

DISCUSSION ON IMPROVED METHOD OF TURBULENCE MODE FOR SUPERCRITICAL WATER FLOW AND HEAT TRANSFER

by

Zhenchuan WANG^{a*}, Guoli QI^a, and Meijun LI^b

^aChina Special Equipment Inspection and Research Institute, Beijing, China

^bChina Coal Research Institute Company of Energy Conservation, Beijing, China

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The turbulence model fails in supercritical fluid-flow and heat transfer simulation, owing to the drastic change of thermal properties. The inappropriate buoyancy effect model and the improper turbulent Prandtl number model are several of these factors lead to the original low-Reynolds number turbulence model unable to predict the wall temperature for vertically heated tubes under the deteriorate heat transfer conditions. This paper proposed a simplified improved method to modify the turbulence model, using the generalized gradient diffusion hypothesis approximation model for the production term of the turbulent kinetic energy due to the buoyancy effect, using a turbulence Prandtl number model for the turbulent thermal diffusivity instead of the constant number. A better agreement was accomplished by the improved turbulence model compared with the experimental data. The main reason for the over-predicted wall temperature by the original turbulence model is the misuse of the buoyancy effect model. In the improved model, the production term of the turbulent kinetic energy is much higher than the results calculated by the original turbulence model, especially in the boundary-layer. A more accurate model for the production term of the turbulent kinetic energy is the main direction of further modification for the low Reynolds number turbulence model.

Keywords: *buoyancy effect, turbulent Prandtl number, improved turbulence model, heat transfer deterioration*

Introduction

Research on convective heat transfer of supercritical fluids has become more important with the development of various supercritical fluid-flow applications, such as supercritical water-cooled reactors (SCWR), trans-critical CO₂ air-conditioning, and heat pump systems. The thermophysical properties of the supercritical fluid vary drastically, the specific heat rises and then decreases rapidly, the density as well as the viscosity decline sharply in the vicinity of the pseudo-critical temperature, as shown in fig. 1. Compared with conventional sub-critical pressure flows, the drastic variations of the thermophysical properties of supercritical fluids near a pseudo-critical temperature will lead to different thermal-hydraulic characteristics [1].

*Corresponding author, e-mail: wangzhenchuan@csei.org.cn

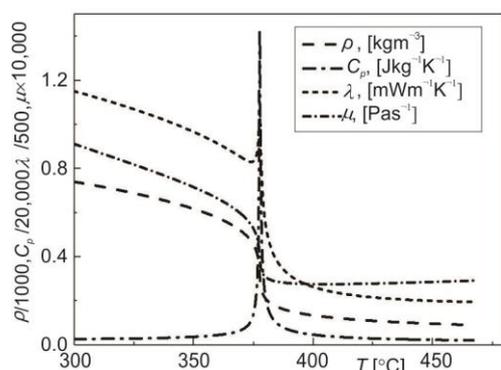


Figure 1. Variation of thermal properties of water at 23.0 Mpa

The special thermal-hydraulic characteristics of supercritical fluids resulting in abnormal heat transfer phenomenon, such as heat transfer deterioration (HTD) condition for convective heat transfer in vertical tube. Compared to those of normal heat transfer, lower heat transfer coefficient values may exist at supercritical conditions, HTD will threaten the security of systems [2]. Numerous heat transfer experiments have been conducted using supercritical water, CO₂, nitrogen, hydrogen, and helium under different operating conditions. A comprehensive understanding of the factors affecting supercritical fluids heat transfer in vertical tubes has been achieved. The heat

transfer regimes could be clarified by dimensionless numbers. For example, Jackson and Hall [1] recognized that the sharp variation of density across the boundary-layer at the pseudo-critical temperature would result in a strong buoyancy effect in the vertical tube, which may heavily change the velocity profiles, reduce the turbulence generation, and cause the heat transfer decrease strongly. Jackson and Hall [3] proposed a non-dimensional parameter, Bo*, to evaluate the influence of buoyancy. Besides, density will change with the variation of the axial temperature and pressure, McEligot and Jackson [4] and Jiang *et al.* [5] proposed non-dimensional parameters, K_{V,T} and K_{V,P}, to evaluate the influence of the thermal acceleration induced by axial temperature variation and the influence of flow acceleration induced by the axial pressure, respectively. In addition, the effect of heat flux, mass-flow rate and diameter on the convective heat transfer of supercritical fluid in vertical heated circular tubes were investigated as well [5-10].

