NUMERICAL STUDY ON LAMINAR FREE CONVECTION HEAT TRANSFER BETWEEN SPHERE PARTICLE AND HIGH PRESSURE WATER IN PSEUDO-CRITICAL ZONE

by

Liping WEI , Youjun LU*, and Jinjia WEI

State Key Laboratory of Multiphase Flow in Power Engineering, Xi´an Jiaotong University, Xi´an, Shaanxi, China

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Supercritical water fluidized bed reactor is a promising new reaction vessel which can effectively gasify wet biomass and efficiently produce hydrogen. Free convection heat transfer from particle in supercritical water is a major basic heat transfer mechanism in a fixed bed or fluidized bed with low superficial velocity. In this paper, numerical study on the steady free convection heat transfer around a single sphere particle in high pressure water of pseudo-critical zone was carried out. Both the Boussinesq approximation method and real properties model (considering variable specific heat, density, viscosity, and conductivity of supercritical water) were incorporated to simulate the flow and temperature field. With respect to Boussinesq approximation, real properties model shows higher vorticity and temperature gradients in the vicinity of the sphere surface, which shows variation of thermo-physical property has remarkable effect on the free convection heat transfer process. High local Nusselt number and high heat transfer rate were observed with real properties model.

Key words: *supercritical water, sphere particle, free convection, heat transfer*

Introduction

Supercritical water fluidized bed reactor (SCWFBR) is a new member of fluidized bed family [1]. It can effectively gasify wet biomass and efficiently produce hydrogen. SCWFBR uses supercritical water (SCW) as fluidization medium and quartz sand as bed materials [2]. Free convection heat transfer from particles in SCW is one of the main heat transfer modes. Due to thermal physical properties of SCW vary sharply in pseudo-critical zone, as shown in fig. 1, the heat transfer characteristics of SCW have to consider the effect of variable properties.

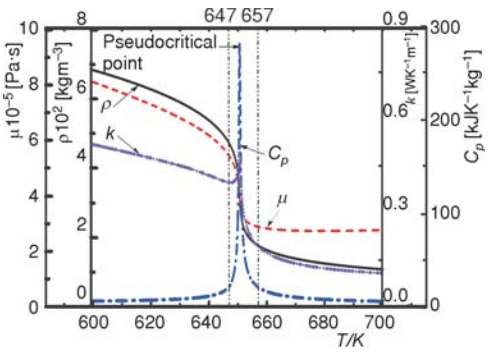

Figure 1. Property of SCW in pseudo-critical zone *P* = 23 MPa

* Corresponding author; e-mail: yjlu@mail.xjtu.edu.cn

However, small number of papers have been published regarding the influence of each thermal physical property on the free convection heat transfer process from sphere in SCW flow.

Free convection heat transfer from a single sphere immersed in stagnant fluids may be considered a simple case of numerous industrially important processes. In addition to the particle fluidization in fluidized bed, many practical applications, such as in metal particle melting, vaporization of fuel droplets, spray drying, and so on, involve the problem free convection from a stationary isolated sphere in fluid. Studies on natural convection over a sphere in infinite fluid have been conducted through theoretical analysis, experimental method, and numerical simulation. The analytical works on natural convective flow over a sphere have been applied to the limited cases by using boundary layer assumptions or asymptotic expansion techniques and Boussinesq approximation. The exact solution of boundary layer is complicated because of the non-linear nature of convective term and coupling of momentum and energy equations [3]. Table 1 lists the related studies about free convection from a sphere in static fluid before the year of 2000. Those previous work enhanced the understanding of the free convection heat transfer from a sphere in different fluid and large wide parameter regime. However, most studies are lim-

Table 1. Collection of literature about free convection from a spherical particle

