SAUDI INTERNATIONAL CONFERENCE
ON NUCLEAR POWER ENGINEERING

Proceedings of SCOPE
13-15 Nov. 2023 – KFUPM
Paper 23053

Numerical Prediction of Natural Circulation Heat Transfer for Supercritical Carbon Dioxide

Abdullah Alasif [1], Andrea Pucciarelli [2] and Afaque Shams [1,3]
1 Mechanical Engineering Department, King Fahd University of Petroleum & Minerals (KFUPM), Saudi Arabia
2 Università di Pisa, Dipartimento di Ingegneria Civile e Industriale, Largo Lucio Lazzarino 2, 56122 Pisa, Italy
3 Interdisciplinary Research Center for Renewable Energy and Power Systems (IRC-REPS), KFUPM, Saudi Arabia
Email(s): Abdullah.asif@kfupm.edu.sa; andrea.pucciarelli@unipi.it ; afaque.shams@kfupm.edu.sa

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 accuracy of computational fluid dynamics models under supercritical conditions. Out of these models, RANS is the most widely used and consumes less computational power relative to other models. In this paper, natural circulation heat transfer of supercritical carbon dioxide will be investigated using RANS approach. To validate the prediction accuracy of RANS model, an extensive comparative study with experimental data is presented in the present paper.*

Keywords: Natural Circulation, Supercritical, CFD

I. Introduction

For decades supercritical fluids have been used in many processes like gasification, fluid extraction, chemical reactions, and oxidation. In addition, the use of supercritical fluids has been deployed in many applications, like power generation, jet engine cooling, and nuclear engineering [1]. For nuclear reactors, many generation IV reactors will consider supercritical fluids either as primary coolants or working fluids in power generation cycles [2]. In addition, since higher temperatures are usually achieved for steam cycles, improvements in the global efficiency of the cycle are achieved as well. The use of supercritical fluids is preferred in thermal processes because of the enhanced properties such as high specific heat and low viscosity [1]. These advantages are caused by the sharp changes in thermophysical properties that happen when moving beyond the critical point. As can be seen from Figure 1, thermophysical properties such as density, viscosity, specific heat, and thermal conductivity change drastically when approaching the critical point. These changes occur around a temperature defined as the pseudo-critical temperature at which the isobaric-specific heat exhibits a maximum [3]. These drastic changes may lead to abnormal heat transfer phenomena [1]. Heat transfer deterioration occurs when a sharp increase in wall temperature is observed, the reason being a decrease in the heat transfer coefficient value from the normal heat transfer case [4]. A second phenomenon that may occur is heat transfer enhancement and it is defined as an increase in the heat transfer coefficient from the base value calculated using well-known correlations (e.g., the Dittus-Boelter correlation) [2]. Many fluids have been studied throughout the years, but a huge part of the literature is focusing on carbon dioxide. Carbon dioxide holds many positive features, for example, it is nonflammable and nontoxic which makes it safer than other fluids. Furthermore, it is widely abundant [3]. In addition, the critical point values (pressure and temperature) are relatively lower when compared to water [2] thus making facilities intrinsically safer and cheaper. Carbon dioxide is thus an interesting surrogate fluid for water; nevertheless, the use of carbon dioxide data as a practical mean to investigate possible thermos-fluid-dynamic behaviors of water requires the development of a similarity theory.

