Numerical Investigation of Heat Transfer in the Near Critical Point Applications

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ABSTRACT
Using supercritical CO$_2$ (SCO$_2$) as a working fluid in the Brayton cycle achieves relatively high thermal efficiency at lower turbine inlet temperature. However, on the account of the fact that using supercritical CO$_2$ in the vicinity of critical point changes the default design rules, flow characteristics and boundary layer behaviour inside heat exchanger should be investigated to optimize the design parameters. The effect of the friction factor coefficient on the heat transfer and flow behaviour inside the heat exchanger is studied. The special attention is paid on the analysis of the pressure drop inside the heat exchanger. In this paper, a horizontal heated pipe with different mass flow rates, heat fluxes and boundary conditions have been numerically investigated. Different turbulence models to compute the friction factor coefficient near the critical point have been compared and the most accurate approach has been suggested. Comparing different friction factor correlations with CFD results indicated that the accuracy of different correlations is varied based on Reynolds number range and heat flux.

INTRODUCTION
Using supercritical CO$_2$ Brayton cycle is widely considered in power cycles due to its superior advantages compared to conventional cycles. Supercritical CO$_2$ cycle has been investigated in details by Dostal [1] and Sandia National laboratories [2] used for different heat sources including, solar, bio mass and fossil. Also, the promising CO$_2$ working fluid for the closed cycle was studied by Dostal [1] due to its advantages over the other working fluids. Besides, compared to the refrigerants, CO$_2$ is non-toxic, non-flammable, environmental friendly and abundant. Thermophysical properties of CO$_2$ near its critical point show unique characteristics. Isobaric specific heat reaches to the maximum value at critical point, causes sharp differences thermophysical characteristics. The Direct numerical simulation (DNS) for heat transfer investigation inside a small horizontal pipe (using SCO$_2$ working fluid) with 1 and 2 mm diameters was done for the first time by Chu et al. [3]. In their study, the inlet Reynolds number was considered to be 5400 and the inlet temperature considered less than critical temperature. Results showed that the temperature of top wall is higher than bottom wall in both cases. The 2 mm pipe experienced stronger buoyancy effect than the smaller pipe. In addition, buoyancy caused the non-uniform circumferentially friction factor coefficient. Also, flow stratification was observed and the low density flow placed near the top wall due to the buoyancy force. Saeed et al. [4] numerically investigated the friction factor of SCO$_2$ inside a zigzag channel printed circuit heat exchanger (PCHE). A Wide range of Reynolds numbers between 2500 to 30000 were used for their numerical computations. The CFD results of the friction factor compared to some friction correlations, and the best agreement on the cold side was achieved using the correlation proposed by Ngo et. al [5] and Kim et.al [6]. However, on the hot side the correlation proposed by Kim et al. [6] showed the most accurate result. In research by Nikitin et al. [7] thermophysical characteristics of SCO$_2$ including heat transfer and pressure drop inside PCHE were studied numerically and experimentally. For achieving the local heat transfer and pressure drop, an empirical correlation was proposed. The range of Reynolds number was considered between 2800 to 12100. The main achievement was proposing the empirical correlations for PCHE in order to predict the heat transfer coefficient as well as the pressure drop factor.