Researchers	Results or range	Study method
Merk and Prins [4]	$\mathrm{Nu} = C(\mathrm{GrPr})^{1/4}$, $\mathrm{Pr} > 1$	Theoretical
Acrivos [5]	Power-law fluids; steady; laminar	Theoretical
Fendell [6]	Small Gr number; steady; laminar	Theoretical
Raithby and Hollands [3]	Laminar	Theoretical
Potter and Riley [7]	High Gr; steady; laminar	Theoretical
Singh and Hasan [8]	Low Gr	Theoretical
Churchill [9]	$\mathrm{Nu} = 2 + (0.589\mathrm{Ra}^{0.25})/[1 + (0.43/\mathrm{Pr})^{9/16}]^{4/9}$ $\mathrm{Gr} < 10^9$, all Pr	Theoretical
Jafarpur and Yovanovich [10]	$\mathrm{Nu} = 2 + (0.600\mathrm{Ra}^{0.25})/[1 + (0.5/\mathrm{Pr})^{9/16}]^{4/9}$ $0 \leq \mathrm{Ra} \leq 10^8$	Theoretical
Kranse and Schenk [11]	$\mathrm{Nu} = 2 + 0.59(\mathrm{GrPr})^{1/2}$, $\mathrm{Pr} = 8.3$, $10^8 < \mathrm{Gr} < 10^9$	Experimental
Schenk and Schenkels [12]	$0 < \mathrm{Gr} < 2\cdot10^5$	Experimental
Jaluria and Gebhart [13]	Thicker boundary upright hemisphere	Experimental
Argyropoulos and Mikrovas [14]	$\mathrm{Nu} = 2 + 10^{-3.746}(\mathrm{GrPr})^{0.878}$; $0.014 < \mathrm{Pr} < 0.219$	Experimental
Fujii *et al*. [15, 16]	$D_\infty/D > 40$; $0.01 < \mathrm{Ra} < 10^6$; $\mathrm{Pr} < 100$; steady; laminar	Numerical
Geoola and Cornish [17, 18]	$\mathrm{Gr} < 12500$; $\mathrm{Pr} < 100$; transient	Numerical
Farouk [19]	$10^{-1} < \mathrm{Ra} < 10^5$	Numerical
Riley [20]	$\mathrm{Pr} = 0.72$ and 0.7; $10^2 \leq \mathrm{Gr} \leq 10^4$; transient	Numerical
Dudek *et al.* [21]	$0.0004 < \mathrm{Gr} < 0.5$; steady-state and transient	Numerical
Takamatsu *et al*. [22]	$D_\infty/D > 60$; $0.7 < \mathrm{Pr} < 120$	Numerical
Jia [23]	$\mathrm{Pr} = 0.72$ and 7.0; $10 \leq \mathrm{Gr} \leq 10^8$; transient	Numerical
Kurdyumov and Linan [24]	A correlation for all Pr	Numerical

ited to the kind of fluid. Recently, Nazar and Amin [25] studied the steady laminar free conduction flow over an isothermal sphere in a micropolar fluid with Prandtl number of 0.7 and 7. Beget *et al*. [26] further presented a numerical analysis of this problem on the effect of Soret/Dufour effects. Yang *et al.* [27] solved full Navier-Stokes equations and the energy equation for transient laminar natural convection heat transfer over an isothermal sphere for a wide range of Grashof numbers ($10^5 < \mathrm{Gr} < 10^9$) and Prandtl numbers (Pr = 0.02, 0.7, 7, and 100). Prhashanna and Chhabra [28] studied the free convection heat transfer from a heated sphere immersed in quiescent power-law fluids with $10 < \mathrm{Gr} < 10^7$, $0.72 < \mathrm{Pr} < 100$, and $0.4 < n < 1.8$. They found that the value of $D_\infty/D = 80$ is adequate to obtain results which are free from domain effects. Other authors studied magnetohydrodynamics natural convection flow on a sphere [29-32].

