SENSITIVITY ANALYSIS OF CFD CODE FLUENT-12 FOR SUPERCRITICAL WATER IN VERTICAL BARE TUBES

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Summary

The ability to use FLUENT 12 or other CFD software to accurately model supercritical water flow through various geometries in diabatic conditions is integral to research involving coal-fired power plants as well as Supercritical Water-cooled Reactors (SCWR). The cost and risk associated with constructing supercritical water test loops are far too great to use in a university setting. Previous work has shown that FLUENT 12, specifically realizable k-ε model, can reasonably predict the bulk and wall temperature distributions of externally heated vertical bare tubes for cases with relatively low heat and mass fluxes. However, sizeable errors were observed for other cases, often those which involved large heat fluxes that produce deteriorated heat transfer (DHT) regimes.

The goal of this research is to gain a more complete understanding of how FLUENT 12 models supercritical water cases and where errors can be expected to occur. One control case is selected where expected changes in bulk and wall temperatures occur and they match empirical correlations' predictions, and the operating parameters are varied individually to gauge their effect on FLUENT's solution. The model used is the realizable k-ε, and the parameters altered are inlet pressure, mass flux, heat flux, and inlet temperature.

1. Introduction

In the 1950s, the idea of using supercritical water appeared to be rather attractive for thermal power industry. The objective was increasing the total thermal efficiency of coal-fired power plants. At supercritical pressures there is no liquid-vapour phase transition; therefore, there is no such phenomenon as Critical Heat Flux (CHF) or dryout. Only within a certain range of parameters a deteriorated heat transfer may occur. Work in this area was mainly performed in the former USSR and in the USA in the 1950s – 1980s [1].

In general, the total thermal efficiency of modern thermal power plants with subcritical-parameters steam generators is about 36 – 38%, but reaches 45 – 50% with supercritical parameters, i.e., with a "steam" pressure of 23.5 – 26 MPa and inlet turbine temperature of 535 – 585°C thermal efficiency is about 45% and even higher at ultra-supercritical parameters (25 – 35 MPa and 600 – 700°C)[1].

On the other hand, SCWRs are a concept being developed by Canada as part of Generation-IV International Forum (GIF), in which SCW is considered as a coolant. Canada's contribution to the Generation-IV nuclear-power reactors entails a CANDU-type reactor design utilizing horizontal pressure tubes and heavy water as a moderator. The main difference between Generation-III CANDU reactors and the new Generation-IV design is the use of SCW as a coolant. Use of a supercritical fluid requires higher pressures, but allows for higher outlet temperatures, and thus an increase in overall plant thermal efficiencies from the current 30-35% to possibly 45-50%

In addition, the main problem with empirical correlations and models developed to date is that only 1-D affects have been captured. Performing experiments that will accurately capture 3-D effects are very expensive; hence an alternative approach is needed. Computational Fluid Dynamics (CFD) studies have been performed in this area in attempts to determine various 3-D effects of heat and mass transfer within fuel sub-channels [2]. Most modeling experts in the nuclear industry support the approach of using CFD codes such as FLUENT to analyze 3-D effects[3][4][5]. However, the accuracy of CFD codes for SCW is not well known at this time [6]. A study on well-known experimental datasets is needed to verify the accuracy of CFD codes versus empirical correlations used for the same purpose.

Design of thermal plants requires knowledge of thermalhydraulic conditions existing within the heat transport system. To determine these conditions, an advanced toolset including CFD codes is necessary. The CFD code must be rigorously tested before it may be deemed accurate enough to be applied to plant simulations. CFD codes are routinely used in the industry in attempts to quantify flow effects at normal operating and accident-type scenarios[2], but none have been validated for use at supercritical conditions. In this paper, assessment of the capability of the CFD code FLUENT-12 to capture heat-transfer phenomena of SCW flowing through a vertical bare tube is performed with the specific objective to determine limitations and capabilities near the pseudocritical point.

2. Methodology

A dataset provided by Kirillov et al. from the Institute for Physics and Power Engineering (Obninsk, Russia) was used for this study [7]. The dataset was previously analyzed using many empirical correlations, where the Mokry et al. correlation showed the best fit within the given operating parameters [8]. FLUENT was also used in a previous analysis and it has shown reasonable predictions for bulk fluid and wall temperature profiles. However sizeable errors occurred for some cases, especially those in the deteriorated heat transfer regime.