In addition to experiments, efforts have been undertaken to develop numerical models, which could get detailed information of the flow field and improve the understanding of turbulent flow and heat transfer [11-17]. Meanwhile, direct numerical simulations (DNS) of fluid at supercritical pressures [18-20] provided detailed information on the flow, turbulence and thermal fields for improvement or modification of the Reynolds averaged Navier-Stokes based models. The accuracy of the turbulence models was verified by comparing the predicted wall temperatures and the experimental data. Previous research results show that the low Reynolds number (LRN) turbulence model [11-14], the Reynolds stress model (RSM) [15], and the SST *k-ω* model [16, 17] could obtain good predictions for some cases. Meanwhile, studies [11-17] illustrated that the turbulence models are not always suitable for predicting the wall temperature under HTD condition for all cases. The drawbacks of the turbulence model are embodied in two aspects, modelling the buoyancy production of turbulent kinetic energy (G_k term) by the simple gradient diffusion hypothesis (SGDH) [21-23], modelling the turbulent thermal diffusion by the constant turbulent Prandtl number [24-29]. With regard to the models for the G_k term, Kim *et al.* [21] used different methodologies for modelling direct production of turbulence through the action of buoyancy. The methodologies have been shown that the effect of buoyancy on turbulence is predominantly due to the indirect effect. Xiong and Cheng [30] compared the results with the DNS data, which are calculated by various models about buoyancy production of turbulent kinetic energy, as well as various models of turbulent heat flux based on a four equation turbulence model. The calculated results

showed that EB-AFM model for both buoyancy production of turbulent kinetic energy and turbulent heat flux was a promising candidate for further optimization. With regard to the models of turbulent Prandtl number, in most of these reports, the turbulent Prandtl number is fixed at a constant value of 0.85~0.9 [31]. However, there is a possibility that turbulent Prandtl number is not a constant value in the HTD analysis, because the fluid property is changed drastically at the near-wall region [32]. Recently, the models which treat turbulent Prandtl number as a variable parameter is reported, while those models are still under developed [24-29]. Mohseni and Bazargan [25] found that a decrease in turbulent Prandtl number results in the wall temperatures decreases under buoyancy deteriorated conditions. Bae [27] proposed a formulation of turbulent Prandtl number varying with physical properties and fluid-thermal variables based on the mixing length theory. Jaromin and Anglart [29] tested the sensitivity of the numerical results to the turbulent Prandtl number using the $k-\omega$ turbulence model, constant of 0.9 and 0.95 were recommended for various operating conditions.

In all the reviewed papers, the two aspects (G_k term and Pr_t) of the model improvement and the relative importance are few studies. In the present paper, heat transfer to supercritical water was numerically studied using AKN LRN $k-\varepsilon$ models [33]. The G_k term was calculated by the model according to the generalized gradient diffusion hypothesis approximation (GGDH) [34], the turbulent Prandtl number using a turbulent Prandtl number model proposed by Kays [32]. Better prediction results were accomplished by the improved turbulence model compare with the experimental data, under normal heat transfer (NHT) condition and HTD condition.

Numerical method and experimental data

Numerical method

The flow and heat transfer is assumed to be steady and axisymmetric. The continuity, momentum and energy governing equations accounting for the temperature-dependent property variations are written in cylindrical co-ordinates:

$$\frac{\partial U}{\partial x} + \frac{1}{r} \frac{\partial (rV)}{\partial r} = 0 \quad (1)$$

$$\frac{\partial U^2}{\partial x} + \frac{1}{r} \frac{\partial (rVU)}{\partial r} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + g\beta(T - T_{ref}) + 2 \frac{\partial}{\partial x} \left[(g + g_t) \left(\frac{\partial U}{\partial x} \right) \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[r(g + g_t) \left(\frac{\partial U}{\partial r} + \frac{\partial V}{\partial x} \right) \right] \quad (2)$$

$$\frac{\partial (UV)}{\partial x} + \frac{1}{r} \frac{\partial (rV^2)}{\partial r} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left[(g + g_t) \left(\frac{\partial V}{\partial x} + \frac{\partial U}{\partial r} \right) \right] + 2 \frac{1}{r} \frac{\partial}{\partial r} \left[r(g + g_t) \left(\frac{\partial V}{\partial r} \right) \right] - 2 \frac{(g + g_t)}{r^2} \quad (3)$$

$$\frac{\partial (Uh)}{\partial x} + \frac{1}{r} \frac{\partial (rVh)}{\partial r} = \frac{\partial}{\partial x} \left[\left(\frac{g}{Pr} + \frac{g_t}{Pr_t} \right) \frac{\partial h}{\partial x} \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[r \left(\frac{g}{Pr} + \frac{g_t}{Pr_t} \right) \frac{\partial h}{\partial r} \right] \quad (4)$$

A variable turbulent Prandtl number model was used instead of a constant Pr_t [32]:

$$Pr_t = \frac{1}{\frac{1}{2Pr_{t,\infty}} + CPe_t \sqrt{\frac{1}{Pr_{t,\infty}} - (CPe_t)^2} \left[1 - \exp \left(-\frac{1}{CPe_t \sqrt{Pr_{t,\infty}}} \right) \right]} \quad (5)$$

The $Pr_{t,\infty} = 0.85$, $C = 0.3$.