Variable properties play an important role for development of heat transfer peculiarities for supercritical water [33, 34]. The aim of this study was to determine the effect of variable properties on the free convection heat transfer from particle in supercritical water. This paper focused on the divergence between Boussinesq approximation and a real properties model (Navier-Stokes equations that considered all thermal physical properties of SCW) for natural convective flow over a solid sphere in SCW. By this way, effect of variable properties of SCW on the free convection heat transfer in pseudo-critical zone was analyzed in details.

Problem formulation

Physical problem

Strictly speaking, the laminar free convection heat transfer from a sphere particle in SCW flow is a transient process. However, as this study focuses on the understanding of the effect of fluid property variation, the transient particle temperature variations are not considered. According to the experimental measurement, the magnitude order of Grashof number for free convective flow transition from laminar to turbulence is around 10^9 [23]. For a laminar free convective flow, axisymmetric flow is observed. In this present work, it was considered that steady laminar heat transfer from particle to SCW flow occurs for particles with constant surface temperature. Figure 2 shows the schematics of the SCW flow passing over a sphere.

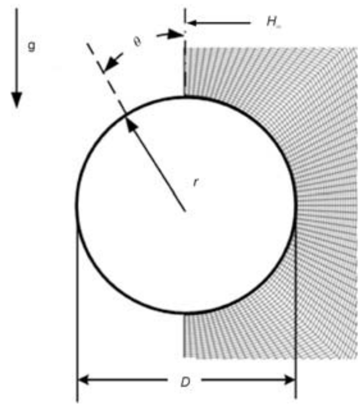

Figure 2. Shows the schematics of the SCW flow passing over a sphere

Mathematical formulation and solution

It is customary to set the thermo-physical properties, except for the density term in momentum equation, as temperature independent and neglect the viscous dissipation. The variation of density with temperature is approximated here through the familiar Boussinesq approximation, *i. e.* $\rho - \rho_\infty = -\rho_\infty\beta(T - T_\infty)$. This leads to the coupling between the momentum and thermal energy equations. This method let the non-linear variation of density become linear with temperature, which reduces the difficulty of solving equations. The control equations of continuity, momentum, energy, and definitions of parameters are shown in tab. 2.

Table 2. Control equations and definitions of parameters

Mass equation	Boussinesq $\nabla\cdot\vec{u}=0$
Momentum equation	$(\vec{u}\nabla)\vec{u}=-\dfrac{\nabla p'}{\rho}+\mu\nabla(\nabla\vec{u})-\vec{g}\beta(T-T_\infty)$
Energy equation	$(\vec{u}\nabla)T=\left(\dfrac{k}{\rho C_p}\right)\nabla(\nabla T)$
Mass equation	Real property model $\nabla\cdot\rho\vec{u}=0$
Momentum equation	$(\vec{u}\nabla)\rho\vec{u}=-\nabla p+\nabla(\mu\nabla\vec{u})-\rho\vec{g}$
Energy equation	$(\vec{u}\nabla)\rho h=\nabla(k\nabla T)$
Grashof number	$\mathrm{Gr}=\dfrac{g\beta\rho^2 d^3\nabla T}{\mu^2}$
Thermal expansion coefficient	$\beta=-\dfrac{1}{\rho_\infty}\left(\dfrac{\partial\rho}{\partial T}\right)$
Vorticity	$\xi=\nabla\vec{u}$
Drag coefficient	$Cd=\dfrac{2F_d}{\pi\rho U^2 R_d^2}=Cd_\mathrm{f}+Cd_\mathrm{p};\quad U=\sqrt{\dfrac{Dg\beta\nabla T}{2}}$
Total drag force	$F_\mathrm{d}=\int_s(\sigma{:}ne_z)\mathrm{d}s$
Viscous drag coefficients	$Cd_1=\dfrac{4\tau_w}{\frac{1}{2}\rho U^2}$
Pressure drag coefficients	$Cd_p=\dfrac{(P_s-P_\infty)}{\frac{1}{2}\rho_\infty U^2}$
Local Nusselt number	$\mathrm{Nu}=\dfrac{D}{T_\mathrm{w}-T_\infty}\dfrac{k_\theta}{k_\infty}\left(\dfrac{\mathrm{d}T}{\mathrm{d}r}\right)_\theta$
Average Nusselt number	$\mathrm{Nu}=\dfrac{D}{2k_\infty(T_\mathrm{w}-T_\infty)}\int_0^\pi k_\theta\left(\dfrac{\mathrm{d}T}{\mathrm{d}r}\right)_\theta\mathrm{d}\theta$

