An Appropriate Numerical Model to Capture Pseudocritical Property Change of Steam Flowing Inside Straight Tube

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Abstract:

The use of supercritical fluids in industries is becoming more and more common due to various reasons such as reduced environmental effects and improved efficiency. Because of the huge cost involved, experimentally investigating heat transfer to supercritical fluids is a difficult affair. Therefore, numerical simulation is an effective tool to investigate heat transfer to supercritical fluids. However, simulating heat transfer to supercritical fluid is a challenging task, mainly because of the abrupt property change near pseudocritical point. In this study, different combinations of CFD solvers, RANS turbulence models and material libraries are evaluated to assess the accuracy of predicting pseudocritical properties of steam flowing inside straight tube. It is found that the combination ofAnsys CFX solver, k-ϵ turbulence model and IAPWS IF-97 material library grossly over-predicts the tube wall temperature. Similarly, the combination of Ansys CFX solver, k-ω turbulence model and IAPWS IF-97 material library accurately predicts the bulk fluid temperature and tube wall temperature only up to a point where pseudocritical point is attained by steam. Beyond that the predicted values start to deflect from experimental values continuously. The most accurate combination turns out to be the Ansys Fluent solver along with NIST REFPROP material library and SST k- ω turbulence model. Both the bulk fluid temperature and tube wall temperature are predicted accurately with this model. Further the wall HTC is also predicted quite accurately with this combination. The percentage deviation in predicting the bulk fluid temperature, tube wall temperature and wall HTC from experimental values are 0.2, 0.5 and 1.07 respectively.

Keywords: CFD; supercritical; HTC; IAPWS; material library

1.0 Introduction:

Supercritical thermal power plants are becoming more famous because of the advantages they offer over subcritical plants, mainly in terms of increased cycle efficiency and reduced environmental effects. In a supercritical power plant, typically the water achieves the supercritical stage inside the lower half of the boiler [1]. The boiler consists of long tubes arranged either vertically or inclined which carry water inside it. As the water moves up inside the tubes, it keeps receiving heat which is generated by burning fuel inside the furnace. Just before reaching the critical temperature, the bulk fluid temperature of water reaches a value where it'sthermophysical properties undergo abrupt changes [2]. This point is called as pseudocritical point and at this point the specific heat capacity of fluid attains its maximum value. During heat transfer to fluids passing through pseudocritical point, the heat transfer coefficient (HTC) may be significantly different from the normal HTC value. In some cases, the HTC is higher than the normal value and in other cases its lower. Depending on the HTC value, the process is termed as either heat transfer enhancement (*hte*) or heat transfer deterioration (*htd*). Boiler designers employ various active and passive methods to avoid *htd* and to prolong the process of *hte*[3-4].

Because of the abrupt changes in thermophysical properties, boiler designers need to be extremely careful while dealing with supercritical fluids.However, experimentally investigating the process of heat transfer to supercritical fluids is an expensive affair, for which there are not many supercritical test facilities available as on date. Therefore, investigating this process numerically is a suitable option for boiler designers. Numerous studies have been done using numerical technique to understand the flow and heat transfer characteristics of supercritical steam in tubes. However, selecting the appropriate turbulence model and capturing the thermophysical properties near pseudocritical point remain as the main challenge in these studies.

Kanungo et al [5] simulated the flow of supercritical steam inside the header of an industrial boiler using commercial CFD solver AnsysFluent. They developed their own material database to account for the property changes of steam, but the database could not encompass the pseudocritical property change of steam. Mao et al. [6] conducted numerical studies on horizontal circular tubes where they used National Institute of Standards and Technology (NIST) REFPROP database for obtaining thermophysical properties and concluded that the SST turbulence model is a better model as the k-ε turbulence model over-predicts fluid temperature and under-predicts wall temperature. Zhao et al. [7] concluded that the SSTk-ω turbulence model is a better model than the realizable k-ε model in simulating supercritical CO_2 flowing through helical tubes. They adapted the same model in simulating supercritical water flow in vertical helical tubes using NIST REFPROP database for thermophysical properties. Mokry et al. [8] developed new correlations for supercritical water HTC for vertical bare tube and compared the results with experimental data. They used NIST REFPROP database for thermophysical properties and found that the k-εturbulence model gives better results compared to the SSTk-ω model.

