Predicting Heat Transfer Rates in Laminar Supercritical Flows using Machine Learning Approaches

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Abstract. Exploiting the heat transfer enhancement characteristics of supercritical fluids to improve heat exchange efficiencies requires an accurate identification of the pseudocritical temperature (TPC) pinch point within the device. Nusselt number (Nu) correlations based on theoretical considerations of constant fluid property or developed based on statistical regression of high-fidelity data have failed to quantify heat transfer rates in the vicinity of TPC adequately (error > 20%) with the disagreement often exacerbated by buoyancy effects. To fill this void, this study assesses the ability of Machine Learning (ML) algorithms (Random Forest and Artificial Neural Network) to predict Nu under laminar heating conditions while being agnostic to the supercritical fluid being employed. High fidelity data needed to train the ML algorithms were generated from steady-state, laminar flow computational fluid dynamic simulations of three supercritical fluids (sCO_2, sH_2O, $sC_{10}H_{22}$) transitioning through their respective TPC. The scenarios encompassed wide variations in: operating pressures, inlet temperatures, wall heat fluxes and mass fluxes in an upward flow tube orientation. When the input data consisted of three non-dimensional parameters based on expert knowledge, both ML algorithms showed improved accuracy in predicting Nu values (Error < 10%).

1. Introduction

In order to exploit the heat transfer enhancement characteristics of supercritical fluids arising from the rapid variation in thermophysical properties in the vicinity of their pseudocritical temperature (TPC), the fluid temperature and pressures with the heat exchange device needs to be controlled precisely. For this, an accurate estimation of the spatially varying heat transfer coefficient (HTC) within the device is necessary. For constant fluid properties, HTC are usually derived from Nusselt number (Nu), which in turn is obtained from the bulk Reynolds (Re), Prandtl numbers (Pr) and/or Grashof numbers (Gr) from well-established correlations. However, formulating similar universal HTC/Nu correlations that are applicable across all the entire supercritical fluids spectrum has been challenging due to heat transfer enhancement (HTE) or heat transfer deterioration (HTD) that has been observed in the vicinity of the TPC. Furthermore, since buoyancy is an important contributor to these effects, the extent of HTE/HTD is dependent on the mass flow rates, imposed heat fluxes and tube orientations [1, 2]. Nonetheless, a bewildering array of supercritical fluid specific, correlations for HTC have been proposed in the literature all of whom have significant uncertainties associated with them in terms of HTC predictions in the vicinity of TPC (generally +/-20 %) [3, 4]. To fill this void, this study assesses the ability of machine learning (ML) algorithms (Random Forest and Deep Neural Network) to predict Nu/HTC under laminar heating conditions while being agnostic to the supercritical fluid being employed. The high fidelity data needed to train the ML algorithms were generated from steady-state, laminar flow computational fluid dynamic simulations of three supercritical fluids (sCO_2, sH_2O, $sC_{10}H_{22}$) transitioning through their respective TPC. The simulations were carried out at sufficient spatial resolutions to generate grid independent, "ground truth" training data for the ML algorithms. The scenarios encompassed wide variations in: operating pressures, inlet temperatures, wall heat fluxes and mass fluxes in an upward flow tube orientation. The thermophysical properties (Φ) of the fluids, normalized by their maximum values across the given temperature range are shown in Figure 1. The TPC of each fluid are readily identified by the location where their specific heats reach their highest value. The different operating conditions investigated in this study are listed in table 1.

