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A computationally light data-driven approach for heat transfer and hydraulic characteristics modeling of supercritical fluids: From DNS to DNN

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ABSTRACT

Power cycles with supercritical fluids show high thermal efficiency and are widely applicable. For instance, supercritical carbon dioxide (sCO_2) is proposed to be deployed in various energy conversion cycles, such as solar thermal, geothermal and nuclear. However, heat transfer deterioration of supercritical fluids in the near-critical region reduces the thermal efficiency and presents a threat to the safety of the system. Therefore, prior identification of such heat transfer deterioration is practically very useful. In addition, hydraulic characteristics (such as wall shear stress) are important for determining pressure drop and the corresponding head loss in designing heat transfer equipment. In the past decade, direct numerical simulation (DNS) has become an important approach to study the heat transfer and hydraulic characteristics of supercritical fluids at moderate Reynolds numbers. The main downside is the extremely high computational burden. In this work, we construct a database including 35 operational conditions (characterized by pipe diameter, inlet pressure, heat flux, and inlet temperature) on sCO_2. Both the wall temperature and the wall shear stress are generated from DNS, dependent on the bulk specific enthalpy. 80% of the data are randomly selected to train a deep neural network (DNN), which fits the training data very well. The rest of the data (20%) are used for validation (strictly separated from training). The DNN fits the validation data even better, demonstrating successful counter-overfitting and the general applicability of the DNN under the operational conditions covered by the database. Training of the DNN takes minutes on a regular computer. Evaluating the wall temperature and the wall shear stress with a given operational condition and bulk specific enthalpy takes negligible time. This shows that DNN is a computationally light approach for heat transfer and hydraulic characteristics modeling of supercritical fluids. Furthermore, we test the trained DNN on an operational condition not considered in the database. The DNN still closely follows the results generated by the DNS. Therefore, a combination of DNS and DNN is able to maintain the modeling accuracy that DNS alone has, and significantly reduce the computational load.

1. Introduction

Supercritical fluids are able to enhance the energy-conversion efficiency. Their applications are found in solar thermal energy [17], geothermal and waste heat recovery [1], heat pump and refrigeration [2]. The Generation-IV International Forum (GIF) has identified six different reactors with the aim of improving thermal efficiency of power cycles by increasing the reactor's outlet temperature (ranging from 650 to 1300 K) [40]. However, structural material may degrade under high temperature and extremely corrosive environment, and safety of nuclear plants cannot be compromised. To circumvent this problem, supercritical carbon dioxide (sCO_2) is one of the alternatives. It can operate in the mid-temperature range (700–1000 K) and improve the plant reliability [1].

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There exist several plant layouts with carbon dioxide as the working fluid, including single and split flow layouts with the options of precompression, recuperation, intercooling, and reheating [13]. Among all these layouts, the recompression layouts have shown great potential in terms of high efficiency [1]. In the recompression Brayton cycle, isobaric heat addition takes place at high pressure, which is far away from the critical point (in the range of 20–25 MPa) and heat rejection takes place in the near-critical pressure (7.5–10 MPa). Fig. 1 shows the temperature-entropy (*T-s*) diagram for the cycle, where heat addition takes place at 20 MPa and heat rejection takes place at 8 MPa. The flow is split at Point 8, and the major part of the fluid is cooled down in the reject heat exchanger (i.e. pre-cooler) in process 8–1. The fluid is compressed isentropically in the compressor (process 1–2) and recompressor (process 8–3). During process 2–3, the major part of the split fluid is heated in the low-temperature recuperator and at point-3; it is mixed up with the fluid coming from the recompressor. Then the fluid is sent to the high-temperature recuperator (process 3–4), where it extracts the heat from the fluid at the low-pressure side (process 6–7). The remaining part of the heat is supplied via an external source such as nuclear during the process 7–8. The isentropic expansion from high-pressure to low-pressure takes place in the turbine in process 5–6 and fluid is passed through the high and low-temperature recuperator for the regeneration purpose. The overall cycle promises high efficiency theoretically, yet might severely suffer from poor heat transfer termed as heat transfer deterioration, which arises in the near-critical region due to significant variation in the thermophysical properties. The severity depends upon the heat and mass flux [42].

Heat transfer deterioration not only reduces the thermal efficiency but also presents a threat to the safety of the system. Prior identification of it will help the engineers to mitigate it. There have been different methods used to investigate the heat transfer characteristics, including experiments [14,41,22,4]. A consensus from these studies is that heat transfer deterioration occurs when the fluid is flowing upward, enhancement occurs during the downward flow and stratification occurs during the horizontal flow. In the recompression Brayton cycle, the pre-cooler is prone to heat transfer deterioration, where sCO_2 gets cooled down. The analytical modeling method has been developed with the aim to rapidly reproduce the experimental results [30,31]. Pandey and Laurien [30] 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.

