

Electronic Supplementary Materials

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Performance analysis and optimization of staggered fin heat exchangers under varying altitudes using machine learning

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Section S1: Simulation Setup

Under laminar flow conditions, the governing equations consist of the following:

(1) The continuity equation

$$\frac{\partial u_i}{\partial X_i} = 0 \quad (S1)$$

(2) The energy equation

$$\rho C_p \frac{\partial (u_i T)}{\partial X_i} = \frac{\partial}{\partial X_i} \left(\lambda \frac{\partial T}{\partial X_i} \right) \quad (S2)$$

(3) The momentum equation

$$\rho \frac{\partial}{\partial X_i} (u_i u_j) = \frac{\partial}{\partial X_i} \left(\mu \frac{\partial u_j}{\partial X_i} \right) - \frac{\partial P}{\partial X_i} \quad (S3)$$

In turbulent flow, the energy equation and momentum are:

$$\rho C_p \frac{\partial (u_i T)}{\partial X_i} = \frac{\partial}{\partial X_i} \left((\lambda + \lambda_t) \frac{\partial T}{\partial X_i} \right) \quad (S4)$$

$$\rho \frac{\partial}{\partial X_i} (u_i u_j) = \frac{\partial}{\partial X_i} \left((\mu + \mu_t) \frac{\partial u_j}{\partial X_i} \right) - \frac{\partial P}{\partial X_i} \quad (S5)$$

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \quad (S6)$$

The turbulence equation used in this study is the RNG k-ε model [Guo et al., 2025]:

$$\rho \frac{\partial}{\partial X_i} (k u_i) = \frac{\partial}{\partial X_i} \left(\alpha_k \mu_{eff} \frac{\partial k}{\partial X_i} \right) + G_k - \rho \varepsilon \quad (S7)$$

$$\rho \frac{\partial}{\partial X_i} (\epsilon u_i) = \frac{\partial}{\partial X_j} \left(\alpha_\epsilon \mu_{\text{eff}} \frac{\partial \epsilon}{\partial X_j} \right) + C_{1\epsilon} \frac{\epsilon}{k} G_k - C_{2\epsilon} \rho \frac{\epsilon^2}{k} - R_\epsilon \quad (\text{S8})$$

The quantities α_k and α_ϵ are the inverse effective Prandtl numbers, respectively for k and ϵ , and $C_{1\epsilon}=1.42$, $C_{2\epsilon}=1.68$, G_k is the turbulent kinetic energy due to the mean velocity gradient. The expression is as follows:

$$G_k = \mu_t \left(\frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i} \right) \frac{\partial u_i}{\partial X_j} \quad (\text{S9})$$

The RNG k- ϵ model is selected due to its superior capability in handling flow separation and streamline curvature, which are dominant features in staggered fin channels. Crucially, the RNG model features an analytically derived differential formula for effective viscosity, enabling better handling of near-wall and low-Reynolds-number effects compared to standard two-equation models. This makes it particularly suitable for the altitude-dependent flow conditions (spanning laminar to transitional regimes) encountered in this study. Similar numerical approaches utilizing the RNG k- ϵ model have been successfully validated in recent studies on complex fin geometries, such as the work by Chen et al. (2021), for predicting flow and heat transfer characteristics.

In the above equation, the effective viscosity $\mu_{\text{eff}} = \mu + \mu_t$. The main difference between the RNG model and the standard one is that the RNG model has an additional term, R_ϵ :

$$R_\epsilon = \frac{C_\mu \rho \eta^3 (1 - \eta/\eta_0) \epsilon^3}{1 + \beta \eta^3} \frac{\epsilon^3}{k} \quad (\text{S10})$$

Here $\eta_0=4.38$, $\beta=0.0121$, $C_\mu=0.0845$, $\eta=S_\epsilon^k$, the modulus of the mean rate-of-strain tensor S is expressed as:

$$S = \left(\frac{1}{2} \left(\frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i} \right) \left(\frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i} \right) \right)^{1/2} \quad (\text{S11})$$

Table S1. Environmental pressure and density at different altitudes

Altitude (m)	Air pressure (kPa)	Density (kg/m ³)	Inlet temperature (K)	Viscosity (Pa s)
0	101.33	1.2257	288.15	1.89E-05
1000	89.87	1.1122	288.15	1.89E-05
2000	78.418	1.0070	288.15	1.89E-05
3000	68.653	0.9096	288.15	1.89E-05
4000	59.897	0.8196	288.15	1.89E-05
5000	52.068	0.7366	288.15	1.89E-05