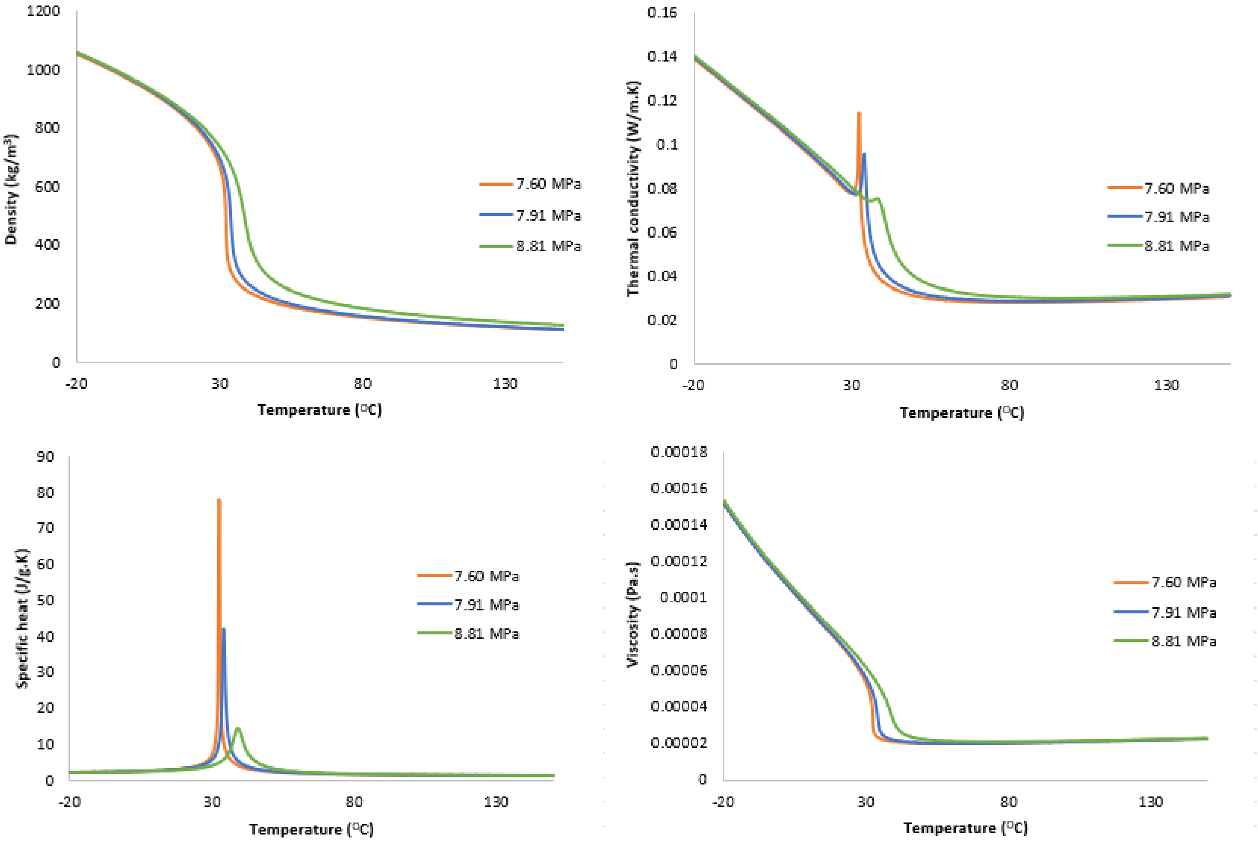

Fig. 1 Thermal physical properties of carbon dioxide at different pressure and temperature values

With the aim to pave the way for the use of surrogate fluids to simulate supercritical water, the University of Pisa recently developed a fluid-to-fluid similarity theory for heat transfer to supercritical fluids showing promising capabilities (see e.g., [5]). Many studies have been done to understand the flow and heat transfer of supercritical fluids inside pipes and channels, in most cases for forced convection conditions. Very few studies were dedicated to understanding the natural convection of supercritical fluids. Natural circulation is important for many applications, especially generation IV nuclear reactors [6]. In fact, passive cooling methods based on natural circulation phenomena are expected to play a relevant role in the design and safety analysis of next generation fission power plants.

The present study aims to investigate the natural circulation heat transfer of supercritical fluids using CFD RANS approaches. In particular, the capabilities of three selected turbulence models are evaluated against a selected experimental data set. The comparison is mainly performed based on the measured and calculated wall temperature trends. The performed analyses allow an understanding of what are the limits and possible improvement path for the selected modeling technique, also providing room for a better understanding of the involved phenomena.

