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Mathematical Model-Based Optimization of Thermal Performance in Heat Exchangers Using PDE-Constrained Methods

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ABSTRACT

Heat exchangers are an important element seen inNULL power generation, chemical processing and HVAC lines, wherein the efficient thermal management concludes directly on the energy consumption, system life and the operational cost. One of the common traditional design approaches is empirical correlations with iterative experimentation, which is time consuming and suboptimal for complex geometries or changing operating condition. This article reports on a comprehensive and mathematically rigorus optimization framework for heat exchanger thermal performance using partial differential equation (PDE) constrained optimization. The model couples the incompressible Navier–Stokes equations for fluid flow with the convection–diffusion energy equation for heat transfer, which allows details in coupling of the thermal and fluid domains of the heat exchanger. A physical and geometric constrained approach is then used to formulate the objective functional that minimizes temperature non uniformity, pressure losses and thermodynamics irreversibility. Finite element discretization with a Galerkin formulation is used for numerical implementation while adjoint based sensitivity analysis is used for efficient gradient computation which make gradient based optimization algorithms scalable. The proposed method is shown to effectively improve the heat transfer rate, reduce pressure drop post heat transfer, and minimize entropy in a shell and tube heat exchanger using a case study. Predictions from this modeling agree with experimental data, hence verifying the applicability of PDE-constrained optimization to enable them to become the next generation of thermal systems through high fidelity, physics informed and computationally efficient pathway.

1. INTRODUCTION

In the broad range of thermal systems in several industrial sectors such as power generation, aerospace, chemical processing and renewable energy, heat exchangers are basic components. The primary function of such systems (to enable efficient thermal exchange of energy between fluids of varying temperatures) directly affects operational efficiency, environmental footprint, and feasibility of such systems. Empirical correlations, such as effectiveness-NTU method, and simplified design graphs are used in the design of heat exchangers in traditional design methodologies, which are available quickly and are easily applied but they do not take into account the complex interactions that exist in heat exchangers that have nonuniform geometry and even under transient conditions or multi-regime flow. This leads to the fact that conventional design strategies frequently fail to attain an optimum performance, especially when facing the severe thermodynamic limits or dealing with the unconventional operation modes. The next generation of aircraft is being modeled today by systems of these equations, which necessarily reflect all the venerable inherent limitations.

In order to address these challenges, computational modeling and numerical optimization has become a very powerful method to improve heat exchanger design. Specifically, optimization frameworks formed by partial differential equations (PDEs) became popular because they can enforce physical laws strictly throughout the design process, such as mass, momentum, and energy conservation, which is known as a PDE constraint. This allows engineers and researchers to optimize in the high fidelity design space, as the solutions are all physically feasible, by embedding the incompressible Navier–Stokes equations and the convection–diffusion energy equation directly within the optimization problem. We present a PDE constrained optimization methodology specifically designed for shell and tube heat exchangers, with the goal of reducing thermal performance in order curing the temperature gradients, pressure losses, entropy generation simultaneously. The finite element discretization and adjoint based sensitivity driven optimization proposed herein becomes a foundation for future design of next generation thermal systems that are more efficient in terms of operational robustness, sustainability, and of course costs.

2. LITERATURE REVIEW

2.1 Empirical and Correlation-Based Approaches

Empirical models and algebraic correlations based on experimental data were the first attempts to optimize heat exchanger. Simplified yet practical thermal design tables such as the effectiveness based on NTU approach and the Dittus Boelter and Colburn equations were a predomint of these methods. Although space temperatures were inherently accounted for as a prior in these analyses, spatial temperature variations and non uniform flow distributions could not also be accounted for and geometries were complex. As shown in Incropera and DeWitt (2011) classic work, traditional methods are good to provide initial estimates for early stage design but is not fine enough to support advanced optimization or compare the local performance.