A prior estimation of heat transfer using correlations is popular for the fluid in the subcritical and high-pressure range. However, their applicability is quite unreliable in the near-critical region. A great amount of efforts have been made on the improvement and development of specific correlations treating the steep variation in the thermophysical properties of supercritical fluids [25,5,19,18]. A detailed benchmark analysis is performed in Pioro et al. [36], showing that most of the correlations are only able to qualitatively predict the rough trend, still far from the actual magnitude. In addition, the large variation in the thermophysical properties also leads to peculiar characteristics of hydraulics. This further results in failure of empirical correlations for skin friction coefficient (linearly proportional to wall shear stress for a given fluid), such as the Colebrook equation [11], which is often used to calculate the pressure drop across the channel and for optimization of pressure drop and heat transfer.

In the past decade, computational fluid dynamics (CFD) has become an important method/tool for thermo-hydraulic research. Reynolds-averaged modeling (RANS) is the most common method considering its low computational costs and readiness in different codes [34,26]. A large number of existing turbulence models have

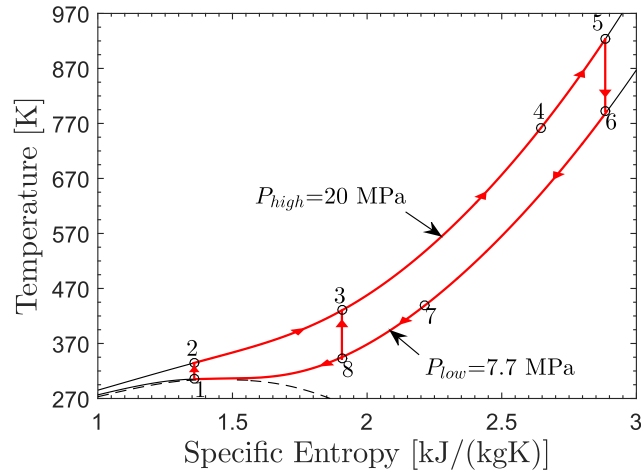

Fig. 1. *T-s* diagram of the recompression Brayton cycle.

been tested for heat transfer of supercritical fluids in simple geometry including water [43] and CO_2 [15]. However, none of them have been proven to be successful. Various low-Reynolds number turbulence models have been systematically assessed by He et al. [15] with the assistance of direct numerical simulations (DNS), which avoids any uncertainties in turbulence modeling and offers a neutral reference. They found out that the model performance is sensitive to the damping function characteristics with respect to buoyancy and flow acceleration. Starting from Bae et al. [3], DNS has delivered plenty of detailed statistics of the flow field, some of which (e.g., the detailed velocity and temperature field) is beyond the reach of experiments [42]. In addition, the experiments are mostly limited to the measurement of the wall temperature, and DNS is able to compute other characteristics, such as the wall shear stress, turbulence intensity and various other turbulence statistics. Therefore, DNS has substantially improved the understanding on the deteriorated heat transfer in the supercritical fluids [28,33,9,29]. The main downside is the heavy computational burden. It is noted that DNS is limited to cases with relatively low Reynolds number, due to the resolution requirement. This situation can be improved with the development of high-performance computing and highly parallel scalable code.

Recently, deep neural networks (DNNs) have received overwhelming attention and demonstrated its capability in capturing the intrinsic relationships hidden in the data in numerous domains [38,12], including fluid dynamics. A multi-layer feedforward neural network has been developed and trained in Scalabrin and Piazza [37] for forced convection heat transfer to sCO_2. Experimental data for training and validation are extracted from 8 publications in literature, including both horizontal and upward pipe orientation. The performance achieved by the neural network is comparable to well-known empirical correlations. Another neural network is proposed in Pesteei and Mehrabi [35] for calculating heat transfer coefficient of sCO_2 in a vertical tube with the diameter of 2×10^{-3} m. Unlike the significant turbulent regime in Scalabrin and Piazza [37], experimental results at low Reynolds numbers ($Re < 2500$) from a single publication [20] are used for training and validation. The available data amount is considerably less than that of Scalabrin and Piazza [37]. In a recent paper [6], an artificial neural network with a single hidden layer is proposed for heat transfer prediction of supercritical water. 5280 data points from experiments are used for training and validation. The performance is clearly better than the well-established correlations.

In this work, for the first time, we link DNS to DNN in modeling the heat transfer and hydraulic characteristics of supercritical flu-