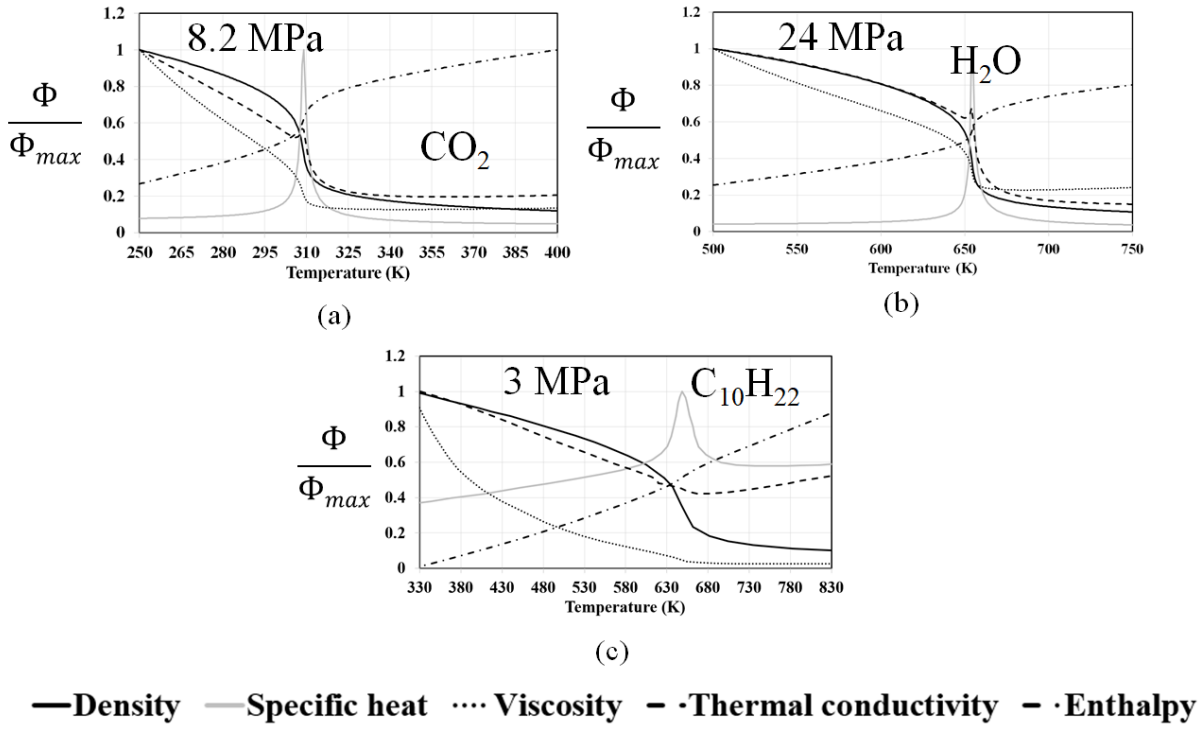

Figure 1. The thermophysical properties (Φ) of the fluids, normalized by their maximum values across the given temperature range. (a) CO_2; (b) H_2O; (c) $C_{10}H_{22}$ (decane).

Table 1. The operating conditions investigated in this study

Fluid	Circular tube diameter (m)	Mass flow rate, G (kg/s)	Inlet temperature T_{inlet} (K)	Wall-flux (W/m^2)	Pressure (MPa)
sCO_2	0.001	3.63E-05	280	3000	8.2
sCO_2	0.002	1.19E-04	300	3000	8.2
sH_2O	0.001	5.39E-05	600	20000	24
sH_2O	0.002	1.11E-04	625	20000	24
sDecane	0.0003	1.00E-05	600	3685	5
sDecane	0.000375	1.00E-05	350	15000	3
sDecane	0.000375	1.00E-05	498	35000	3
sDecane	0.000375	8.00E-06	350	30000	5

In all of the scenarios, we ensured that the fluids transitioned through their respective TPC.

2. Materials and Methods

Ground truth data for training the ML algorithms were obtained from laminar, steady-state simulations were carried out employing the commercial code ANSYS FLUENT 19.1 [5]. 3D geometries of circular pipes were resolved using 485,000 hexahedral cells and simulated after ensuring that grid-independent results were obtained at this resolution across all scenarios. We ascertained that grid-independent results

were obtained at this resolution at all inlet Re, tube diameters, and heat fluxes examined in this study by first ensuring that when constant properties were involved, the Nu converged to 4.36 (according to theoretical considerations when buoyancy was neglected). Second, the computed wall temperature profiles (the primary simulation output of interest) were also ensured to numerically converge, and they did not change with any further increase in mesh resolution.

In order to compute the Nusselt number (Nu) and heat transfer coefficient (h), the local wall temperature (T_{WALL}) must be obtained first. For a specified heat flux Q, T_{WALL} was computed as:

$$T_{WALL} = \frac{Q\Delta n}{k_f} + T_f \tag{1}$$

where q is in W/m^2, Δn is the normal distance from the wall to the centroid of the first cell adjacent to the wall, and k_f and T_f are the fluid thermal conductivity and the fluid temperature adjacent to the wall, respectively. The local heat transfer coefficient (h) was then estimated from T_{WALL} using the relation:

$$h = Q/(T_{WALL} - T_{BULK}) \tag{2}$$

In Equation (2), T_{BULK} is the local fluid bulk temperature estimated from the local bulk enthalpy (H_x) as:

