CFD and Machine Learning based Simulation of Flow and Heat Transfer Characteristics of Micro Lattice Structures

Disha Deb¹, Harish Rajan¹, Rajiv Kundu¹ and R Mohan¹*

¹School of Mechanical Engineering
Vellore Institute of Technology, Chennai
*Corresponding author
E-mail address: mohan.r@vit.ac.in

Abstract
In this paper, systematic CFD analysis using ANSYS Fluent was carried out to generate the dataset for developing the Machine Learning model, which predicts the average final temperature of water and the pressure drop from the set of input parameters considered for applications. There are six micro lattice structures, kagome, tetrahedral, pyramidal, hexagonal, windward bent and hexagonal-windward bent, modelled for this study using FUSION 360 by Autodesk. The study of heat transfer between liquid water and the micro lattice structures realized with the independent variables, initial fluid flow velocity, lattice temperature, and fluid temperature as well as lattice materials and its different structures. About 2146 output data of average final fluid temperature and the pressure drop were collected from the CFD simulations by varying input parameters. To predict the output parameter against the set of input parameters, Machine Learning model with regression based classification algorithm was adopted while training the ML model. The quality metric of the ML model was calculated using residual sum of squares method. The final average temperature of the fluid and pressure drop as predicted by the ML model is closer to simulated data.

Keywords: Micro lattice; Heat Transfer; Computational Fluid Dynamics; Dataset; Machine Learning

Nomenclature
\( \rho \) – density \((\text{kg/m}^3)\)
\( V \) – velocity vector
\( p \) – pressure \((\text{Pa})\)
\( \nabla \) - differential operator \((\text{Cartesian coordinates})\)
\( \mu \) – viscosity \((\text{N-s/m}^2)\)
\( T \) – temperature \((\text{K})\)
\( k \) – thermal conductivity \((\text{W/m-K})\)
\( c_p \) – \( \text{J/kg-K} \)
\( \Phi \) – dissipation function representing work done against viscous forces

1. Introduction
Cooling has always been an integral part of industries and machineries that generate heat on a regular basis. Central cooling system, HVACs in power plants, heavy industries such as distilleries, food processing, refinery etc., require heat exchangers for cooling fluid that in turn is used to keep optimum operating conditions for power producing units. Water is used in many large-scale industries where it absorbs the excess heat from the machineries and then sent to a heat exchanger for cooling the incoming hot fluid without mixing the hot and cold fluid. However, these conventional heat exchangers such as shell and tube, chevron plate heat exchangers incur high pressure drops without significant rise in temperature drop and hence pumping cycles are larger [1-2].

Advancements in manufacturing techniques, especially in additive manufacturing techniques, makes it possible to create uniform and periodic microstructures called micro lattices. Micro lattice is widely being researched due to its potential as a material to build the bodies of airplanes, automotive and other industries due to its very low density and an impressive compressional strength [3-8]. Apart from using micro lattices as building materials, it also has a
number of potentials in the industries for its heat transfer properties [9-11]. Engineering application like air conditioning systems, electric vehicles, aircraft industries require novel methods of heat transfer demands that an increase in the surface area for heat transfer does not cause a significant increase in the weight and space occupied and do not cause a high pressure drop. Although, the problem of using lightweight materials having high specific surface area with moderate pressure drop as heat exchangers was solved with the use of metal foams; Ghosh in his study concluded that with increasing porosity heat transfer decreases [12].

In most of the existing heat transfer devices, an increase in surface area for increased temperature drop is accompanied by a considerable increase in pressure drop. Every heat transfer device has a maximum limit for the pressure drop since an increased pressure drop requires increased pump work. Bai et al. in their study of metallic core structures concluded octet-truss (lattice core) as a significant improvement in heat transfer characteristics over metal foam [13]. Moreover, studies by Saha et al and Kim, et al. reinforced the idea of using micro lattices as a heat exchanging devices due to their excellent specific stiffness and strength and high heat transfer capabilities with minimal flow resistance and moderate pressure drop [10-11]. Hence, micro lattices were chosen by us as a suitable heat exchanging device for doing heat transfer simulations.