These equations are solved using a finite volume method. The thermo-physical property of SCW was calculated from IAPWS-IF97 equations [35]. The boundary conditions included specified uniform far field temperature and velocity profile, no-slip condition and specified temperature at the particle surface, axisymmetry condition along the centerline, and fully developed exit conditions. The convective terms were discretized using second-order upwind scheme. The SIMPLEC algorithm was used to handle the pressure-velocity coupling. Typical values of under-relaxation factors were set from 0.1 to 0.5. A convergence criterion of 10^{-6} for each scaled residual component was specified for the relative error between two successive iterations.

Grid

The domain zone of calculated zone and grid size have strong influence on the simulated results. A larger domain zone is needed for the small Grashof number case because of strong viscous reaction and thick boundary layer [17, 21, 28]. The domain size can be determined by the rate of computed zone height to sphere particle diameter (H_∞/D). Table 3 shows effect of three domain size on the simulated results at a certain condition with particle surface temperature of 657 K and flow temperature of 647 K at far field. As the domain size rate changes from 30 to 40, the resulting changes in the values of Cd_p, Cd_f, Cd, and Nu are found to be 0.93%, 0.09%, 0.023%, and 0.3%. It is adequate to use the value of H_∞/D = 30 to get simulated results which are free from domain effects.

Table 3. Effect of domain size on simulated results

Gr	H_∞/D	Cd_p	Cd_f	Cd	Nu
$3.76\cdot10^3$	25	0.640	1.103	1.743	7.161
	30	0.642	1.106	1.74	7.071
	40	0.636	1.107	1.744	7.049
129	25	2.207	3.837	6.044	3.357
	30	2.030	4.059	6.089	3.558
	40	2.034	4.064	6.098	3.568

Three different girds were created to choose an appropriate grid for domain size of H_∞/D = 30. The principles for determination of grid size are that the grid should be fine enough to solve the steep gradient and avoid infinite computing time to convergence. The grid in radial direction is continuously stretching, by which the grid size is refined near the sphere surface. Table 4 shows the effect of grid size on the simulated results and three cases of grid were chosen in the simulated results. Case 2 is used in this work because it is fine enough and costs relatively less CPU time to reach convergence.

Table 4. Effect of grid size on simulated results (Gr = $3.76\cdot10^3$, H_∞/D = 30)

R_∞/R	Grid ($r_\mathrm{i} \times R_\mathrm{i}$)	Cd_p	Cd_f	Cd	Nu
Case 1	200 × 400	0.640	1.106	1.749	7.071
Case 2	200 × 300	0.642	1.123	1.765	7.087
Case 3	100 × 300	0.580	1.156	1.736	6.942

Validation

There are no experimental data, correlations, or simulation results for SCW flowing over a sphere. Reviews of previous studies on the free convection heat transfer from a sphere, as shown in the introduction section, reveals that the most of previous simulations were conducted based on the Boussinesq approximation. In order to validate the model mentioned in this paper, average Nusselt numbers are obtained in the early stage by simulation with Boussinesq approximation. Boussinesq approximation assumes fluid density to be constant in all terms of the mo-