Section S2: Mesh Generation and Model Validation

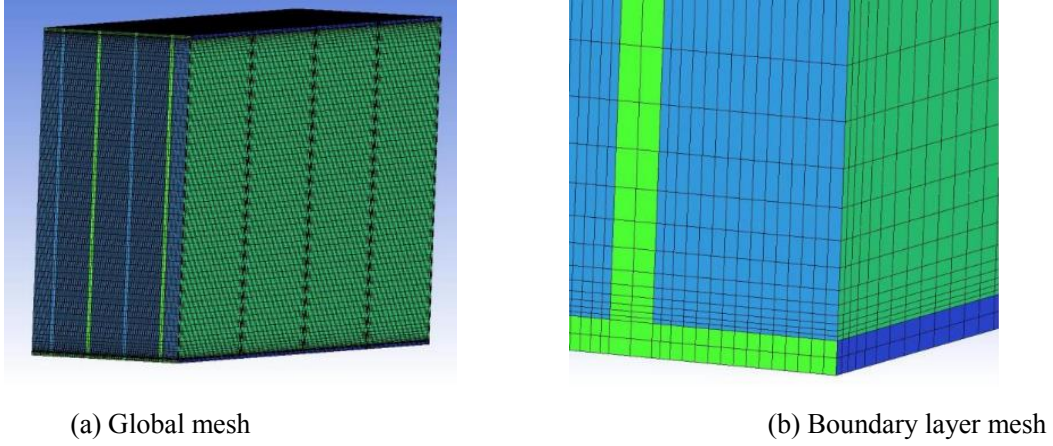


Fig. S1. Mesh generation schematic using ICEM

Section S3: Machine Learning Modeling

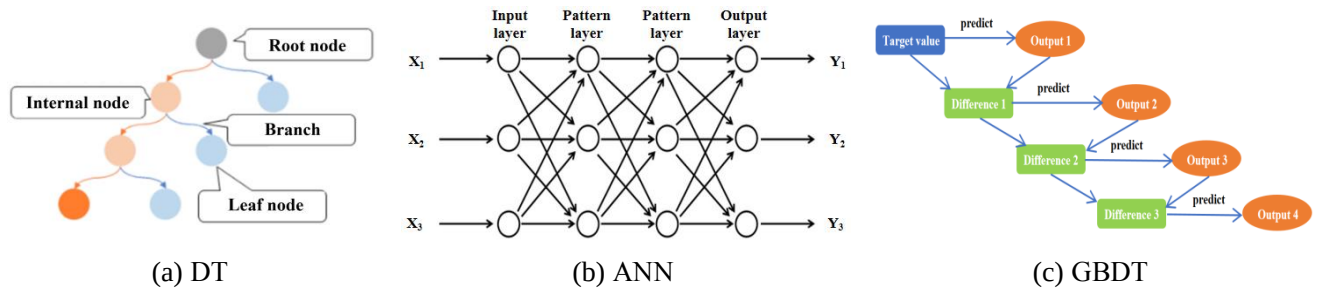


Fig. S2. Principles of the selected modeling approaches (DT, ANN, and GBDT)

The DT model, characterized by its hierarchical structure and rapid training efficiency, provides an intuitive visualization of nonlinear relationships between geometric parameters and performance metrics. Its embedded feature importance ranking offers physically interpretable insights into parameter contributions [Zhao et al., 2025]. The ANN demonstrates universal approximation capabilities through flexible network architecture design. By adaptively configuring hidden layer nodes, ANN effectively captures complex nonlinear mappings between high-dimensional geometric features and multiphysics responses, making it particularly suitable for engineering applications requiring millisecond-level real-time predictions [Foukalas, 2025]. The GBDT, as an ensemble of decision trees, iteratively optimizes predictions by minimizing residuals through gradient descent. This approach significantly reduces bias compared to standalone DT models, while its ability to identify critical feature interactions enhances robustness, particularly in small sample scenarios [Xu et al., 2025]. Collectively, these three methodologies exhibit distinct strengths: DT emphasizes interpretability, ANN excels in high-dimensional nonlinear representation, and GBDT reinforces robustness and generalization when data are scarce.