With the advent of Artificial Intelligence seeping into each and every aspect of technology, it is only a matter of time that Industry 4.0 will seep into heat transfer applications [14]. Therefore, in this paper, an attempt was made to create a dataset from the results of CFD analyses and apply the concept of Machine Learning (ML) into the data gathered. An ML model was trained based on the dataset and the model that provides a near-accurate prediction of dependent variables i.e., average final fluid temperature and pressure drop to the user is displayed through a Graphical User Interface screen. The GUI also has provision to select the various input parameters with input values. This helps the user in deciding the lattice structures that suits their requirement best for any kind of heat exchanging applications.

2. Methodology

In this paper, systematic CFD analysis using ANSYS Fluent for generation dataset and Machine Learning for prediction of desired output based on generated dataset for training and validation of model were adopted for heat transfer applications. The figure 1 represents the methodology implemented in this study.

2.1 Deciding lattice structures for CFD analyses

Lattice structures are available in a variety of different shapes having different anisotropic properties. Bai et al. conducted a heat transfer performance analysis of Kagome, Pyramidal, Tetrahedral, Windward-bent, staggered pin-fin, staggered slanted pin-fin lattice structures among other structures such as metallic foam and rectangular corrugated cellular structures [9]. Yang et al. similarly conducted comparative study between Kagome and tetrahedral truss-cored lattice sandwich panels to bring out the inner flow pattern, heat transfer properties and...
concluded that better heat transfer occurred kagome. However, the pressure drop was found to
be twice than Tetrahedral [15]. Hexagonal shaped metallic lattice and prismatic cellular
honeycombed structures were studied [16-18].

In this study, six micro lattice structures kagome, pyramidal, tetrahedral, hexagonal, windward-
bent, Hexagonal-Windward were chosen for studies and create dataset. These models were
modelled in Autodesk Fusion 360 [19]. Ansys FLUENT was used as a CFD tool to conduct fluid
flow through the lattice frame.

2.2 Modelling of Micro lattices in Fusion 360

The lattice models were designed using Autodesk Fusion 360. The 3D Geometry feature during the
Sketch mode makes modelling structures much easier. Figures 2(a), 3(a), 4(a), 5(a), 6(a), 7(a) show
the modeled unit lattice structures. The unit structures have been repeatedly placed on a straight line
to obtain the microlattice core structure as shown in figures 2(b), 3(b), 4(b), 5(b), 6(b), 7(b). The
lattices have been modelled to fit into a 3mm×1mm×2mm enclosure, 3mm being the length from the
leading edge upto the trailing edge, 2mm being the height and 1 mm being the width. The structures
modelled are as from figure 2-7. The surface areas of these models are shown in Table 1 to
depict the relative size of these structures compared to its surroundings.

Figure 2 : Kagome Lattice (a) Unit Cell (b) Assemble Lattice

Figure 3 : Tetrahedral Lattice (a) Unit Cell (b) Assembled Lattice

Figure 4 : Pyramidal Lattice: (a) Unit Cell (b) Assembled Lattice

Figure 5 : Hexagonal Lattice: (a) Unit Cell (b) Assembled Lattice
Figure 6: Windward Lattice: (a) Unit Cell (b) Assembled Lattice

Figure 7: Hexagonal Windward-bent: (a) Unit Cell (b) Assembled Lattice

Table 1: Surface area of micro lattice

| Structure          | Surface Area (m²) |
|--------------------|-------------------|
| Kagome             | 2.868563e-05      |
| Pyramidal          | 2.491382e-05      |
| Tetrahedral        | 8.56743e-05       |
| Hexagonal          | 3.11926e-05       |
| Windward Bent      | 9.814e-05         |
| Hexagonal-Windward Bent | 9.237491e-05 |

The designed models were imported into ANSYS Workspace. A cuboidal enclosure was provided in Design Modeler. A cushion of 0.5mm was provided between the enclosure walls and the microlattice. The enclosure is made to provide an extra passage for the fluid to flow smoothly into the ambient space otherwise reverse flow of fluid can take place which could result in floating point exception. Hence the extension at the outlet ensures the upstream flow of fluid is not affected by any boundary condition during outflow.