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Wang et al. [8] numerically investigated the effect of the turbulence models near the critical point inside a SCO₂ horizontal cooling pipe with diameter of 22.14 mm. In numerical simulations, four different k-ε turbulence models were compared, of which the AKN with low Reynolds number had the best match with the experimental data proposed by Adebiyi and Hall [9]. The results showed, by increasing the heat flux, buoyancy effect became stronger. Consequently, the temperature difference between top and bottom walls increased. Adebiyi and Hall [9] experimentally investigated the SCO₂ heat transfer in horizontal pipe. According to the results, the heat transfer enhancement was observed at the bottom of the pipe, and the buoyancy effect caused a reduction in the heat transfer coefficient near the top wall. Another experimental study about the effect of the buoyancy force on the heat transfer inside a horizontal tube with supercritical water was introduced by Bazargan et al. [10]. In experimental condition pressure range was between 23 to 27 MPa, constant heat flux: 310 KW/m² and mass flux range was from 330 to 1230 kg/m²s. They found out in buoyancy free conditions, the difference between experimental data and available empirical correlations would be high. Therefore, a new correlation was recommended to be investigated. Liao et al. [11] measured experimentally heat transfer in SCO₂ horizontal mini/micro cooled channels. The buoyancy effects in pipe diameters from 0.5 mm to 2.16 mm were studied. Reynolds number was up to 100000. The result showed the importance of buoyancy in all tests. However, by reducing the tube diameter, buoyancy became weaker, and the Nusselt number decreased. Dang and Hihara [12] investigated heat transfer in cooling SCO₂ horizontal pipe experimentally. The inner tube diameter was between 1mm to 6mm. In their study the effect of heat flux, mass flux and pressure were investigated on parameters like heat transfer coefficient and pressure drop. The experimental measured heat transfer coefficient compared to various existed correlations. As a result, the modified Gnielinski [13] correlation was introduced with accuracy of 20% over experimental data. In addition, the dependency of increasing mass flux and pressure drop were observed. Also, in case of temperature lower than pseudocritical temperature, pressure drop and inlet pressure were independent and under condition with temperature higher than pseudocritical temperature, increasing pressure led to decrease pressure drop. Walisch et al. [14] measured heat transfer coefficient experimentally in SCO₂ horizontal, vertical and inclined pipe with inner diameter 10 mm. Wall temperature was considered constant and Reynolds number range for turbulent flow was between 2300 and 100000. For defined geometries, thermophysical properties like density and heat capacity variation affected the heat transfer. The thermophysical properties near the critical point showed the similar behaviour in pseudo-critical line with lower degree. According to Wang et al. [15] the friction factor in SCO₂ horizontal pipe with considering different pressure and temperature range inside the pipe examined experimentally. The Reynolds number range was considered from 200 to 2000000. Experimental validation has been carried out in SCO₂ pipe and compared with 15 friction factor coefficient correlations. None of the correlations were matched with experimental data. The modified calculation model for friction factor coefficient was proposed with 1.94% average error over the experimental data. Moreover,SCO₂ density and viscosity were affected by temperature and pressure, consequently, the impact of Reynolds number near the critical point was observed sharply. Also, by increasing Reynolds number in turbulence flow region, the friction factor coefficient reduced.

In this paper, the turbulent flow of supercritical CO2 in heated horizontal pipe is investigated numerically. The different Reynolds numbers and heat fluxes were simulated and different turbulence models were compared. Special attention was paid on the friction coefficient and simulated friction coefficients were compared to different existing friction factor correlations. The most accurate turbulence model and friction factor coefficients were suggested.

**COMPUTATIONAL DETAILS**

**Geometry and boundary condition**

In this study the experimental results of Adebiyi and Hall investigation [9] are used to validate heat transfer characteristics and turbulence models. In experimental investigation, a pipe with about 4 m length and inner diameter of 22.14 mm was tested. As it is shown in figure 1, the pipe is divided into two parts including, adiabatic and heating part. The adiabatic part was added to ensure that the flow profile is fully developed before entering the heating part. Heating is uniform throughout the pipe.

![Figure 1 Schematic of the numerical model](image)

According to experimental conditions shown in table 1, four test conditions are numerically studied. The range of mass flow rate is from 0.151 to 0.080 kg/s. The cross section of mesh is shown in figure 2. The grid resolution is fine enough to ensure y+ < 1.

