

LESSONS LEARNED FROM THE APPLICATION OF CFD MODELS IN THE PREDICTION OF HEAT TRANSFER TO FLUIDS AT SUPERCRITICAL PRESSURE

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Abstract

Based on previous and recent work on the subject, the paper summarizes the results obtained in the assessment of various CFD codes and models against experimental data related to heat transfer with fluids at supercritical pressure. The aim of the work is to summarise the lessons learned in this regard, drawing conclusions about model suitability. The results discussed address different codes, models, fluids and geometrical conditions. In particular, experiments with both water and carbon dioxide are considered, the FLUENT and the STAR-CCM+ commercial codes were used together with two different in-house codes adopting different k - ϵ , k - ω and k - τ models. Experimental data related to circular and non-circular ducts are addressed.

1. Introduction

Heat transfer to supercritical fluids represents an important issue for the design of new generation nuclear reactors, making use of supercritical fluids as primary or secondary coolant. Models for the analysis of heat transfer and fluid dynamics are required for application in the prediction of the complex phenomena occurring owing to the changes of properties exhibited at the transition across the pseudo-critical temperature and even before this threshold. Heat transfer, in particular, shows phenomena of enhancement and deterioration that must be carefully considered with a view to keeping the surface temperature of heater rods of a nuclear reactor within reasonable limits.

Reviews of experimental data available for comparison with models and engineering correlations have been published in recent years [1-3], with the aim of providing a sound basis for designing Generation IV reactors involving supercritical fluids. Actually, interesting studies in relation to heat transfer deterioration because of buoyancy or acceleration effects were performed decades ago [4-11]; this interesting body of older data is presently reconsidered in the new perspective of the present needs for nuclear reactor design, together with updated information being provided by recent studies (see e.g., [12-16]), for refining or validating engineering correlations and CFD models (see e.g., [18-23]).

The Universities of Manchester, Aberdeen and Pisa cooperated in the last years in an effort devoted to assessing presently available CFD codes against relevant experimental data [23-26]. Various low-Reynolds models implemented in in-house and also commercial codes were considered, reaching meaningful conclusions about the present state-of-the-art in the field. The cooperation is still ongoing and producing new data to be provided to the scientific community in order to establish the present needs in terms of model improvement.

The conclusions reached so far in the research are reported here to try to highlight the relevant lessons learned.

2. Pis'menny et al. (2006) data for supercritical water

A purposely developed in-house code was applied by Sharabi [24-25] in the prediction of experiments conducted by Pis'menny et al. [12] at the National Technological University of Ukraine. The experiments investigated turbulent heat transfer in vertical circular tubes for water in a gas-like state or affected by mixed convection in both upward and downward flows, at an operating pressure of 23.5 MPa. The test section was made by thin stainless steel tubes with an inner diameter of 6.26 mm. Uniform heating by direct or alternating electric current was used and thermocouples were placed at the inlet and the outlet of the tube and along its outer surface to measure fluid and wall temperatures.

The in-house code adopted solved the flow balance equations by different two-equation RANS models in axi-symmetric geometry using the finite volume technique. The turbulence models used were: the k - ϵ models by Jones and Launder (JL) [27], Launder and Sharma (LS) [28], Lam and Bremhorst (LB) [29], Chien (CH) [30], Yang and Shih (YS) [31], Abe, Kondoh and Nagano (AKN) [32], the k - ω model by Wilcox (WI) [33] and the k - τ model by Speziale (SP) [34].

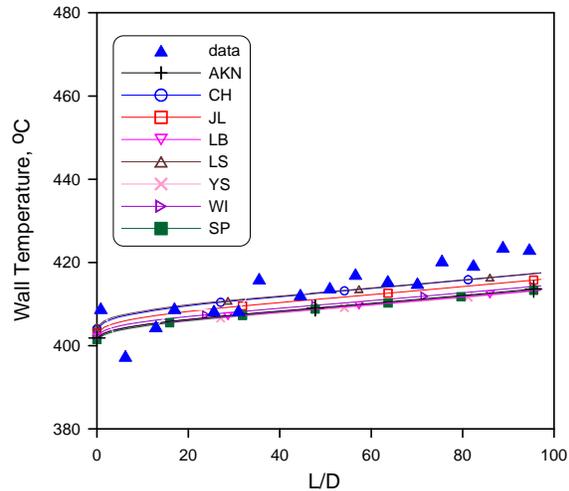
Figure 1 reports the typical behaviour shown by the models considered. In particular, the following considerations can be drawn from the presented data and the complete analysis is reported in references [24-25]:

- all the models considered are reasonably able to simulate the observed heat transfer conditions in downward flow and in upward flow at low heat flux to mass flux ratio;
- the k - ϵ models are able to detect the occurrence of heat transfer deterioration when the wall temperature exceeds the pseudo-critical value; nevertheless, they tend to overestimate the wall temperature after deterioration, over-responding to the decrease in turbulence kinetic energy, and, furthermore, do not show a sufficient recovery after the temperature peak;
- the k - ω and k - τ models exhibit a lower ability to capture deterioration, though the latter model does show deterioration, but very much delayed along the pipe length.