Kirillov et al. experiments with SCW data can be used to benchmark the ability of the FLUENT code in solving heat- and mass-transfer problems within the supercritical region. These experiments consist of a 4-m long vertically-oriented tube of inner and outer diameters of 10 mm and 14 mm, respectively. The tube was made of stainless steel with an average surface roughness of 0.7 μm.

Supercritical water was pumped upwards through the test section at four different mass fluxes of 200, 500, 1,000 and 1,500 kg/m^{2}s. The test section was heated with an electrical current flowing through the tube wall. The heat flux was varied between 73 and 1,256 kW/m^2. All runs had an inlet pressure of 24±0.1 MPa. For each value of mass flux, the inlet temperature was varied so that the enthalpy increase along the heated length of the tube also varies. The inlet temperature was set to less than 25°C from the pseudocritical point in each test to capture specifics of approaching the pseudocritical point. Some of the low heat flux cases were modeled so that the pseudocritical point is located just upstream of the test-section outlet. Table 1 lists uncertainties in measured and calculated parameters.

Table 1: Uncertainties in Parameters [7]**.**

Parameter	**Maximum Uncertainty**
Test-section power	±1.0%
Inlet pressure	±0.25%
Wall temperature	±3.0%
Mass flow rate	±1.5%
Heat loss	≤3.0%

In order to clearly see where errors or unexpected changes in bulk and wall temperature distributions occur, an existing case will be selected and its parameters varied individually. For example, six calculations of the case will be performed with operating pressures increasing incrementally from 22 to 27 MPa while all other parameters remain constant. This will allow the effects that different pressures have on the calculations to be observed separately from others such as mass and heat fluxes. Previous work has shown the realizable k-ε model with a 2m mesh to most accurately reproduce experimental results. Therefore an existing case with a reasonable prediction by FLUENT-12 was chosen as a control case.

3. Numerical Results and Analysis

Many parameters were studied for the sensitivity analysis, but before starting the comparison, the effect of the convergence criteria had to be gauged. Best results were yielded with a convergence criteria of 10^{-6} for all residuals; Comparison between the wall and bulk fluid temperature distributions with convergence levels from 10^{-3} to 10^{-6} yielded no significant different between 10^{-4} and 10^{-6}, where the maximum deviation was about 1% as shown in Figure 1. This allows for studies to be conducted on a lower convergence level without sacrificing accuracy. By dropping the convergence by an order of magnitude, processing time could be reduced by hours per case which could be useful for mid-range computing power. High-end computing systems will experience less of improvement in computational time.

In order to understand FLUENT's response to different pressures in and around the supercritical region, a number of cases were solved with pressures ranging from 22 to 25 MPa. The temperature distributions along the wall as well as the bulk fluid temperature were plotted for each case. Figure shows the reduction in wall temperatures as the pressure is increased well beyond the critical point. This is due to the fact that the 22 and 23 MPa cases involved water which has already developed past the pseudocritical point and into the dense gas-like region. As a result the water in these regions has considerably low thermal conductivities which effectively insulate the inner surface of the tube, raising the temperatures dramatically.

An interesting effect observed is that once the pressure reaches 23.5 MPa, changes in the wall temperature distribution for subsequent pressures becomes minimal. This is likely due to the fact that very few changes occur in the properties of the water in the region which is past the critical point but before the pseudocritical point. From a design standpoint this shows that there is little benefit to increasing the pressure beyond 23.5 or 24 MPa in the proposed designs.