Though numerous numerical investigations are done by various groups to understand the heat transfer characteristics of supercritical steam, there still exists room to find an optimum combination of turbulence model and material database which can accurately capture the pseudocritical property change of steam. In the present study, multiple numerical simulations are performed to assess the accuracy of the model in terms of property prediction of supercritical steam near pseudocritical point. A combination of CFD solvers, Reynolds Averaged Navier-Stokes (RANS) turbulence models and material libraries are used to carry out the simulations.The predicted properties are compared with experimental data and an optimum numerical model is proposed which can capture the pseudocritical property change of steam accurately. This combination of turbulence model and material database can be of great help to boiler designers in simulating the performance of boilers.

2.0 Geometry and Numerical Scheme:

The geometry considered for this numerical study is a straight tube of 4 m length and 10 mm internal diameter. This geometry is similar to the one used by Mokry et al [9] in their experiments.Similar to their experimental conditions, in this simulation also steam enters the tube through the inlet, receives heat from the heated cylindrical wall and exits the tube through outlet. The flow domain for numerical simulation is discretised in AnsysMesher with predominantly hexahedral mesh elements. Adequate number of prism layers is generated near the tube wall to ensure that the y^+ value in numerical simulation remains near unity.

2.1 Numerical Solver:

The simulations are performed using Ansys Fluent 18.1 and Ansys CFX 19, which are finitevolume based commercial CFD solvers. The governing equations are the conservation of mass, conservation of momentum (Navier-Stoke equations) and conservation of energy. To solve the flow equations, pressure based segregated algorithm SIMPLEC (Semi-Implicit Method for Pressure Linked Equations-Consistent) is used. SIMPLEC is based on a predictor-corrector approach. To discretise the pressure and diffusion terms in the governing equation, a second-order central differencing scheme is used and to discretise the convective terms a second-order upwind scheme is used.A combination of turbulence models and material database, as will be discussed in subsequent sections, are used for simulations. The convergence criteria for iterative calculations used in the CFD simulations are as follows. The minimum root mean square residual is 1e-04 for flow and the turbulence parameters and 1e-06 for energy parameters.

2.2 Material and Boundary Conditions:

As discussed above, the supercritical state of steam is simulated by using both Ansys Fluent and Ansys CFX. In Ansys Fluent, the real gas model based on NIST material library is used as the material library. The real gas model uses the NIST thermodynamic and transport Properties of Refrigerants and Refrigerant Mixtures Database Version 9.1 (REFPROP v9.1) to evaluate thermodynamic and transport properties. The REFPROP v9.1 database is a shared library that is dynamically loaded into the solver [10]. For simulation using ANSYS CFX, the material library used is the one by International Association for the Properties of Water and Steam Industrial Formulation 1997 (IAPWS IF-97).IAPWS IF-97 is used to develop thermophysical properties of steam and water. IAPWS IF-97 helps to avoid iterative calculations of thermodynamic properties of water and steam when two properties are given as two independent variables. The IAPWS-IF97 is much faster than the previous equations of state such as the IAPWS-95 and IFC-67. Presentlythe IAPWS-95 and IAPWS-IF97 are considered to be the best equations of state for calculating thermodynamic properties of water and steam, which can be used for industrial and scientific uses all over the world, except for some special cases [11].

For numerical simulations, the experimental conditions of Mokry et al. [9] are prescribed as boundary conditions. Mokry et al. [9] conducted experiments with supercritical steam over a wide range of parameters, as listed in Table-1. A combination of mass flux, wall het flux, steam inlet temperature and pressure are selected from Table-1 and are prescribed as boundary conditions in simulations. In all the simulation cases, the wall of the tube is treated as a rough wall with average wall roughness value as 63 µm.

