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Numerical Investigations on Supercritical Heat Transfer Characteristics of Environmental Friendly Refrigerants

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Abstract

The heat transfer of supercritical fluids is a vastly growing field, specifically to find suitable alternatives to replace conventional R134a, which can be beneficial for climate change. Most of the experimental and numerical investigations have been conducted to explore supercritical water, carbon dioxide and R134a as heat transfer working fluids. Hydrofluoroolefin (HFO) and refrigerants blends have been considered the most environment-friendly refrigerants to replace Chlorofluorocarbons (CFCs), Hydrochlorofluoro-carbons (HCFCs) and Hydrofluorocarbons (HFCs). Their main advantage of zero Ozone Depletion Potential (ODP) and comparatively lower Global Warming Potential (GWP) have attracted growing amount of attention to mitigate environmental issues. This work adopts the computational method and takes the environmentally friendly refrigerants to investigate the heat transfer characteristics under widely used shear-stress transport (SST) model. A comprehensive comparison was performed at reduced pressure of 1.10 for supercritical fluids R515A, R1234ze(E) and R134a. The peaks of heat transfer coefficient occurred in the vicinity of pseudo critical temperature for all of these considered fluids; however, R134a resulted in higher heat transfer coefficient, Reynolds number and Prandtl number in comparison with R515A and R1234ze(E). The higher heat transfer coefficient of supercritical fluid R134a is owing to its thermophysical properties and the specific heat plays crucial role in the heat transfer of supercritical fluids. Owing to environmental issues, R515A can be a considerable replacement of R134a. R1234ze(E) is also promising alternative to R134a; however, safety issues should thoroughly concern its mild flammable characteristics.

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Keywords

Heat Transfer, Supercritical Fluids, Simulations, R515A, R1234ze(E), Environmental Friendly Refrigerants

1. Introduction

Supercritical fluids have wide range of industrial applications owing to the substantial impact of their heat transfer characteristics [1]-[8]. Supercritical fluids, in comparison with conventional fluids, have attracted growing amount of attention because of relatively higher heat transfer rate and lower exergy losses [9]. The thermophysical properties of supercritical fluids considerably vary near the critical (T_c) or pseudo critical temperature (T_{pc}). The heat transfer coefficient, owing to dramatic variations near pseudo-critical point, depends upon pressure, tube diameter, flow direction, heat flux and type of working fluid [10]. Therefore, this results in complex heat transfer characteristics which may account for heat transfer enhancement or deterioration [11].

Most of the experimental and numerical investigations have been conducted to explore supercritical water and carbon dioxide (sCO$_2$) [12]-[18]. Dang and Hihara [19] [20] investigated the effects of tube diameter on heat transfer coefficient of sCO$_2$ under cooling conditions and proposed the modified Gnielinski equation. Zhang and Hu [2] measured the effects of buoyancy and tube diameter for sCO$_2$. The influence of mass flux, pressure and tube diameter were plotted against heat transfer coefficient and pressure drop. Further to that, dimensionless diameter was incorporated in the development of correlation which can precisely estimate heat transfer in large-diameter tube. Wang and Guan [21] computationally investigated underlying mechanism of buoyancy effects for supercritical carbon dioxide flowing through large horizontal tube. At higher heat flux, the buoyancy is more pronounced and can cause considerable difference in the temperature at top and bottom walls. Zahlan and Groeneveld [22] performed extensive experimental tests for sCO$_2$ under vertical conditions.

However, supercritical organic fluids have not been thoroughly investigated for in tube heat transfer. Zhao and Jiang [23] examined that fluid temperature, mass flux and pressure can considerably impact the in-tube cooling heat transfer and flow of supercritical fluid R134a. Experimental data predicated (using the least square curve-fitting method) a modified Gnielinski's correlation which can give heat transfer coefficient within ±15% accuracy. Wang and Tian [24] conducted experimental investigations for supercritical fluid R134a flowing through micro-fin and smooth tube under horizontal position. These measurements under different mass fluxes, heat fluxes and pressures suggested that micro-fin tube resulted in higher heat transfer coefficient than that of smooth tube. Herein, buoyancy criteria of $\dfrac{Gr_b}{\text{Re}_b^2}\left(\dfrac{\rho_b}{\rho_w}\right)\dfrac{x}{d}$ were suggested to accurately predict results.

Further to that, micro-fin tube can significantly reduce the buoyancy effects. In more recent work, Wang and Tian [25] suggested that internally ribbed tube resulted in higher heat transfer coefficient than that of smooth tube under similar working conditions.

Kang and Chang [26] performed experiments for steady-state and transient-pressure in upward flow of supercritical fluid R134a. The study suggested that pressure transient rates have slight impact upon heat transfer rate. Cui and Wang [27] experimentally examined supercritical fluid R134a for different flow directions in a vertical tube. The data suggested good heat transfer in downward flow as compared to upward direction. He and Dang [28] [29] experimentally investigated supercritical fluid R245fa in vertical tube under heating condition. The experimental results revealed 70% data can be calculated by Yamagata's correlation within ±30% accuracy. The experimental data of supercritical fluid R1233zd(E) showed good agreement with Petukhov's correlation. In comparison with supercritical fluid R245fa, supercritical fluid R1233zd(E) can bring higher heat transfer coefficient. Jiang *et al.* [30] compared supercritical fluid R-22 and ethanol using smaller tube (1.004 mm) under higher heat flux (110 - 1800 $kW \cdot m^{-2}$). Ethanol was suggested for better flow and heat transfer performance; therefore, it's reasonable for cooling applications in combustion chambers.