II. Recent Supercritical CO_2 Numerical Analyses

Predicting heat transfer to supercritical fluids is rather a challenging task. Up to date, no developed model is able to suitably predict heat transfer in large ranges of operating conditions though some improvements were achieved for some selected experimental databases (see e.g., the works performed at the University of Pisa described hereinafter). This statement is also supported analysing some of the latest papers concerning recent numerical studies involving CO_2. Wahidi et al. [7] analyzed the heat transfer and flow of supercritical carbon dioxide using CFD. The study was done using the RANS approach by ANSYS FLUENT. Simulations were 3D and the RNG k-ε turbulence model was used. The results were validated with correlations rather than experimental data. It was deduced that to stabilize the flow, a certain heat input value must be imposed. In addition, working at minimum supercritical pressures yields less instability in the flow. Till now there are no turbulence models that can predict fairly the flow of supercritical fluids in the mixed convection regime. For this reason, Bae [8] proposed a computational model for the buoyancy influenced flows for supercritical fluids. The developed model can fairly predict DNS data for mixed convection flows. However, if buoyancy is greatly affecting the flow the model produces inaccurate results. Wang et al. [9] investigated the flow of supercritical carbon dioxide under Poiseuille-Rayleigh-Benard convection. The effect of Reynolds and Rayleigh numbers on the flow was investigated using ANSYS FLUENT mainly focusing on the flow characteristics rather than the heat transfer features. Srivastava and Basu [10] studied the heat transfer of supercritical carbon dioxide in an inclined natural circulation loop. The model used was a rectangular loop modeled in ANSYS FLUENT with the RNG k-ε turbulence model. It was found that inclination reduces the rate of circulation and heat transfer coefficient. In addition, the buoyancy parameter was found to be the most feasible parameter to identify the beginning of flow-induced heat transfer deterioration. Biradar et al. [11] investigated the use of supercritical and subcritical carbon dioxide in passive solar water heaters in natural circulation conditions. The system was simulated using ANSYS FLUENT with the RNG k-ε turbulence model. Results suggested that, in this case, using supercritical carbon dioxide instead of water enhances the mass flow rate, efficiency, and heat transfer substantially.

III. Considered Experimental Data

Li et al. [6] investigated experimentally, the natural circulation heat transfer of supercritical carbon dioxide. A rectangular loop was used for the experimental setup; a sketch of the facility is reported in Figure 2.

The loop is 1000 mm in width and 1500 mm in height. Pipes with 4 mm inner diameter and 1 mm thick were used. The whole loop is covered with 50 mm thick thermal insulation. High purity carbon dioxide was used as a working fluid and the loop was vacuumed before filling the carbon dioxide to avoid any influence from different fluids. The fluid first passes through a vertical section where it is heated up by DC heaters and it is later cooled in a horizontal refrigerator. The test section lies in the vertically heated section with a height of 800 mm. T-type thermocouples are arranged at every 50mm in the test section to measure the outer wall temperature. To measure the bulk inlet and outlet temperatures, two thermistors (PT100) were used. The experimental setup was tested for stability and repeatability by measuring multiple times some parameters during operations, the fluctuations in parameter values were found to be negligible. The experiment was performed at different operating pressures, filling masses, cooling temperatures, mass and heat fluxes. Heat transfer deterioration was observed to occur and existing correlations for forced convection supercritical carbon dioxide heat transfer were tested against the experimental data. Unfortunately, they failed to reproduce the experimental data for natural circulation. The authors thus introduced a new parameter to existing correlations which improved the predicting capabilities for the addressed natural convection data set. The experimental data provided by Li et al. [6] in their study will be used to validate the simulation results of this work.

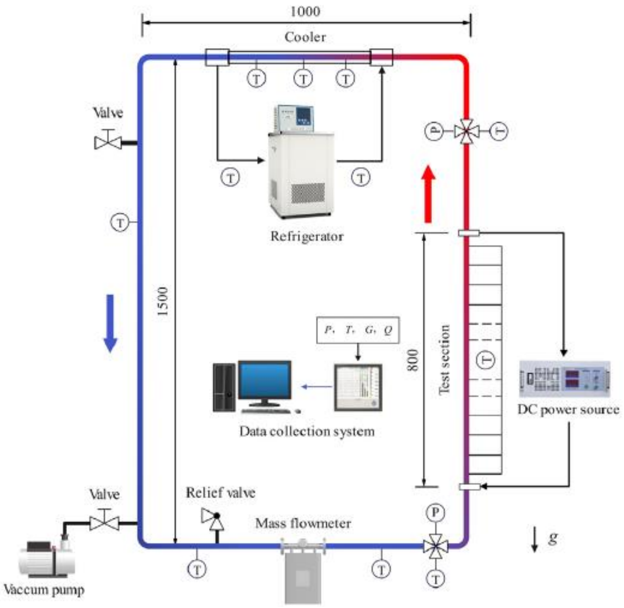

Fig. 2 Schematic diagram of the experimental system. Taken from [6]

IV. Methodology

During the last decade, several CFD analyses of heat transfer to supercritical fluids were performed at the University of Pisa adopting the RANS approach. After stating that no available turbulence models could suitably predict heat transfer deterioration phenomena, a modified Lien et al. [12] model adopting the Algebraic Heat Flux Model (AHFM) for the sake of calculating the turbulent heat flux contribution was developed at the University of Pisa [13]–[15].

