Applied Thermal Engineering 131 (2018) 815–824

Contents lists available at ScienceDirect

Applied Thermal Engineering

journal homepage: www.elsevier.com/locate/apthermeng

Research Paper

Heat transfer prediction of supercritical water with artificial neural networks

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HIGHLIGHTS

- This paper proposes an ANN for heat transfer prediction of supercritical water.
- 5280 data points from experiments are used to train and validate the ANN.
- Counter-overfitting techniques are taken to achieve more general applicability.
- The performance of the ANN is much better than well-established correlations.
- This paper opens numerous opportunities in supercritical fluids research.

ARTICLE INFO

Article history:
Received 26 May 2017
Revised 8 November 2017
Accepted 16 December 2017
Available online 19 December 2017

Keywords:
Supercritical fluid
Heat transfer
Artificial neural network
Overfitting

ABSTRACT

Supercritical fluids have been under intensive investigation due to their broad applications in the domain of energy conversion. They are able to significantly increase the efficiency of thermal cycles. However, abrupt changes of thermophysical properties of the supercritical fluids have been observed near the critical point, causing heat transfer deterioration that is challenging to predict. This largely thwarts the technology development with the supercritical fluids, making accurate prediction of heat transfer the fundamental issue to address. In this paper, we propose to train an artificial neural network (ANN) based on 5280 data points collected from published experimental results, for the heat transfer prediction of supercritical water. Validation (strictly separated from training) shows that the mean error percentage and its standard deviation are both below 0.5%. Furthermore, a series of tests, including operational conditions out of the training and validation data, are performed in comparison with four well-established correlations. The results demonstrate that the performance of the ANN is considerably better than the correlations. Training of the ANN takes less than an hour on a regular computer, and the prediction takes several milliseconds. This is the first time that ANNs are trained for general heat transfer prediction of supercritical water. This paper should open further opportunities in the supercritical fluids research to be pursued jointly by the fluid dynamics community and the computer science community.

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1. Introduction

In the quest for efficiency enhancement in energy conversion, supercritical fluids are attractive options. Schuster et al. [49] have investigated the supercritical Organic Rankine Cycles (ORC), which primarily use the low-temperature heat sources (such as geothermal energy, solar desalination and waste heat recovery) and the supercritical organic fluids. The thermal efficiency is improved by more than 8%, compared with the subcritical state. Chen et al. [8] have proposed a supercritical Rankine Cycle (SRC) based on zeotropic mixture working fluids, which shows 10–30% enhancement in the thermal efficiency over the conventional subcritical ORC. In addition, Zhang and Yamaguchi [59] have shown that a solar thermal collector based on supercritical carbon dioxide

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https://doi.org/10.1016/j.applthermaleng.2017.12.063
1359-4311/Published by Elsevier Ltd.

(sCO_2) achieves an annually-averaged collector efficiency of 60%, which is much higher than that of a normal water-based solar collector.

The applications of the supercritical fluids are not limited to the low-temperature heat sources. The idea of using supercritical fluids in the power plants has been intensively explored since the 1960s [25]. The supercritical and ultra-supercritical coal-fired power plants have shown superiority over their subcritical counterparts. Various advanced technologies can be coupled to these supercritical power plants to increase the efficiency as well as reduce carbon emissions [56,6]. Moreover, the Supercritical Water Cooled Reactor (SCWR) is one of the nuclear reactor candidates suggested by Generation-IV International Forum (GIF) [48]. It is estimated that the SCWR is able to achieve a thermal efficiency of about 45%, compared to about 33% for the current Light Water Reactor (LWR) [45]. In addition to the land-based power plants, the SCWR is expected to be used in marine vessels (ships and submarines) as well. The water used as coolant is compatible to the operating environment of the vessels. The main advantages of using supercritical water are compact design of heat exchangers, elimination of the dry-out problem, exclusion of steam separators, high power density, a smaller core and better fuel economy [5].

For supercritical fluids, often the Brayton or supercritical Rankine cycle is suggested. In both the cycles, either heat rejection or heat addition takes place at constant pressure in the near-critical region [13]. This region is prone to heat transfer deterioration due to the abrupt changes of thermophysical properties, as evidenced by the erstwhile experiments tracing back to the 1960s [52,1,55,17]. The tube wall temperature significantly increases due to the poor heat transfer between the tube wall and the bulk fluid. The heat transfer deterioration not only reduces the thermal efficiency but also presents a threat to the safety of the system. Therefore, prior identification of such a problem will help the engineers to mitigate it. Along this direction, advanced correlations considering non-constant properties have been developed based on the experimental data [26,3,20] and are still extensively used after half a century.