Xiong and Gu [31] performed experiments and numerical simulations to evaluate the intermittent heating effects for supercritical fluid R134a. After analyzing experimental data and simulation models, SST k-ω model was suggested to accurately predict heat transfer enhancement as well as heat transfer deterioration. The decrease in velocity for near-wall region can cause heat transfer deterioration. Liu and Xu [32] compared nine turbulence models with experimental results of sCO_2 passing through helical tube and suggested the Shear Stress Transport model for best prediction to heat transfer characteristics. The comparisons of various turbulent models were performed in previous research works for different supercritical fluids including sCO_2 [32] [33] [34] [35] [36], supercritical water [37]-[42], supercritical methane [43], supercritical nitrogen [44], supercritical fluid R134a [31] [45] [46] and supercritical fluid R1234ze(E) [1]. These findings suggested good agreement between simulations (performed by SST k-ω model) and experimental data. This model can provide most accurate prediction to heat transfer coefficient, wall and bulk temperatures [36]; therefore, the present simulations of supercritical fluid R515A were performed using SST k-ω model.

R515A is non-flammable and azeotrope replacement of R134a [47], and the mixture information is shown in Table 1. It has a lower global warming potential (GWP) of 403 than that of R134a (1300 GWP of R134a). R515A /R1234yf system was suggested to lower emissions and increase energy efficiency as compared to R744 system [48]. In this context, the potential alternatives are being investigated regarding heat transfer behavior, cyclic performance and safety problems. The heat transfer characteristics are almost similar. Moreover, the environmental issues caused by R134a can be mitigated with these potential eco-friendly alternatives.

Table 1. Refrigerants information.

Refrigerant	R515A [49]	R1234ze(E) [1]	R134a [50]
Critical pressure (MPa)	3.5581	3.6349	4.059
Critical temperature (K)	381.31	382.51	374.45
ODP	0	0	0
GWP	387	<10	1340
T_{pc} at 1.1 P_c	386.2	387.5	379.0
Safety Classification	A1-non Flammable	A2L-Mildly Flammable	A1-non Flammable

However, most of the studies have explored their flow boiling or condensation heat transfer. There are few investigations at supercritical pressure, which attempted to evaluate the feasibility of HFO. R134a has been widely used for the organic Rankine cycle due to its better thermal performance. But global environmental issues demand to replace of the existing R134a with environment-friendly refrigerants which can serve potential alternatives. In this regard, R515A and R1234ze(E) have been compared with R134a at reduced pressure (P/P_{cr} = 1.10). This work is a step forward to study and explore the environment-friendly refrigerants. The simulations performed in this study can provide details about heat transfer of supercritical fluids under different mass fluxes, heat flux and tube diameters.

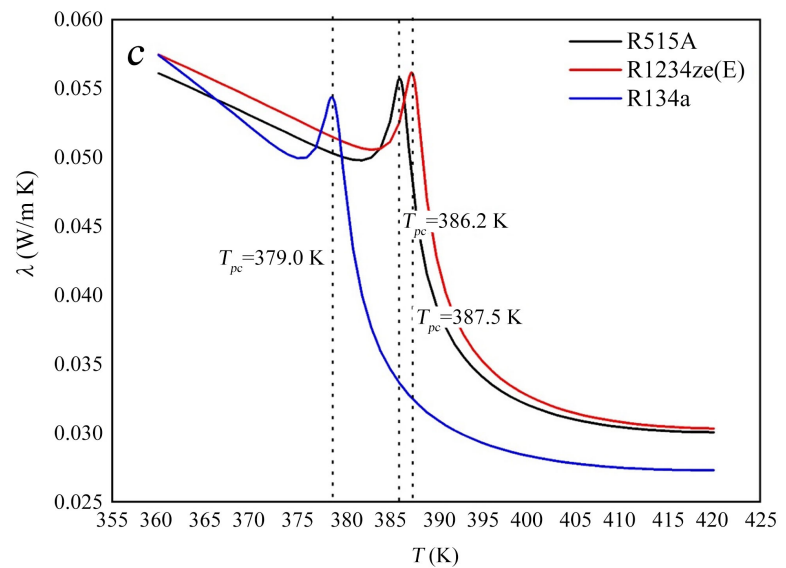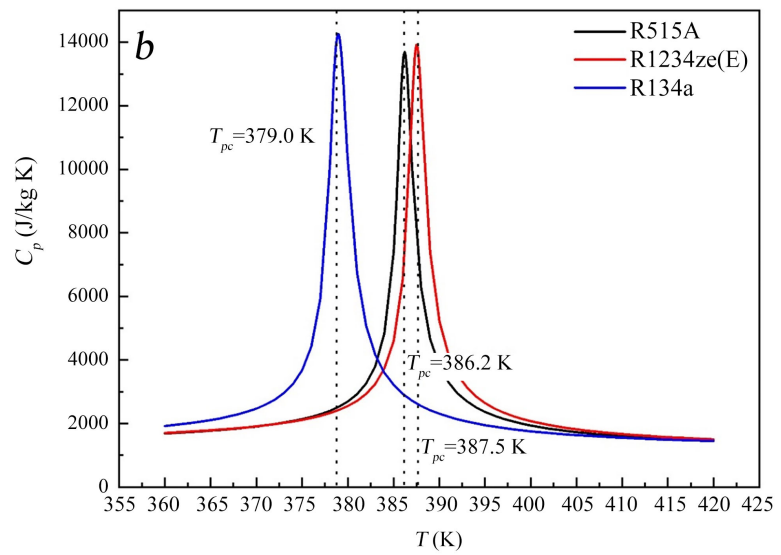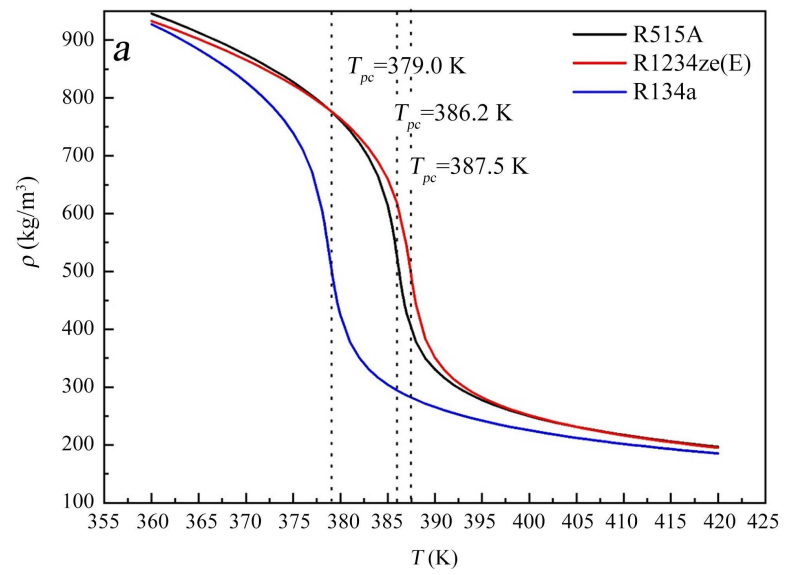## 2. Numerical Simulations

