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Numerical Prediction of Heat Transfer for Supercritical Carbon Dioxide in Horizontal Circular Tubes

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Abstract – *Due to their high specific heat, low viscosity, and good diffusivity, supercritical fluids have the potential to be ideal coolants. However, understanding the heat transfer for fluids under supercritical conditions has been a challenge. To understand the peculiar heat transfer characteristics, a wide range of experiments with different ranges of parameters and geometrical configurations has been conducted. The generated experimental data can be used as a reference to expand and assess the prediction capabilities of computational fluid dynamics (CFD) models under supercritical conditions. Out of these models, Reynolds-Averaged Navier-Stokes (RANS) modeling approach is the most widely used one and requires less computational power compare to other modeling approaches. This work aims to study the heat transfer characteristics of supercritical Carbon Dioxide (SCO_2). The current work is focused on the numerical modeling of SCO_2 in horizontal tubes using different RANS model. Various flow conditions are modeled to study the impact on the heat transfer coefficient. A large temperature variation is also expected in some conditions due to stratification. To validate the results, an extensive comparative study with experimental data has been performed.*

Keywords: CFD, Supercritical, Heat transfer deterioration, Turbulence models, Carbon dioxide

I. Introduction

Supercritical fluids are fluids that are working above the defined critical pressure and temperature. Operating at supercritical conditions gives the fluid many advantages like high specific heat and low viscosity to be used in multiple applications. These fluids can be used in power generation, jet engine cooling, and coolants in nuclear reactors [1]. Many generation (IV) design concepts are considering the use of supercritical fluids as coolants and working fluids in Rankine and Brayton cycles [2]. Out of many fluids available, carbon dioxide is often preferred for experimental analyses because of its abundance, and it being a nontoxic and nonflammable fluid [3]. Furthermore, carbon dioxide's critical pressure and temperature are substantially lower than water which makes it a favorable fluid [2]. However, supercritical fluids have one main disadvantage which is the drastic change in thermophysical properties such as dynamic viscosity, specific heat, thermal conductivity, and density near the critical region. These drastic changes happen around a temperature defined as the pseudo-critical temperature [3]. These drastic changes lead to abnormal heat transfer. Two phenomena of heat transfer are associated with these changes, which are heat transfer enhancement and heat transfer deterioration [1]. Heat transfer enhancement happens when the heat transfer coefficient is higher than the normal heat transfer coefficient which is expected and evaluated from well-known correlations, for example, the Dittus-Boelter correlation [2]. Heat transfer deterioration happens when there is a sudden increase in wall temperatures which is the result of the heat transfer coefficient being lower than the coefficient in the case of normal heat transfer [4]. Understanding and predicting the heat transfer of supercritical fluids has been a challenge, therefore many experiments have been conducted to understand the nature of mass and heat transfer in the critical regime. However, conducting experiments is costly and dangerous at critical pressure and temperature. Hence many researchers have shifted their interest to Computational Fluid Dynamics (CFD) solutions. Mainly there are three approaches of CFD: Reynolds-Averaged Navier-Stokes Simulation (RANS), Large Eddy Simulation (LES), and Direct Numerical Simulation (DNS). RANS is the most used method due to its wide availability in common commercial codes (e.g., CFX, Ansys Fluent, and STAR-CCM+). Moreover, RANS consume less computational power compared to LES and DNS. However, it is the least accurate [5]. Therefore, RANS models need to be validated with experimental data when investigating supercritical behavior. Many attempts have been made to investigate the behavior of supercritical fluids using RANS. Different geometries, fluids, and boundary conditions have been tested. This work aims to assess the predictability and accuracy of RANS models in the case of horizontal flow of supercritical carbon dioxide inside a tube. The data will be validated with a recent experimental study.