The model reckons on the Lien et al. [12] model for what concerns the k and ε equations and the eddy viscosity definition. Nevertheless, it considers the additional production term of turbulence and dissipation due to buoyancy: G_k and G_ε respectively.

They are:

$$G_k = g_i\overline{\rho' t'} = -\rho\beta g_i\overline{u_i' t'} \qquad (1)$$

$$G_\varepsilon = -\frac{\varepsilon}{k}\rho\beta g_i\overline{u_i' t'} \qquad (2)$$

where the $\overline{u_i' t'}$ contributions are calculated by adopting the AHFM correlation. AHFM firstly was proposed by Launder [16] and was successfully adopted, in slightly different shapes, by many research groups as a sound method for the calculation of the turbulent heat flux. The adopted AHFM correlation considered in the present paper is reported below.

$$\overline{u_i' t'} = -C_t\frac{k}{\varepsilon}\left(C_{t1}\overline{u_i' u_j'}\frac{\partial T}{\partial x_j} + C_{t2}\overline{u_j' t'}\frac{\partial u_i}{\partial x_j} + C_{t3}\beta g_i\overline{t'^2}\right) \qquad (3)$$

The following settings were considered.

$$C_t = 1;\ C_{t1} = 0.113;$$

$$C_{t2} = 0.113;\ C_{t3} = \max\left(0, e^{\frac{h_w^*}{2.5}} - 0.4\right) \qquad (4)$$

Where ε is the turbulence dissipation rate, k is turbulent kinetic energy, ρ is the density, u is the velocity, g is the gravitational constant, T is the temperature and β is coefficient of volume expansion. The adopted coefficients are the results of a long tuning process based on the analysis of tens of experimental conditions adopting different fluids. In particular, h_w^* is the dimensionless wall enthalpy, a parameter that turned out to be relevant in a similarity theory for supercritical fluids recently proposed at the University of Pisa. The reader is remanded to [17] for a deeper description.

Eventually, the $\overline{u_i' t'}$ contributions were adopted for the calculation of the turbulent Prandtl number as well.

$$Pr_{tur} = -\frac{\upsilon_t}{\overline{u_r' t'}}\frac{\partial T}{\partial x_r} \qquad (5)$$

Where Pr_{tur} is turbulent Prandtl number and υ_t kinematic turbulent viscosity.

This way, the constant Pr_{tur} hypothesis usually adopted by turbulence models (see e.g., the Lien k-ε [12] and the SST k-ω models [18]) is not necessary and an improved thermal field prediction is expected.

The model proved to predict sufficiently well heat transfer phenomena occurring for several supercritical fluids (e.g., water, carbon dioxide, R23) for mass fluxes up to 600-700 kg/m^{2}s especially when heat transfer deterioration is led by buoyancy phenomena. Limited improvements were instead achieved for higher mass fluxes, in particular when huge heat fluxes were applied leading to deterioration phenomena mainly ruled by flow acceleration.

The model was never tested for low mass flux conditions such as the ones investigated by Li et al. [6] in their work. This application will thus be an interesting benchmark to understand the capabilities of the developed model in such operating conditions.

Moving towards the discretization of the addressed domain, the pipe was simulated considering a two-dimensional domain taking advantage of the axisymmetric nature of the problem. A constant axial dimension of about 4.4 mm was adopted to predict the axial development of the wall temperature. Radial wise, the nodalization in the vicinity of the wall was instead refined in order to reach a y+ value smaller than 1 for the first cell next to the wall, as requested by the adopted low y$^+$ approach. The total cell count was about 20 thousand cells. A sample of the adopted nodalization is reported in Figure 3.