2.1. Physical Model

Thermophysical properties of supercritical fluids vary considerably near pseudo-critical point, as shown in **Figure 1**. The thermophysical properties of supercritical fluids R515A, R1234ze(E) and R134a at different temperatures and pressures were taken from REFPROP 9.1 and were plotted using OriginPro tools. Therefore, it is crucial to investigate the supercritical heat transfer in the vicinity of T_{pc} under different pressure rates. A 3D physical model is employed in the simulations to consider the effects of buoyancy for supercritical fluids, as shown in **Figure 2**. Most of the commercial heat exchangers, which are employing organic Rankine cycle, are using horizontal flow direction rather than vertical [1] [2] [25]. Therefore, the present simulations adopted horizontal flow to explore the heat transfer. An adiabatic section (200 mm) is considered to eliminate the entrance effect, and constant heat flux boundary (q) is used for the wall (1000 mm) with different diameters. The relevant refrigerants information regarding critical parameters has been described in **Table 1**.

2.2. Mathematical Model

The detailed mathematical model is described below [35].

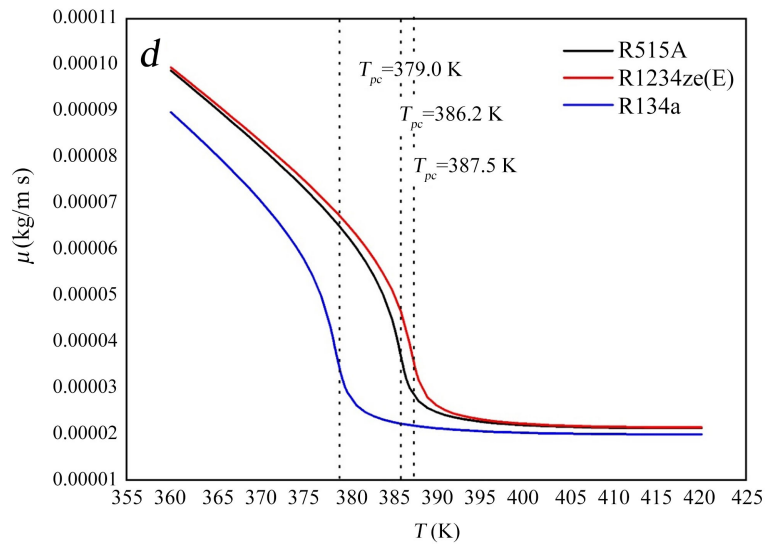The continuity equation is described as:

Figure 1. Supercritical R515A, R1234ze(E) and R134a at reduced pressure of 1.10 (a) Density (b) Specific heat (c) Thermal conductivity (d) Viscosity (REFPROP 9.1).
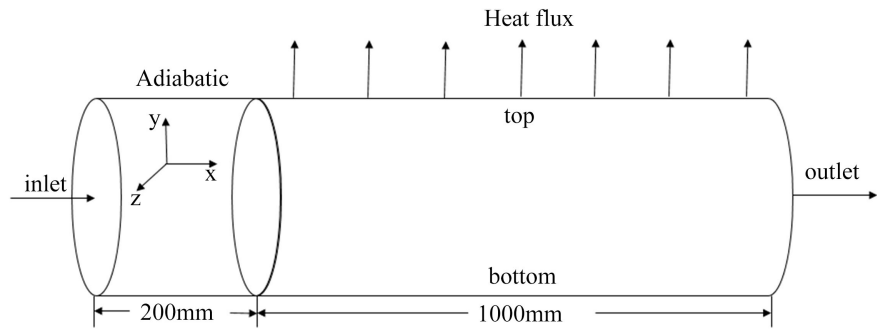