The turbulent kinetic energy and dissipation rate equations in the AKN turbulence model are:

$$\left[\frac{\partial(Uk)}{\partial x} + \frac{1}{r} \frac{\partial(rVk)}{\partial r} \right] = \frac{\partial}{\partial x} \left[\left(g + \frac{g_t}{\sigma_k} \right) \frac{\partial k}{\partial x} \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[r \left(g + \frac{g_t}{\sigma_k} \right) \frac{\partial k}{\partial r} \right] + P_k + G_k - \rho \varepsilon \quad (6)$$

$$\left[\frac{\partial(U\varepsilon)}{\partial x} + \frac{1}{r} \frac{\partial(rV\varepsilon)}{\partial r} \right] = \frac{\partial}{\partial x} \left[\left(g + \frac{g_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x} \right] + \frac{1}{r} \frac{\partial}{\partial r} \left[r \left(g + \frac{g_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial r} \right] + C_{\varepsilon 1} f_1 \frac{\varepsilon}{k} (P_k + G_k) - C_{\varepsilon 2} f_2 \frac{\varepsilon^2}{k} \quad (7)$$

The GGDH approximation [34] was used to model the buoyancy production of turbulent kinetic energy (gravitational production) is:

$$G_k = -\overline{\rho' u' g_x} = -c_\theta \beta \rho g_x \left(\frac{k}{\varepsilon} \right) \left[\mu_t \left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x} \right) \frac{\partial T}{\partial r} + \left(2\mu_t \frac{\partial u}{\partial x} - \frac{2}{3} \rho k \right) \frac{\partial T}{\partial x} \right] \quad (8)$$

where $g_x = -g$ for upward flow, $g_x = g$ for downward flow, and $c_\theta = 0.3$.

As a contrast, the SGDH used in the original turbulence model is:

$$G_k = -\overline{\rho' u' g_x} = \beta g_i \frac{\mu_t}{Pr_t} \frac{\partial T}{\partial x} \quad (9)$$

In the present study, the computational domain was discretized into a structured grid, typically, 2500×60 (axial \times radial) for the HTD cases. The mesh was carefully adjusted on the axially and radially direction to ensure the near-wall flow features were properly resolved. The PISO scheme was used for coupling the pressure and the velocity fields, the second-order upwind method was used to solve density, momentum, turbulent kinetic energy, specific dissipation rate, and energy equations. All thermal properties were calculated by the NIST Standard Reference Database.

Experimental data

The experimental data in the papers of Mokry *et al.* [7] and Gu *et al.* [10] were used for the comparison, with the fluid-flowing upwards in a uniformly heated vertical tube. The test section was a circular tube with an inner diameter of 10 mm, the heated length is 4000 mm and 2500 mm for the experiment of Mokry *et al.* [7] and Gu *et al.* [10], respectively. The working fluid was supercritical water and the experiment pressure was 23.0, 24.1, and 25.0 MPa. The experimental data and set-up are shown in tab. 1. The Case 1 is a NHT case in Mokry *et al.* [7] and Case 2 to Case 7 are HTD cases in Gu *et al.* [10].

Table 1 Operating conditions

Case	Pressure [MPa]	T_{in} [K]	Mass flux [$\text{kgm}^{-2}\text{s}^{-1}$]	Heat flux [kWm^{-2}]	Reference
1	24.1	615.55	498	190	[7]
2	23.0	576.15	600	700	[10]
3	23.0	576.15	1000	700	[10]
4	23.0	576.15	1000	1000	[10]
5	25.0	576.15	600	700	[10]
6	25.0	576.15	1000	1000	[10]
7	25.0	576.15	1000	1000	[10]

Results and discussion

Comparison of predicted wall temperature with experimental results

Figure 2 shows the comparison of the experimentally data with the calculated results generated by improved AKN LRN turbulence models. The G_k term is modelled by GGDH model and the Pr_t is not a constant but using the Kays's turbulent Prandtl number model. As shown in fig. 2, the trend of results calculated by the improved turbulence model is consistent with the experimental data under the HTD conditions. The temperature trend in all the cases