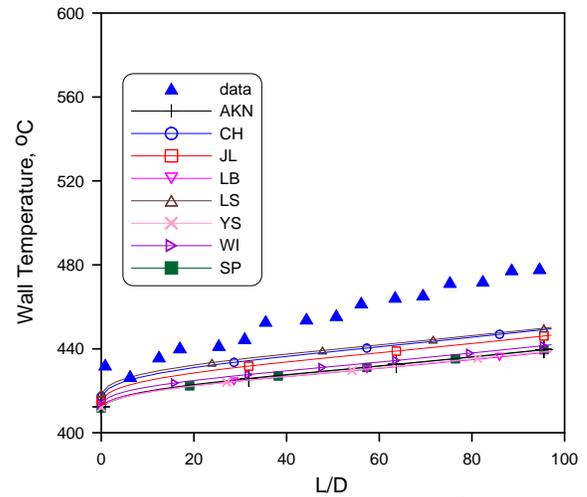
As it will be shown later on, this situation is characteristic of the capabilities of models currently available and has been confirmed in the analysis of other data, with different fluids and geometries. The impression is that k - ϵ models have to differing extents the right ingredients for predicting deterioration, though with a consistent overestimation of this effect.

In relation to the causes at the root of the observed behaviour, it was noted that deteriorated heat transfer is predicted to be induced by laminarisation consequent to a decreased turbulence production by shearing. This is clearly shown in Figure 2, where the axial and radial distributions of velocity and turbulence kinetic energy are reported; it can be noted that the distortion of the velocity profile from the classical forced flow to mixed convection has a corresponding effect on turbulent kinetic energy, causing a big drop in its values close to the wall. This is at the root of heat transfer deterioration, shown in the corresponding plot of wall temperature in Figure 1f.

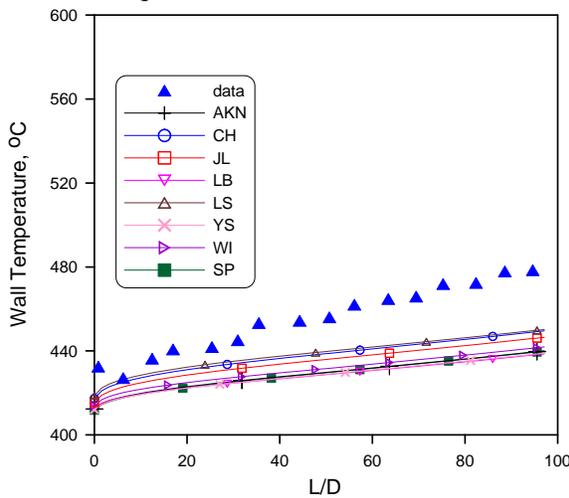
The same data were the subject of analyses by different models implemented in the STAR-CCM+ code [35-36]. The results showed that the V2F [37] model has also a response similar to the ones of the low Reynolds number k - ϵ models considered (Figure 3a,b); expectedly, models making use of wall functions (as the "All y^+ " one), are not able to reproduce the onset of deterioration. On the other hand, the standard "low-Re" k - ϵ model implemented in the code [38] produced results similar to the ones observed from other similar models.



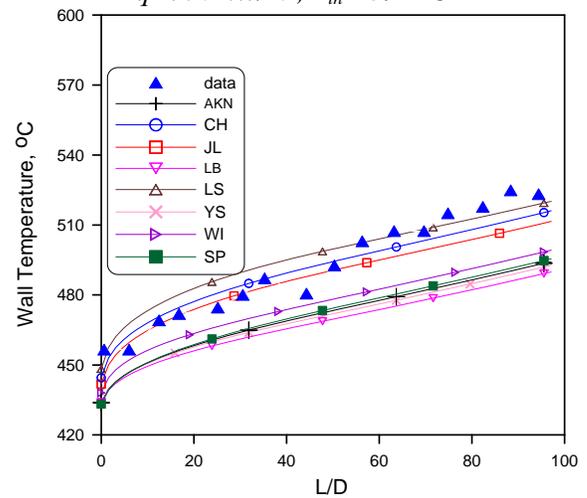
a) upward flow, $G=2193 \text{ kg}/(\text{m}^2\text{s})$,
 $q=433 \text{ kW}/\text{m}^2$, $T_{in}=391 \text{ }^\circ\text{C}$



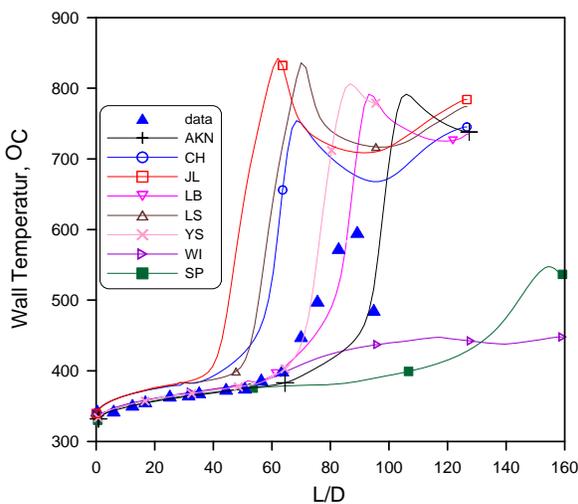
b) upward flow, $G=2193 \text{ kg}/(\text{m}^2\text{s})$,
 $q=750 \text{ kW}/\text{m}^2$, $T_{in}=391 \text{ }^\circ\text{C}$