Figure 2. 3D physical model.

$$\frac{\partial}{\partial x_i}\left(\rho u_i\right) = 0 \tag{1}$$

The momentum equation is described as:

$$\frac{\partial}{\partial x_j}\left(\rho u_i u_j\right) = \frac{\partial}{\partial x_j}\left[\mu_{eff}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\mu_{eff}\frac{\partial u_k}{\partial x_k}\right] - \frac{\partial p}{\partial x_j} + \rho g_i \tag{2}$$

The energy equation is described as:

$$\frac{\partial}{\partial x_i}\left(\rho u_i c_p T\right) = \frac{\partial}{\partial x_i}\left(\lambda \frac{\partial T}{\partial x_i}\right) + \Phi \tag{3}$$

where μ_{eff} describes effective viscosity coefficient, and Φ describes energy dissipation.

The turbulent kinetic energy equation is described as [1] [35]:

$$\frac{\partial}{\partial t}\left(\rho k\right) + \frac{\partial}{\partial x_i}\left(\rho k u_i\right) = \frac{\partial}{\partial x_j}\left(\Gamma_k \frac{\partial k}{\partial x_j}\right) + G_k - Y_k + S_k \tag{4}$$

The dissipation rate equation is described as:

$$\frac{\partial}{\partial t}(\rho\omega) + \frac{\partial}{\partial x_i}(\rho\omega u_i) = \frac{\partial}{\partial x_j}\left(\Gamma_\omega \frac{\partial \omega}{\partial x_j}\right) + G_\omega - Y_\omega + D_\omega + S_\omega \qquad (5)$$

where G_k and G_ω denotes the generation of k and ω, Γ_k and Γ_ω denotes the effective diffusivity of k and ω, respectively, Y_k and Y_ω denotes the dissipation of k and ω due to turbulence, D_ω defines the cross-diffusion term, S_k and S_ω are user-defined source terms.

2.3. Boundary Conditions

ANSYS FLUENT was employed for 3D simulation of turbulent flow. The thermophysical properties of supercritical fluids at different temperatures were taken from REFPROP 9.1 and input by piecewise-linear function. SST model was adopted for present simulations owing to relatively accurate results for a range of supercritical fluids. This model has been widely used for predicting reliable results. The detailed working conditions are described in Table 2. The reference values including inlet velocity are computed from inlet for each case using ANSYS FLUENT. The following boundary conditions were adopted: mass flow inlet, outflow boundary, and constant wall heat flux. SIMPLE algorithm is used for pressure and velocity coupling.

The bulk temperature and heat transfer coefficient were calculated as follows:

$$T_b = \int_0^A \rho u T \mathrm{d}A \Big/ \int_0^A \rho u \mathrm{d}A \qquad (6)$$

$$h = \frac{q}{T_b - T_w} \qquad (7)$$

where T_b is the bulk temperature, T_w is the wall temperature, u is the local velocity and A is the cross-sectional area of the tube.

2.4. Mesh Independence Verification and Model Validation

ANSYS ICEM is used to generate high-quality hexahedral mesh as shown in Figure 3. Keeping all the working conditions same, h is plotted for different mesh sizes as illustrated in Figure 4. The deviation in h values obtained from different mesh sizes is trivial and further details have been described in Table 3. A reasonable compromise is to use *mesh* 2 for further simulations which can bring satisfactory accuracy and calculation speed.
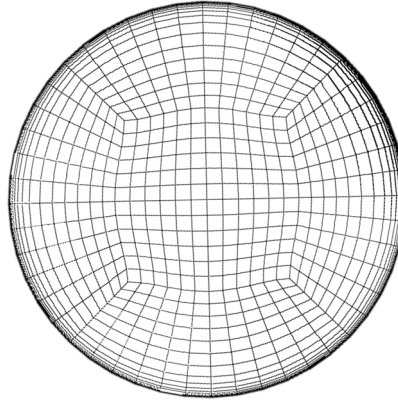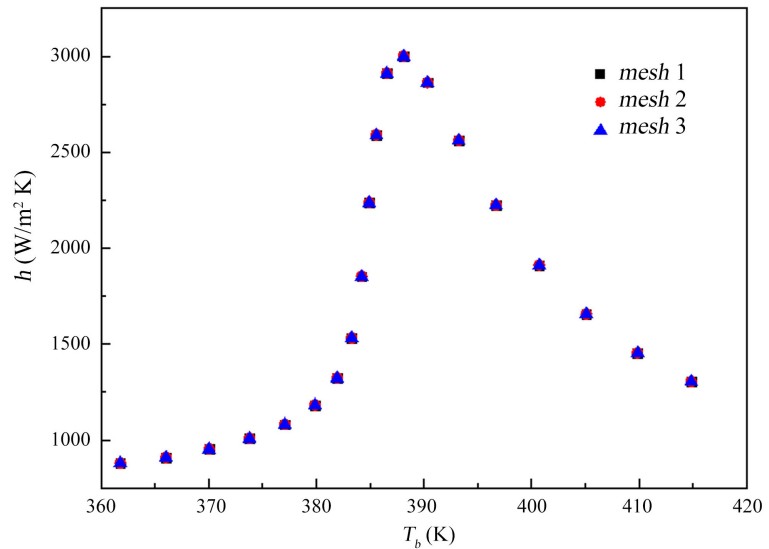
The model verification is performed against experimental data presented by Dang and Hihara [19] and Jiang and Hu [1]. The present simulations resulted in a reliable heat transfer performance and better consistency with the experimental results (Figure 5) and can be employed for supercritical fluids.