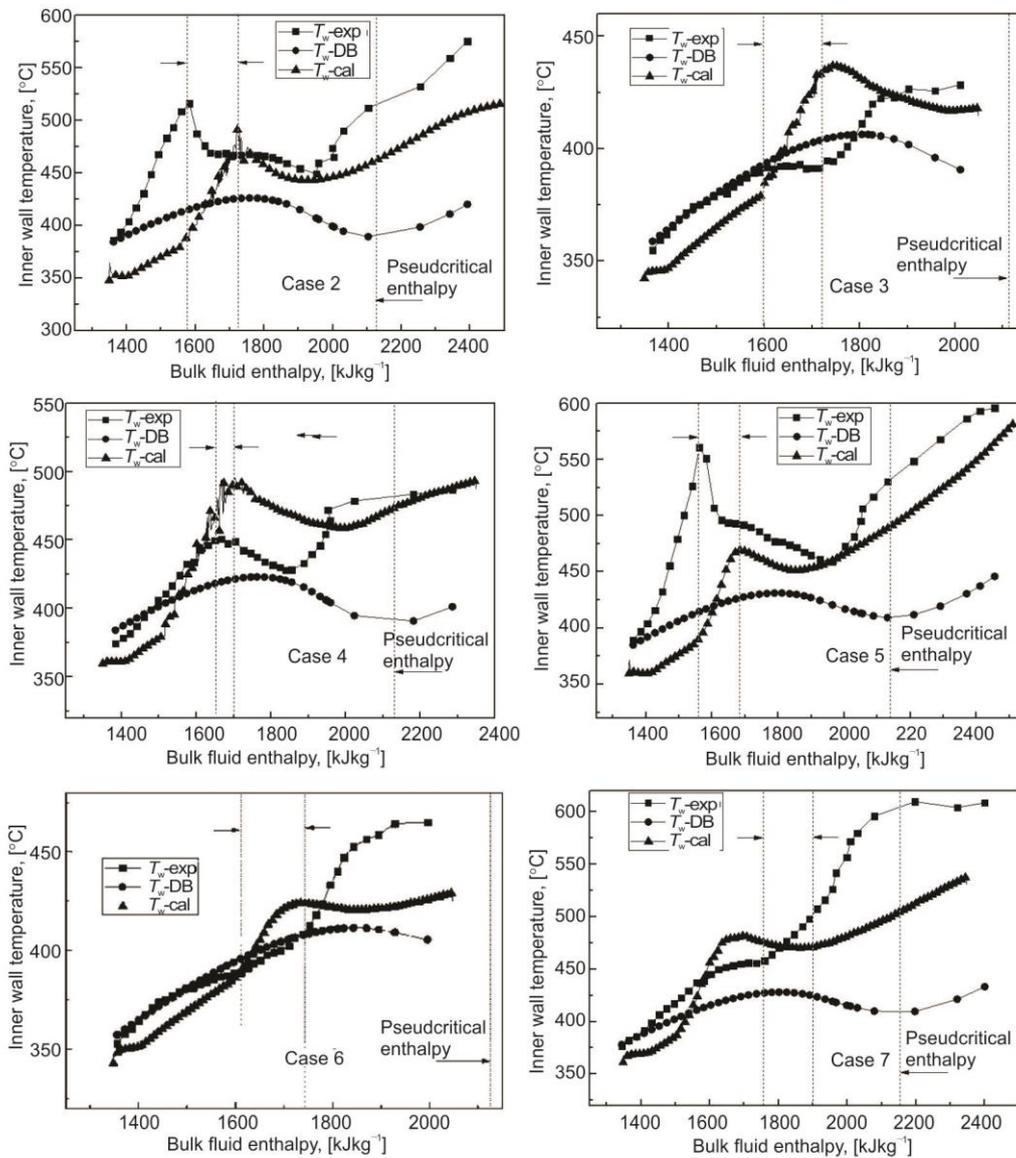


Figure 2. Comparison of temperature by improved model and D-B equation with experimental data

(Case 2 to Case 7) shown in fig. 2 is not linear, the heat transfer is deteriorated by the buoyancy effect. The cases in fig. 2 could be classified into two categories, one (Case 2, Case 4, and Case 5 – Series 1) with a peak temperature value and the other cases (Case 3, Case 6, and Case 7 – Series 2) with a sudden rise in temperature when the fluid temperature closed to the pseudocritical temperature. The definition of the prediction accuracy of bulk fluid enthalpy between the numerical results and experimental data is the difference in peak position or the difference in temperature sharply rising point. The prediction accuracy of bulk fluid enthalpy is about ± 200 kJ/kg for all the cases in fig. 2. As shown in fig. 2, the results calculated by the D-B equation could get the temperature trend qualitatively in some cases, while the empirical correlation is not suitable for all the HTD cases. The results calculated by the D-B equation show the heat transfer is drastically deteriorated by the buoyance effect.

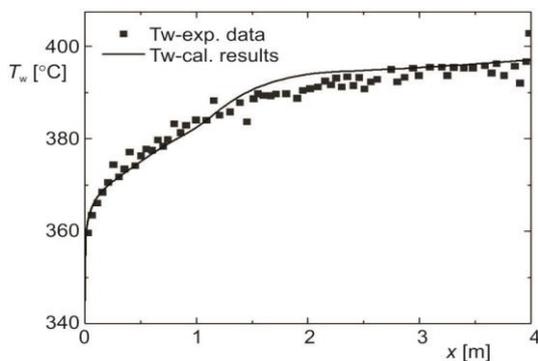


Figure 3. Comparison of temperature for NHT cases

Figure 3 shows the comparison results simulated by the improved turbulence model and the experimental results in Mokry *et al.* [7] under NHT condition. The improved turbulence model could reproduce the experimental temperature results very well in NHT case, the wall temperature difference between simulation results and experimental data is within $\pm 3\%$. The improved turbulence model does not change the prediction accuracy of the original model, which means there is no need to change the G_k term model and the turbulent Prandtl number model under the calculation of NHT conditions.