2.3 Performing CFD analyses on the structures using ANSYS Fluent

The flow and heat transfer characteristics of the micro lattice structure is modeled as three-dimensional, steady, incompressible laminar flow. For the lateral surface of the enclosure, zero gradient boundary conditions and free slip velocity was assumed. The generated CAD model of the lattice structure is meshed in Ansys Workspace. Meshing is a very important factor in deciding the accuracy of the simulation results. Finer the meshes, more accurate are the results and coarser the meshes, faster are the results obtained. ANSYS feature of meshing imported models was opted. The built in smart default mesh settings automatically provide a resolution that can save time while giving dependable solutions. The numerical simulations were carried out in ANSYS Fluent and the results of the simulations were analyzed using ANSYS CFD-Post. The governing equations are discretized using Finite volume method and the diffusion terms in the momentum and energy equations are evaluated using second order schemes. The incompressible flow is modeled using a pressure based solver with double precession. The residuals for the continuity, momentum and energy equations are set to a small value of 10⁻⁶. The viscous dissipation and radiation effects in the flow are neglected.

2.3.1 Governing equations
The governing equations for the steady state 3-D laminar flow are given as follows:

\[ \nabla \cdot \mathbf{V} = 0 \]  \hspace{1cm} (1)

\[ \rho \left[ \frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V} \cdot \nabla) \mathbf{V} \right] = -\nabla p + \mu \nabla^2 \mathbf{V} + \rho f \]  \hspace{1cm} (2)

\[ \rho c_p \left[ \frac{\partial T}{\partial t} + (\mathbf{V} \cdot \nabla) T \right] = k \nabla^2 T + \phi \]  \hspace{1cm} (3)

Equations (1), (2) and (3) represent the differential form of conservation of mass, linear momentum and energy respectively for an incompressible fluid.

2.3.2 **Boundary conditions**

Inlet boundary conditions are velocity of fluid ranging from 0.01 – 0.05 m/s, gauge pressure of 200 Pa, fluid temperature ranging from 350-390 K, solid domain temperature ranging from 290-320 K and no reverse flow at outlet.

Maloney et al. in their experimental study of fabricating a cross-flow heat exchanger packed with Nickel micro-lattice structure concluded a laminar flow region inside the micro lattice structure due to decreasing inner diameter [20]. Based on their results and since the dimensions of our micro lattices were relatively much smaller than the surrounding flow domain, the flow was safely assumed as laminar. The energy model was selected to allow heat transfer between the lattice core and the fluid. For the analysis, the case assumed was that the lattice walls were initially isothermally heated. Liquid water was chosen as the fluid for the analysis since it is the most commonly used fluid in industries.

Water at an initial temperature higher than the initial temperature of the lattice is made to flow at a fixed velocity across the lattice structures. Heat transfer between the fluid and the lattice occurs by three methods – conduction between the walls and the fluid in contact with the walls, by convection within the fluid domain and by thermal radiation. The convective heat transfer coefficient is chosen as 10W/m²K and emissivity is chosen as 0.4. Based on Xiong et al. recommendations for metallic micro lattice structures, three variations were provided for lattice material (aluminium, copper, nickel) for each lattice [21]. The materials are already available in FLUENT materials database. Standard initialization was done with respect to the inlet. Different solvers coupled, SIMPLE, SIMPLEC were tested and coupled solver was chosen since it provided fastest convergence among others. After the completion of the analysis, the contours of the outlet were studied to find final average temperatures of the fluids. The pressure drop was calculated by Surface Integrals from the Reports.

2.4 **Collecting data from analyses and preparing dataset**

The results obtained from the numerical simulations were recorded into a dataset. The dataset contains independent and dependent parameters. The independent parameters consist of various initial working conditions like velocity, fluid temperature, lattice temperature, material of the micro lattice and the shape of the micro lattice used. These parameters are considered independent because they can be controlled independently in most of the applications. The final fluid temperature and the pressure drop are chosen as the dependent variables. In order to have ample data for both training and testing, analyses were performed with five variations of initial velocity, lattice temperature and fluid temperature and three variations of lattice material
(aluminium, copper, nickel). A portion of the dataset with the independent and dependent parameters is depicted in Table 2.