Table-1: Range of steam parameters considered in simulation

Mass flux (kg/m^2s)	**Heat flux (kW/m^2)**	**Inlet temperature (°C)**	**Inlet pressure (bar)**
499-1499	236-681	341-350	239-242

The parameters turbulent intensity (the ratio of root-mean-square of the velocity fluctuations to the mean flow velocity) and hydraulic diameter are used to specify the turbulence at boundaries. Ansys [10] recommends to use the following formula to have a gross estimation of the turbulent intensity for flow inside ducts,

$$I = \frac{U'}{U_{avg}} = 0.16\left(Re_{D_H}\right)^{\frac{-1}{8}},$$

where I is the turbulence intensity, U' is the root-mean-square of the velocity fluctuations, U_{avg} is the mean flow velocity and Re_{D_H} is the Reynolds number of the flow based on hydraulic diameter. Using the above formula it is calculated that for a flow with a Reynolds number of 50,000 the turbulent intensity value is close to 4% [10]. Therefore, in all the simulation cases, a turbulent intensity of 5% has been assigned at the boundaries.

3.0 Results and Discussion:

The results of CFD simulation using Ansys CFX solver along with k-ε turbulence model and k-ω turbulence model are compared with experimental data of Mokry et al. [9] and the same is shown in Fig.1. The material database used in these simulations are IAPWS IF-97 material library.The mass flux and wall heat flux prescribed in this simulation are 500 kg/m^2 and 335 kW/m^2 respectively. The inlet temperature and pressure of steam in this simulation are 350 ^{0}C and 242 bar respectively. As it can be observed in Fig.1(a), when the turbulence model is k-ε, the predicted wall temperature is distinctly different from experimental values. Similarly, in Fig.1(b), when the turbulence model is k-ω, the predicted values of both wall temperature and bulk fluid temperature are close to experimental values only up to an axial distance of roughly 1.5 m. Beyond 1.5 m axial distance, the predicted values start to deflect from experimental values. This is to be noted that the axial distance of 1.5 m in the tube corresponds to attainment of pseudocritical point for the given inlet conditions.Therefore, the numerical model does not predict pseudocritical property change of steam accurately. The trends in Fig.1 indicate that the k-ω turbulence may be better model compared to k-ε turbulence model, though the material library could be improved in order to address the inaccuracy in prediction after axial distance of 1.5 m.

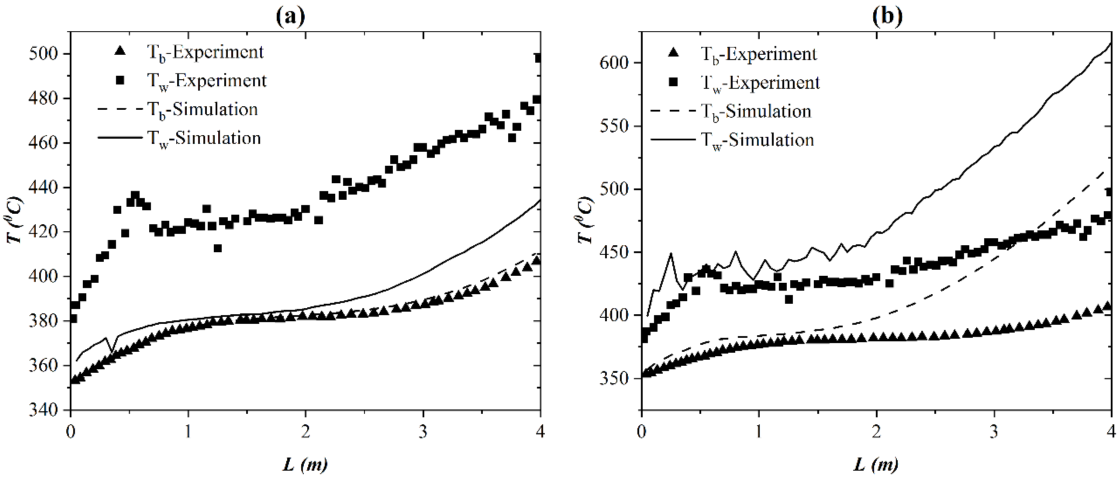

Fig.1: Comparison of CFD simulated data using ANSYS CFX solver along with IAPWS IF97 material library and experimental data. (a) k-ε turbulence mode (b) k- ω turbulencemodel.