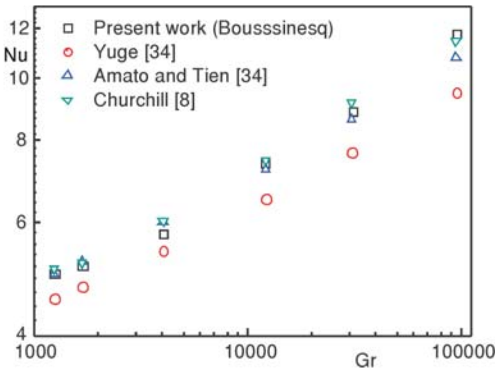

Figure 3. Comparison of average Nusslet number obtained by simulation with correlations

mentum equation except the body force term. All properties are evaluated at fluid film temperature, T_m, defined as $(T_w + T_\infty)/2$. Figure 3 shows the comparison of average Nusselt number obtained by simulation with correlations that were presented by different authors [9, 36]. It is clear that the trend of the simulation results keeps consistent with those correlations. The predicted values of Nusselt number by simulation have a agreement with that calculated by Amato and Tien's and Churchill's correlations within deviation generally within ±5%, and Yuge's correlation within deviation within –15%. However, the present famous correlations are useless for supercritical fluid. Next subsections will show the flow and heat transfer details for free convection heat transfer in SCW flow, which reflects the reasonableness of real properties model used in this paper.

Results and discussion

The special heat transmission of SCW fluid mainly depends on the effect of severe property variation, especially in the pseudo-critical zone. The present paper is devoted to the effect of the variation of SCW fluid properties on the heat transfer process. In this work, steady laminar free convection flow field for SCW flowing over a sphere particle are conducted based on two methods of real properties model and Boussinesq approximation. In order to clearly understand the difference between two models or the effect of variable properties, the SCW thermal physical properties for Boussinesq approximation are determined at the far field temperature in next sections. The dimensionless parameters (Nusselt number, Grasof number, Reylied number, and so on) are all calculated at the temperature in the far field.

Flow field

Figure 4 compares the streamline contours near the sphere surface in the pseudo-critical zone. Fluid is pushed towards the hot sphere by buoyant force and a steady-state buoyant

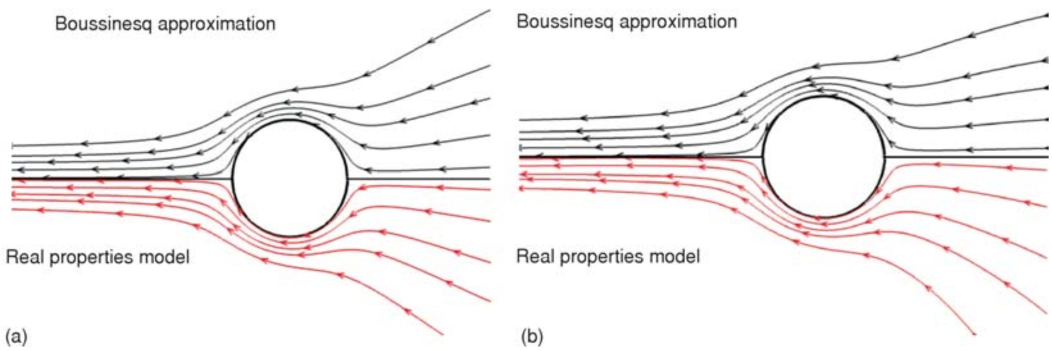

Figure 4. Effect of property variation on streamline; (a) P = 23 MPa, T_w = 657 K, T_∞ = 647 K; (b) P = 23 MPa, T_w = 667 K, T_∞ = 637 K

plume formed with hot fluid rising. The general shapes of the flow field did not change significantly at rear hemisphere even if all variable properties are considered. The similar steady plume above sphere has been reported in literatures [23, 27]. However, the flow streamlines near the leading hemisphere occupied larger flow areas when all variable properties were incorporated in calculation, which means that more fluid around the sphere is driven by buoyancy force toward the leading hemisphere. This phenomenon can also be achieved at a high Grasholf number, as shown in literatures [23, 27, 28]. This is attributed to the dramatic decrease in the density of SCW near the pseudo-critical point, which results in a stronger buoyancy force with an increasing sphere surface temperature. At the same time, fig.4(a and b) show that the larger temperature difference between sphere surface and far field leads to stronger buoyancy force and free convection.