Section S4: Comparison Results of Machine Learning Models

Table S2. Key hyperparameter settings for the machine learning models

Model	Parameter	Value
DT	Max depth	24
	Min samples split	3
	Min samples leaf	2
GBDT	Number of estimators	336
	Learning rate	0.1638
	Max depth	2
	Min samples split	12
	Min samples leaf	2
ANN	Number of hidden layers	2
	Neurons per layer	192, 64
	Activation function	Tanh
	Learning rate	0.0025
	Batch size	64
	Epochs	147

Table S3. Performance comparison of different machine learning models

Model	Dataset	Pressure Drop (R ²)	Pressure Drop (RMSE)	Heat Transfer Coefficient (R ²)	Heat Transfer Coefficient (RMSE)
DT	Training	0.979	5.271	0.991	3.715
	Validation	0.839	9.483	0.980	5.059
	Testing	0.949	8.232	0.976	5.968
ANN	Training	0.993	3.106	0.996	2.578
	Validation	0.974	3.789	0.981	5.103
	Testing	0.983	4.744	0.985	4.718
GBDT	Training	0.996	2.416	0.998	1.524
	Validation	0.990	2.335	0.999	1.300
	Testing	0.998	1.673	0.999	1.164

As illustrated by the comprehensive regression analysis in Fig. S3, the results demonstrate that GBDT achieves the best overall performance. In the training set, it attains $R^2 = 0.996$ and $RMSE = 2.416$; the validation set yields $R^2 = 0.990$ and $RMSE = 2.335$; and the test set shows $R^2 = 0.998$ and $RMSE = 1.67$. The scatter points nearly overlap with the ideal fit line, indicating that GBDT not only captures training data patterns effectively but also generalizes exceptionally well to unseen data, exhibiting strong robustness. ANN ranks second, with the training set producing $R^2 = 0.993$ and $RMSE = 3.106$; the validation set delivering $R^2 = 0.974$ and $RMSE = 3.789$; and the test set showing $R^2 = 0.983$ and $RMSE = 4.744$. DT exhibits relatively weaker performance, with the training set achieving $R^2 = 0.979$ and $RMSE = 5.271$; the validation set showing a significant decline with $R^2 = 0.839$ and $RMSE = 9.483$; and the test set delivering $R^2 = 0.949$ and $RMSE = 8.232$. The substantial drop in R^2 and increase in RMSE on the validation set suggest a high risk of overfitting, limiting its generalization capability. Based on these results, GBDT is selected as the optimal surrogate model for pressure-drop prediction. Its exceptional predictive accuracy, combined with outstanding generalization capability, makes it the most suitable choice among the evaluated models.