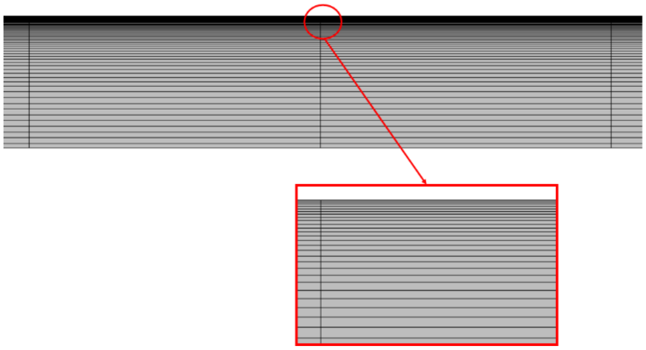

Fig. 3: Sample and near wall magnification of the adopted nodalization.

A uniform heat flux is assumed at the wall, conjugated heat transfer is thus neglected in similarity with other works in the available literature. Eventually thermodynamic properties for the supercritical CO_2 were provided by adopting the REFPROP10 tool (NIST package) and were implemented assuming that pressures drops were negligible, and pressure could be considered almost constant along the heated section.

V. Results

In the present section, the comparisons between the experimental data by Li et al. [6] and the predictions provided by the adopted turbulence model developed at the University of Pisa (here labeled as "Current UniPi Model) are reported. The predictions obtained adopting the Lien et al. [12] and the SST k-ω [18] are reported as well for the sake of comparison.

The selected conditions provide an attractive benchmark for the adopted turbulence model. Particularly, the operating pressures straddle between 7.60 and 8.81 MPa, (i.e., between 1.02 and 1.2 times the critical pressure) thus allowing for investigating the capabilities of the model in addressing different quantitative and qualitative properties trends transition from liquid-like to gas-like conditions. In addition, since the inlet temperatures are very close to the pseudo-critical temperature, all the addressed cases involve the crossing of the pseudo-critical threshold both in the wall and bulk. Eventually, because of the relatively low mass fluxes, buoyancy induced heat transfer deterioration is expected, thus allowing for further validation of the model against this class of heat transfer phenomena.

As can be observed, the proposed figures allow for drawing some general lessons.

The Lien et al. [12] k-ε model usually overestimates the wall temperature trend. Temperature increases dramatically since the beginning once the pseudo-critical temperature is exceeded at the wall. The model thus predicts a stronger heat transfer deterioration phenomenon compared to the addressed experimental conditions. In addition, it cannot predict any heat transfer recovery (or final restoration after deterioration see e.g., [19]). In fact, after a first peak, the wall temperature is stabilized for a while and then starts increasing again but with a milder slope, usually overestimating the experimental value by more than 20°C.

The SST k-ω, instead, usually predicts a single peak right at the beginning of the heated section and later moves towards normal/enhanced heat transfer, thus resulting in a global underestimation of the measured trends.

The predictions provided by the Lien et al. [12] k-ε and the SST k-ω are in accordance with the lessons drawn at the University of Pisa. In fact, k-ε models are usually observed to strongly overestimate deterioration and the wall temperature trends while the SST k-ω usually predicts improved heat transfer conditions, thus leading to wall temperature underestimations.

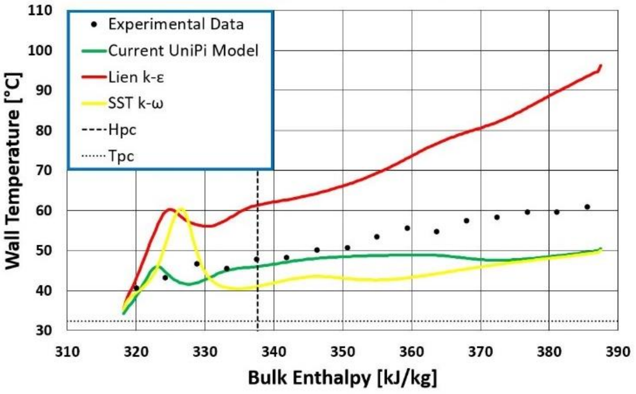

Fig. 4 CO_2 at a supercritical pressure of 7.60 MPa. Comparison between experimental data and CFD results for G= 162 kg/m^{2}s, q"= 14.14 kW/m^2, Tin=32.57°C.