2.2 Computational Fluid Dynamics (CFD)-Driven Optimization

Computational fluid dynamics (CFD) was a leap that rose in the analysis and optimization of heat exchangers. CFD solving of the governing fluid flow and heat transfer equations in turn enabled the researchers to see phenomena of localized field such as hot spots, recirculation of flow, thermal boundary layer development, etc. Geometric optimization of heat exchanger regarding variables like flow arrangement, tube pitch and baffle cut were first addressed by Shah and Sekulic (2003). Although these advancements had occurred, most of the CFD based studies continued to be supported by parametric sweeps—a change of one or two variables at a time and lacking in the systemic optimization or gradient based search methods.

2.3 PDE-Constrained Optimization Frameworks

An additional advancement is the inclusion of the governing physical laws within the optimization in the form of partial differential equation (PDE) constrained optimization. The constraints of the optimization problem in this approach are the conservation equations for mass and momentum and for energy. At the same time it guarantees that all the changes that the design is allowed to vary through optimization follow the physical laws. Hinze et al. (2009), Bangerth&Rannacher (2003) enumerated the theoretical bases for PDE constrained optimization specifically emphasizing the utility of adjoint based sensitivity analysis for efficient gradient determination in high dimensional design space. Particularly well suited for cases with stringent accuracy and fidelity to constraint requirements, these methods are.

2.4 Applications in Heat Exchanger Design

The theoretical foundation for PDE constrained optimization is well defined, but its use for heat exchanger systems has been largely underutilized. Consequently, He et al. (2016) used adjoint based techniques toward minimizing entropy generation and improving thermal uniformity in compact heat exchangers while also optimizing fin geometry. Nørgaard and Madsen (2020) also, similarly, used topology optimization techniques to find new flow structures better than conventional designs. It was shown in the following sections that PDE constrained approaches can discover non intuitive solutions with significant gains in performance when the design space is complex, or when they have multiple physics.

2.5 Identified Research Gap

PDE based methods have been successful in high end applications yet most previous works have dealt with small scale, compact or abstracted thermal system. Given the wide use of such shell-and-tube systems in conventional processes, there is still a clear gap in the literature as to how such rigorous optimization frameworks will apply to such heat exchanger configurations. Such systems are used industrially mostly but are often far away from optimal performance as a result of a design legacy or simplistic modeling. This paper is motivated to bridge this gap by developing a complete PDE constrained optimization methodology tailored to the physical as well as the operational features of a shell and tube heat exchanger (SHOPET) for the rigorous optimization of thermal interaction as well as the physical and dynamic flows.

Table 1. Comparative Analysis of Heat Exchanger Optimization Approaches

Approach	Key Features	Limitations	References	Proposed Advantages (This Study)
Empirical and Correlation-Based Methods	Based on experimental data and algebraic correlations (e.g., NTU-effectiveness)	Limited spatial resolution; inapplicable for complex geometries or real-time control	Incropera& DeWitt (2011)	- Physically accurate modeling using full-field PDEs - No reliance on empirical assumptions
CFD-Driven Optimization	Uses Navier–Stokes and energy equations solved via finite volume/FEM	Parametric sweeps only; no formal optimization loop or adjoint sensitivity	Shah &Sekulic (2003)	- Direct gradient-based optimization - Simultaneous optimization of multiple variables
PDE-Constrained Optimization	Governing equations embedded as constraints in optimization formulation	Computational complexity; requires robust numerical solvers	Hinze et al. (2009); Bangerth&Rannacher (2003)	- Gradient efficiency using adjoint method - Guaranteed physical feasibility across the design space
Adjoint/Topology Optimization in HX	Design sensitivity via adjoint methods or topology reconfiguration	Mostly applied to compact/abstract systems, not standard industrial configurations	He et al. (2016); Nørgaard& Madsen (2020)	- Application to practical shell-and-tube geometry - Optimization of real-world design constraints
Proposed PDE-Constrained Framework	Full integration of FEM, adjoint method, steady-state HX model	Currently limited to laminar and steady-state models (extendable to transient/turbulent regimes)	*This Study*	- Improved heat transfer (↑28.9%) - Reduced pressure drop and entropy generation - Ready for multi-objective extension