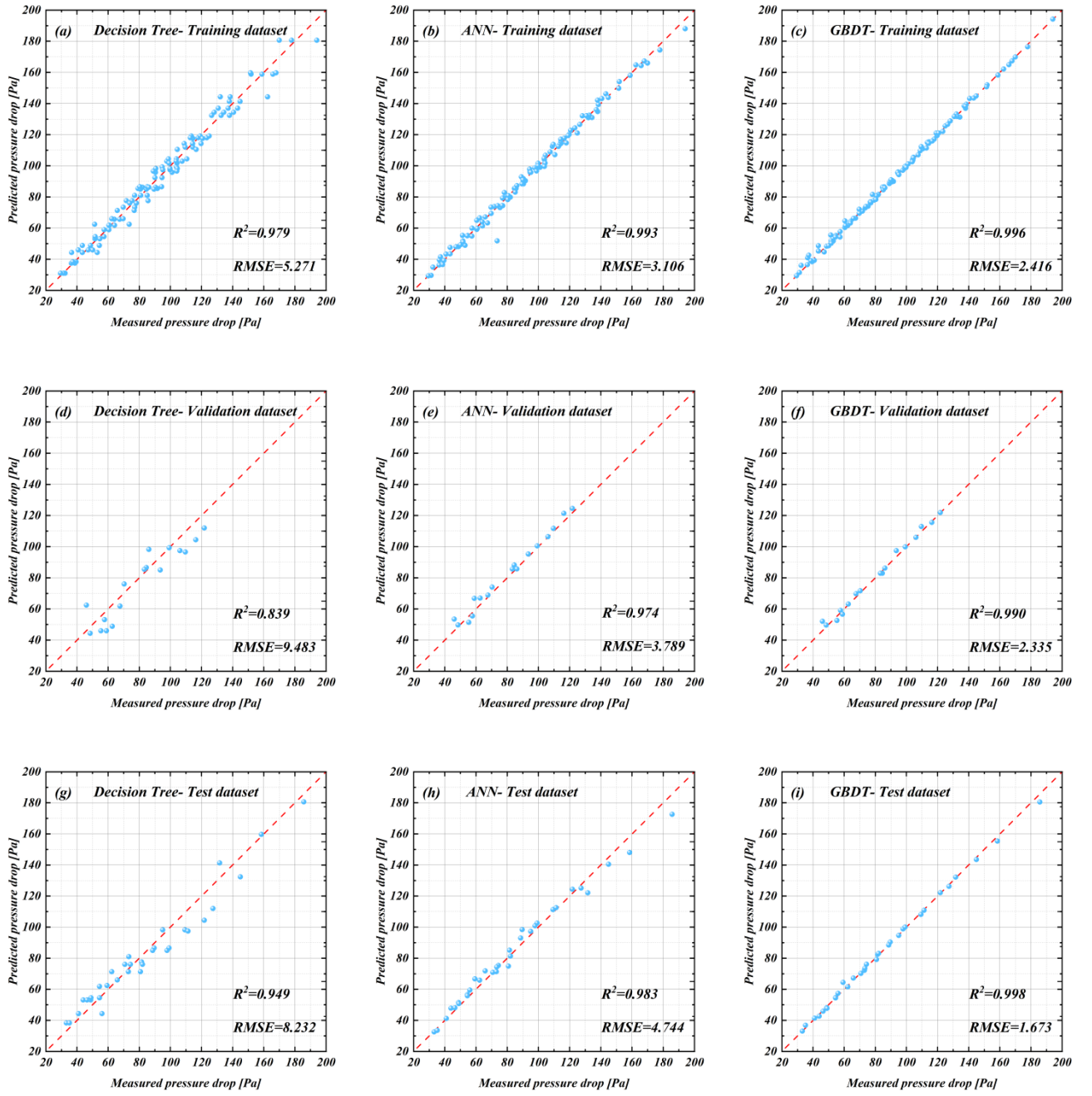


Fig. S3. Comparison of predicted pressure drop values from different machine learning models with simulation results