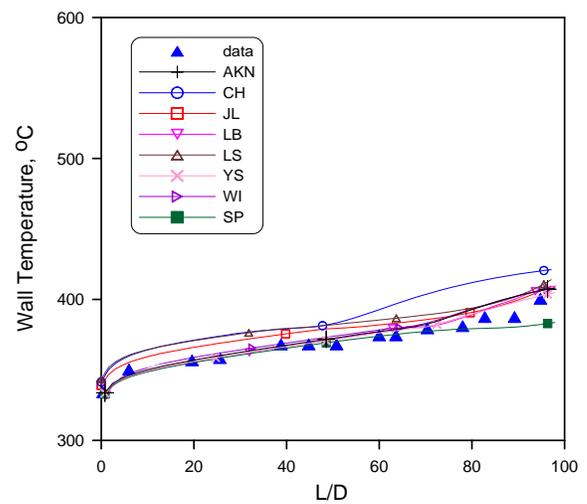
c) upward flow, $G=2193 \text{ kg}/(\text{m}^2\text{s})$,
 $q=750 \text{ kW}/\text{m}^2$, $T_{in}=391 \text{ }^\circ\text{C}$



d) upward flow, $G=2193 \text{ kg}/(\text{m}^2\text{s})$,
 $q=1172 \text{ kW}/\text{m}^2$, $T_{in}=393 \text{ }^\circ\text{C}$



e) upward flow, $G=509 \text{ kg}/(\text{m}^2\text{s})$,
 $q=390 \text{ kW}/\text{m}^2$, $T_{in}=300 \text{ }^\circ\text{C}$



f) downward flow, $G=509 \text{ kg}/(\text{m}^2\text{s})$,
 $q=390 \text{ kW}/\text{m}^2$, $T_{in}=300 \text{ }^\circ\text{C}$

Figure 1. Typical results obtained for Pis'menny et al. (2006) data by an in-house code [24]

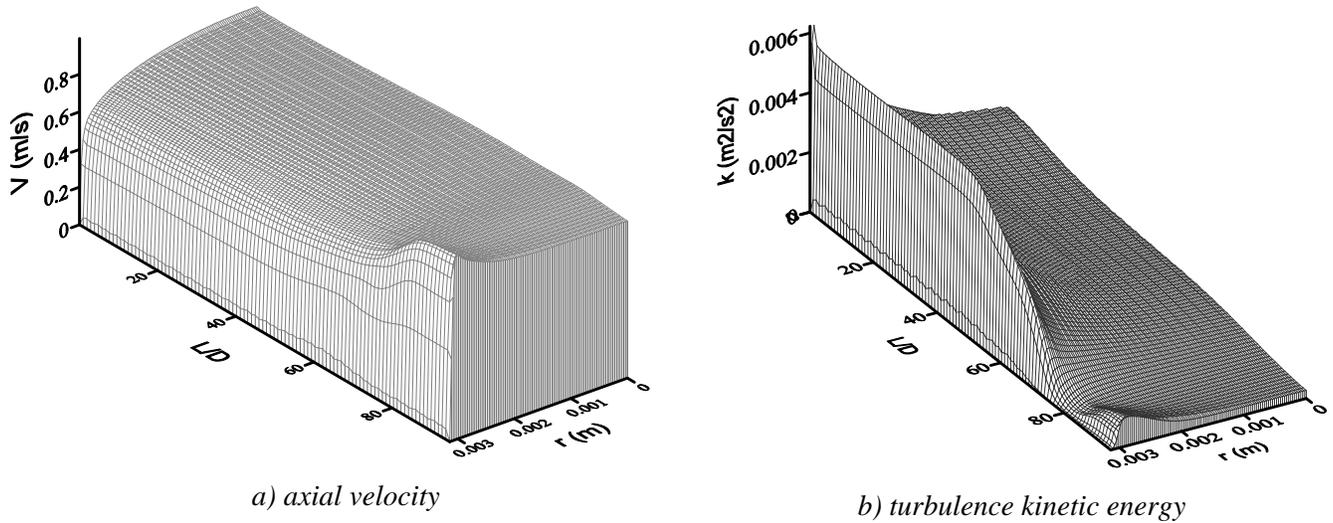
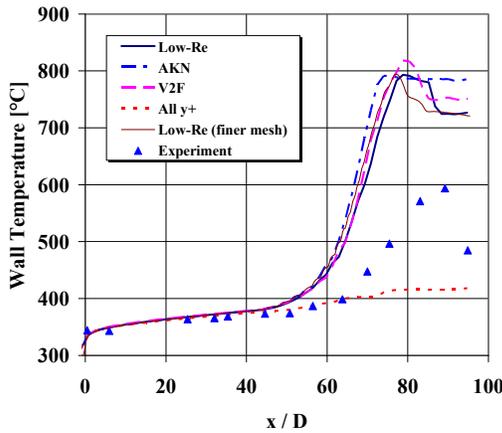
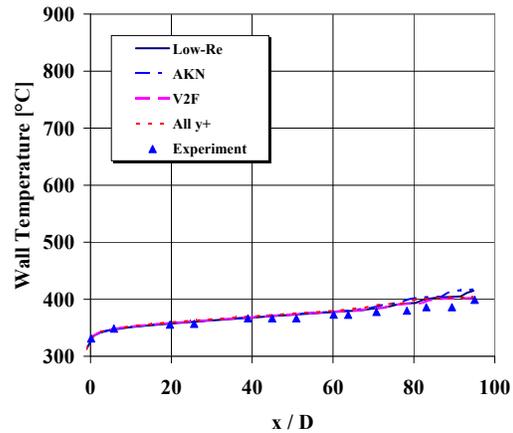