Figure 5 shows the effect of all property variation on surface vorticity magnitude in pseudo-critical zone. The surface vorticity increases over the leading hemisphere and then reduces over the rear after it reaches a peak value in both calculations. However, the magnitude of surface vorticity for real properties model is always higher than results obtained based on Boussinesq approximation. At the same time, the position of surface vorticity maximum value for real properties is in the back of that of Boussinesq approximation model. This is attributed to a severe decrease in fluid viscosity near the pseudo-critical point for SCW flow, which leads to high momentum diffusivity and a thinner boundary layer thickness. Therefore, there is a large radial gradient of tangential velocity near the sphere surface, which is equal to the surface vorticity in magnitude. A decrease in viscosity results in a decrease of viscous drag coefficient, which induces high tangential velocity around the sphere. The similar phenomenon of thinner flow boundary caused by decreasing fluid viscosity was obtained in forced convection flow from a sphere in plasma flow [37]. On the contrary, the Boussinesq approximation ignores variable viscosity in momentum equation, which gives rise to a distortion of simulation.

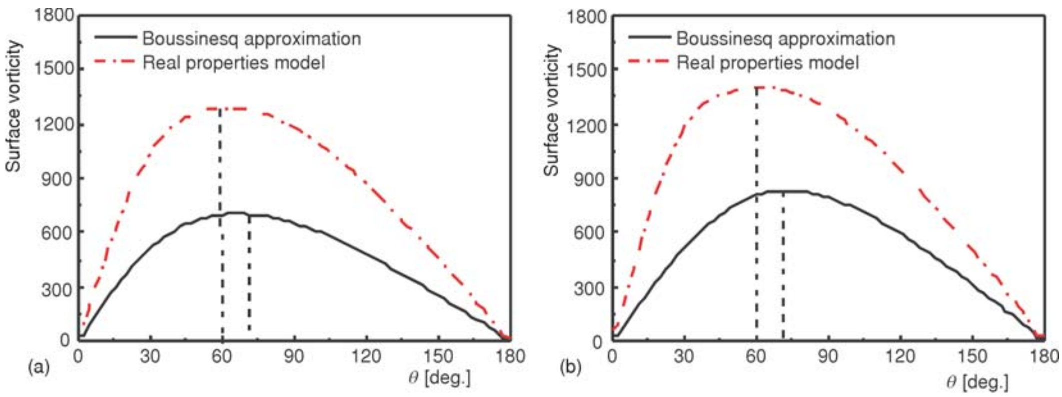

Figure 5. Effect of property variation on surface vorticity; (a) P = 23 MPa, T_w = 657 K, T_∞ = 647 K; (b) P = 23 MPa, T_w = 667 K, T_∞ = 637 K

Temperature field and local Nusselt number

Figure 6 compares the temperature contours based on Boussinesq approximation with real properties model in pseudo-critical zone. Generally, the shapes of temperature contours for two models are similar. However, when all property variation is incorporated in the computa-

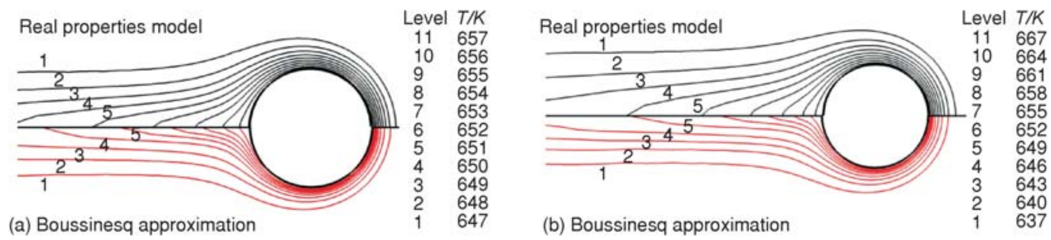

Figure 6. Effect of property variation on temperature contour; (a) P = 23 MPa, T_w = 657 K, T_∞ = 647 K; (b) P = 23 MPa, T_w = 667 K, T_∞ = 637 K