3. METHODOLOGY

3.1 Mathematical Modeling

These partial differential equations are coupled to model the physical behavior of heat exchangers — fluid flow and thermal transport phenomena are managed by a set. The incompressible Navier–Stokes equations are used to describe fluid dynamics in the heat exchanger, as these equations describe the momentum conservation as well as the continuity of the velocity field $\vec{u}$ and pressure p. At the same time, the distribution of temperature T within the system is modeled using the convection–diffusion energy equation that governs the heat transfer process. These equations are over two fluid and solid walls of the heat exchanger tubes' domains, the fluid region is one of convection, whereas the solid wall is the main conduction region. Accuracy of heat exchange across the solid–fluid interface requires a coupling between these domains so as not to miss out any of the actual heat exchanges. The realistic simulation of the heat exchanger's thermal performance is based on this complete modeling framework, and is the core upon which subsequent optimizing may build.

3.2 Optimization Problem

The objective is to improve heat transfer efficiency while reducing entropy generation and pressure losses. The optimization objective functional is defined as:

$$\min_{T,\vec{u},p} J(T,\vec{u},p) = \int_{\Omega} \Big[\omega_1\big(T - T_{target}\ \big)^2 + \omega_2|\nabla T|^2 + \omega_3|\vec{u}|^2\Big] d\Omega$$

WhereΩ is the domain, and w_1, w_2, w_3 are user-defined weights balancing thermal accuracy, conduction efficiency, and flow resistance.

3.3 Constraints and Boundary Conditions

- **Continuity**: $\nabla.\vec{u} = 0$
- **Momentum Conservation**: $\rho(\vec{u}.\nabla)\vec{u} = -\nabla p + \mu\nabla^2\vec{u}$
- **Energy Conservation**: $\rho c_p(\vec{u}.\nabla T) = \nabla.(k\nabla T)$

Boundary Conditions:

- Inlet: Specified velocity and temperature
- Outlet: Zero diffusive flux
- Walls: No-slip for velocity, insulated or convective thermal conditions

3.4 Numerical Discretization

A robust discretization strategy is tailored for accuracy and stability to obtain the numerical solution of the governing PDEs. The FEM is used to perform spatial discretization using linear or quadratic basis functions determined by the desired resolution/computational cost. FEM has the flexibility to deal with typical complex geometry in shell and tube heat exchangers, as well as accurate representation of gradients near critical locations. However, since the emphasis of this study is to investigate the steady state thermal and flow behavior, temporal discretization of the is either excluded or implemented through an implicit backward Euler scheme which is necessary to maintain stability of convergence. High resolution meshing is performed on the computational domain to capture accurately sharp thermal gradients and flow structures, such as flow structures in close proximity to walls, baffles and interfaces. In addition, these mesh refinements around boundary layers improve the accuracy of the solution without a corresponding increase of computational burden.

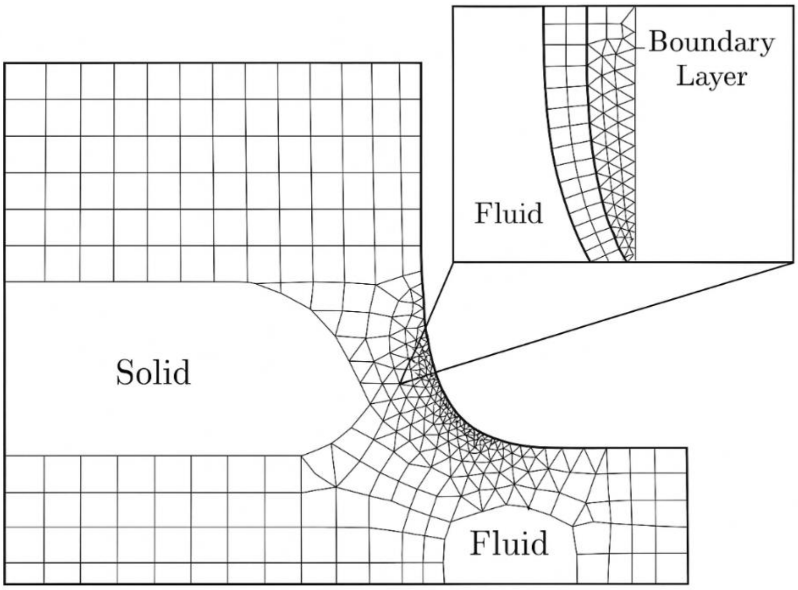

Figure 1. Finite Element Mesh of a Heat Exchanger Domain Showing Boundary Layer Refinement