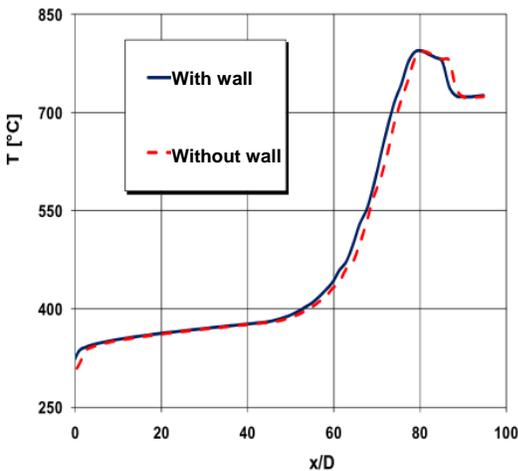
Figure 2. Axial and radial distribution of velocity and kinetic energy for the case in Figure 1f (Yang and Shih model, upward flow, $G=509 \text{ kg}/(\text{m}^2\text{s})$, $q=390 \text{ kW}/\text{m}^2$, $T_{in}=300 \text{ }^\circ\text{C}$) [24]



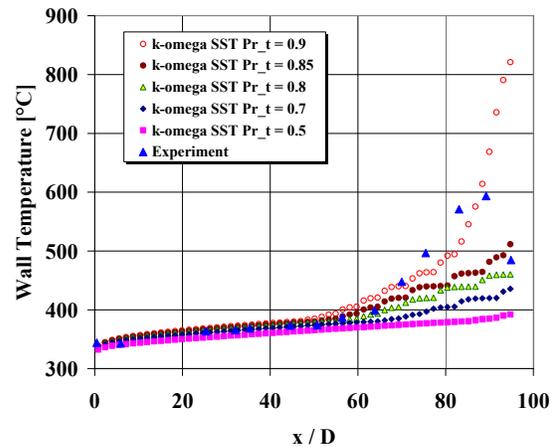
a) $q=390 \text{ kW}/\text{m}^2$, $G= 509 \text{ kg}/(\text{m}^2\text{s})$, $T_{in}=300 \text{ }^\circ\text{C}$, upward flow [35]



b) $q=390 \text{ kW}/\text{m}^2$, $G= 509 \text{ kg}/(\text{m}^2\text{s})$, $T_{in}=300 \text{ }^\circ\text{C}$, downward flow [35]



c) $q=390 \text{ kW}/\text{m}^2$, $G= 509 \text{ kg}/(\text{m}^2\text{s})$, $T_{in}=300 \text{ }^\circ\text{C}$, upward flow [39]



d) $q=390 \text{ kW}/\text{m}^2$, $G= 509 \text{ kg}/(\text{m}^2\text{s})$, $T_{in}=300 \text{ }^\circ\text{C}$, upward flow

Figure 3. Results obtained by the STAR-CCM+ code for Pis'menny et al. (2006) data

Later analyses on the same data by STAR-CCM+ showed that the inclusion of a model for the wall was relatively ineffective in improving the predicted behaviour [39], shedding light on the minor effect played by axial heat conduction along the wall on wall temperature (Figure 3c). Finally, a recent application to the same data of the SST $k-\omega$ model [40] produced relatively poor results and a strong influence of the assumed turbulent Prandtl number, which was not noted with other models (Figure 3d).

3. Kim et al. (2005) data for supercritical carbon dioxide

Kim et al. [13] made use of carbon dioxide at 8 MPa in a 1.2 m long test section heated by DC current and preceded by an adiabatic section of 0.8 m. The flow was upward and conditions of aided mixed convections were established in the channel. The geometry of the tubes varied, including circular, triangular and square cross section pipes with hydraulic diameters of 7.8, 9.8 and 7.9 mm, respectively, made of Inconel 625 with a thickness of 1 mm. Thermocouples were silver-soldered on the outer pipe surface every 30 mm along the heated length. The experimental conditions addressed in the simulations [25] involve an inlet temperature of 15 °C, a mass velocity of 314 kg/m²s and heat fluxes of 20, 23 and 30 kW/m². The obtained results are shown in Figure 4 and Figure 5.

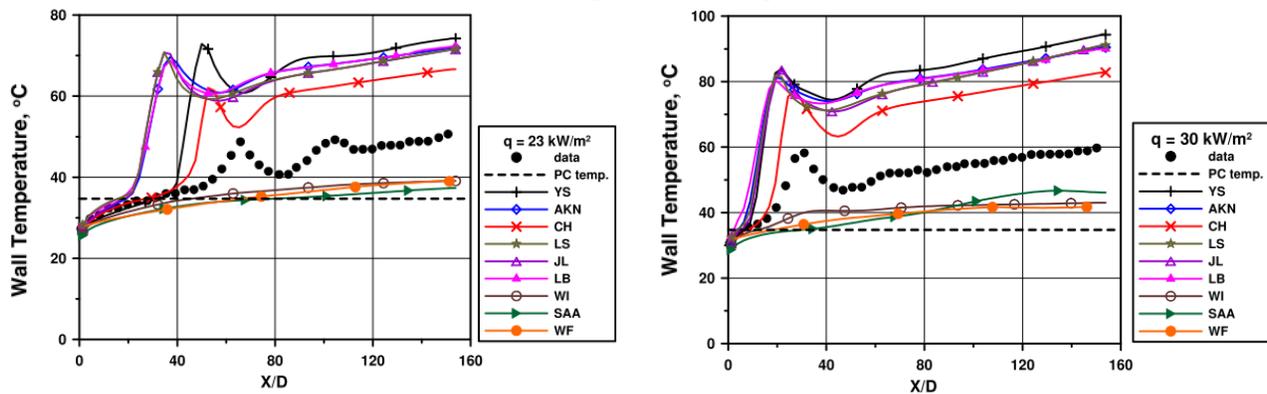
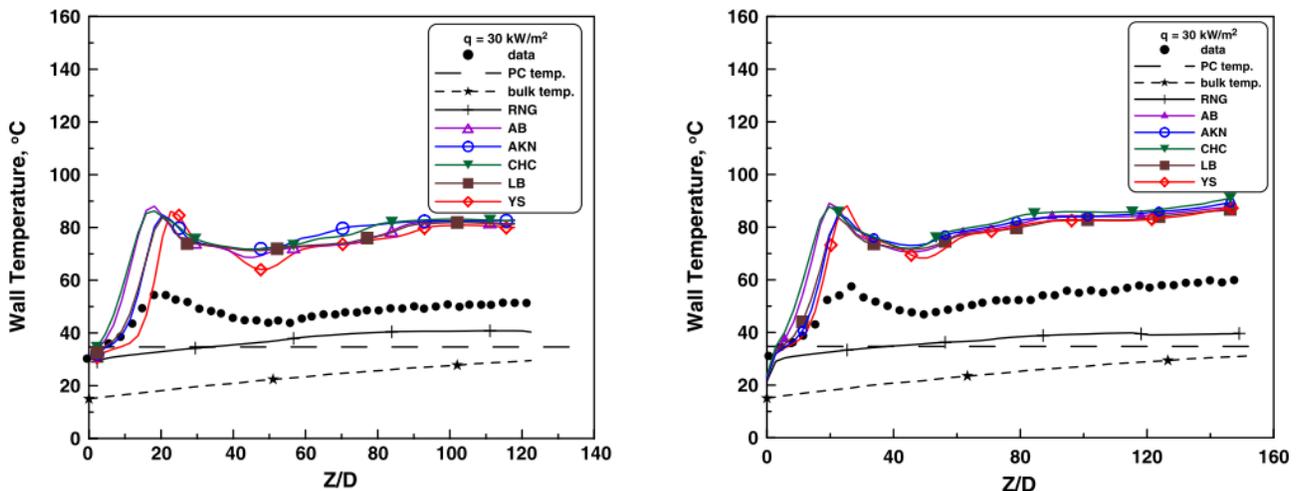