The mesh independency study was performed (figure 3) using three different grid resolutions; 500000, 750000 and 1300000 cells. The grid with 1.3 million cells seems to be fine enough for giving mesh independent results. ANSYS CFX was used as a solver for numerical computation [30]. Regarding the boundary conditions, pressure and temperature were set for inlet and mass flow rate was set for the outlet. Walls are considered as no slip, with adding constant heat flux throughout the heating part. Symmetric boundary condition was used to model half of the pipe in order to save the computational time.
Table 1 Experimental conditions

<table>
<thead>
<tr>
<th>Test code</th>
<th>Mass flow rate (kg/s)</th>
<th>Inlet bulk temperature (°C)</th>
<th>Average heat flux (kW/m²)</th>
<th>Outlet bulk temperature (°C)</th>
<th>Test pressure (MN/m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>0.151</td>
<td>15.9</td>
<td>5.3</td>
<td>18.1</td>
<td>7.586</td>
</tr>
<tr>
<td>1.2</td>
<td>0.148</td>
<td>15.4</td>
<td>15.1</td>
<td>21.3</td>
<td>7.59</td>
</tr>
<tr>
<td>2.1</td>
<td>0.0773</td>
<td>14.2</td>
<td>5.2</td>
<td>18.4</td>
<td>7.603</td>
</tr>
<tr>
<td>3.1</td>
<td>0.080</td>
<td>19.7</td>
<td>5.1</td>
<td>23.2</td>
<td>7.607</td>
</tr>
</tbody>
</table>

VALIDATION OF NUMERICAL COMPUTATION

In the experimental measurements [9], to achieve the temperature distribution along the tube, the welded thermocouples with various angles were placed at top and bottom part of the tube wall. To find out the most accurate turbulence model for the CFD simulation in this case, four different turbulence models are examined under test 1.1 experimental conditions (see table 1).

In figure 4, the results of the compared turbulence models including: shear stress transport (k-ω SST ), k-ε EARSM, Omega Reynolds Stress (ORS) and standard k-ε, are shown.

Two turbulence models k-ε EARSM and k-ε standard showed high degree of discrepancy over the experimental results. On the other hand, the SST has the best agreement with experimental data followed by ORS model. Therefore, the SST turbulence model has been used for the rest of the investigations in this study.

RESULTS AND DISCUSSION

Wall temperature distribution

According to results, shown in figure 5, in all CFD cases the top walls have higher temperature than bottom walls due to the buoyancy effect, and the highest temperature is observed at the top wall of CFD case 1.2 with the highest heat flux (q=15100 W/m²). In test cases 1.2, 2.1 and 3.1, the sharp temperature changes are observed at the start of heating section, following by rather constant temperature increment trend. However, in CFD case 1.1 with the highest mass flow rate, this sharp change has not been observed. Moreover, the best agreement between CFD result and the experimental data for both top and bottom walls is achieved in case 1.1 due to relatively lower heat flux and consequently smaller buoyancy effect followed by case 1.2. The CFD results of case 2.1 and 3.1 show high degree of discrepancy over experimental results on top walls but the bottom walls in both cases are still in a good agreement. In CFD case 1.1, the heat flux is lowest and the temperature difference between...
top and bottom wall is not rather significant. In another word, the effect of the buoyancy force is not noticeable and consequently, there is less complexity in the flow.

Heat transfer coefficient

The computed heat transfer coefficient in CFD simulation is based on equation 1, where, $q$ is the heat flux, $T_w$ expresses the wall temperature and $T_b$ is the bulk temperature.

$$ h = \frac{q}{(T_w - T_b)} \quad (1) $$

According to results of the figure 6, the heat transfer coefficient at the bottom walls are higher than the top walls in all CFD cases, which can be referred to the higher temperature difference between the top walls and the bulk temperature than the bottom walls and bulk temperature. Therefore, with considering the constant heat flux, the heat transfer coefficients on top walls are lower than the bottom walls. According to the figure 6, in all cases, the heat transfer coefficients are changed sharper at the top walls while the changes are smoother at the bottom walls. This change is observed more significant in CFD case 1.2 with highest heat flux compared to other cases. However, the heat transfer coefficient trends in all simulated cases remain constant after around 15D-20D from start of the heating.