To address the issue of inaccuracy in prediction after 1.5 m axial distance, additional simulations are performed with NIST REFPROP material library. The CFD solver in these simulations are Ansys Fluent as NIST REFPROP material library is not available to Ansys CFX solver. The turbulence model used here is SSTk-ω.Two cases are simulated here with mass and heat flux values as 500 kg/m^2,335 kW/m^{2}and 1002 kg/m^2,681 kW/m^{2}respectively. In first case the inlet temperature and pressure of steam are prescribed as 350 ^{0}C and 242 bar respectively. In the second case, the inlet temperature and pressure of steam are prescribed as 350 ^{0}C and 239 bar respectively.The results of CFD simulation using the above combinations compared with experimental data of Mokry et al.[9] and the same is shown in Fig.2. In Fig.2(a) and Fig.2(b), both the tube wall temperature and bulk fluid temperature values are predicted very accurately, in comparison to experimental values. Even after attainment of pseudocritical point at about 1.5 m axial distance also, the model is able to predict the steam properties accurately.

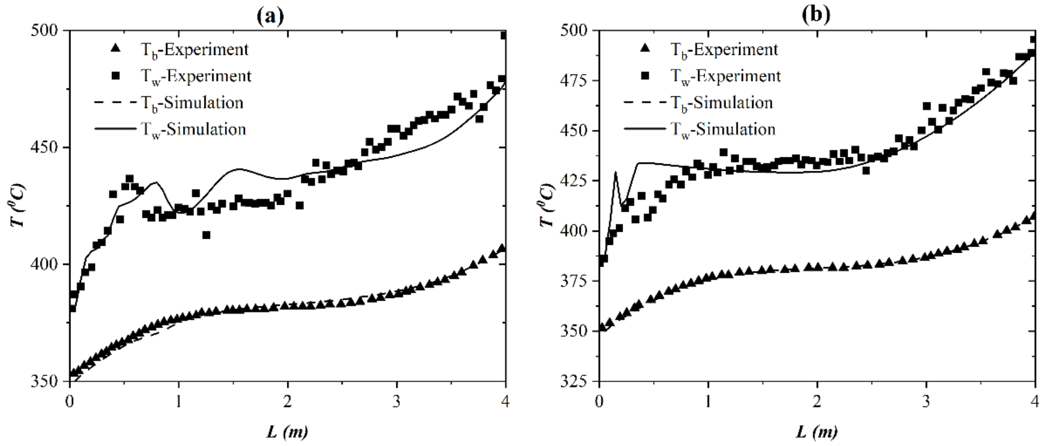

Fig.2: Comparison of CFD simulated data using ANSYS Fluent solver along with NIST REFPROP material library and SST k-ε turbulence mode, with experimental data. (a) 500 kg/m^2, 335 kW/m^2 (b1002 kg/m^2,681 kW/m^2.

After establishing that the combination of Ansys Fluent solver, NIST REFPROP material library and SST k-ω turbulence model is the optimum one to predict pseudocritical properties of steam, the HTC values are predicted for the case of 500 kg/m^2,335 kW/m^2 and 1002 kg/m^2,681 kW/m^2. The predicted values are compared with experimental values and are shown in Fig.3. Here also, the predicted values of HTC by this numerical model are very close to experimental values. Therefore, this numerical model is able to predict pseudocritical property change of steam accurately.