Figure 4. Results obtained by an in-house code for Kim et al. (2005) circular tube data [25]



a) triangular channel

b) square channel

Figure 5. Results obtained by the FLUENT code for Kim et al. (2005) non-circular tube data [26]

It can be noted that the use of an in-house code and FLUENT [41] confirmed previous findings about the capability of k - ϵ models in predicting heat transfer deterioration even in 3D conditions and with a different fluid, but sometimes with a marked overestimate of wall temperature. The conclusions were extended also to other low-Re models (as the Cheng et al. [42] model, CHC; note that SAA has the same meaning as SP in previous plots). The intrinsic incapability of wall functions (the case labelled RNG since this k - ϵ model was used in the bulk fluid) in detecting deterioration phenomena and the poor behaviour of the k - ω and k - τ models were also confirmed.

4. Watts (1980) data for supercritical water

Watts data [11] are the subject of an extensive work [43-46] being carried out in the frame of the IAEA CRP on "Heat Transfer Behaviour and Thermo-hydraulics Codes Testing for SCWRs". The interest of these data is in the broad range of conditions over which they were obtained, involving both upward and downward flow and showing deteriorated heat transfer also at temperatures well below the pseudo-critical one. In this respect, these data added an interesting contribution to the understanding of model behaviour.

Watts' experiments were conducted in a uniformly heated pipe, having a diameter of 25.4 mm and length of 2 m. A unheated length of 0.78 m was located upstream the test section. The operating pressure of the fluid was 25 MPa and the heat flux ranged from 175 to 400 kW/m², with values of the inlet temperature equal to 150, 200, 250, 300 °C and inlet mass fluxes from 200 to 1000 kg/(m²s). A natural circulation loop was used to produce the flow and the test section was heated by electrical current. The inside tube temperatures were inferred by the measurement of the outside surface values, considering heat conduction in the pipe wall.

In a first phase of the work [23, 43], the data were simulated extensively by the SWIRL code [44], allowing to test the performance of the Yang and Shih [31], the Abe, Kondo and Nagano [32] and the Launder and Sharma [32] models. This revealed again a general capability of these k - ϵ models to quantitatively reproduce deteriorated heat transfer in upward flow at temperatures lower than the pseudo-critical one (see e.g., Figure 6). Considering the previous experience, obtained mainly in comparison with deteriorated conditions across the pseudo-critical threshold, this finding represented an interesting additional information. Despite the encouraging behaviour shown by models in such cases, quantitative inadequacies are still present even under non-deteriorated conditions related to upward flows, indicating an incomplete description of turbulence effects; as already noted, downward flow seemed easier to reproduce (Figure 7).

An interesting conclusion from the work is indicated by the results in Figure 8, which show a general deterioration of heat transfer in upward flow, with respect to pure forced convection conditions (calculated assuming zero gravity), and a general enhancement in downward flow. The work also confirmed the overestimation of wall temperature in deteriorated heat transfer cases in which the fluid temperature is crossing the pseudocritical threshold. A partial comparison of the results from SWIRL with those obtained by the STAR-CCM+ and the FLUENT codes, with available k - ϵ models, confirmed these findings (Figure 9 and Figure 10), motivating a thorough application of these codes.

At the time of writing, the work of systematic application of these two commercial codes is close to completion [45-46]. Some relevant results obtained by STAR-CCM+ are reported in Figure 11 and Figure 12, confirming that k - ϵ models are capable of providing quantitatively correct estimates of wall temperature for deteriorated heat transfer for temperatures below the pseudo-critical value, while the agreement is much worse when this limit is exceeded. On the other hand, the SST k - ω model [40] seems unable to even detect the onset of deterioration in the cases addressed. Similar conclusions are reached using FLUENT, as shown in Figure 13, which illustrates again the typical behaviour of k - ϵ models in predicting deterioration with wall temperatures below the pseudo-critical temperature.