II. Literature Review

Pu et al. [6] numerically investigated the mixed convection heat transfer of supercritical CO_2 inside small horizontal tubes. The study was done by using a commercial code. The turbulence model used was the k-ω shear stress transport (SST) model. It was found that buoyancy has a significant effect on heat transfer even with horizontal flow inside small diameter tubes. In addition, a remarkable difference in heat transfer coefficient was noticed between the bottom and top sides of the tube at high heat fluxes. Mao et al. [7] did an interesting work analyzing the thermal performance of supercritical carbon dioxide flowing horizontally inside ribbed tubes. The analysis was done by CFD using Ansys Fluent with k-ω (SST) turbulence model. Different types of ribs were investigated. It was deduced that ribbed tubes can significantly decrease the effect of heat transfer deterioration at low temperatures. In addition, the triangular shaped ribs can enhance the heat transfer more than circular or rectangular ribs. Furthermore, smaller size ribs and medium pitch are more desirable to enhance the turbulent heat transfer. Wang et al. [8] analyzed the heat transfer of supercritical carbon dioxide in a highly buoyant flow. Three cases were investigated with three

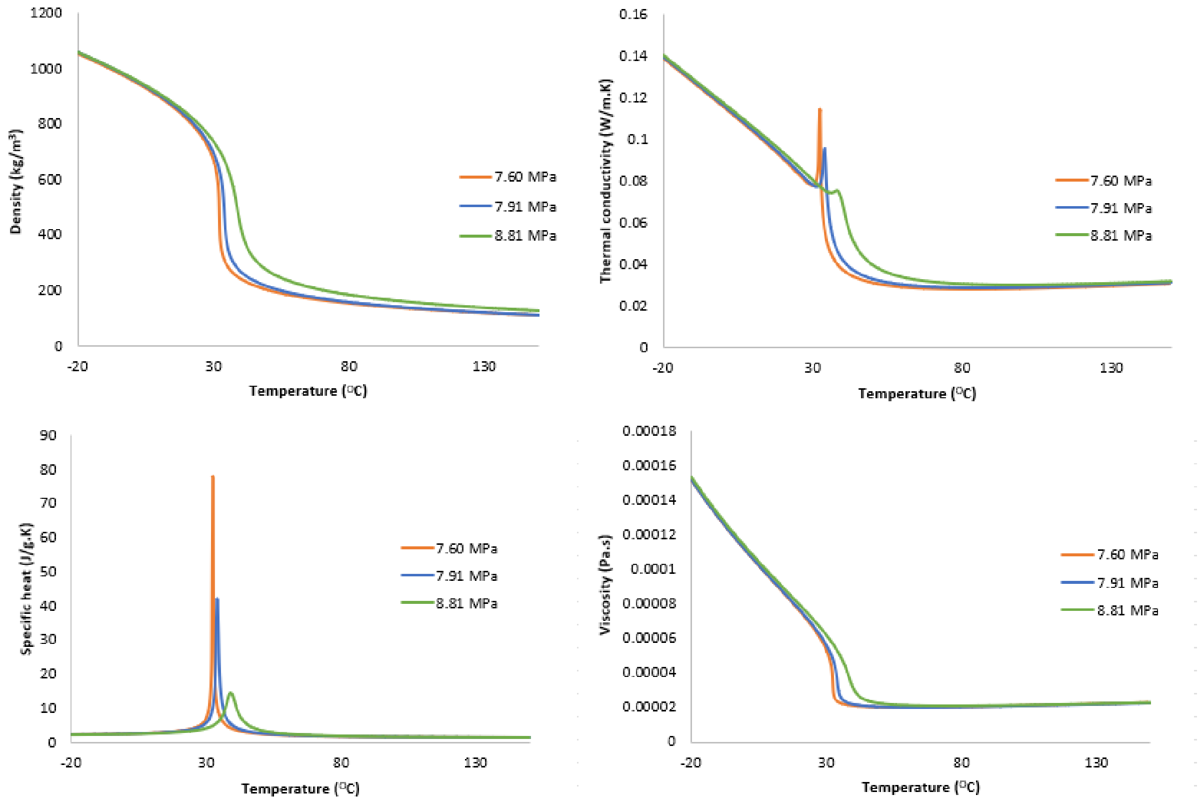

Fig. 1. Thermal physical properties of carbon dioxide at different pressure and temperature values [20]