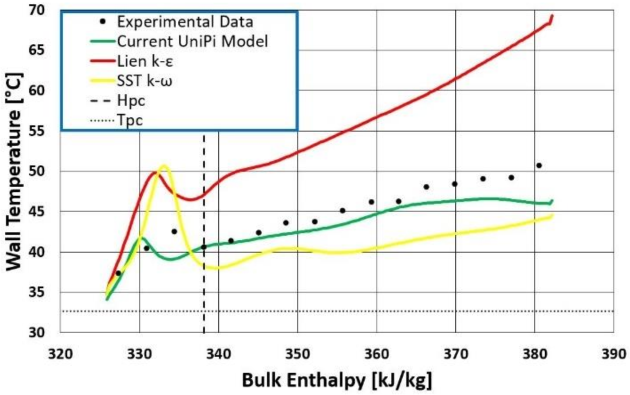

Fig. 5 CO_2 at a supercritical pressure of 7.67 MPa. Comparison between experimental data and CFD results for G= 129.2 kg/m^{2}s, q"= 9.16 kW/m^2, Tin=32.56°C.

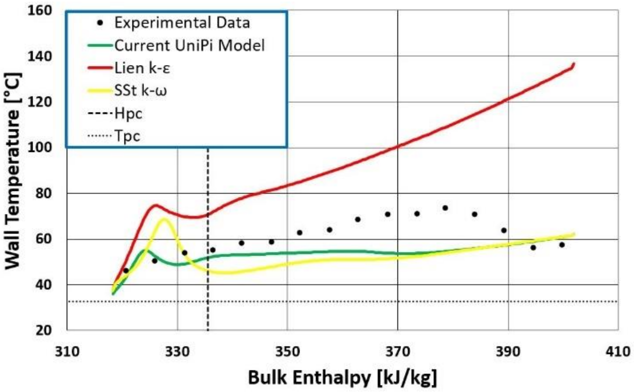

Fig. 6 CO_2 at a supercritical pressure of 7.68 MPa. Comparison between experimental data and CFD results for G= 183.1 kg/m^{2}s, q"= 19.31 kW/m^2, Tin=32.45°C.

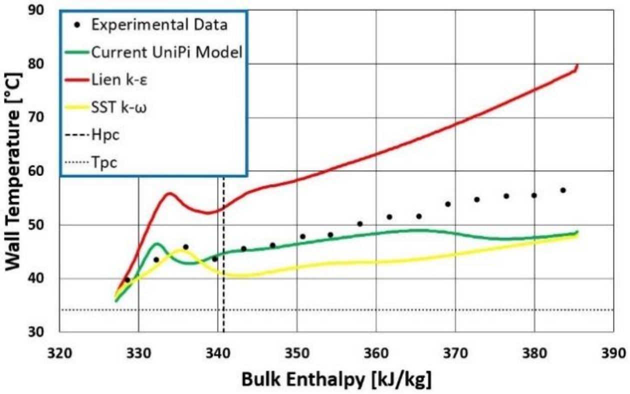

Fig. 7 CO_2 at a supercritical pressure of 7.91 MPa. Comparison between experimental data and CFD results for G= 145.6 kg/m^2s, q"= 10.68 kW/m^2, Tin=33.8°C.

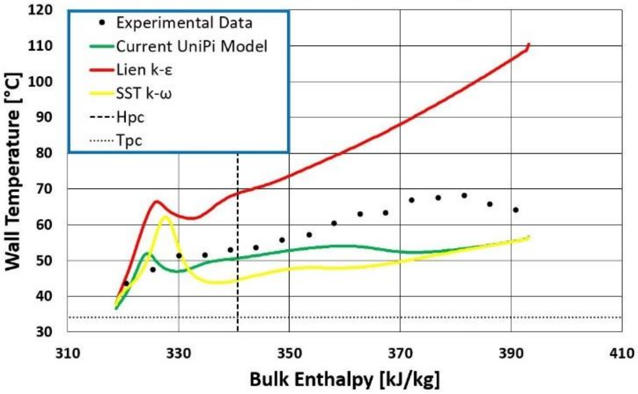

Fig. 8 CO_2 at a supercritical pressure of 7.91 MPa. Comparison between experimental data and CFD results for G= 170.9 kg/m^2s, q"= 16.02 kW/m^2, Tin=33.5°C.