Table 2. Working conditions considered for comparison analyses.

case	d (mm)	L (mm)	P (MPa)	G (kg/m^2 s)	q (kW/m^2)
1	4.12	1000	$P/P_{cr} = 1.10$	240	−10
2	4.12	1000	$P/P_{cr} = 1.10$	240	−50
3	9.44	1000	$P/P_{cr} = 1.10$	240	−50
4	9.44	1000	$P/P_{cr} = 1.10$	600	−50

Table 3. Mesh independence for different cell numbers.

mesh	Cell number	h
mesh 1	2467584	0%
mesh 2	1862784	0.02%
mesh 3	1257984	0.06%

Figure 3. Details of mesh.

Figure 4. Mesh independence for different cell numbers.

3. Results

R1234yf and R1234ze(E) have been suggested as drop-in replacements for R134a in many previous research works. The performance parameters and heat transfer characteristics are almost similar. Moreover, the environmental issues caused by R134a can be mitigated with these potential eco-friendly alternatives [51]-[56]. In this section, heat transfer characteristics at supercritical pressure are investigated using wider range of operating conditions. The comprehensive comparison was performed at reduced pressure of 1.10 for supercritical fluids R515A, R1234ze(E) and R134a, as shown in **Figure 6-8**.
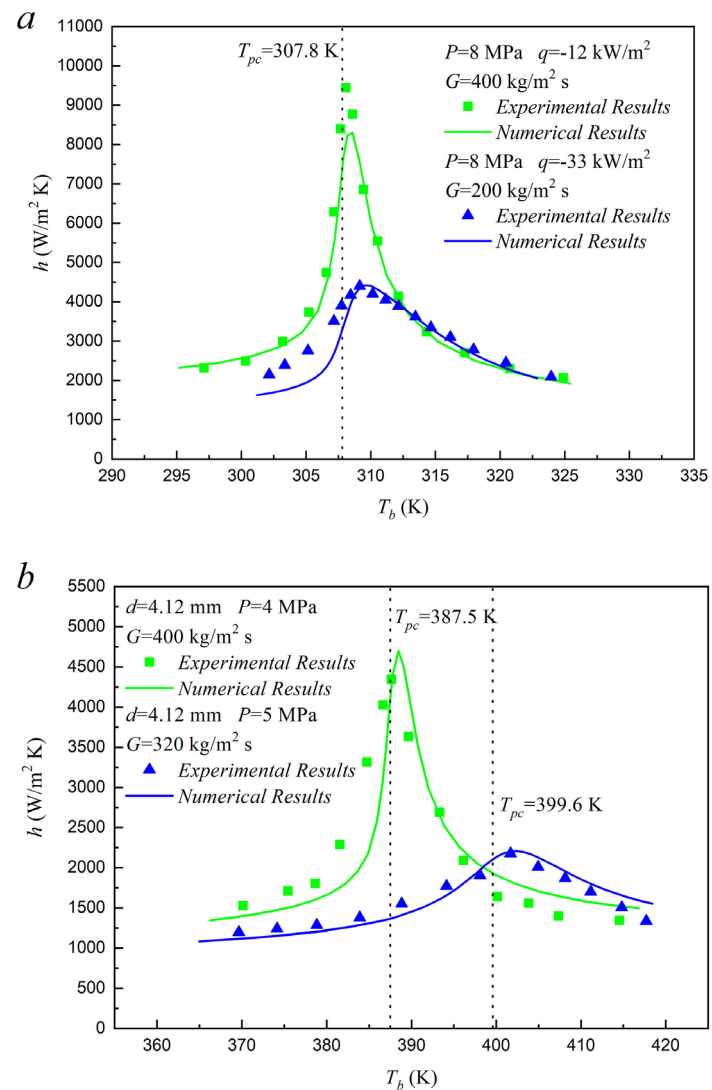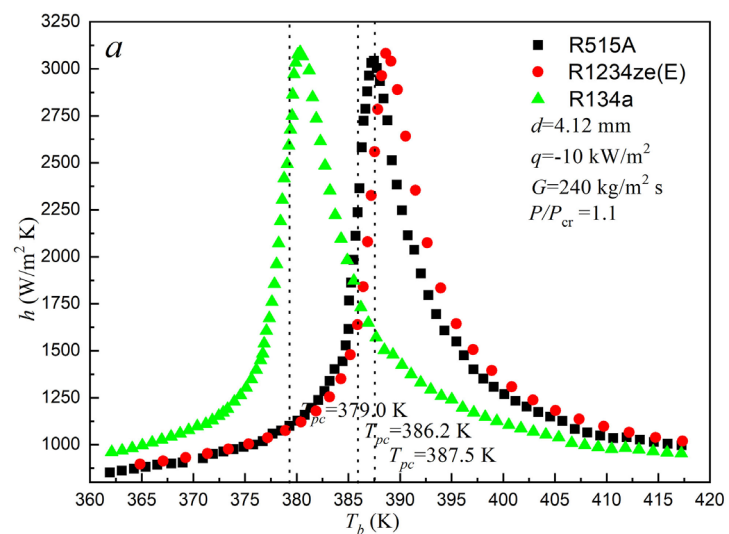