different diameters. RANS approach was used with the Abe-Kondoh-Nagano (AKN) k-ε turbulence model. The simulations showed that high buoyancy can significantly increase heat transfer deterioration not only locally but also on the overall heat transfer and the affected region decreases when the tube diameter increases. Li et al. [9] investigated the convective heat transfer for the flow of supercritical carbon dioxide inside a counter-flow tube in tube heat exchangers. The analysis was done using RANS and k-ω SST turbulence models. ANSYS CFX software was used. From the results, it was found that the k-ω model can produce more accurate results at large mass fluxes and high inlet temperatures. However, the k-ε model is more accurate at low mass fluxes and low inlet temperatures. Huang et al. [10] simulated the flow of supercritical carbon dioxide in horizontal U-tubes. RANS approach with four turbulence models were tested. Out of different turbulence models, the renormalization group (RNG) k-ε model was the most reliable for this case. The results suggested that the centrifugal force in the U-section enhanced the heat transfer when the bulk temperature was near the pseudo-critical temperature. Furthermore, the centrifugal force can restrict the effect of flow acceleration and buoyancy. Li et al. [11] analyzed the heat transfer of supercritical carbon dioxide flowing in horizontal concave tubes. Ansys Fluent was used for the analysis with the k-ω SST turbulence model. The results indicated that the heat transfer coefficient in a concave tube is larger than in normal horizontal tubes. The same behavior is observed near the pseudo-critical temperature however the results contradict the predictions from empirical correlations. Wang et al. [12] simulated the flow of supercritical carbon dioxide in a horizontal tube subjected to non-uniform heat flux. The simulation was done using RANS with the k-ε turbulence model since the results generated using the latter model were close to experimental data. The effect of operating pressure was investigated, and it was found that the maximum heat transfer coefficient decreases as pressure increases and the local heat transfer at the circumference increases as the pressure approaches the critical pressure. Wang et al. [13] analyzed the horizontal flow of supercritical carbon dioxide in large tubes. RANS method with different k-ε turbulence models were used for the analysis. The researchers found that the AKN low-Reynolds number model has the best prediction and is the closest to experimental data. It was deduced that the buoyancy effect increases as the heat flux increases and heat transfer deterioration appears. Sharma et al. [14] investigated the heat transfer of supercritical carbon dioxide in sub-channels. RANS with RNG k-ε turbulence model has been used for the analysis. The researchers investigated the effect of increasing the pressure above the critical point and deduced that the pressure has no main effect on heat transfer if the bulk temperature is significantly higher than the pseudo-critical temperature. In addition, the effect of heat flux on heat transfer coefficient was studied and it was found that the coefficient increases as heat flux increases. Cai et al. [15] numerically studied the heat transfer in a micro-tube heat exchanger between supercritical fluids and water. RANS approach with the SST k-ω turbulence model was used for this study. It was found that the heat transfer characteristics are similar at low and high Reynold numbers and if mass flux is increased, the heat transfer coefficient of carbon dioxide increases. Furthermore, in agreement with many previous studies, the effect of buoyancy is significant in the heat transfer of supercritical carbon dioxide even at small tube diameters and at low Reynolds numbers: buoyancy induces heat transfer enhancement at the upper part of the tube and deterioration in the lower part.

III. Methodology

This section will explain the physical model and the equations used by the software to predict the wall temperature.

III.A. Geometry

The physical model is a 3D model built using the ANSYS tool Design modeler and it is a replica of the test pipe used by Theologou et al. [16] in their experimental study. The pipe diameter is 4 mm with a heated length of 2.04 m; in addition, an adiabatic (unheated) length at the entrance of 350 mm is included. The flow direction is along the z-axis and gravity is applied along the negative y-axis.

III.B. Equations and Numerical Model

Ansys Fluent was used for the numerical solution. The following are the governing equations for the numerical method [7].

The continuity equation is:

$$\frac{\partial}{\partial x_i}(\rho u_i) = 0 \tag{1}$$

The momentum equation is:

$$\frac{\partial}{\partial x_i}(\rho u_i u_j) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left[(\mu + \mu_t)\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + \frac{\partial}{\partial x_j}\left(-\rho\overline{u_i' u_j'}\right) + \rho g_i \qquad (2)$$

The energy equation is:

$$\frac{\partial}{\partial x_i}(\rho u_i T) = \frac{\partial}{\partial x_i}\left[\left(\frac{\mu}{Pr} + \frac{\mu_t}{Pr_t}\right)\frac{\partial T}{\partial x_j}\right] \qquad (3)$$

where ρ is the density, P is the static pressure, u is the velocity, μ is the viscosity, μ_t is the turbulent viscosity, g is the gravitational constant, T is the temperature, Pr is the Prandtl number, and Pr_t is turbulent Prandtl number.

