Would LBM then be more advantageous for PHFHEs?

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2. Thermal LBM Instabilities and High Peclet Numbers.

The candidate identified issues with numerical instabilities in thermal LBM simulations for high Peclet numbers (Pe = 682), which is critical for heat transfer. The candidate also noted that stabilization methods exist but were outside the scope of your research.

- What specific stabilization methods for thermal LBM would you suggest for future research, and how would their implementation affect the computational cost and overall efficiency of the LBM model?
- Do you believe resolving these instabilities could change the overall conclusion about LBM's unsuitability for PHFHEs from a heat transfer perspective, or would other factors still play a dominant role?

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3. Possibilities for Local Mesh Refinement in LBM.

The candidate highlighted that OpenFOAM gained a significant advantage due to its ability to perform local mesh refinement, a feature absents in LBM. The candidate also mentioned that local refinement in LBM is possible but wasn't included in comparison.

- Please explain how local refinement of the computational network works in LBM and why its use is not as common as in FVM
- How would the implementation and optimization of local mesh refinement in LBM affect the computational efficiency of the LBM model for PHFHEs, and could it significantly reduce the differences in computational times compared to OpenFOAM, especially for domains with complex geometric details (like gaps between fibers)?
- How would local LBM refinement integrate with the "binary mask" for geometry definition that you cited as an LBM advantage?

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4. Detailed Analysis and Remediation of Issues in Inline Arrangements.

In thesis is the significant discrepancy between experimental and numerical results for inline arrangements, attributed to differences between ideal and actual structures.

- What specific methods would you propose for more detailed quantification and characterization of manufacturing imperfections and thermal expansion of fibers in inline arrangements? Could these imperfections be modeled in OpenFOAM to better bridge the gap between simulations and experiments?

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5. Practical Implications and Limitations of the Pareto Front for Industrial Partners.

The candidate effectively used the Pareto front concept to explore the design space and identify suitable trade-offs between heat transfer and pressure drop.

- How exactly does the industrial partner can interpret and utilize the Pareto front in practice when making design decisions, especially when other factors such as cost,

weight, or manufacturing complexity, which are not directly part of the Pareto front's objective functions, need to be considered?

- In which cases would you recommend transitioning from the Pareto front to a more traditional optimization with a defined cost function (multi-objective optimization), and how could such a cost function be robustly formulated for PHFHEs?

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6. The potential application of surrogate models.

In the conclusion of the thesis, the candidate suggests the possibility of using surrogate models to replace physically oriented models.

- How close are we now to replacing CFD modelling with surrogate models? Can these models be trained using experimental data alone, or will a physical model always be necessary for training?

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7. Laminar versus turbulent flow.

The candidate states that one reason for using PHFHE is the high heat transfer coefficient inside the fibers due to laminar flow. In classical tube flow theory, however, heat transfer is higher in turbulent flow.

- Why does the flow in the PHFHE have a higher transfer coefficient inside the fibers due to the laminar flow?