Effect of buoyancy on turbulence production

Figure 4 shows the temperature comparison of the experimental data and simulation results. As shown in fig. 4, the original turbulence model seriously underestimate the buoyancy effect on the heat transfer to the fluid. The original turbulence model could not catch the temperature trend qualitatively. The buoyancy effect has a large impact on the production of turbulence kinetic energy, which is necessary to model the buoyancy effect by a more accurate model, such as GGDH. Figure 5 shows the radial direction buoyancy production of turbulence kinetic energy (G_k term) in Case 2 calculated by the original AKN LRN turbulence model (solid point) and the improved turbulence model (hollow point). The G_k term in the improved turbulence model is much higher than the results calculated by the original AKN LRN turbulence model, especially in the near-wall region. The intensity of the turbulence in the near-wall region will affect the development of the turbulent flow and then the heat transfer rate. The low prediction of the G_k term leading to the peak value simulated by the original turbulence model is extremely higher than the experimental results.

Figure 6 shows the turbulent kinetic energy field simulated by the original turbulence model and the improved turbulence model for Case 2. The size of the tube in the flow direction is scaled down by a factor of one hundred to show the global trend of the turbulent kinetic energy. The turbulent kinetic energy calculated by the original model severely underestimated the turbulence flow, which led to the overestimate of wall temperature, as shown in

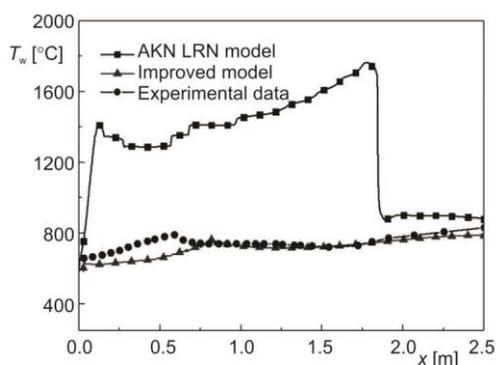


Figure 4. Comparison of temperature results for numerical simulation and experimental data

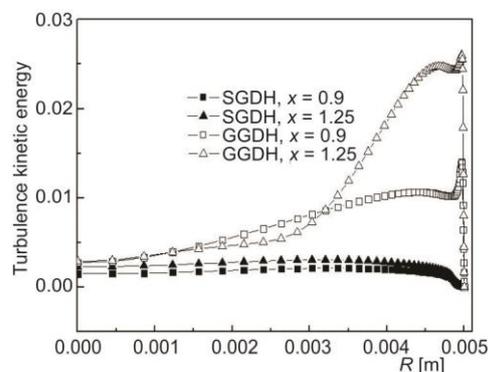


Figure 5. Buoyance production of turbulence kinetic energy calculated by SGD and GGD

fig. 4. As shown in fig. 6(b), the turbulent kinetic energy decreased first and then increased, which led to a low wall temperature in the middle of the tube. The turbulence production and dissipation are affected by the buoyance effect, while the original turbulence model was unable to catch the evolution of the turbulent flow accurately.

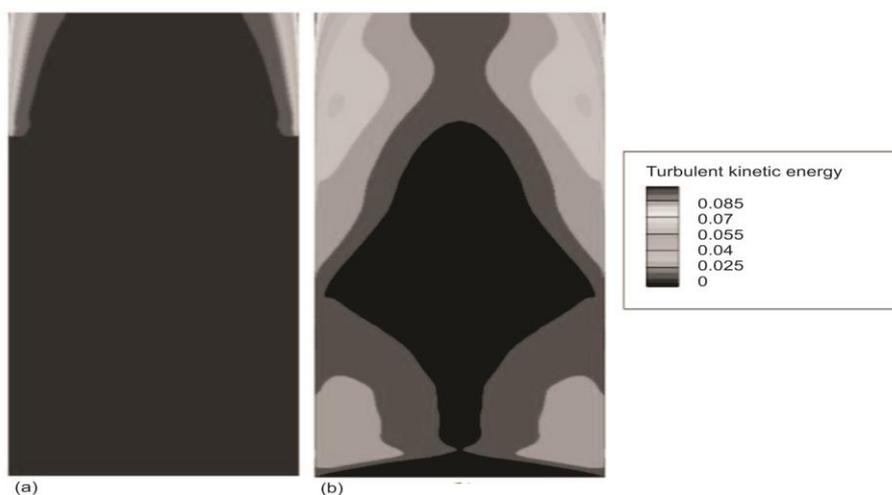


Figure 6. Comparison of turbulent kinetic energy by different turbulence model (a) original turbulence model, (b) improved turbulence model

Effect of turbulence Prandtl number model

The turbulent Prandtl number is defined as the ratio of the turbulent eddy viscosity to the turbulent thermal diffusivity, which is about equal to a constant value, normally taken as a constant of 0.85 in many two-equation eddy viscosity models. The constant value of turbulent Prandtl number is not suitable for the numerical simulation of supercritical fluid due to the drastically variation of thermal properties especially when the temperature near the pseudo-critical temperature. The effect of turbulent Prandtl number on the accuracy of the turbu-

lent model is investigated in this section. The buoyancy production of turbulent kinetic energy was modelled by GGDH approximation, two turbulent Prandtl number model were used, Kays's Prandtl number model and Bae's turbulent Prandtl number model.

The Bae's turbulent Prandtl number model is a function of fluid-thermal variables as well as physical properties, which is derived by Reynolds analogy.