Figure 5. Model validation by comparing previous experimental data (a) Dang and Hihara [19] and (b) Jiang and Hu [1].
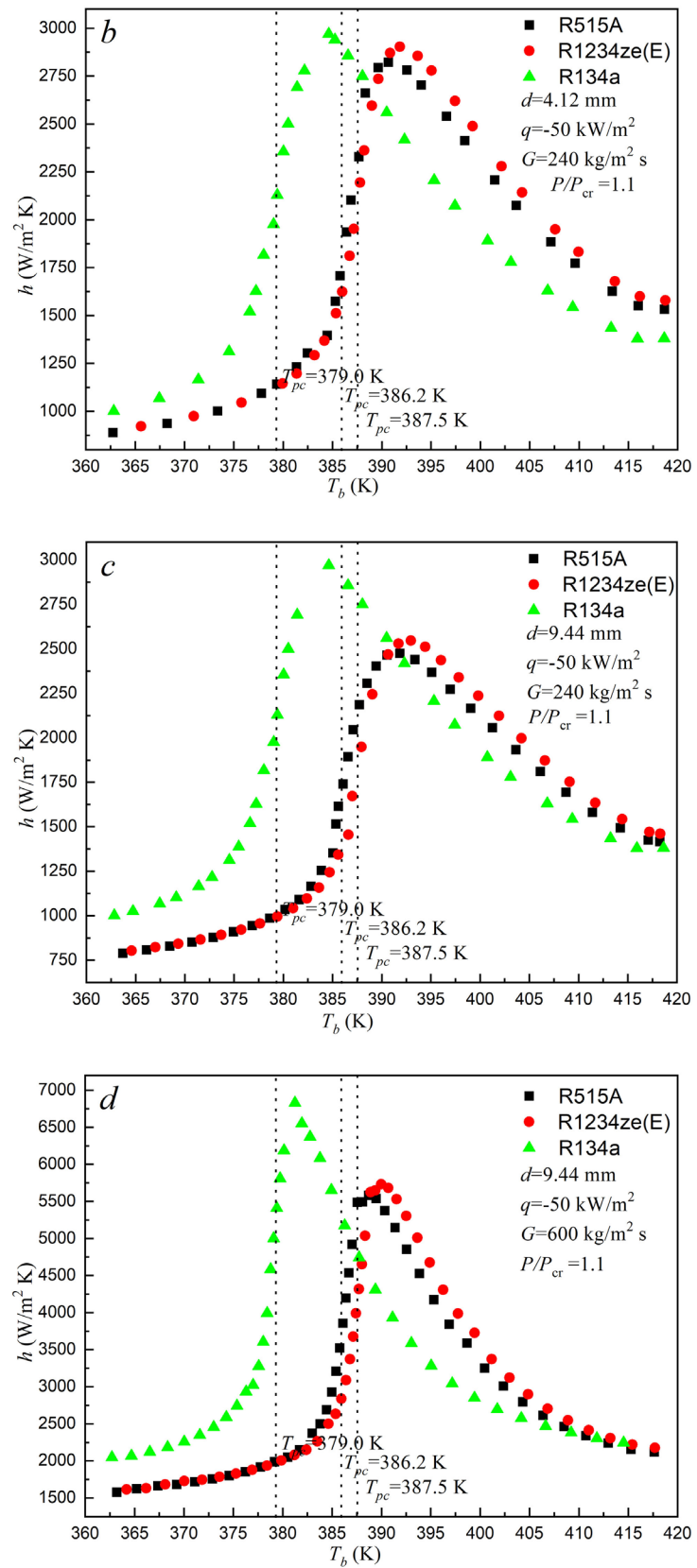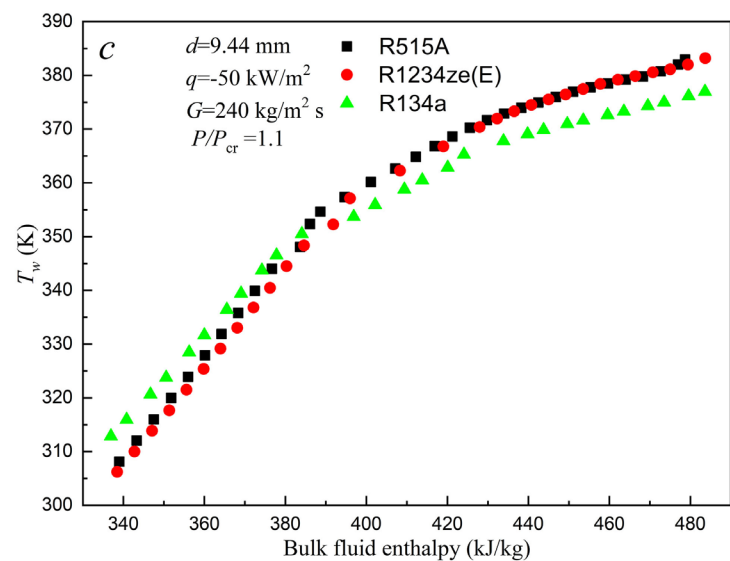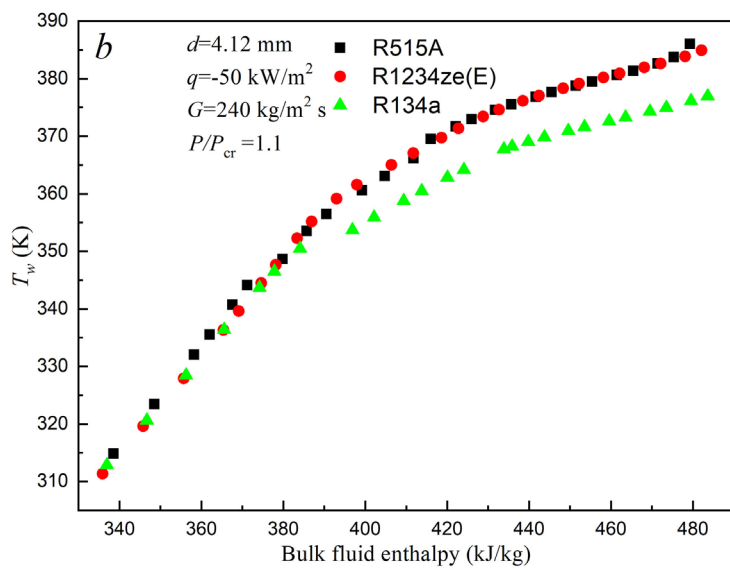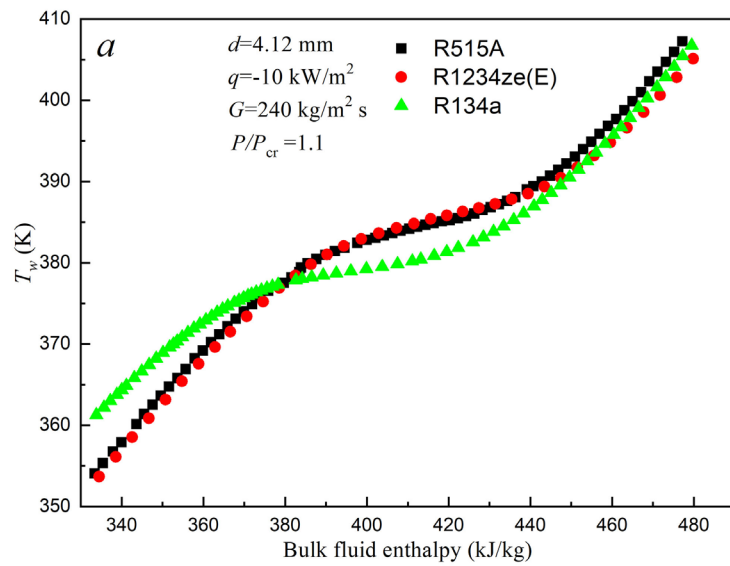
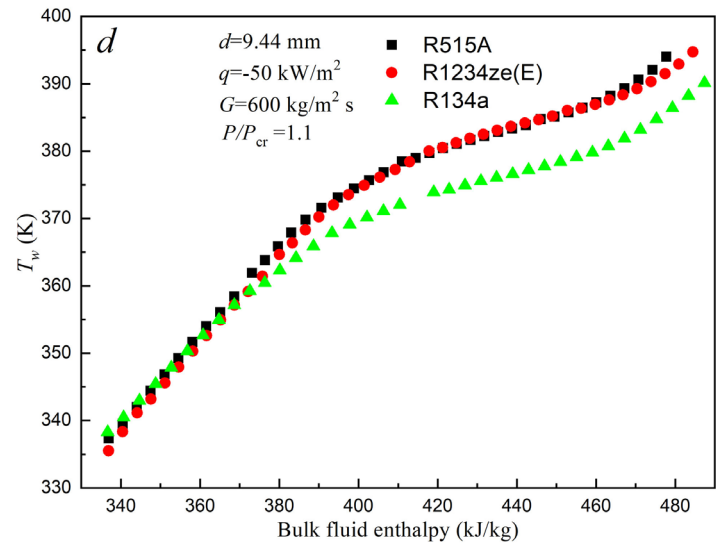**Figure 6.** Comparison of heat transfer coefficient for supercritical fluids R515A, R1234ze(E) and R134a.
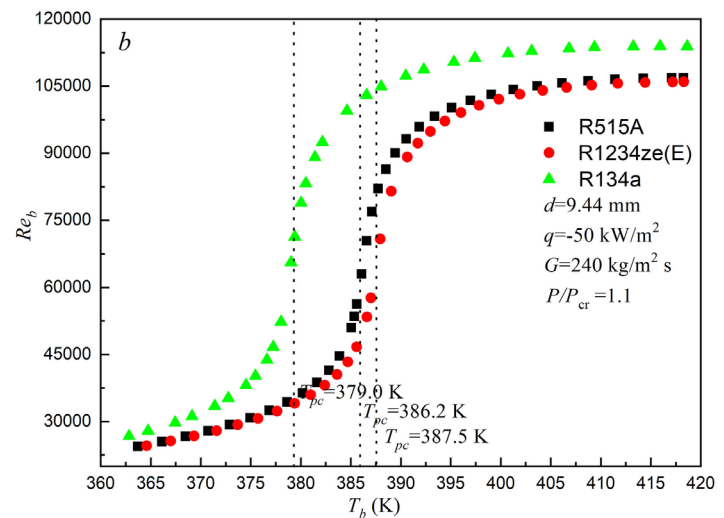
Figure 7. Comparison of T_w for supercritical fluids R515A, R1234ze(E) and R134a.