$$H_x = H_{in} + Q*\pi*d*x/G \tag{3}$$

Where, G is the mass flow in Kg/s and H_{in} the enthalpy corresponding to inlet temperature (obtained from REFPROP [6]), x is the distance from the inlet, and d is the tube diameter (in m). The local bulk temperature (T_{BULK}) was evaluated from the estimated local bulk enthalpy (H_x) (cf. Figure 1). The thermal conductivity (K_{BULK}) corresponding to the bulk temperature was then estimated (cf. Figure 1) and used to calculate the Nusselt number (Nu) from the expression:

$$Nu = hD/k_{BULK} \tag{4}$$

The different bulk non-dimensional numbers of interest in heat transfer scenarios: Reynolds number (Re), Prandtl number (Pr), and modified Grashof number (Gr*) were also computed at each axial spatial location along the tube (200 locations per simulation). Consequently, simulations of the entire set of operating scenarios listed in Table 1 generated 1,600 data sets of: Nu, Re, Pr and Gr*. To demonstrate the challenge with obtaining a correlation for Nu using statistical regression techniques, Nu variations are shown as a function of Gr*/Re and Gr*/Re$^{2.7}$ in Figure 2. These are common non-dimensional parameters used in Nu correlations to quantify the effects of buoyancy in HTE. The scatter in the data encompassing all three supercritical fluids, clearly highlights the challenge of formulating a correlation using statistical regression alone. To alleviate this shortcoming, we employed two ML algorithms: Random Forest (RF) and Artificial Neural Networks (ANN) to assess their ability to uncover the relationship among the different non-dimensional variables: Nu, Re, Pr and Gr*.

ANNs are universal approximators that are able to perform complex regression tasks and identify the interactions between input and output variables. The important structural characteristics of ANN are: (i) an input layer, that in data from the selected input features (Re, Pr and Gr*); (ii) a hidden layer that builds the representation for the desired output (Nu), and (iii) an output layer that holds the prediction of the output variables (Nu) based on the previous calculations.

RF is a decision tree based ML-regression algorithm [7]. For regression tasks, this algorithm builds a fix number of decision trees that are each fed independent subsets of data. Each tree uses a random selection of input features and grows the trees to obtain predictions. Once all trees are finished, the mean predicted value is estimated and chosen as the resulting prediction. Using this approach is advantageous, as a low bias is introduced in the final solution, and the contribution of each input feature to the target value can be estimated.

Minimum and maximum values of the non-dimensional variables across the 1,600 data points were: Re [55, 2300]; Pr [0.9, 10.3]; Gr* [58, 2×10^8]. To facilitate the ML process, all of the input parameters were normalized [0, 1] by dividing the values with the maximum value of the corresponding variable. A 80/20 data split was applied for training and testing for both ANN and RF models.

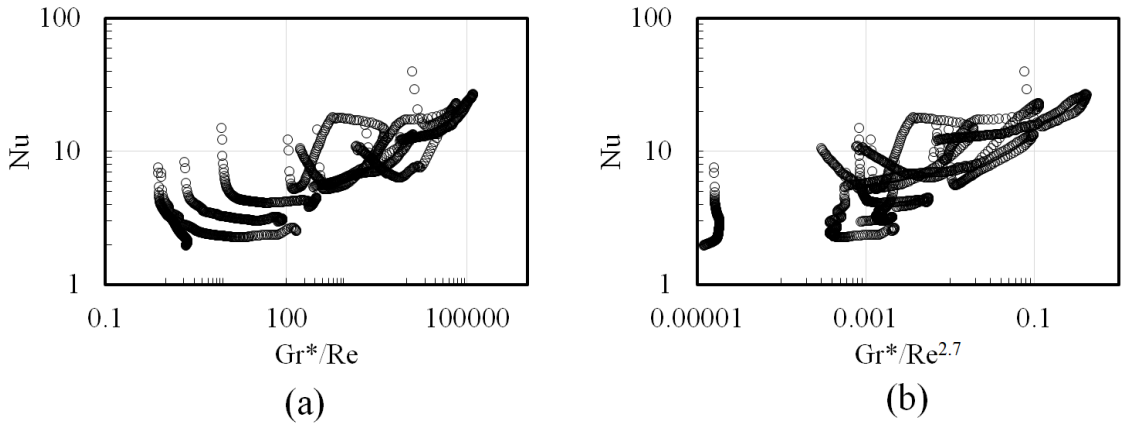

Figure 2. Relationships among the different non-dimensional parameters ascertained from the CFD simulations. (a) Nu versus Gr*/Re; (b) Nu versus $Gr^*/Re^{2.7}$.