This $Pr_{t,0}$ is a function of some incremental variations, the $Pr_{t,0}$ expression is:

$$Pr_{t,0} = \frac{1 + \frac{u}{\rho} \left| \frac{\partial \rho}{\partial y} \right| / \left| \frac{\partial u}{\partial y} \right| + \frac{l}{\rho} \left| \frac{\partial \rho}{\partial y} \right|}{1 + \frac{T}{\rho} \left| \frac{\partial \rho}{\partial y} \right| / \left| \frac{\partial T}{\partial y} \right| + \frac{T}{c_p} \left| \frac{\partial C_p}{\partial y} \right| / \left| \frac{\partial T}{\partial y} \right| + \frac{l}{c_p} \left| \frac{\partial C_p}{\partial y} \right| + \frac{l}{\rho} \left| \frac{\partial \rho}{\partial y} \right| + \frac{lT}{\rho C_p} \left| \frac{\partial \rho}{\partial y} \frac{\partial C_p}{\partial y} \left(\frac{\partial T}{\partial y} \right)^{-1} \right|} \quad (10)$$

While Bae [28] then introduced two functions which is analogous to a damping function:

$$h_1 = 1 - \exp\left(-\frac{y^+}{A^+}\right), \quad h_2 = 0.5 \left[1 + \tanh\left(\frac{B - y^+}{10}\right) \right], \quad y^+ = \frac{\left(\frac{\tau_w}{\rho}\right)^2 y}{\nu}$$

Finally, Bae's turbulent Prandtl number model was then defined:

$$Pr_t = \sigma_t - h_1 h_2 (\sigma_t - Pr_{t,0}) \quad (11)$$

Figure 7 shows the temperature comparison predicted by the Kays's turbulent Prandtl number model (Kays's Pr_t model) and Bae's turbulent Prandtl number model (Bae's Pr_t model). The buoyancy production of the turbulent kinetic energy is moulded by GGDH. In Series 1 (Case 2, Case 4, and Case 5), the temperature distribution has a large difference, the difference in Series 2 (Case 3, Case 6, and Case 7) is relatively small. The difference of the calculated results between the two models is concentrated in the area where the fluid temperature exceeds the pseudocritical temperature. The figures show that the Kays's Pr_t model is more suitable for the operating conditions which the present paper concerns about. When the supercritical water bulk temperature is close to the pseudo-critical temperature, the Bae's Pr_t model gets a very low wall temperature.

Profiles of turbulent kinetic energy predicted by the AKN model with different turbulent Prandtl number model are compared in Figs. 8 and 9 for Case 2 and Case 4. The global trend of the turbulence kinetic energy is similar to each other, which is simulated by different Pr_t model, the turbulent kinetic energy has a lower value in the middle of the tube which leads to the peak wall temperature value in those poison as shown in fig. 2. However, the turbulent kinetic energy simulated by the Bae's Pr_t model is higher than the Kays's Pr_t model in the outlet section. As shown in fig. 7, the wall temperature simulated by the Bae's Pr_t model is lower than the Kays's Pr_t model in the outlet section.

Figure 10 shows the results of turbulence kinetic energy production due to the buoyance (G_k term), and the turbulence Prandtl number for different cross-section is shown in fig. 11. The trend of G_k term calculated by different models is similar, the magnitude is equivalent. The difference of wall temperature between the different models is caused by the turbulent Prandtl number, owing to the same G_k term model (GGDH) adopted in the turbulence model. As shown in fig. 11, lower turbulent Prandtl number predicted by Bae's Pr_t model in the core region results in higher turbulent thermal diffusion, leading to the heat transfer increases and the wall temperature decreases in the outlet section.