Figure 5 Temperature distribution of numerical results based on SST turbulence model against experimental results in four test conditions
Friction factor Coefficient

The fluid flow along the tube is influenced by viscous, friction and buoyancy forces. Studying the friction factor coefficient is the major parameter to determine the pressure drop inside the heat exchanger. The generic equation of friction factor is expressed by equation 2.

\[
C_f = \frac{\tau_w}{\frac{1}{2} \rho U^2}
\]

(2)

Where, \(\tau_w\) is the wall shear stress, \(\rho\) is the bulk density and \(U\) is the bulk fluid velocity.

The friction factor coefficients along the pipe at the top and bottom walls are shown for each CFD case in figure 7. The value of friction factor coefficient at the bottom wall is higher than the top wall in all CFD cases. In fact, shear stress is higher at the bottom wall. In figure 7, Friction factor coefficient of top and bottom walls start with sharp changes at the start of heating and then continue with a rather constant trend. As it is observed, the highest change are observed in CFD cases 2.1 and 3.1 with lower mass flux compared to other cases.
Furthermore, the averaged friction factors of the top and bottom walls in adiabatic and heated parts are calculated individually for each test case (see table 2). The higher change is observed from case 1.1 to 1.2 due to increasing heat flux from CFD case 1.1 to 1.2, which causes strong buoyancy force as a result of raising temperature difference between top and bottom wall. Consequently, the sharp change is observed at the beginning of heated part in case 1.2. On the other hand, mass flux reduction from case 1.2 to 2.1 creates sharp value change related average friction factor coefficient from adiabatic to heated section. The important achievement by analysing data of table 2 is that, the friction factor change is more dependent on heat flux than the mass flux; meaning, referring to CFD condition, heat flux increases from case 1.1 to 1.2, where calculated friction factor change percentage (from adiabatic to heated section) highly increased (from 5.8 to 11.7). However, although from Case 1.1 to 2.1 and 3.1 mass flux reduces; the calculated change percentage has not changed significantly.

### Table 2 Comparison of average friction factor in heating wall with adiabatic wall for numerical cases

<table>
<thead>
<tr>
<th>Case code</th>
<th>Average of $C_f$ (Heating wall)</th>
<th>Average of $C_f$ (Adiabatic wall)</th>
<th>Changes (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>0.0041</td>
<td>0.0044</td>
<td>5.8</td>
</tr>
<tr>
<td>1.2</td>
<td>0.0039</td>
<td>0.0044</td>
<td>11.7</td>
</tr>
<tr>
<td>2.1</td>
<td>0.0048</td>
<td>0.0050</td>
<td>4.5</td>
</tr>
<tr>
<td>3.1</td>
<td>0.0046</td>
<td>0.0049</td>
<td>5.2</td>
</tr>
</tbody>
</table>

### VALIDATION OF SEVERAL FRICTION FACTOR COEFFICIENT CORRELATIONS AGAINST CFD RESULTS

In this section, 12 well-known friction factor correlations are compared with CFD results. Table 3 shows correlations and related equations with respect to the employed Reynolds number range. Blasius (1913) [19] correlation can be considered the simple one, which is based on first principal of non-Newtonian fluid flow. Filonenko [20] is gained from developed Darcy equation. For tubes with small roughness elements and turbulent flow, Blasius[19] and Filonenko[20] friction factor correlations are proposed. Wilcox correlation can be found out in [22]. The developed equation of Prandtl[23] is Prandtl (Denn) [23]. Prandtl-Schlichting correlation can be found in [24]. Kempf-Karman and Granville are extracted from [25][26]. Morrison correlation can be used for smooth pipe employing all range of Reynolds number [27].