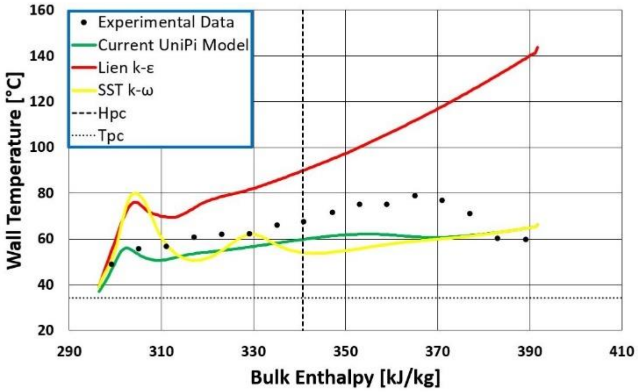

Fig. 9 CO_2 at a supercritical pressure of 7.91 MPa. Comparison between experimental data and CFD results for G= 198.8 kg/m^2s, q"= 23.83 kW/m^2, Tin=31.7°C.

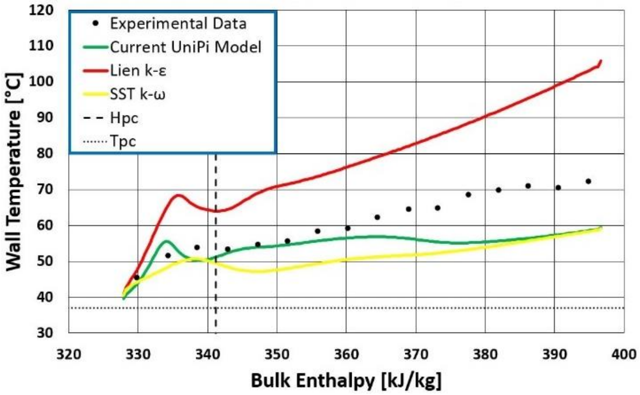

Fig. 10 CO_2 at a supercritical pressure of 8.45 MPa. Comparison between experimental data and CFD results for G= 164.1 kg/m^2s, q"= 14.21 kW/m^2, Tin=36.35°C.

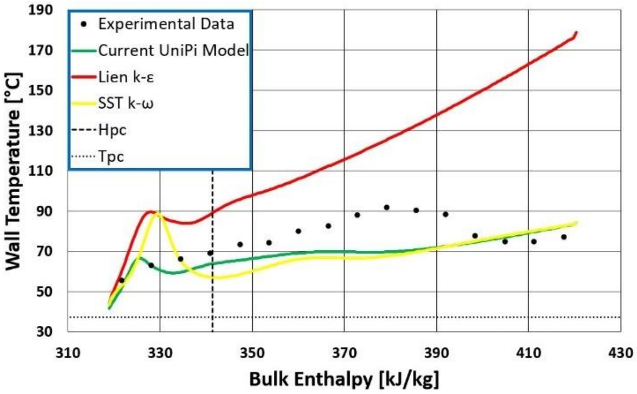

Fig. 11 CO_2 at a supercritical pressure of 8.49 MPa. Comparison between experimental data and CFD results for G= 189.9 kg/m^2s, q"= 24.25 kW/m^2, Tin=35.885°C.

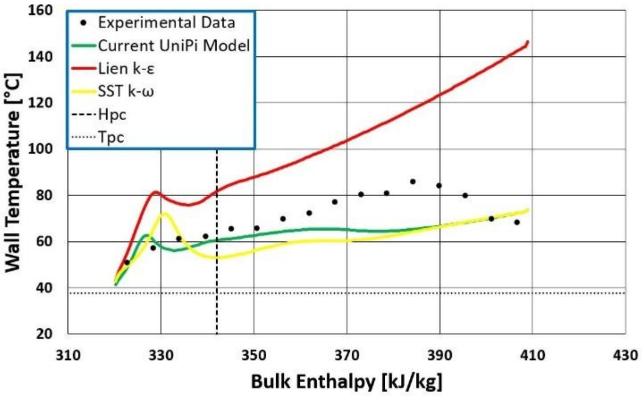

Fig. 12 CO_2 at a supercritical pressure of 8.59 MPa. Comparison between experimental data and CFD results for G= 182.9 kg/m^2s, q"= 20.43 kW/m^2, Tin=36.385°C.