| Lattice structure | Material    | Inlet velocity (m/s) | Inlet gauge pressure (Pa) | Lattice initial temperature (K) | Fluid initial temperature (K) |
|-------------------|-------------|----------------------|---------------------------|--------------------------------|------------------------------|
| Kagome            | Copper      | 0.01                 | 200                       | 290                            | 350                          |
| Kagome            | Aluminium   | 0.01                 | 200                       | 290                            | 350                          |
| Kagome            | Nickel      | 0.01                 | 200                       | 290                            | 350                          |
| Pyramidal         | Copper      | 0.01                 | 200                       | 290                            | 350                          |
| Pyramidal         | Aluminium   | 0.01                 | 200                       | 290                            | 350                          |
| Pyramidal         | Nickel      | 0.01                 | 200                       | 290                            | 350                          |
| Tetrahedral       | Copper      | 0.01                 | 200                       | 290                            | 350                          |
| Tetrahedral       | Aluminium   | 0.01                 | 200                       | 290                            | 350                          |
| Tetrahedral       | Nickel      | 0.01                 | 200                       | 290                            | 350                          |
| Hexagonal         | Copper      | 0.01                 | 200                       | 290                            | 350                          |
| Hexagonal         | Aluminium   | 0.01                 | 200                       | 290                            | 350                          |
| Hexagonal         | Nickel      | 0.01                 | 200                       | 290                            | 350                          |
| Windward          | Copper      | 0.01                 | 200                       | 290                            | 350                          |
| Windward          | Aluminium   | 0.01                 | 200                       | 290                            | 350                          |
| Windward          | Nickel      | 0.01                 | 200                       | 290                            | 350                          |
| Hex-windward      | Copper      | 0.01                 | 200                       | 290                            | 350                          |
| Hex-windward      | Aluminium   | 0.01                 | 200                       | 290                            | 350                          |
| Hex-windward      | Nickel      | 0.01                 | 200                       | 290                            | 350                          |

2.5 Training ML model on the data

Machine Learning involves training a model to make predictions of any future data by making it learn first from the existing data. This field has grown immensely developing newer, faster and efficient algorithms to make a computer system smarter in the way it predicts data. Since the computer is being shown which label to treat as the predicted outcome, this form of learning is termed as Supervised Learning. In this study, supervised learning method (Linear Regression) is used to train the computer and to make predictions on the required data parameters [22]. In this study, supervised machine learning approach has been adopted with use of Jupyter, a web based application to predict the outcome from the set of training data. Sklearn, Pandas, NumPy and Tkinter packages are part of Machine learning model development. Multi output regression was used to get the desired results from the set of training data [23-25]. The data set was divided into training and testing in the 4:1 ratio.

2.5.1 Jupyter notebook - integer encoding

The initial dataset had many string data-type values such as, lattice material and lattice shape. In order for the prediction model to work, the dataset has to be converted into a NumPy matrix. And the limitation is NumPy can only take integer or float values hence the string values needed to be converted to an equivalent integer value. The raw data frame is shown in figure 8 and the
integer encoded data frame is provided in figure 9. A multi-output regression model was trained using the modified dataset.

![Integer encoded data frame](image)

**Figure 8**: Raw Dataset

![Integer encoded data frame](image)

**Figure 9**: Integer encoded data frame

### 3. Results and Discussion

#### 3.1 Formation of Data set

The test conditions for the copper micro lattices of Kagome, Pyramidal, Tetrahedral Windward-Bent, Hexagonal and Hexagonal-windward are (i) working fluid as water, (ii) lattice temperature 330°K, (iii) fluid temperature 390°K (iv) inlet velocity 0.05 m/s and (v) inlet gauge pressure 200 Pa. The figures 10-15 shows the temperature contours obtained after simulation of micro lattice assemblies with above test conditions. The extracted average temperature of Kagome, Pyramidal, Tetrahedral Windward-Bent, Hexagonal and Hexagonal-windward are 332.5°K, 368°K, 359.5°K, 385°K, 368.5°K and 369°K respectively and are tabulated as part of dataset. Similarly, data set were formed by varying input parameters such as velocity from 0.01 to 0.05 in steps on 0.01 m/s and lattice temperature 290°K to 330°K with steps 10°K and lattice material
of aluminium, nickel while keeping inlet pressure constant at 200 Pa. Also, the pressure drop was calculated in Fluent using area weighted average under Surface Integrals. Table 3 represents few sample data sets out of 2146 data collected from simulations.