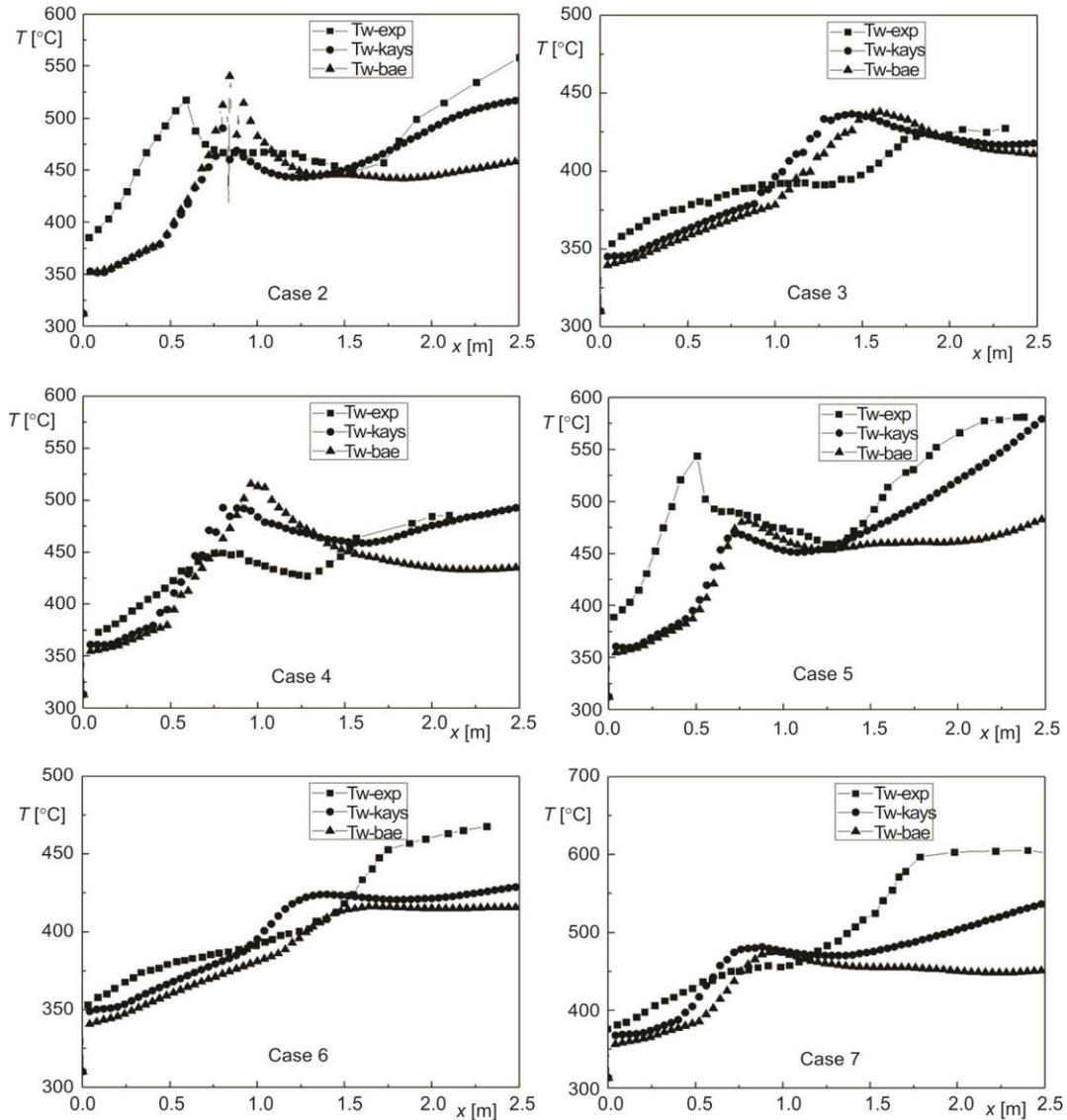


Figure 7. Predictions of temperature with various turbulent Prandtl number model

Conclusions

The heat transfer of supercritical water-flowing upward in a vertical tube with an inner diameter of 10 mm for various heat fluxes is investigated and numerically simulated using AKN LRN turbulence model. The buoyance production of turbulent kinetic energy is modelled by the Generalized Gradient Diffusion Hypothesis, the turbulent Prandtl number is not a constant value but a turbulent Prandtl number model concerning the variation of thermal properties. The main findings are summarized as follows.

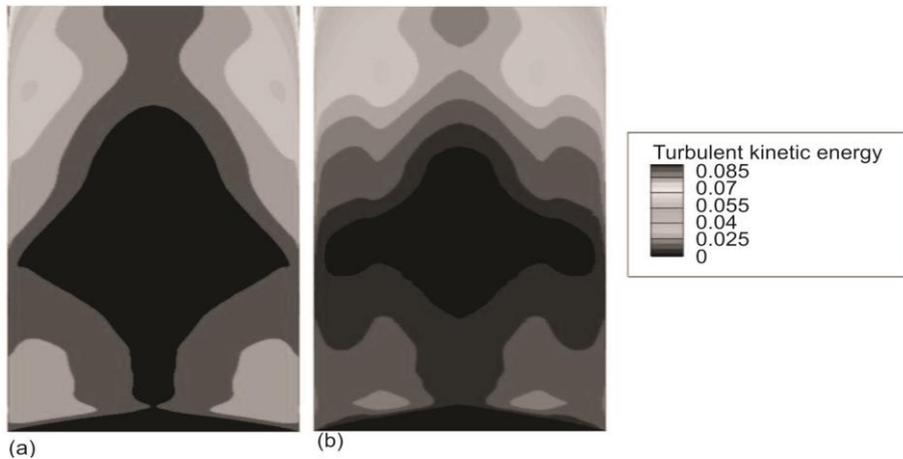


Figure 8. Comparison of turbulence kinetic energy by different Pr_t model for Case 2
 (a) Kays's Pr_t model, (b) Bae's Pr_t model