3. Results and Discussion

Nu predictions are shown against their true values in Figure 3 along with R^2 values and percent error in the predictions. The ANN model consisted of four hidden layers, with the first two containing 96 neurons each and the last two containing 32 neurons each, and utilized a nonlinear activation function. The RF model that used 100 estimators, performed exceptionally well, achieving an R^2 value of 1. As shown in Figure 3 (b, d) the RF model effectively captured the relationships between Re, Pr, and Gr* in predicting Nu, nearly across the entire range. Notably, while the model was not extensively hyperparameter-tuned, it still demonstrated remarkable accuracy, highlighting the robustness of the chosen features in driving Nu predictions. The distributions of percent error in Nu predictions shown in Figures 3c and 3d indicate an improved performance using the RF algorithm where most of the errors are within +/-5%.

To better understand the effects of each parameter, a heat map was generated, as shown in Figure 4. In the figure, each parameter has a perfect correlation of 1 with itself, represented by dark red. Gr* and Nu exhibit the highest correlation at 0.8, followed by Nu and Re. This is aligned with the trends anticipated based on heat transfer expert knowledge as shown in Figure 2. Pr on the other hand is weakly correlated with Nu indicating that it may not play a significant role in developing universal heat transfer correlations for laminar supercritical heat transfer. Additional insights are obtained from the SHAP plots shown in Figure 4 (c and d) that is an indicator of overall impact of the feature across all samples in the dataset. The ML algorithms are seen to be most sensitive to low values of Gr*.

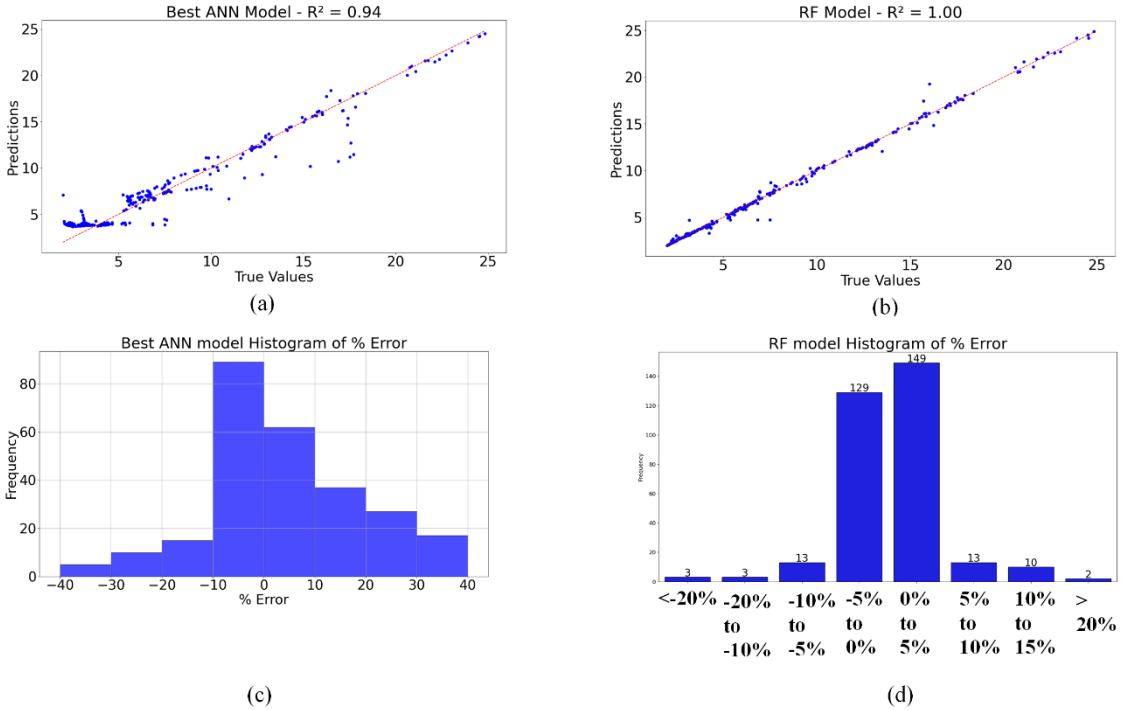

Figure 3. Nu predictions versus Nu true values (a) ANN; (b) RF. Percent error in Nu predictions (c) ANN; (d) RF.