tions the temperature gradients become higher than that of Boussinesq approximation. Wen and Jog [37] believed that low thermal conductivity results in a fact that energy is confined to a smaller radial distance around sphere, as they studied a forced convection from a sphere in plasma. Things are different for the present case. There are peaks of thermal conductivity and specific heat for SCW in pseudo-critical temperature point [35]. The temperature distribution is the results of competition of heat conductivity in fluid (depends on thermal conductivity) and the heat storage capacity of fluid (depends on specific heat). Figure 7 shows that the local Nusselt number obtained by real properties model is higher than by Boussinesq approximation model, which provides further evidence for this point. The increase in the temperature gradient is due to a thinner thermal boundary layer, which is caused by elevated thermal conductivity and specific heat by increasing surface temperature. More energy is transferred from sphere particle surface to fluid in response to an increase in fluid conductivity. However, fluid with higher specific heat can store more energy, which makes diffusion of energy confined to a smaller radial distance and results in a higher temperature gradient.

The Boussinesq model can't reflect the real density variation trend and ignore the variation of other properties. So the use of Boussineq model results in unsuitability of this widely used model for predicting quantitatively free convection heat transfer from a sphere in high pressure water in pseudo-critical zone. The present real properties model shows a more accurate and reasonable prediction.

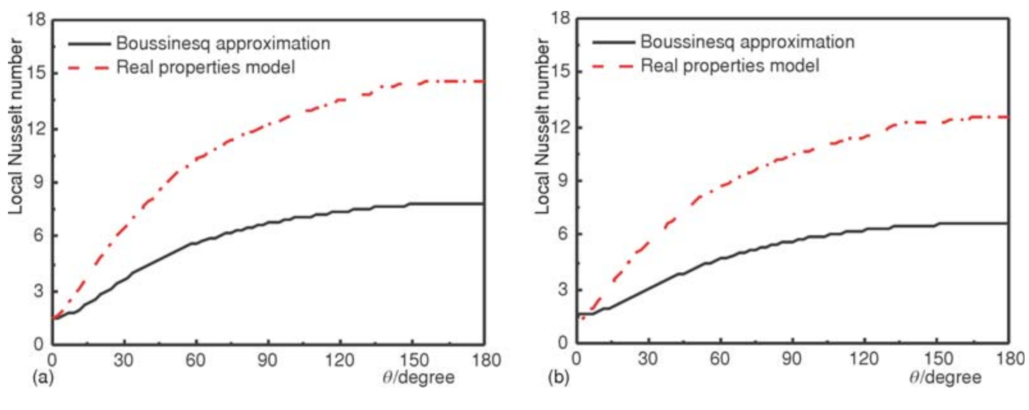

Figure 7. Effect of property variation on local Nusselt number; (a) P = 23 MPa, T_w = 657 K, T_∞ = 647 K; (b) P = 23 MPa, T_w = 667 K, T_∞ = 637 K