Figure 10: Temperature contour – Kagome

Figure 11: Temperature contour for Pyramidal

Figure 12: Temperature Contour for Tetrahedral

Figure 13: Temperature Contour for windward bent
Figure 14: Temperature Contour for Hexagonal

Figure 15: Temperature Contour for Hexagonal-Windward

| Lattice structure | Material | Inlet velocity (m/s) | Inlet gauge pressure (Pa) | Initial temperature (K) | Fluid initial temperature (K) | Avg. final fluid temperature (K) | Pressure drop (Pa) |
|-------------------|----------|----------------------|----------------------------|----------------------------|-------------------------------|----------------------------------|-------------------|
| Kagome            | Copper   | 0.01                 | 200                        | 290                        | 350                           | 330.5                            | 0.0330772         |
| Kagome            | Aluminium| 0.01                 | 200                        | 290                        | 350                           | 330.5                            | 0.0330772         |
| Kagome            | Nickel   | 0.01                 | 200                        | 290                        | 350                           | 342.5                            | 0.0330772         |
| Pyramidal         | Copper   | 0.01                 | 200                        | 290                        | 350                           | 380                              | 335.0             | 0.0394501         |
| Pyramidal         | Aluminium| 0.01                 | 200                        | 290                        | 350                           | 350                              | 327.5             | 0.0394501         |
| Pyramidal         | Nickel   | 0.01                 | 200                        | 290                        | 350                           | 350                              | 337.5             | 0.0394501         |
| Tetrahedral       | Copper   | 0.01                 | 200                        | 290                        | 350                           | 350                              | 318.25            | 0.1367691         |
| Tetrahedral       | Aluminium| 0.01                 | 200                        | 290                        | 350                           | 350                              | 318.0             | 0.1277518         |
| Tetrahedral       | Nickel   | 0.01                 | 200                        | 290                        | 350                           | 350                              | 350               | 318.5             | 0.1277518         |
| Hexagonal         | Copper   | 0.01                 | 200                        | 290                        | 350                           | 350                              | 318.5             | 0.1277518         |
| Hexagonal         | Aluminium| 0.01                 | 200                        | 290                        | 350                           | 350                              | 318.5             | 0.1277518         |
| Hexagonal         | Nickel   | 0.01                 | 200                        | 290                        | 350                           | 350                              | 318.5             | 0.1277518         |
| Windward          | Copper   | 0.01                 | 200                        | 290                        | 350                           | 350                              | 318.5             | 0.1277518         |
| Windward          | Aluminium| 0.01                 | 200                        | 290                        | 350                           | 350                              | 318.5             | 0.1277518         |
| Windward          | Nickel   | 0.01                 | 200                        | 290                        | 350                           | 350                              | 318.5             | 0.1277518         |
| Hex-windward      | Copper   | 0.01                 | 200                        | 290                        | 350                           | 350                              | 318.5             | 0.1277518         |
### 3.2 Predicted Values and Quality Metric

The final test dataset was used to predict values which can then be compared with the actual values. RSS (Residual Sum of Squares) was also calculated for the model as a quality metric. The real values are shown in figure 16 and the predicted values are shown in figure 17.

|               | Aluminium | 0.01 | 200  | 290  | 350  | 319.0 | 0.0386259 |
|---------------|-----------|------|------|------|------|-------|------------|
| Hex-windward  | Nickel    | 0.01 | 200  | 290  | 350  | 320.5 | 0.0386259 |

**Figure 16**: Simulated values

**Figure 17**: Predicted values
Figure 18: RSS values for temperature and pressure

As can be seen in figure 18, the RSS (Residual Sum of Squares) values for temperature and pressure are quite low and hence the model has a good quality metric [26].

3.3 Graphical User Interface (GUI) using Tkinter

A graphical user interface (GUI) using Tkinter was made as a deployment of ML model. The user interface has been made as simple as possible and it asks the user for the required inputs. These inputs are fed into the trained model and the predicted values of temperature and pressure will be displayed in readable manner. The deployed GUI is shown below in figure 19.

Figure 19: Graphic User Interface

Overall performance of the machine learning model is satisfactory and can be used for any practical industrial applications. The data set is based on numerical simulation. However, actual data may not be the same as obtained, since different environmental factors in physical setups can affect the results.

4. Conclusions

In this paper, artificial intelligence approach was adopted to train the machine learning model based on dataset obtained from CFD simulation of micro lattice assemblies that can be used in various heat transfer applications. Based on the mean RSS values obtained on the dependent variables from model, it is inferred that the ML model works satisfactorily. The model can be further improved by adding more data into the dataset and data from the experimental data. With the help of the regression model, one can predict the final fluid temperature and the pressure drop that can be expected from a particular lattice structure made with aluminium, copper or nickel working under a specific initial fluid velocity, initial fluid temperature and initial lattice temperature. This will be useful to get an idea on which microlattice structure suits a particular application.

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