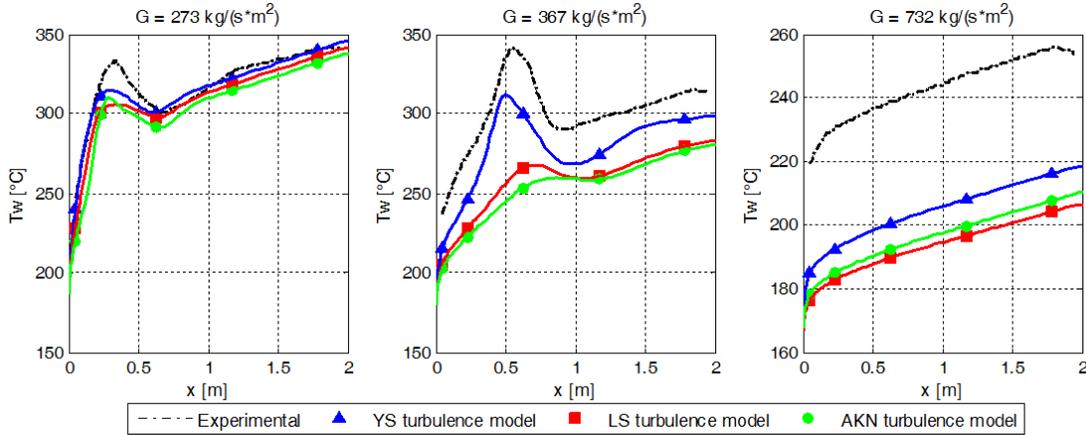


Figure 6. Comparison between experimental and calculated inner wall temperature for Watts (1980) data obtained by the SWIRL code with different turbulence models [23] ($q = 255 \text{ W}/\text{m}^2$, $T_{in} = 150^\circ\text{C}$, upward flow)

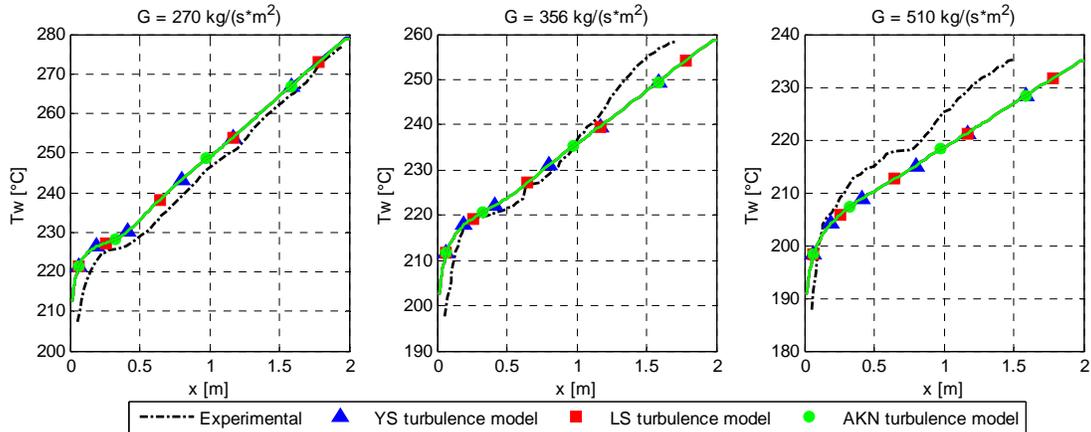


Figure 7. Comparison between experimental and calculated inner wall temperature for Watts (1980) data obtained by the SWIRL code with different turbulence models [23] ($q = 255 \text{ W}/\text{m}^2$, $T_{in} = 150^\circ\text{C}$, downward flow)

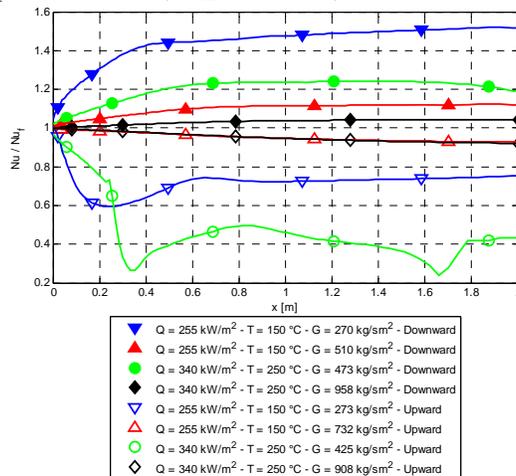


Figure 8. Ratio of the Nusselt numbers for upward or downward flow to the one for pure forced convection for Watts (1980) data, calculated by SWIRL with the YS turbulence model [23]