Nusselt number

Based on the presented analysis effect of variable properties on flow and temperature field is obvious for free convective heat transfer from a sphere in SCW flow. In order to analyze predominant effect of the thermo-physical property on free convective heat transfer of SCW passing over a particle, the simulations conducted in this work by varying density and another property with temperature while the rest properties are maintained constant as values in the far field. For simplicity, we call those model fluid as real properties flow (all four variable properties are considered), variable specific heat flow (only variable specific heat and density are considered), variable conductivity flow (only variable conductivity and density are considered), variable density flow (only variable density is considered), and variable viscosity flow (only variable viscosity and density are considered). Figure 8 shows the effect of each property on the Nusselt number. The trends of Nusselt number varying with Grashof number for variable property flow are in accordance with the results by Boussinesq approximation. It can be seen from the fig. 8 that the divergence between real properties flow and variable specific heat flow is within –10%. The average Nusslet numbers obtained for variable conductivity flow are greater than that of variable density flow. So the main factors enhances the heat transfer from particle to flow are the variation of specific heat and thermal conductivity. The variable density stratification not only forms buoyancy force but also affects on the flow and heat transfer. The Boussineq approximation just focuses on the effect of density on the forming buoyancy force, which results in incorrect predictions for present problem. What's more, the relationship between Grashof number and Nusselt number for free convection heat transfer from a sphere particle in SCW flow is nearly linear in logarithmic coordinates.

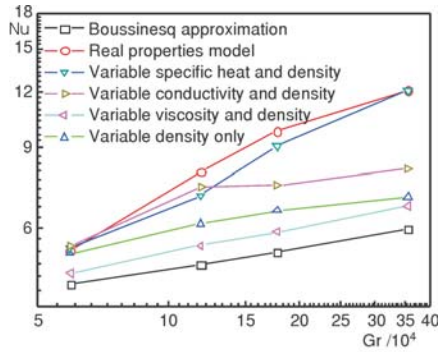

Figure 8. Effect of property variation on average Nusselt number, *P* = 23 MPa

Conclusions

The laminar free convection heat transfer from sphere particle in SCW was studied by numerical method. A computational model considering the thermo-property variation of SCW was developed successfully to describe the flow and heat transfer phenomena. Good agreement on Nusselt number was found between the simulation of Boussinesq approximation and correlations. The real properties model used in this paper shows a more accurate and reasonable prediction. Simulation results show that variation of viscosity plays a major role in the determination of flow field variation. Compared to Boussinesq approximation, magnitude of surface vorticity for real properties model is higher, which relates a thinner boundary layer for SCW flow. High temperature gradient and high heat transfer rate in the vicinity of the particle surface were observed based on real properties model. The increasing trend of Nusselt number mainly depends on variation of specific heat and conductivity. The relationship between Grashof number and Nusselt number for variable property flow is nearly linear in logarithmic co-ordinates.

Acknowledgments

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Nomenclature

Cd – drag coefficient
Cd_f – viscous drag coefficient
Cd_p – pressure drag coefficient
C_p – special heat, [$Jkg^{-1}K^{-1}$]
D – diameter of sphere particle, [mm]
D_∞ – diameter of computed zone, [mm]
e_z – unit vector along he flow direcrion
F_d – drag force, [N]
Gr – Grash of number
$\vec{g}$ – acceleration to gravitation
H_∞ – height of computed zone, [mm]
h – enthalpy, [Jkg^{-1}]
k – conductive coefficient, [$Wm^{-1}K^{-1}$]
Nu – Nusselt number
n – normal direction along the sphere surface
R_i – radius grid number of domain
r_i – particle wall grid number
P – pressure, [MPa]
Pr – Prandtl number
p' – pressure variation
Ra – Rayleigh number
T – temperature, [K]
U – characteristic velocity, [ms^{-1}]
$\vec{u}$ – velocity, [ms^{-1}]

Greek symbols

θ – streamwise angle, [deg.]
μ – viscosity, [Pa·s]
ρ – density, [kgm^{-3}]
σ – stress tensor, [Nm^{-2}]
τ – wall shear stress, [Nm^{-2}]
ζ – vorticity

Subscripts

d – drag
f – viscous coefficient
m – film temperature
p – pressure coefficient
w – wall surface
∞ – far field

Acronyms

SCW – supercritical water
SCWFBR – supercritical water fluidized bed reactor

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