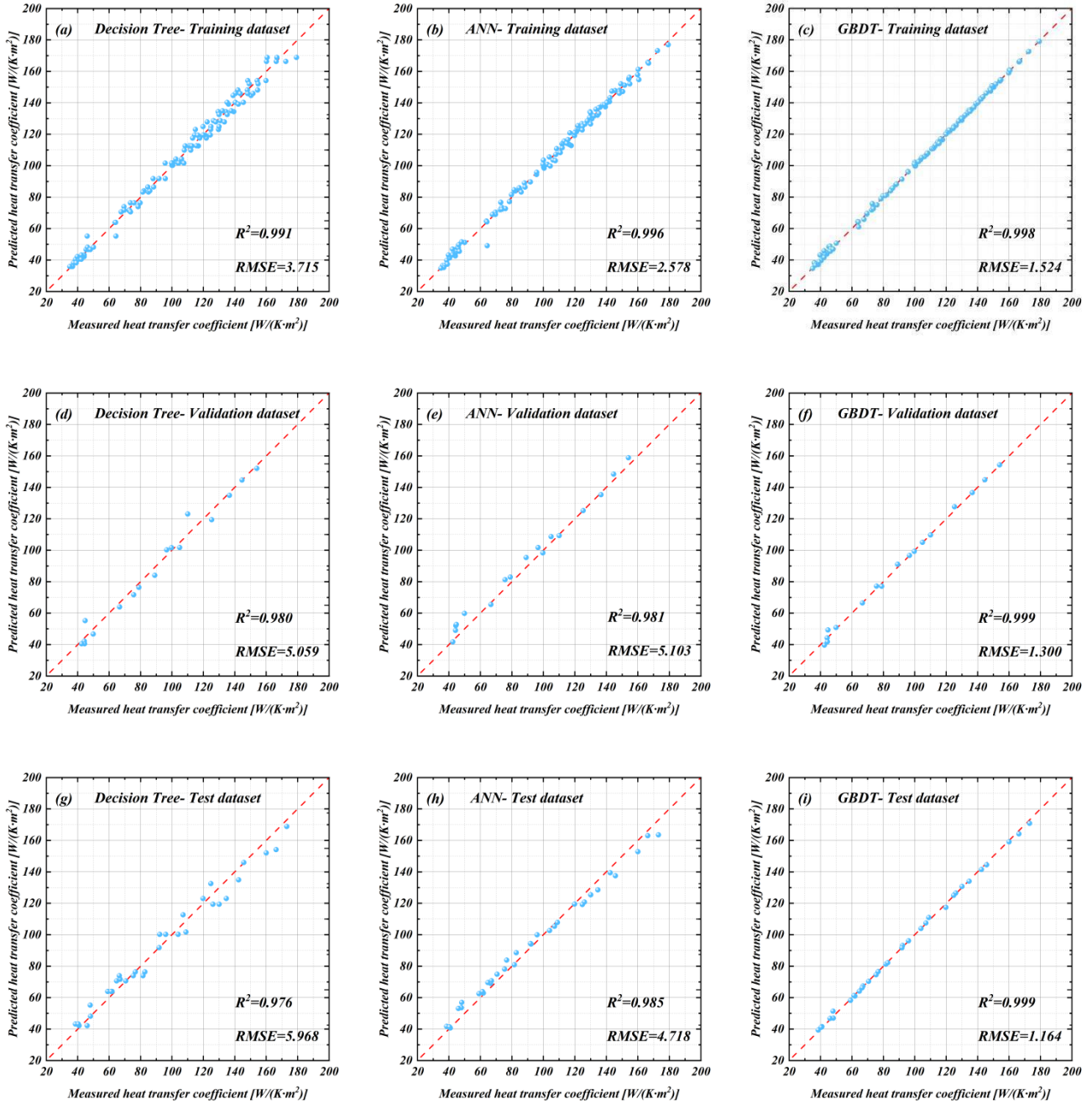


Fig. S4. Comparison of predicted heat transfer coefficient values from different machine learning models with simulation results

As can be seen from Fig. S4, there are obvious differences in the prediction performance of the three models (DT, ANN, GBDT) on the training set, validation set, and test set when predicting heat transfer coefficients: DT shows extremely high fitting accuracy on the training set ($R^2 = 0.991$, $RMSE = 3.715$), but its precision significantly decreases on the validation set ($R^2 = 0.980$, $RMSE = 5.059$) and test set ($R^2 = 0.976$, $RMSE = 5.968$), reflecting a serious overfitting problem; ANN has an R^2 of 0.996 and an RMSE of 2.578 on the training set, with R^2 values of 0.981 and 0.985, and RMSE values of 5.103 and 4.718 on the validation set and test set respectively—its generalization ability is better than that of DT but still has some fluctuation; GBDT, by contrast, maintains excellent and stable performance on all three datasets, achieving $R^2 = 0.998$, $RMSE = 1.524$ on the training set, R^2

= 0.998, RMSE = 1.823 on the validation set, and $R^2 = 0.999$, RMSE = 1.164 on the test set. This not only confirms GBDT's high fitting degree but also its extremely small errors in validation and testing, fully demonstrating stronger generalization ability and robustness. Combined with its previously proven superior performance in predicting pressure drop, GBDT demonstrates consistently outstanding performance in predicting both key thermal-fluid indicators (pressure drop and heat transfer coefficient), with near-perfect R^2 values (approaching 1.0), minimal RMSE errors, and robust resistance to overfitting across all evaluation datasets. These characteristics confirm its reliability as a predictive model, so GBDT is selected as the surrogate model for subsequent multi-objective optimization tasks—its computational efficiency paired with high prediction precision makes it an ideal choice for efficiently guiding the optimization process while maintaining solution accuracy. For a clear quantitative comparison, the detailed performance metrics (R^2 and RMSE) of the three models across all datasets are summarized in Table S3. Furthermore, the predictive uncertainty of the machine learning surrogate models was rigorously quantified through these metrics across the training, validation, and testing datasets. As shown in Table S3, the GBDT model consistently maintained R^2 values near 1.0 and low RMSE values (e.g., 1.164 for the heat transfer coefficient in the test set), demonstrating that the impact of data-driven uncertainty on the subsequent multi-objective optimization is negligible. This high level of predictive stability ensures that the final optimized results are robust and reliable for practical applications.

Section S5: Multi-objective Optimization of Pressure Drop and Heat Transfer Coefficient

Table S4. Quantitative comparison of pressure drop and heat transfer coefficient before and after optimization

Altitude (m)	Pressure Drop Baseline	Pressure Drop Point 1 Change	Pressure Drop Point 2 Change	Heat Transfer Coefficient Baseline	Heat Transfer Coefficient Point 1 Change	Heat Transfer Coefficient Point 2 Change
0	82.75	-0.6%	-16.8%	88.40	+23.3%	+0.3%
1000	78.76	-0.5%	-16.7%	85.08	+23.1%	+0.2%
2000	74.89	-0.3%	-16.6%	81.77	+23.0%	-0.0%
3000	71.14	-0.0%	-16.8%	78.50	+23.0%	-0.2%
4000	67.53	0.0%	-16.7%	75.28	+22.9%	-0.3%
5000	64.04	-0.1%	-16.8%	72.10	+22.7%	-0.5%

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