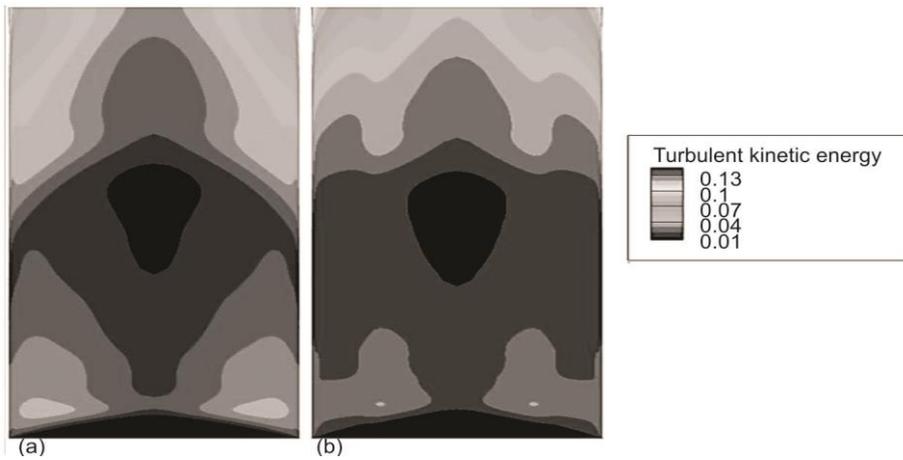


Figure 9. Comparison of turbulence kinetic energy by different Pr_t model for Case 4
 (a) Kays's Pr_t model, (b) Bae's Pr_t model

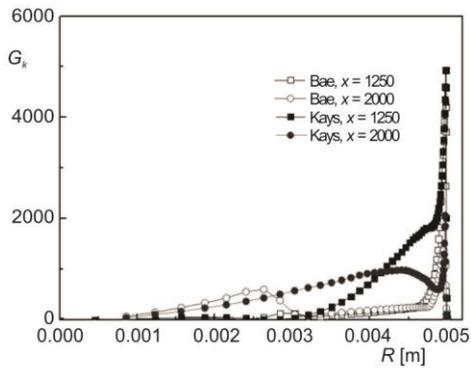


Figure 10. Turbulent kinetic energy production due to buoyance

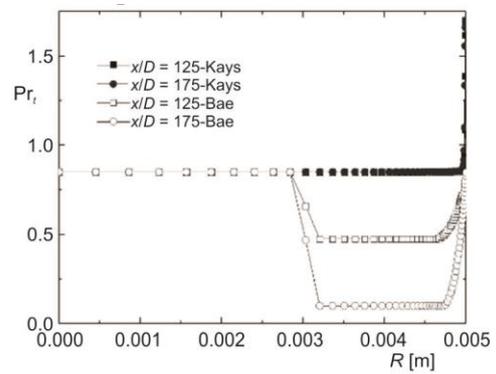


Figure 11. Profiles of turbulence Prandtl number for different cross-section

- The original AKN LRN turbulence model is incapable in quantitatively predict the turbulent flow and heat transfer of supercritical water under HTD conditions. The original turbulence model greatly underestimated the buoyancy production of turbulent kinetic energy and misuse a constant value of turbulent Prandtl number especially near the pseudo-critical temperature.
- An improved method has been used in the present paper, G_k term modelled by the GGDH model and Kays's turbulent Prandtl number model was used for obtaining the turbulent thermal diffusivity. The improved turbulence model is capable in quantitatively predictions of wall temperature under HTD conditions.
- The model for G_k term is very important for simulation of supercritical water-flow and heat transfer in vertical tube. It is necessary to use the GGDH or more accurate model for modelling the buoyance production of turbulent kinetic energy.
- The turbulent Prandtl number is the second factor for the disability of the original turbulence model under the HTD conditions. A very low turbulent Prandtl number in the core region will lead to a low temperature which is not correspondent with experimental results. Further modifications for the LRN turbulence models need to be made by carefully selecting the turbulent Prandtl number model.

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Nomenclature

Bo^*	– non-dimensional buoyancy parameter	T	– temperature, [°C]
C_p	– specific heat at constant pressure, [Jkg ⁻¹ K ⁻¹]	U	– axial velocity, [ms ⁻¹]
D	– tube diameter, [m]	u	– axial turbulent velocity fluctuation, [ms ⁻¹]
g	– gravitational acceleration, [m ² s ⁻¹]	V	– radial velocity, [ms ⁻¹]
Gr^*	– Grashof number	v	– radial turbulent velocity fluctuation, [ms ⁻¹]
h	– enthalpy, [Jkg ⁻¹ K ⁻¹]	x	– axial co-ordinate [m]
Kv_T	– non-dimensional flow acceleration parameter	y^+	– dimensionless wall distance
Kv_p	– non-dimensional flow acceleration parameter	<i>Greek symbols</i>	
k	– turbulence kinetic energy, [m ² s ⁻²]	β	– coefficient of thermal expansion, [–]
Nu	– Nusselt number	δ_t	– thermal boundary
Pe	– Peclet number, (=Nu/RePr)	ε	– dissipation rate, [m ² s ⁻³]
Pr	– Prandtl number	μ	– molecular viscosity
Pr_t	– turbulent Prandtl number	μ_t	– turbulent viscosity
p	– pressure, [MPa]	ρ	– fluid density, [kgm ⁻³]
Re	– Reynolds number		
r	– radial co-ordinate, [m]		

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