Figure 8. Comparison of the dimensionless numbers for supercritical fluids R515A, R1234ze(E) and R134a.

The peaks of h occurred in the vicinity of T_{pc} for these considered fluids, however, R134a resulted in higher heat transfer coefficient in comparison with R515A and R1234ze(E). Herein, specific heat plays crucial role in the heat transfer of supercritical fluids. R134a has comparatively higher specific heat as shown in **Figure 1**. The higher heat transfer coefficient of supercritical fluid R134a is owing to its thermophysical properties.

In order to study the influence of flow rate on the supercritical heat transfer process, different flow rates were selected in the 9.44 mm diameter heat exchange tube, and their convective heat transfer coefficients were compared and analyzed. The effect of mass flow on the heat transfer process is shown in **Figure 6(c)** and **Figure 6(d)**. When the heat flux and tube diameter of the supercritical heat exchange process remains unchanged, it can be seen that the supercritical heat transfer coefficient increases with the increase of the mass flow rate. When

the diameter of the heat exchange tube is the same, the larger flow rate causes the Reynolds number to increase, so that the thickness of the boundary layer on the inner surface of the heat exchange tube decreases during fluid flow. As a result, the fluid heat transfer coefficient can be improved.

Tube geometry, concerning different diameter, was considered for further simulations. The heat transfer coefficient may slightly lower with relatively large diameter tube as demonstrated in Figure 6(b) and Figure 6(c). The ratio of boundary layer flow with total stream becomes lower in case of large diameter tube and this can slightly decrease the h. The considered range of heat flux in the present simulations showed slight impact upon h (Figure 6(a) and Figure 6(b)). The rest of the simulations were performed under heat flux of 50 kW/m^2.

The influential nondimensional parameters (Figure 8) have been illustrated to further comprehend the heat transfer ability. Al the nondimensional parameters showed considerable influence of pseudo critical temperature, specifically in the vicinity of T_{pc}. It can be seen from Figure 8(a) that these supercritical fluids are affected by the buoyancy in heat exchange tubes for the considered conditions. Richardson numbers are from 0.1 to 10, as a result, the heat transfer process was affected by natural convection and force convection.

R134a showed beneficial values of Reynolds number and Prandtl number under the same operating conditions. Owing to environmental issues, the present simulations suggest that R515A is a considerable replacement of R134a. Table 1 showed that the GWP of R134a is more than three times higher. Both R515A and R134a have safety classification of A1-non Flammable. R1234ze(E) is also promising alternative to R134a, however, safety issues should thoroughly concern the flammability.

4. Conclusions

Hydrofluoroolefin and refrigerants blends have been attracting huge attentions owing to their environment-friendly characteristics. These can replace CFCs, HCFCs and HFCs, because the heat transfer characteristics are almost similar. The present simulations attempted to investigate supercritical fluids R515A, R1234ze(E) and R134a under cooling conditions flowing through horizontal tube. Herein, this work investigated the influence of different heat fluxes, mass fluxes and tube diameters as follows:

- The increase in mass flux can enhance the heat transfer owing to increase in Reynolds number. The influence of G is considerably prominent around T_{pc}, specifically when the T_b is slightly higher than T_{pc}. Higher values of G resulted in increased Re with thin boundary layer, consequently, increase in heat transfer and higher h values.
- The 9.44 mm diameter tube showed slightly lowered heat transfer coefficient than that of 4.12 mm. For the considered range of heat flux, heat transfer coefficient changed slightly.
- A comprehensive comparison was performed at reduced pressure of 1.10 for

supercritical fluids R515A, R1234ze(E) and R134a. The peaks of heat transfer coefficient occurred in the vicinity of pseudo critical temperature for all of these considered fluids, however, R134a resulted in higher heat transfer coefficient, Reynolds number, Prandtl number and Nusselt number in comparison with R515A and R1234ze(E).

- Owing to environmental issues, the present simulations suggest that R515A is a considerable replacement of R134a. R1234ze(E) is also promising alternative to R134a; however, safety issues should thoroughly concern its mild flammable characteristics.

Further investigations are required to thoroughly explore the heat transfer characteristics of potential alternatives in cooling and heating conditions. The effect of vertical tube and flow directions can also be considered. The simulations are reliable enough; however, experimental investigations under actual conditions can strongly affirm the results.

Acknowledgements

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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Nomenclature

A	cross-sectional area (mm^2)	R	tube radius (mm)
c_p	specific heat [J/(kg K)]	Re	Reynolds number
$\bar{c}_p$	average specific heat [J/(kg K)]	Ri	Richardson number
d	diameter (mm)	T	temperature (K)
G	mass flux [kg/(m^2 s)]	u	fluid velocity (m/s)
Gr	Grashof number	v	velocity (m/s)
h	heat transfer coefficient [W/(m^2 K)]		*Greek symbols*
i	enthalpy (J/kg)	λ	Thermal conductivity [W/(m K)]
k	turbulent kinetic energy (m^2/s^2)	μ	viscosity (g/m s)
$\dot{m}$	mass flow rate (kg/s)	ρ	density (kg/m^3)
Nu	Nusselt number		*Abbreviations / Acronyms*
P	pressure (MPa)	GWP	Global Warming Potential
Pr	Prandtl number	LB	Lattice-Boltzmann
q	heat flux (kW/m^2)	ODP	Ozone Depletion Potential
Q	heat exchange amount (kW)	SST	Shear Stress Transport
r	radial coordinate (mm)		