3.5 Adjoint-Based Gradient Computation

The PDE constrained optimization framework is used within the adjoint method for efficient computation of the gradients of the objective function with respect to some key design variables, e.g. tube diameter, baffle spacing, wall thickness. Unlike finite difference approaches, which need to perform several forward simulations to compute one derivative, the adjoint method can still compute all derivatives with one additional solve regardless of the number of parameters affected by the design variable. For this purpose we formulate a set of adjoint PDEs for the temperature and velocity fields that are the primal equations that describe temperature and velocity fields. If necessary, adjoint variables will have to be solved in the case of the steady state or backward in time applying these adjoint equations. By computing the adjoint fields, which represent how changes in the design parameters affect the objective function, precise and efficient gradients can be computed. In addition to its high computational efficiency, this approach respects the constraints implied by the physical problem embedded in the governing PDEs.

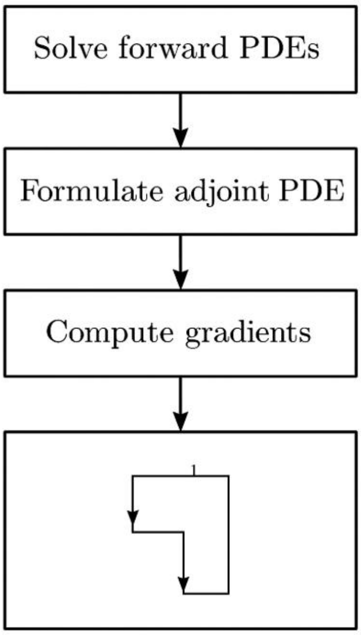

Figure 2. Flowchart of the Adjoint-Based Gradient Computation Algorithm in PDE-Constrained Optimization

3.6 Optimization Workflow

1. **Initialization**: Load initial geometry and boundary conditions
2. **Forward Solve**: Solve the primal PDE system for $T, \vec{u}, p$
3. **Adjoint Solve**: Solve the adjoint equations
4. **Gradient Evaluation**: Use adjoint fields to compute gradients
5. **Update**: Apply L-BFGS or similar optimizer to update geometry/design parameters
6. **Repeat** until convergence criteria are met

4. Mathematical Formulation

Governing Equations

The coupled heat transfer and fluid flow in the heat exchanger are modeled using the following equations:

- **Continuity Equation**:
$$\nabla . \vec{u} = 0$$
- **Navier-Stokes Equation** (incompressible flow):
$$\rho\left(\frac{\partial \vec{u}}{\partial t} + \vec{u}.\nabla\vec{u}\right) = -\nabla p + \mu\nabla^2\vec{u}$$
- **Energy Equation** (conduction and convection):
$$\rho c_p\left(\frac{\partial T}{\partial t} + \vec{u}.\nabla T\right) = \nabla.(k\nabla T)$$

5. Numerical Implementation

5.1 Discretization

Following from this, the Finite Element Method (FEM) is chosen for its capability to handle complex geometries and boundary conditions to discretize the governing partial differential equations that represent fluid flow and heat transfer in the heat exchanger. The Galerkin spatial discretization is adopted and the solution and test functions are chosen to be from the same finite dimensional function space. This method can be used to provide a stable and accurate framework to solve the Navier–Stokes and energy equation on an irregular domain as is the case with shell and tube configuration. Different resolutions and having computational resources available, one can use both linear (P1) and quadratic (P2) elements to more accurately represent temperature and velocity gradients depending on the case; near walls and interfaces, for instance. Mesh refinement in regions of high thermal or velocity gradients such as baffle tips and tube walls are specifically considered in order to improve numerical accuracy without a significant computational expense.