In this analysis, both the RNG k-ε and the SST k-ω turbulence models will be used since both models are the most recommended to yield better results when dealing with supercritical fluids as evident from the literature review.

The two equations for RNG k-ε model are:

Turbulence kinetic energy equation is:

$$\frac{\partial}{\partial x_i}(\rho u_i k) = \frac{\partial}{\partial x_j}\left(\alpha_k \mu_{eff}\frac{\partial k}{\partial x_j}\right) + G_k + G_b - \rho\varepsilon - Y_M + S_k \qquad (4)$$

Turbulence dissipation rate is described as:

$$\frac{\partial}{\partial x_i}(\rho u_i \varepsilon) = \frac{\partial}{\partial x_j}\left(\alpha_\varepsilon \mu_{eff}\frac{\partial k}{\partial x_j}\right) + C_{1\varepsilon}\frac{\varepsilon}{k}(G_k + G_b) - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} + S_\varepsilon \qquad (5)$$

Where ε is the turbulence dissipation rate, k is turbulent kinetic energy, G_k is the generation of turbulence kinetic energy due to the gradients of the mean velocity, G_b is the generation of turbulence kinetic energy because of buoyancy, Y_M is the contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate, α_k is the inverse effective Prandtl number for k, α_ε is the inverse effective Prandtl number for ε, and S_k and S_ε are user-defined source terms.

The SST k-ω turbulence model equations are:

$$\frac{\partial}{\partial x_i}(\rho u_i k) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + G_k - Y_k \qquad (6)$$

$$\frac{\partial}{\partial x_i}(\rho u_i \omega) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\omega}\right)\frac{\partial \omega}{\partial x_j}\right] + G_\omega - Y_\omega + D_\omega \qquad (7)$$

Where ω is the specific turbulent dissipation rate, σ_k is the turbulent Prandtl number for k, and σ_ω is the turbulent Prandtl number for ω and D_ω is the cross-diffusion term. For more details about the turbulence models the reader is referred to [17].

III.C. Enhanced Wall Treatments and y^+ Values

In the present study, three approaches will be considered. Firstly, the SST k-ω turbulence model will be tested with a fine mesh near the wall to resolve the viscous sublayer. Ideally, the y^+ should be approximately one everywhere. Secondly, the same mesh will be used with the RNG k-ε model. Finally, a coarser mesh with large y^+ values of 50 or more will be tested with the RNG k-ε model and the Enhanced Wall Treatment (EWT) method. To read more about Fluent's enhanced wall treatment the reader is referred to [17].

III.D. Carbon Dioxide Properties

Properties of carbon dioxide are extracted from NIST (National Institute of Standards and Technology) [18] dataset which is incorporated within Ansys Fluent and these properties are updated every iteration based on the temperature.

III.E. Boundary Conditions and Dataset for Validation

The data generated by the work of Theologou et al. [16] will be used for validation. The experimental facility used by the aforementioned study is called SCARLET (Supercritical CARbon dioxide Loop at IKE StuTTgart). The test section is heated by a DC power source and 40 temperature sensors are used on the top, middle, and bottom surfaces of the pipe. Similar boundary conditions have been considered and are listed in Table 1.

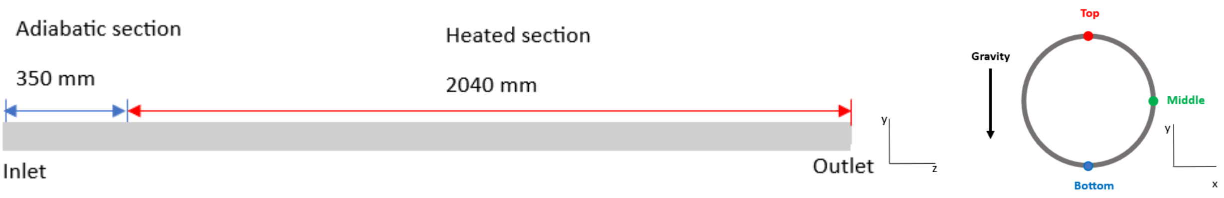

Fig. 2. A schematic of the test pipe

Table I Boundary Conditions

Boundary condition	Value	Unit
Inlet Temperature	5	°C
Operating Pressure	7.75	MPa
Mass flux	400	kg/m^{2}s
Heat flux	50	kW/m^2