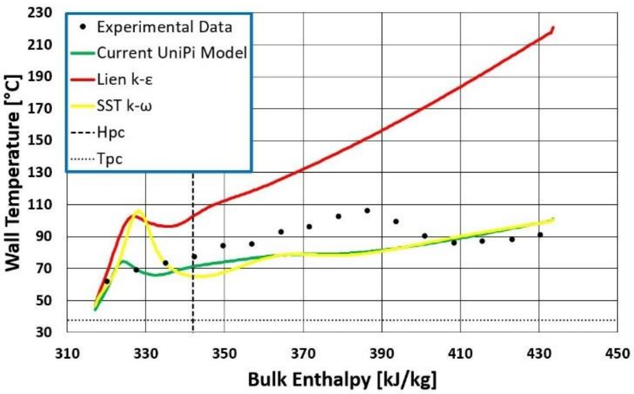

Fig. 13 CO_2 at a supercritical pressure of 8.73 MPa. Comparison between experimental data and CFD results for G= 200.5 kg/m^{2}s, q"= 29.43 kW/m^2, Tin=36.6°C.

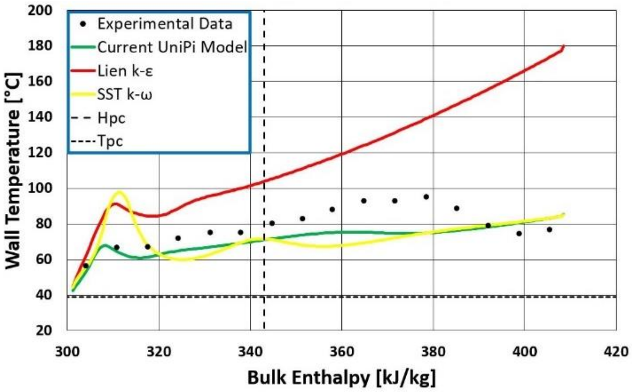

Fig. 14 CO_2 at a supercritical pressure of 8.81 MPa. Comparison between experimental data and CFD results for G= 207.4 kg/m^{2}s, q"= 28.03 kW/m^2, Tin=34.8°C.

The model developed at the University of Pisa usually provides the best estimations especially for the first part of the heated section; after the recovery phase, instead, the prediction turns to be closer to the one provided by the SST k-ω model, probably owing to the good heat transfer capabilities predicted by both the models in that very region. The obtained improved predictions are mainly due to the use of AHFM for the estimation of the turbulent heat flux contributions and of the buoyancy turbulence production terms. The model is indeed able to predict sufficiently well the initial wall temperature increase, also reporting a small wall temperature peak. On the other hand, after the initial deterioration phase, the model seems to predict an early recovery phase thus predicting lower wall temperature trends with respect to the experimental values in the second half of the test section. The observed discrepancies are especially larger for higher pressures and heat fluxes. This is probably to be connected with a highly strong predicted impact of buoyancy phenomena that after the initial deterioration, may impact positively on heat transfer eventually leading to heat transfer recovery and wall temperature decrease.

VI. Conclusion

The performed analyses allow to understand and test the limits and capabilities of the selected turbulence models on a new set of experimental data. The considered operating conditions are indeed very interesting since they address a sufficiently wide range of operating pressure. In addition, the fluid exceeds the pseudo-critical threshold both at the wall and in bulk thus providing room for the occurrence of different heat transfer phenomena. While the selected k-ε and k-ω models provide limited results, reporting respectively strong overestimations and underestimations of the experimental trends, the UniPi model allowed for improved predictions. This is mainly due to the use of AHFM to predict the turbulent heat flux contributions and the buoyancy production trends. While improvements are definitively needed before claiming a sufficiently good prediction is achieved, the AHFM is confirmed to be a sound tool to be considered for the improvement of numerical predictions of heat transfer when adopting the RANS approach. In future studies, the set of parameters adopted by the UniPi model will be updated trying to improve the quality of the predictions of this model both in the presently considered experimental data set and against other experimental results.

Acknowledgments

Siemens is gratefully acknowledged for making this work possible by releasing the STAR-CCM + code.

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