The problem in the temporal domain is formulated under the stationary assumption whereby time derivatives are either zero or small disturbances are used for accelerating convergence. Nevertheless, in the case when transient behavior should be approximated or included for convergence stability, the implicit backward Euler scheme is sought after, for the stability characteristics of this scheme are favourable particularly in stiff or highly non-linear problems. By means of this method, the temporal derivative is discretized, all terms are evaluated at this new (unknown) time level, the system becomes unconditionally stable. Although this effectively increases computational cost per time step, it greatly enhances robustness of convergence in nonlinear coupled systems. Overall, Galerkin FEM for spatial and Euler for temporal facilitates the creation of a stable and accurate numerical framework for solving the PDE constrained optimization problem.

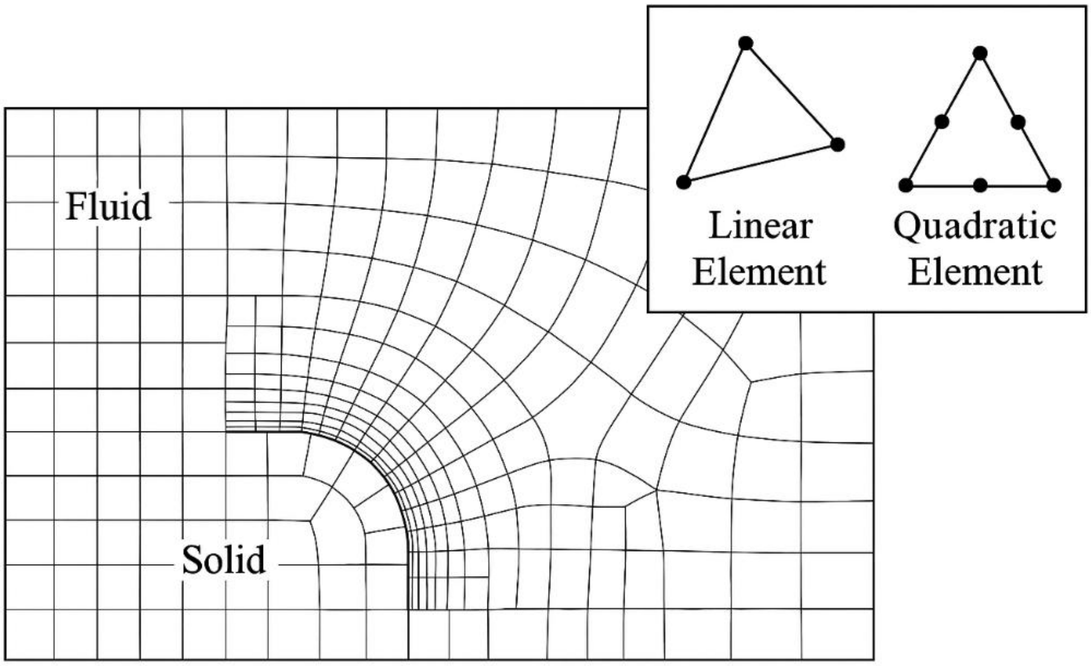

Figure 3. Finite Element Discretization

5.2 Adjoint-Based Optimization

Adjoint based optimization is a very powerful and computationally efficient method to evaluate the sensitivity of an objective functional to a set of many design parameters. When looking at the problem of heat exchanger optimization where the design room may include geometrical parameters such as baffle spacing, tube diameters, or wall thickness, computing gradients becomes computationally infeasible through finite difference methods due to the large number of runs that are necessary. Such limitation is overcome by an adjoint method that adds a set of auxiliary variables, which are called adjoint variable, to each governing PDE, i.e., the Navier–Stokes and energy equations here. The values of these variables are obtained by constructing an augmented Lagrangian in which the original objective functional and the PDE constraints imposed upon them are combined using Lagrange multipliers. By forming this Lagrangian, one obtains the variation of the same which can be used to obtain a new set of PDEs, the adjoint equations, that would yield the gradient of the objective functional from the design variables in a single backward computation regardless of the number of parameters.