IV. Results

To investigate the pipe flow incorporating the buoyancy effect, three wall temperature values are measured around the pipe (top, middle, and bottom). The results of the simulation are shown in Figure 3 and Figures 5 to 9. Different turbulence models had differently predicted the wall temperatures at different locations. The y^+ values achieved for the SST k-ω were below 0.98. For the RNG k-ε model without EWT the y^+ ranged approximately between 0.60-1.42 and with EWT the values were approximately 50-325.

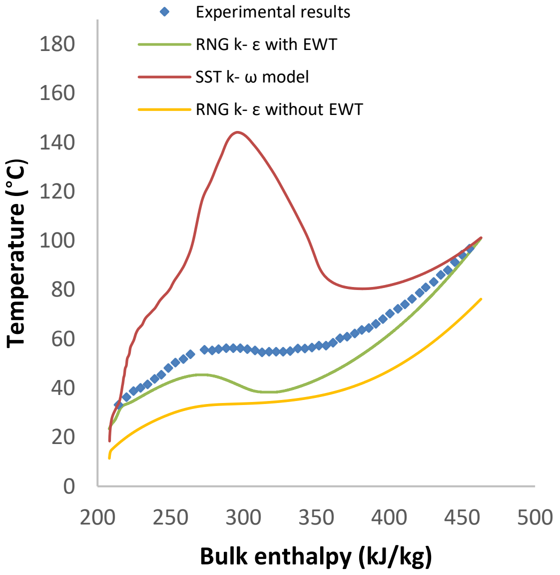

Fig. 3. Wall temperature measured at the top of the pipe.

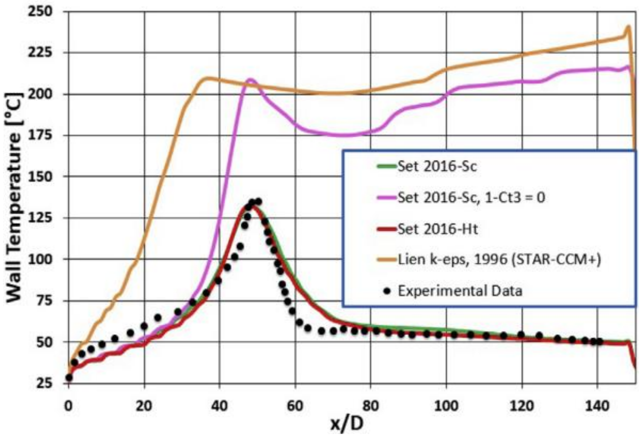

Fig. 4. Figure from the study [19] *for supercritical carbon dioxide*

Figure 3 shows the wall temperature vs bulk enthalpy variation at the top of the horizontal pipe. It is observed that the SST k-ω adequately predicted the wall temperature at the entrance of the pipe, however, once the temperature reached the pseudo-critical temperature the model tends to overestimate the deterioration, and higher values of wall temperature are reported. After that, the temperature starts to recover from the deterioration and the calculated wall temperature starts to match the experimental results. As the top region of the horizontal pipe is expected to be at the highest temperature, this over-predictive behavior is present. This behavior is not present at the middle or lower region of the pipe, as will be discussed later. This shows that the SST k-ω model has limitations in modeling the flow near the supercritical region while the results before and after match with the experimental data. It is also worth noting that the previous modeling efforts reported in the literature have shown similar trends of overprediction [19]. Figure 4 shows such a case where the flow is overpredicted by more than 50 °C by different turbulence models. It can be further noted that once the pseudo critical region affects the temperature, it remains higher till the end of the test section. However, in the current work, the temperature reduces back to the experimental values towards the pipe outlet.