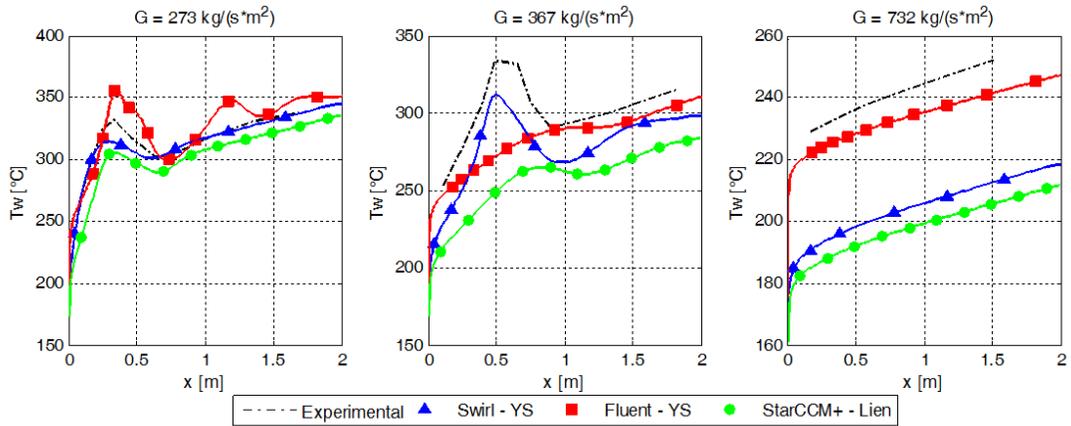


Figure 9. Comparison between experimental and calculated inner wall temperature for Watts (1980) data obtained by different codes ($q = 255 \text{ W/m}^2$, $T_{in} = 150^\circ\text{C}$, upward flow) [23]

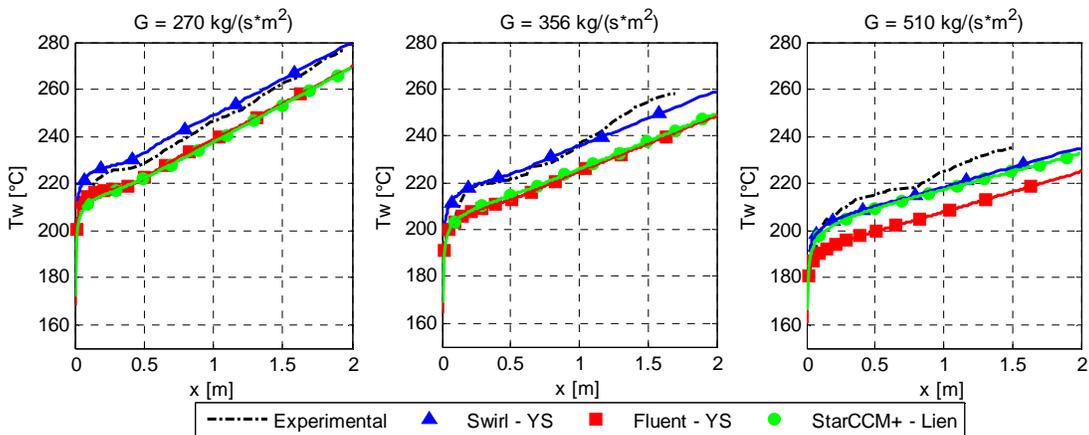


Figure 10. Comparison between experimental and calculated inner wall temperature for Watts (1980) data obtained by different codes ($q = 255 \text{ W/m}^2$, $T_{in} = 150^\circ\text{C}$, downward flow) [23]

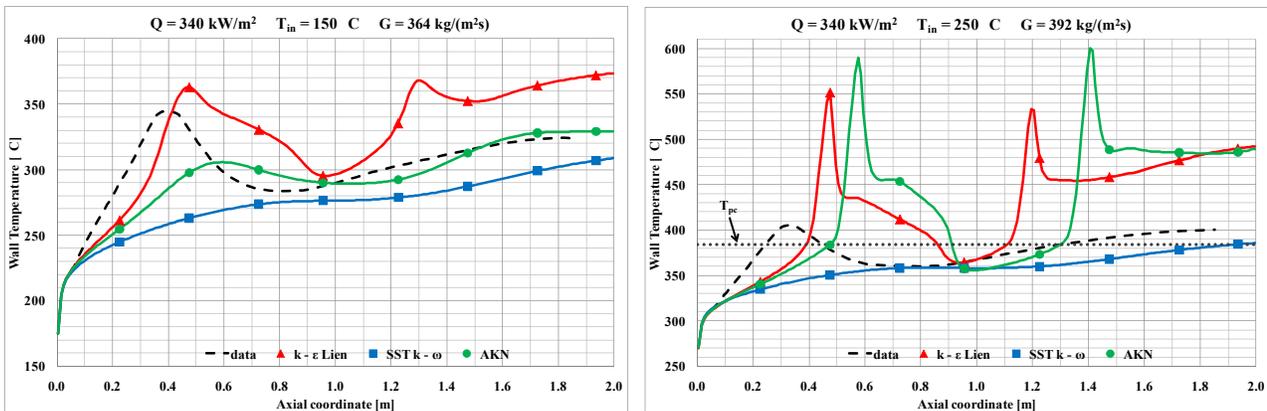


Figure 11. Comparison between experimental and calculated inner wall temperature obtained by the STAR-CCM+ code with different models for upward flow [45]