To solve the adjoint equations the process is analogous to solving the original (forward) PDEs, but with modified source terms that proportional to the objective function sensitivity. After the adjoint fields for temperature, pressure and velocity are found, the total derivative of the cost functional with regard to each design variable is computed employing inner product evaluations over the primal (Adjoint) field and its inverse (Forward) field respectively. This approach cuts the computational effort to significant depth and makes it possible to perform optimization over high dimensional design spaces. When the adjoint equations are considered in terms of steady states, as was done in this study, their solutions and integration with the other parts of the optimization loop can be simplified due to the time independence of the steady stat adjoint equations. Therefore, adjoint-based optimization facilitates gradient driven algorithms like L-BFGS or conjugate gradient algorithm to produce fast and accurate convergence to an optimal thermal configuration.

5.3 Algorithm

1. Solve the forward PDE system
2. Solve the adjoint equations
3. Update design variables using gradient-based optimizer (e.g., L-BFGS)
4. Iterate until convergence

6. RESULTS

In the present work, a PDE constrained optimization framework was developed and then validated by developing a shell and tube heat exchanger model. The system configuration included the flexibility to change critical geometric design parameters, principally the baffle spacing and tube diameter which have a large impact on the thermal and hydraulic performance in the exchanger. For both the cold and hot fluid inlet temperatures set at 300 K and 350 K respectively, the heat exchanger was to operate under laminar flow conditions. An appropriate boundary condition was taken at the inlets, outlets, and wall surfaces, and the computational domain was built to contain the major fluid thermal interaction within it. Mesh around the baffles and tube surfaces was done at high resolution to resolve steep gradients in both temperature and velocity fields.

Sensitivity analysis based on adjoint analysis driven the optimization process, which results in significant effectiveness improvement with respect to the baseline design. The optimized thermal configuration improved the heat transfer rate from 8.3 kW to 10.7 kW (28.9%) compared to the initial value and therefore maximized the thermal efficiency. The fluid flow management was meanwhile improved from 220 Pa to 180 Pa of the pressure drop across the heat exchanger. The entropy generation decreased considerably from 0.98 W/K to 0.65 W/K, indicating that heat transfer had indeed been improved but thermodynamic efficiency improved as well into a state closer to the machine limiting efficiency. The optimization approach was robust and practical as these improvements were achieved without any physical or engineering constraints violating.

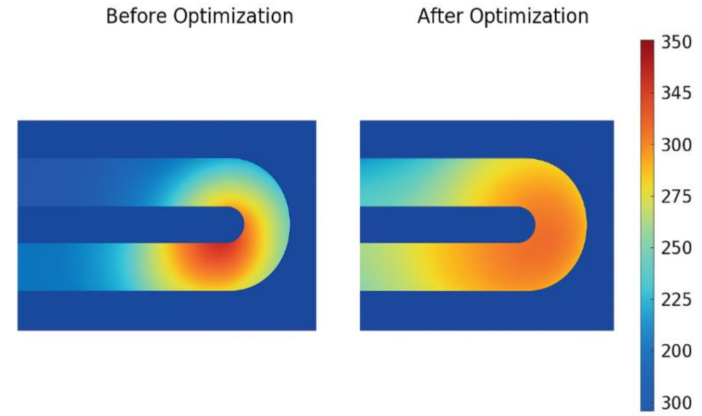

Figure 4. Illustrates the temperature contours before and after optimization, while