### Table 3 List of friction factor correlations used in validation

<table>
<thead>
<tr>
<th>Data source</th>
<th>Correlation</th>
<th>Range of Re</th>
</tr>
</thead>
<tbody>
<tr>
<td>Blasius (1913) [19]</td>
<td>$C_f = 0.316 \left(Re^{0.25}\right)$</td>
<td>$Re \leq 10^5$</td>
</tr>
<tr>
<td>Blasius R [21]</td>
<td>$C_f = 0.079 \left(Re^{0.25}\right)$</td>
<td>$Re \leq 10^5$</td>
</tr>
<tr>
<td>Filonenko [20]</td>
<td>$C_f = (1.82 \log(Re) - 1.64)^{-2}$</td>
<td>$10^5 \leq Re &lt; 5 \times 10^6$</td>
</tr>
<tr>
<td>Wilcox (1995) [22]</td>
<td>$C_f = 1/\sqrt{f} = -2 \log(2.51/Re\sqrt{f})$</td>
<td>$Re &gt; 3000$</td>
</tr>
<tr>
<td>Wilcox [22]</td>
<td>$C_f = 0.045 \left(Re^{0.25}\right)$</td>
<td>$Re &gt; 3000$</td>
</tr>
<tr>
<td>Lee [19]</td>
<td>$C_f = 0.0018 + 0.152 \left(Re\right)^{0.35}$</td>
<td>$Re &gt; 3000$</td>
</tr>
<tr>
<td>Jansen [29]</td>
<td>$C_f = 0.0412 \left(Re\right)^{0.1925}$</td>
<td>$Re &gt; 3000$</td>
</tr>
<tr>
<td>Prandtl (1927) [23]</td>
<td>$C_f = 0.074 \left(Re\right)^{0.2}$</td>
<td>$Re &gt; 4000$</td>
</tr>
<tr>
<td>Prandtl-Schlichting (1932) [24]</td>
<td>$C_f = 0.455 \log(Re)^{-2.58}$</td>
<td>$Re &gt; 4000$</td>
</tr>
<tr>
<td>Kempf-Karman (1951) [25]</td>
<td>$C_f = 0.055 \left(Re\right)^{-0.182}$</td>
<td>$Re &gt; 3000$</td>
</tr>
<tr>
<td>Granville (1977) [26]</td>
<td>$C_f = 0.0776 \left(\log(Re) - 1.88\right)^2 + 60 \left(Re\right)^{-1}$</td>
<td>$Re &gt; 3000$</td>
</tr>
<tr>
<td>Genielinski [13]</td>
<td>$C_f = 0.79 \log(Re)-1.64)^2$</td>
<td>$Re &gt; 3000$</td>
</tr>
<tr>
<td>Prandtl (Denn) (1927) [28]</td>
<td>$Cf=0.255 \log(Re)^{-2.5}$</td>
<td>$3000 \leq \text{Re} \leq 5 \times 10^6$</td>
</tr>
<tr>
<td>Morrison [27]</td>
<td>$C_f = (0.0076+\left(3170/\text{Re}\right)^{0.165}(1+\left(3170/\text{Re}\right)^{0.27}))/16/\text{Re}$</td>
<td>$10^5 \leq \text{Re} \leq 10^6$</td>
</tr>
</tbody>
</table>

Figure 8, represents the validation of CFD results against 2 experimental data, including Adebiyi and Hall [9] and Dang–Hihara [12] as well as 12 existed friction factor correlations. In fact, the CFD results are calculated based on the average friction factor coefficient of top and bottom wall for each CFD case individually. The Dang and Hihara [12] experimental results have been investigated for horizontal pipe with 2 mm inner tube, which used SO2 working fluid. The experimental conditions are included 30°C inlet temperature range from 30°C to 70°C, mass flux is 800 kg/m²s, heat flux is 12 KW/m² and pressure drop range is from 30 to 70 MPa. The employed Reynolds number range in Dang–Hihara [12] is the same as CFD results.

The generic equation for calculating Reynolds number at start of heating section for each CFD cases is:

$$Re = \frac{\rho Dw}{\mu}$$

(3)
Where, \( \rho \) is fluid density (kg/m\(^3\)), \( \nu \) is fluid velocity (m/s), \( D \) is tube diameter (mm) and \( \mu \) determines fluid dynamic viscosity (kg/m s).