For the RNG k-ε model with EWT, the temperature is underestimated, and an enhancement of heat transfer after the deterioration is predicted at a level that is lower than the experimental data. However, for the model without EWT, the wall temperature at all locations is underestimated by a relatively large margin. For RNG k-ε models, the same behavior is noticed in the middle and bottom regions, shown in Figure 5 and Figure 6 respectively, however, for the SST k-ω model, the predicted values are underestimated in the middle and bottom region, unlike the top region.

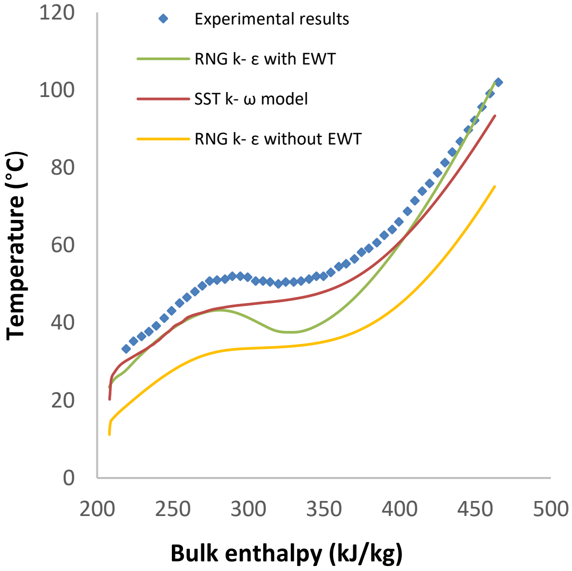

Fig. 5. Wall temperature measured at the middle of the pipe.

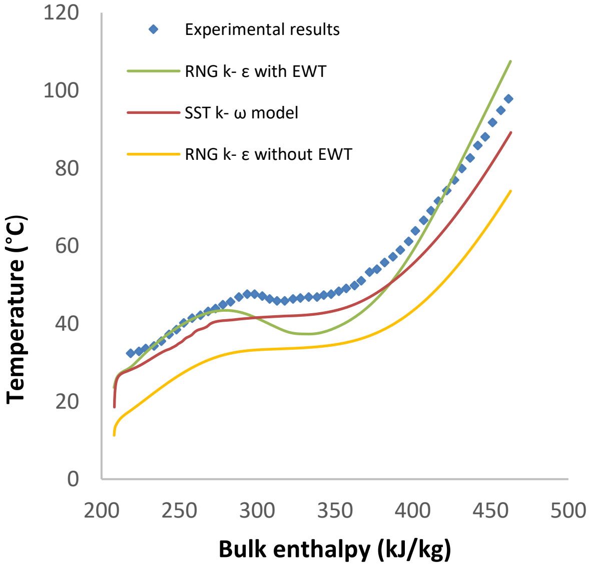

Fig. 6. Wall temperature measured at the bottom of the pipe.

Figures 7 to 9 are used to compare the performance of each model at the top, middle, and bottom regions of the pipe. As the horizontal pipe is non-axisymmetric due to the buoyancy effect, some variation is expected between the temperature prediction at the three regions. A comparison of all experimental reference data shows that the highest temperature indeed occurs at the top region and the lowest at the bottom region.

It is evident from Figure 7 that the SST k-ω model predicts the buoyancy adequately, hence the difference between the three regions. In contrast, Figure 8 shows that the RNG k-ε models neglect the buoyancy effect since the difference between the three regions is negligible, even when compared to the experimental data. Also, a consistent underprediction is observed in comparison to the experimental data. From Figure 9 for k-ε RNG with EWT, the experimental and numerical results are in better close agreement. Underestimations are observed for the bulk-enthalpy region 300-400 kJ/kg but the overall performance looks the best results among the considered approaches.