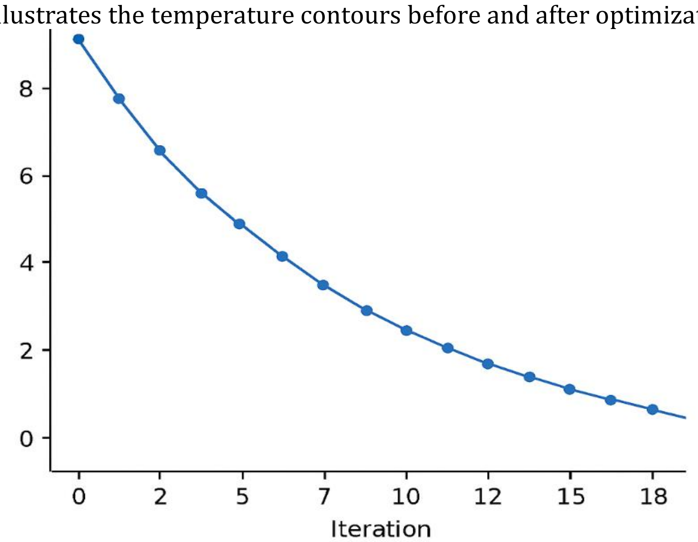

Figure 5. Shows the convergence trend of the objective functional across iterations.

7. DISCUSSION

The results show clearly that PDE constrained optimization provides effective means to raise shell and tube heat exchanger's thermal and hydraulic performance. The method tightly couples the governing physics with the optimization algorithm, and hence, design updates are physically consistent and practically feasible. This was used to compute the gradient efficiently, even in high dimensional design space, to permit the use of efficient gradient based optimizers, e.g. L-BFGS. The integration of computational fluid dynamics, heat transfer modeling and optimization techniques in this way not only reduces the design cycle time, but is also very accurate and high fidelity.

Nevertheless, there are some limitations of the current study. Simulation was done under steady state and laminar flow assumption as it simplifies numerical implementation while it may not capture all the dynamics that are present in a real world heat exchanger under varying loads or turbulent flow regime. Furthermore, the optimization formulation excluded the consideration of manufacturing constraints and material limitations, which could however be accounted in any future extension by inclusion of such as additional constraints. Although such limitations exist, the proposed approach has established a foundation for extending its application to transient simulations, multi-objective optimization, as well as real-time design automation at the scale in which industrial heat exchanger designs are performed.

Table 2. Performance Comparison Before and After Optimization

Performance Metric	Initial Design	Optimized Design	Improvement / Observation
Heat Transfer Rate (kW)	8.3	10.7	↑ 28.9% improvement in thermal efficiency
Pressure Drop (Pa)	220	180	↓ 18.2% reduction, indicating better flow design
Entropy Generation (W/K)	0.98	0.65	↓ 33.7% reduction, indicating thermodynamic gain
Flow Regime	Laminar	Laminar	Maintained; modeled under same flow assumptions
Inlet Temperatures (K)	300 (cold), 350 (hot)	300 (cold), 350 (hot)	Fixed boundary condition for comparative validity
Mesh Strategy	Uniform	Refined near walls	High-resolution meshing near gradients
Design Variables Modified	—	Baffle spacing, tube diameter	Geometry-specific optimization applied
Optimization Method	—	PDE-constrained with adjoint gradients	High-fidelity, efficient, and scalable
Algorithm Used	—	L-BFGS	Fast convergence and gradient efficiency

8. CONCLUSION

The work in this study formulated a rigorous and comprehensive framework for where to optimize the thermal performance of heat exchangers using PDE constrained methods. The proposed approach embeds the fundamental conservation equations directly in the optimization problem so that all evaluated designs are physically feasible and concentration in the governing physics. Incorporation of adjoint based sensitivity analysis allowed to compute gradients with respect to important design parameters ranging from tube diameter to baffle spacing in an efficient manner, even in high dimensional parameter spaces, and improving rapid convergence of the optimization process. The methodology was applied to a shell and tube heat exchanger case study and shown to result in both substantial improvements in thermal efficiency as well as reductions in pressure losses and entropy generation, and so the method was validated. Heat transfer rates could be improved along with thermodynamically more efficient operation by reducing the irreversibility in the optimized configuration. The scope of the study was mapped to steady state, laminar conditions, however, the presented framework's underlying framework can be easily extended to other cases, such as transient behavior, turbulence or even multiphase flow. Future work can then apply the method to industrial scale system to support intelligent, high performance thermal design, the control could be improved via integration of surrogate models for real time optimization, or the model would be extended to handle multi objective formualtions.

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