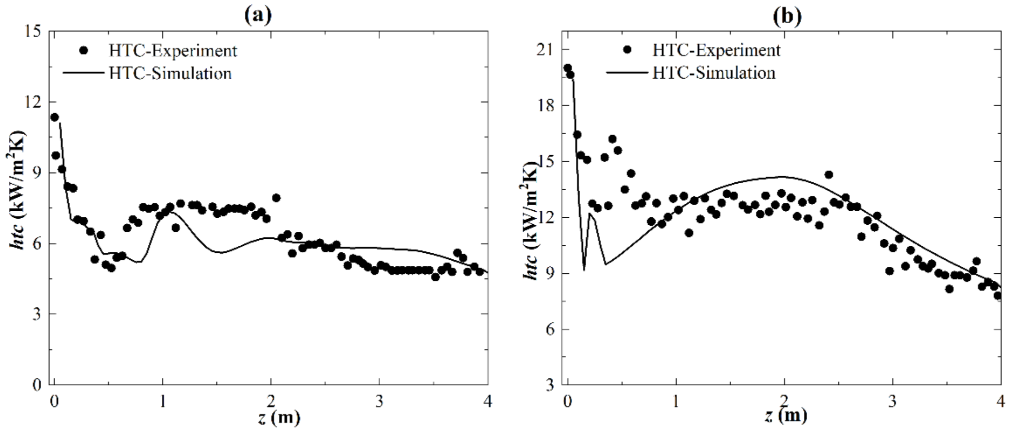

Fig.3: Comparison of predicted values of HTC by using AnsysFluent solver,NIST REFPROP material library and SST k- ω turbulence model with experimental data(a) 500 kg/m2, 335 kW/m^2 (b1002 kg/m^2,681 kW/m^2.

The absolute values of T_b, T_w and HTC as predicted in CFD simulation using AnsysFluent solver, NIST REFPROP material library and SST k- ω turbulence model are compared with experimental values in Table-3. As it can be seen, the maximum deviation in prediction is 1.07% and therefore it can be safely concluded that the combination of AnsysFluent solver, NIST REFPROP material library andSST k- ω turbulence model is the optimum combination available presentlyto carry out simulation of supercritical steam flow in tubes.

Table-3: Comparison of absolute values of T_b, T_W and HTC predicted by simulation with experimental data.

	Average value		
	Tb (° C)	**Tw (° C)**	**HTC (kW/m^2 K)**
Experiment	379.46	437.82	12.06
CFD	381.33	440.01	11.93
% Deviation	**0.2**	**0.5**	**-1.07**

4.0 Conclusions:

In the present study, different combinations of CFD solvers and numerical schemes are evaluated to assess the accuracy of predicting pseudocritical properties of steam flowing inside straight tube. Commercial CFD solvers Ansys Fluent and Ansys CFX are used in the simulations and the experimental data of Morky et al. [9] are used for comparison. The RANS two-equation turbulence models k-ε and k-ω are used in the study. The IAPWS IF-97 and NIST REFPROP material libraries used to simulate the supercritical steam flow. From the simulations, it is found that the combination ofAnsys CFX solver, k-ϵ turbulence model and IAPWS IF-97 material library grossly over-predicts the tube wall temperature. Similarly, the combination of Ansys CFX solver, k-ωturbulence model and IAPWS IF-97 material library accurately predicts the bulk fluid temperature and tube wall temperature till an axial distance of roughly 1.5 m. After this distance the predicted values start to deflect from experimental values continuously. The axial distance of 1.5 m in tube corresponds to attainment of pseudocritical point for given inlet conditions. Therefore, the numerical model does not predict pseudocritical property change of steam accurately. The most accurate combination turns out to be the AnsysFluent solver along withNIST REFPROP material library and SST k- ω turbulence model. Both the bulk fluid temperature and tube wall temperature are predicted accurately with this model. Further the wall HTC is also predicted quite accurately with this combination. The percentage deviation in predicting the bulk fluid temperature, tube wall temperature and wall HTC from experimental values are 0.2, 0.5 and 1.07 respectively. Therefore, the numerical model consisting of Ansys Fluent solver along with NIST REFPROP material library and SST k- ω turbulence model is capable to predicting pseudocritical property change of steam.

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Nomenclature:

CFD	Computational Fluid Dynamics
HTC	Heat Transfer Co-efficient
htd	Heat transfer deterioration
hte	Heat transfer enhancement
NIST	National institute of standards and technology
SST	Shear Stress Transport
RANS	Reynold’s Averaged Navier-Stokes
SIMPLEC	Semi-Implicit Method for Pressure Linked Equations-Consistent
IAPWS	International Association for the Properties of Water and Steam

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