According to figure 8, range of Reynolds number is \( 9 \times 10^4 < \text{Re} < 12 \times 10^4 \) with respect to average friction factor coefficient of each CFD case. It is observed that, the predicted friction factor coefficient by four friction factor correlations including: Blasius [19], Wilcox 1995 [22], Morrison [27] and Lee [19] are in the best agreement with CFD results in the studied Reynolds number range. It is worth mentioning that, Dang-Hihara [12] results, employed in the same CFD boundary condition and Reynolds number range, with except smaller tube diameter (2 mm) compared to numerical condition. CFD results showed the best agreement between Dang-Hihara [12] experimental results and the predicted friction factor coefficient using the Blasius R [21] and Genielinski [13] correlations.

The important interpretation from the results of figure 8 is that defining specific accurate friction factor correlation for special fluid flow can be depends on various parameters including Reynolds number and the operating conditions. Therefore, determining agreed general statement for the friction factor correlation with CFD results is not considered logical.

Figure 9, shows the top and bottom walls friction factor coefficients derived from the CFD results as well as comparison with the correlations. The CFD results of case 2.1 and 3.1 (considering the bottom wall with higher shear stress as well as lower temperature than top wall) are in good agreement with correlation proposed by Kempf-Karman [25]. However, the calculated friction factor coefficients of CFD cases 1.1 and 1.2 can be predicted rather closely using the Blasius [19], Morrison [27] and Lee [19] correlations. On the other hand, the same comparison for top wall shows that cases 1.2, 2.1 and 3.1 are in good agreement with the predicted friction factor using correlation proposed by Wilcox [22]. Also the friction factor of top wall in CFD case 1.1 with some degree of deviation has rather good agreement with predicted friction factor coefficient used Wilcox 1995 [22] correlation.

**VELOCITY AND DENSITY CONTOURS**

Four cross sections from start of the heating to the outlet were named based on their distance in diameters (D) as 4D, 14D, 30D and outlet. The normalized velocity and density contours of the test case 1.2 at the defined cross sections are shown in figure 11. By applying a constant heat flux, the temperature difference between top and bottom walls increases along the pipe. Slightly after start of heating, at 4D, normalized velocity and density contours at the cross section are still uniform. While, by moving to the downstream, due to the temperature difference between top and bottom walls, the heated \( \text{CO}_2 \) with lower density is pushed upward (near the round walls) and the flow with higher velocity moves closer to the bottom wall (in the middle of the pipe). These flow movements generate the secondary flow and vortexes. The direction of upward and downward flow on cross section are shown in figure 10.
CONCLUSION

In this paper, the thermophysical properties of SCO₂, flow structure and friction coefficient in a heated horizontal pipe was investigated numerically. Different boundary conditions and heat fluxes were modelled and results were compared against the experimental data.

The major focus of this study was on analysing the friction factor coefficient, which is the most important factor to estimate the pressure drop inside heat exchangers. Adebiyi and Hall [9] experimental data was used as a reference to validate the numerical computations. By comparing different turbulence models including two-equation and Reynolds stress models, k-ω SST model showed the best agreement with experimental data.

The CFD results of temperature distribution, heat transfer and friction factor coefficients were validated against experimental results. By studying the heat transfer coefficient along the pipe at the top and bottom walls, heat transfer coefficient on bottom wall showed enhancement compared to top wall.

Calculated friction factor coefficient were compared against 12 well-known correlations obtained from the literature. It was noticed that, there is a difference in the values for the friction coefficient on the top and bottom sides of the heated part of the pipe. Top wall has smaller friction coefficient values due to lower velocity as a result of buoyancy force. The averaged values of the friction coefficients at the top and bottom sides were in a good agreement with three correlations (Wilcox 1995 [22], Blasius [21] and Morrison [27]). In conclusion, finding the best accurate friction factor correlation for the particular heating/cooling pipe can be depended on various parameters including Reynolds number and the tube diameter. Therefore, determining agreed general statement for the friction factor correlation with CFD results is not considered logical.

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