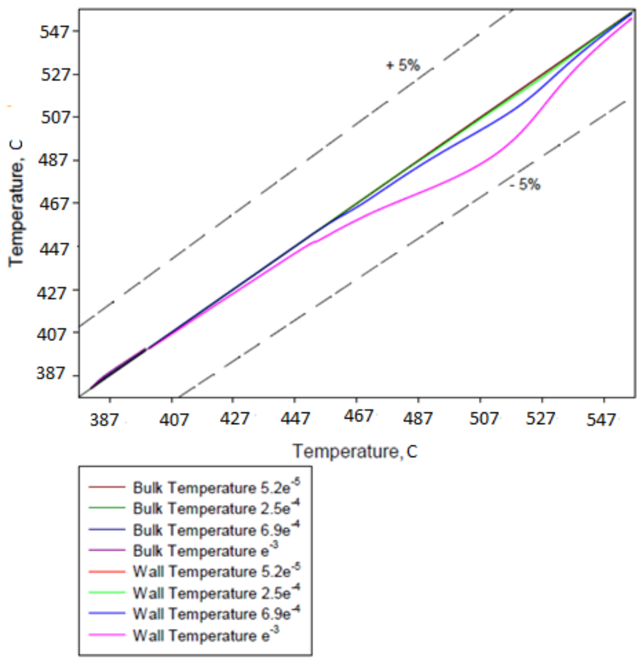

Figure 1: Comparison of various Convergence Criterions to a Convergence Criterion of e^-6

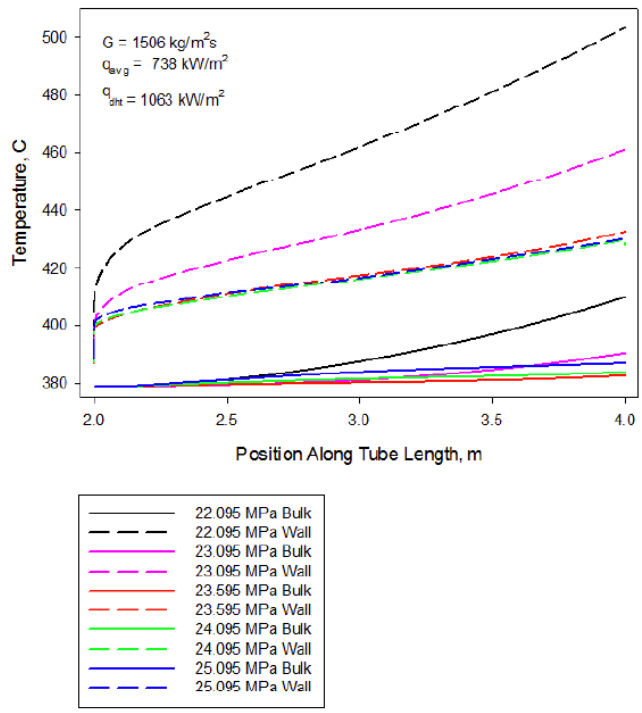

Figure 2: Bulk and Wall Temperature Distributions with Various Pressures

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While the wall temperature distributions calculated by FLUENT all produced similar shapes, the bulk temperature distributions were observed to be much different than one would expect. Figure 2shows a steadily increasing bulk temperature along the length of the tube for the 22 and 23 MPa cases but very different distributions for other pressures. This is unexpected as the very high wall temperatures for these cases would indicate that a lot of the heat was not transferred to the fluid. Furthermore, the bulk temperature for the 23.5 MPa case is observed to remain nearly the same throughout the tube while the 24 and 25 MPa cases initially increase but taper off three quarters of the way through the tube. One possible explanation of the results obtained is FLUENT's interpretation of the property changes, specifically the spike in specific heat, which occur in and around the pseudocritical point. To test this hypothesis NIST was used to determine the corresponding pseudocritical point temperatures for each pressure used. The data obtained can be found in theTable 2.

At a temperature that is right at the pseudocritical point. Because a very large spike in the specific heat of the fluid occurs at the pseudocritical point very little temperature change can be seen in the bulk fluid for this case. This effect can also be observed in the 24 and 25 MPa cases in the form of a plateau in bulk fluid temperature as they approach their respective pseudocritical points. This would indicate that the large, although brief, spike in specific heat of the fluid at the pseudocritical point has a very dramatic effect on FLUENT's calculation of the solution.