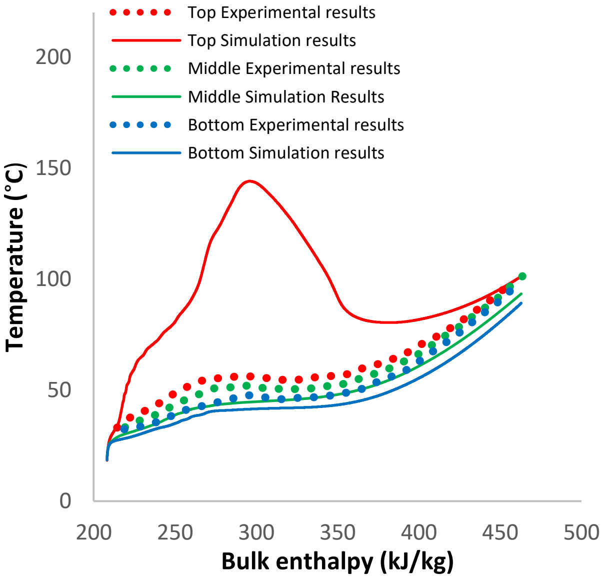

Fig. 7. Wall Temperatures prediction for SST k-ω turbulence model

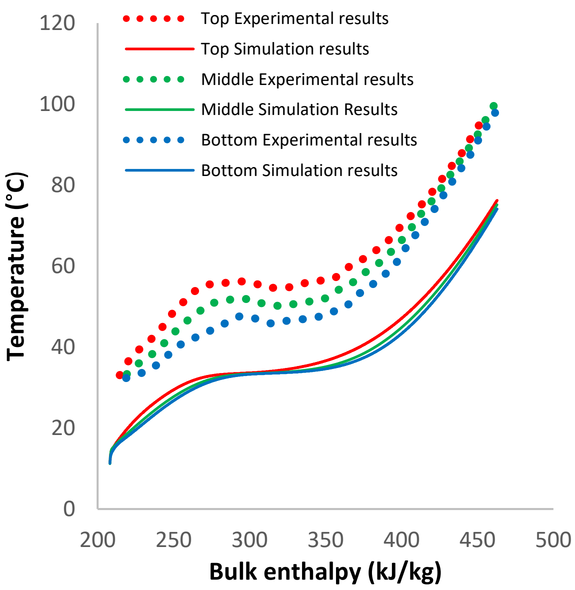

Fig. 8. Wall Temperatures prediction for k-ε RNG turbulence model without EWT.

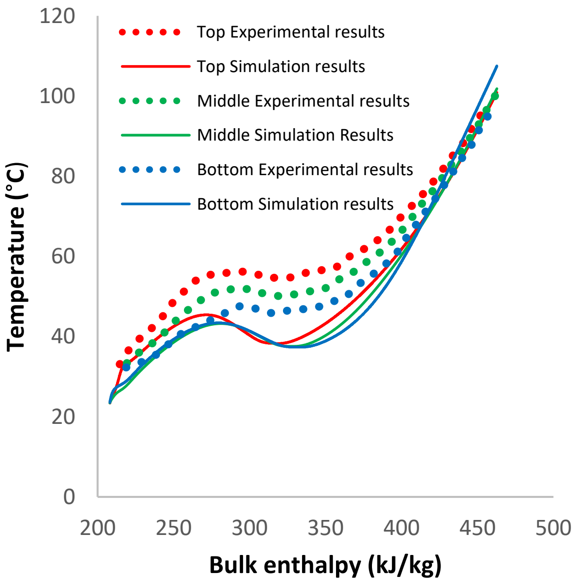

Fig. 9. Wall Temperatures prediction for k-ε RNG turbulence model with EWT.

V. Conclusions

An assessment of the predictability for wall temperatures of widely known RANS-based turbulence models under supercritical conditions has been studied. Three regions have been investigated to understand the effect of buoyancy on horizontal flow inside pipes. The results are compared to an experimental study done under similar conditions. From the results, the following has been concluded:

- The SST k-ω turbulence model reported differences in wall temperatures between different regions which implies the effect of buoyancy on heat transfer is well captured however in the top region huge overestimation of deterioration is noticed.
- The behavior of the increase of wall temperatures in all three regions was adequately predicted by both RNG k-ε models. However, both models underestimated the values of wall temperature as compared to the experimental reference.
- The RNG k-ε model with EWT underestimated the deterioration and enhancement of heat transfer. However, it shows better predictions in the middle and bottom regions especially after and before deterioration.
- Comparing the three models, the RNG k-ε model without EWT is the least accurate. This is probably due to its intrinsic limits in dealing with buoyant flows as well as the near wall treatment of flow and heat transfer.

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