Recently, the attention on the SCWR concept and thermal cycles for renewable energy has encouraged more studies on heat transfer of supercritical fluids. Supercritical carbon dioxide has similar properties to supercritical water, with scaled-down values. Therefore, most of the recent experiments have been conducted on the sCO_2 with a low operating pressure at laboratory scale, to gain fundamental knowledge of supercritical fluids. McEligot and Jackson [32] have studied the heat transfer deterioration in sCO_2 and found out that the main reasons for heat transfer deterioration are radial property variations, relaminarization brought by flow acceleration and the effect buoyancy. The heat transfer of sCO_2 are investigated in Kim et al. [23] and Liu et al. [28] by experiments. They have conducted series of experiments in the pressure range of 7.75–8.85 MPa (the critical pressure is 7.38 MPa for CO_2) with different mass and heat flux combinations. They observed heat transfer deterioration at high heat flux and low mass flux when the fluid properties changed drastically. Analytical modeling method has also been developed by different authors with the aim to reproduce experimental results [29,36,37]. Pandey and Laurien [36] suggested a two-layer modeling theory, which divides the wall-bounded flow into a laminar sub-layer and a turbulent layer. Both layers can be targeted and modeled separately.

Besides the experiments and correlations, computational fluid dynamics (CFD) is an important tool providing tube-insight information, which is difficult to derive from experiments. Large efforts have been made in the past to predict the heat transfer of supercritical water and CO_2 with CFD [18,44,57]. However, CFD studies using turbulence models seem to be unreliable at the supercritical pressure. Bypassing the uncertainties in the turbulence modeling, direct numerical simulation (DNS) is an attractive tool for fundamental research. Starting from Bae et al. [2], DNS has delivered plenty of statistics and improved the understanding on the deteriorated heat transfer in the supercritical fluids [38,39,9]. However, as a result of the resolution requirement from the high Reynolds number and the high Prandtl number near the pseudo-critical point, DNS is still limited to theoretical studies far from real applications.

Artificial neural networks (ANNs) have been successfully applied in a number of domains [14,53,12,58]. Recently, they have received overwhelming attention [47,10]. Among the limited studies that investigate heat transfer of supercritical fluids with ANNs, most target supercritical CO_2. A multi-layer feedforward neural network has been developed in Scalabrin and Piazza [46] for forced convection heat transfer to supercritical CO_2. Experimental data from 8 publications in the literature are used for training and validation, including both horizontal and upward pipe orientation. The performance achieved by the neural network is similar to (slightly better than, as stated by the authors) correlations. The flow patterns and heat transfer performances are quite different in horizontal and vertical pipes. For supercritical fluids, deteriorated heat transfer and recovery are expected in the vertical upward flow, while flow stratification occurs in the horizontal flow. There is no discussion on how the ANN should be trained to take account of both orientations. An ANN is proposed in Pesteei and Mehrabi [40] for calculating local heat transfer coefficient of supercritical CO_2 in a vertical tube with the diameter of 2 mm at low Reynolds numbers (<2500). Empirical results from a single source are used for training and validation. The operational conditions for this ANN are highly restricted. The ANNs from both the studies above are only used for supercritical CO2.

In a more recent paper [11], an ANN is trained with in-house experimental data for a supercritical boiler design. The authors report 100% prediction accuracy for the training data at a deviation level of $\pm 7\,^{\circ}C$, which drops to about 80% in the validation. From these results, there seems to be a high chance of overfitting – the most critical issue in ANNs. That is, the ANN fits the training data too closely by capturing the local features. However, it has difficulty in generalization, since the global heat transfer features of the supercritical fluids are not captured. No counter-overfitting techniques are discussed in the paper. Overfitting renders the trained ANN practically much less useful, not only in the fluid dynamics, but also for all other domains. In addition, the major issue with these papers deploying ANNs in heat transfer prediction of supercritical fluids is that no evidence is presented on whether the abrupt heat transfer deterioration in the near-critical region is captured, which is the key technical challenge in the heat transfer prediction of supercritical fluids.

Main contributions: In this paper, for the first time, we propose to train an ANN with experimental data for general heat transfer prediction of supercritical water. Mass flux, heat flux, pressure, tube diameter, and bulk specific enthalpy are the five input parameters. The tube wall temperature is the output to be predicted. A number of techniques are implemented for counter-overfitting, which is the key technical issue preventing the ANN from being generalized and making it practically less useful. Validation is strictly separated from training. Tests including the input parameters out of the range of the input parameters for the training and validation data are conducted. The results show that the ANN is able to achieve high-precision heat transfer prediction of supercritical water. The performance is significantly better than the widely used correlations. Training of the ANN takes less than an hour on a regular computer. Prediction of one temperature with the ANN takes several milliseconds, as compared with several seconds using a correlation. This paper opens numerous research opportunities on deploying ANNs (including convolutional neural networks, deep