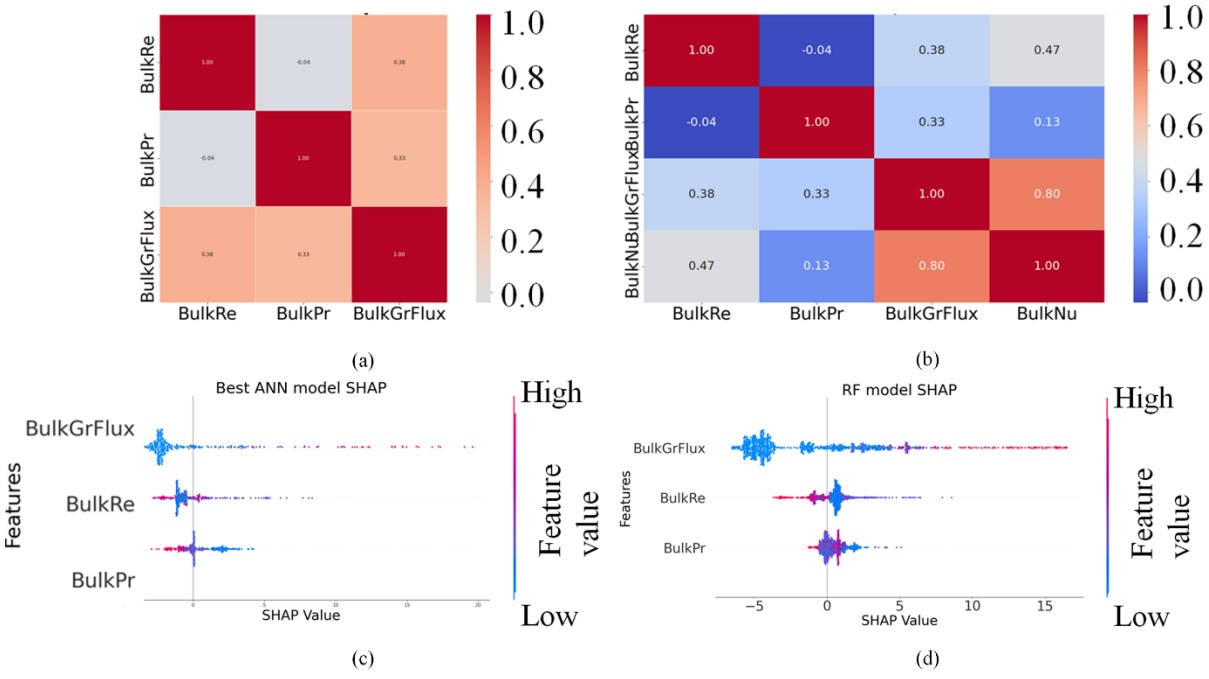

Figure 4. Heat map showing the relationships between each variable (a) ANN; (b) RF; SHAP plots (c) ANN; (d) RF.

4. Conclusions

Accurate estimations of HTC during supercritical heat exchange is challenging due to strong thermophysical property variation in the vicinity of the TPC. Furthermore, buoyancy induced heat

transfer augmentation or deterioration can occur resulting from turbulence enhancement or relaminarization of flows adjacent to the walls. Consequently, formulating robust, accurate correlations even in the laminar regime has proved to be challenging. However, heat transfer domain expertise accumulated over the years have identified key non-dimensional variables influencing heat transfer rates including: Re, Pr and Gr*. Capitalizing on this prior knowledge, this paper explores the ability of two ML algorithms, ANN and RF in uncovering the complex inter-relationships between these key variables and Nu. Since the use of non-dimensional variables implies that the uncovered relationships need to be fluid agnostic, data from three supercritical fluids (sCO_2, sH_2O, $sC_{10}H_{22}$) transitioning through their respective TPC were employed as training data. The scenarios encompassed wide variations in: operating pressures, inlet temperatures, wall heat fluxes and mass fluxes in an upward flow tube orientation. The training data set did indeed highlight the very complex inter-relationships among the variables deeming the development of a correlation via statistical regression to be challenging. Both ML algorithms were able to successfully unveil the hidden relationships between the variables with an improved performance obtained from the RF algorithm (where the differences between the true and predicted Nu values was within +/-5%). Furthermore, heat maps of the predictions clearly showed that the strongest correlations were between Nu and Gr* followed by Nu and Re in alignment with domain knowledge. Pr on the other hand is weakly correlated with Nu indicating that it may not play a significant role in developing universal heat transfer correlations for laminar supercritical heat transfer.

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