Table 2: Pseudocritical Point Temperatures for Corresponding Pressures

Inlet Pressure (MPa)	Pseudocritical Temperature (^{o}C)
22.095	374.06
23.095	377.83
23.595	379.71
24.095	381.58
25.095	385.24

4. Conclusion

A sensitivity study was performed to determine the effective range of FLUENT's capabilities in predicting supercritical water behavior in bare tube. The following remarks can be made in regard to the research preformed:

- Simulations can be completed to a lower convergence level without sacrificing accuracy of calculation.
- FLUENT can predict wall and bulk fluid temperatures at mass fluxes higher than 300 kg/m^{2}s and when temperatures do not exceed 2000^{o}C, the limit for NIST REFPROP's database.
- Raising the pressure beyond 23 MPa, does not yield significant difference in temperature profiles in the prediction of FLUENT.
- Heat transfer variance yielded a maximum of about 1600 kW/m^2 before reaching the temperature limits for REFPROP. No lower limits were found for heat flux.

5. REFERENCES

[1] Igor Pioro, "NUCLEAR POWER AS A BASIS FOR FUTURE ELECTRICITY PRODUCTION IN THE WORLD: PART 1. GENERATION III AND IV REACTORS," University of Ontario Institute of Technology, Oshawa, Canada, 2011.

[2] M. Sharabi and W. Ambrosini, "Transient 3D Stability Analysis of SCWR Rod Bundle Subchannels by a CFD Code," in *International Conference on Nuclear Engineering (ICONE-16)*, Orlando, 2008.

[3] M. V. Holloway and D. E. Beasley, "Investigation of Swirling Flow in Rod Bundle Subchannels Using CFD," in *International Conference on Nuclear Engineering (ICONE-16)*, Miami, 2006.

[4] A. Muhana and D. R. Novog, "Validation of FLUENT for Prediction of Flow Distribution and Pressure Gradients in a Multi-Branch Header Under Low Flow Conditions," in *International Conference on Nuclear Engineering (ICONE-16)*, Orlando, 2008.

[5] J.M Pietralik and B. A. Smith, "CFD Application to FAC in Feeder Bends," in *International Conference on Nuclear Engineering (ICONE-16)*, Miami, 2006.

[6] G.V. Vanyukova et al., "Application of CFD-Code to Calculations of Heat Transfer in a Fuel Bundle of SCW Pressure-Channel Reactor," in *4th International Symposium on Supercritical Water-Cooled Reactors*, Heidelberg, Germany, 2009, p. 9.

[7] P.L. et al. Kirillov, "Experimental Study on Heat Transfer to Supercritical Water Flowing in Vertical Tubes," in *Nuclear Energy Systems for Future Generation and Global Sustainability (GLOBAL-2005)*, 2005, 2005.

[8] H Zahlan, D C Groeneveld, and S Tavoularis, "Look-up Table for Tran-Critical Heat Transfer," in *The 2nd Canada-China Joint Workshop on Supercritical Water Cooled Reactors (CCSC 2010)*, Toronto, ON, Canada, 2010.

[9] National Institute of Standards and Technology. (2007) Reference Fluid Thermodynamic and Transport Properties (REFPROP 8.0).

[10] B. E. Launder and W. P. Jones, "The Calculation of Low Reynolds Number Phenomena with a Two-Equation Model of Turbulence," *International Journal Heat and Mass Transfer*, vol. vol. 16, no. no. 6, pp. 1119-1130, 1973.

[11] F. Menter, "Two-Equation Eddy-Viscosity Turbulence Models for Engineering Applications," *AIAA Journal*, vol. vol. 32, pp. 1598-1605, 1994.

[12] B. A. Gabaraev, Y. N. Kuznetsov, I. L. Pioro, and R. B. Duffey, "Experimental Study on Heat Transfer to Supercritical Water Flowing in 6-m Long Vertical Tubes," in *International Conference on Nuclear Engineering (ICONE-15)*, Nagoya, Japan, 2007.

[13] B.V. Dyadyakin and A.S. Popov, "Heat Transfer and Thermal Resistance of Tight Seven-rod Bundle, Cooled with Water Flowing at Supercritical Pressures," vol. vol. 11, pp. 244-253, 1977.

[14] S. Gupta, A. Farah, K. King, S. Mokry, and I. Pioro, "Developing New Heat-Transfer Correlation for SCW Flow in Vertical Bare Tubes," in *International Conference on Nuclear Engineering (ICONE-18)*, Xi'an, 2010.

[15] D. Wilcox, "Simulation of Transition with a Two-Equation Turbulence Model," *AIAA Journal*, vol. vol. 32, no. no. 2, pp. 247-255, 1994.