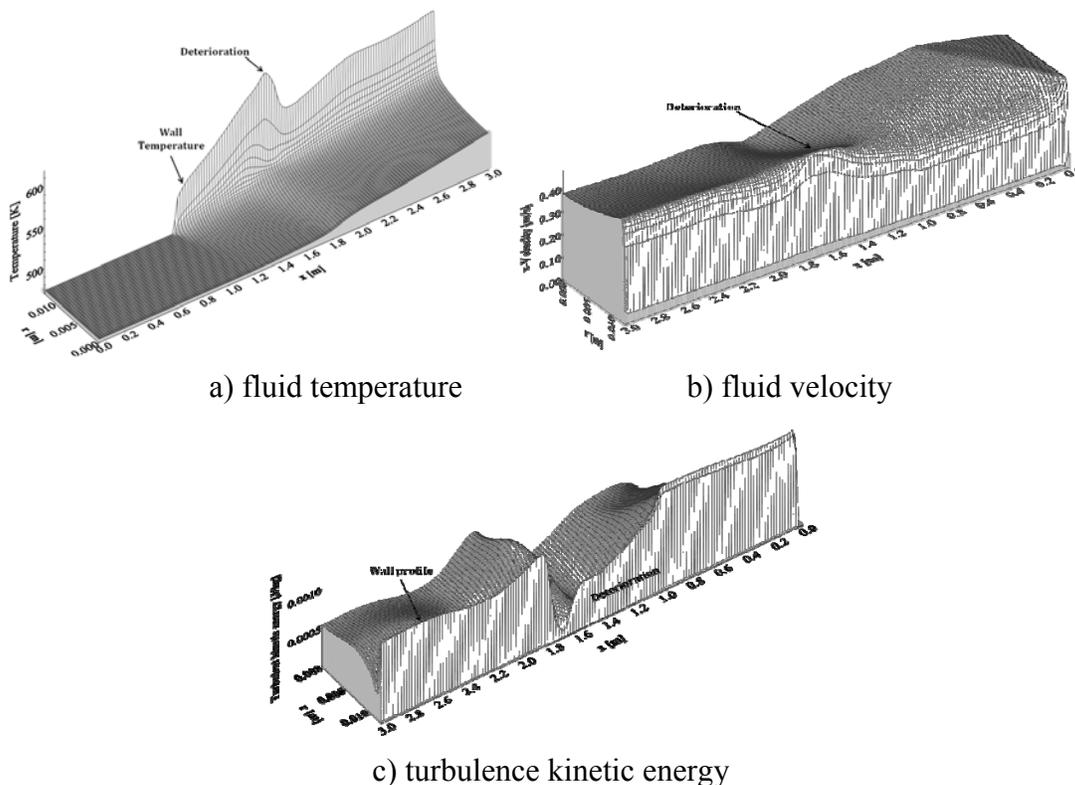


Figure 12. Radial and axial distributions of fluid temperature, velocity and turbulent kinetic energy along the channel as evaluated by STAR-CCM+ with standard Low-Re $k-\epsilon$ model (upward flow, $q=250 \text{ W/m}^2$, $T_{in} = 200 \text{ }^\circ\text{C}$, $G = 340 \text{ kg/(m}^2\text{s)}$) [45]

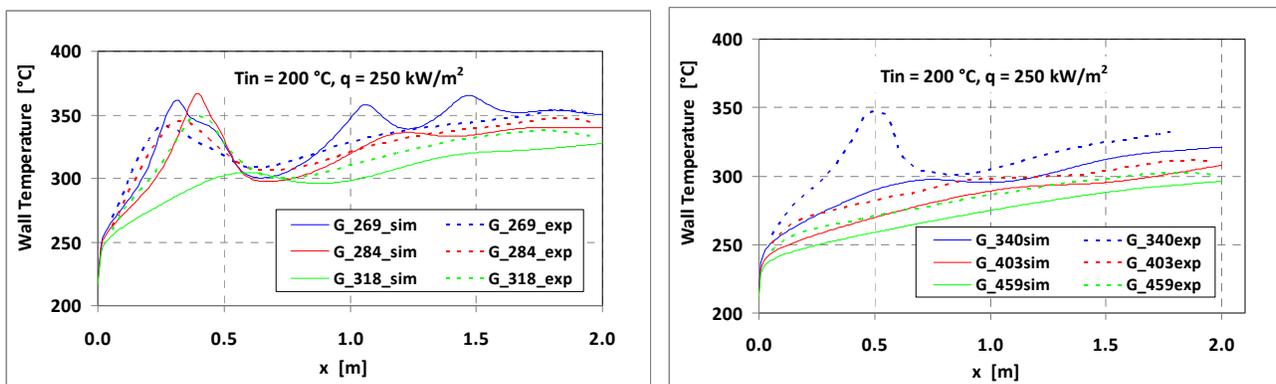


Figure 13. Comparison between experimental and calculated inner wall temperature obtained using the FLUENT code with the YS model for upward flow [46]

5. Conclusions

The work jointly performed by the Universities of Manchester, Aberdeen and Pisa in the frame of their cooperation, starting with the PhD study of Medhat Sharabi [25] and continuing with the joint co-tutoring of MSc and BSc students, has addressed a broad range of operating conditions. The result of this work is a meaningful picture concerning the present capabilities of CFD models in predicting heat transfer to supercritical fluids, clearly showing the areas requiring further improvement.

In particular, it was found that:

- low-Re k - ϵ models generally have good capability in reproducing deteriorated heat transfer when the wall temperatures are below the pseudo-critical threshold; the mechanism acting in this case is clearly the laminarisation due to the reduction of turbulence production by shearing associated with the effects of buoyancy on the radial velocity profile;
- the major flaw exhibited by k - ϵ models is that they overestimate observed wall temperature when deterioration occurs with the temperature exceeding the pseudo-critical value at the wall and in the boundary layer; also in this case, the mechanism causing deterioration is mainly laminarisation, accompanied and made even worse by the sharp changes in fluid properties near the wall;
- the reproduction of heat transfer in non-deteriorated cases by k - ϵ models is sometimes excellent and sometimes poor; the reasons for this inconsistent behaviour are not completely understood and require further investigation concerning the details of the model assumptions adopted;
- on the other hand, within the limits of the analyses performed, k - ω models were not found to be effective enough in reproducing heat transfer deterioration; this conclusion will be better supported by work to be performed with more direct comparison with published data in which the SST k - ω model was found to have better performance [20].

A further valuable result of the studies made by the three Universities in cooperation is the involvement of young students and researchers in joint work on these fascinating and challenging aspects of heat transfer in support to the design of Generation IV reactors.

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