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Deposited on: 22 November 2021
Heat Transfer of Supercritical Carbon Dioxide in a Tube-in-Tube Heat Exchanger-A CFD Study

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Date: 22 November 2021
Abstract

For better design and optimization of the heat exchanger (HX), forced convective heat transfer and flow characteristics of supercritical carbon dioxide (SCO2) in a water-cooled experimental counter-flow tube-in-tube HX were studied numerically with three-dimensional Reynolds-averaged Navier-Stokes equations and shear stress transport (SST) turbulence model by using computational fluid dynamics method in ANSYS CFX. With a sole tube model of the HX, effects of SCO2 inlet pressure, mass flux, tube diameter and wall heat flux on SCO2 mean heat transfer coefficient (MHTC) were investigated. Influences of turbulence models and discretisation schemes of the advection terms in the SST model, wall temperature of conservative and hybrid values in CFX-Post on MHTC were clarified, and buoyancy effect in the horizontal HX was explored. The SST model can achieve better agreement with the experimental MHTCs of SCO2 than the other models. The buoyancy effect can improve MHTC by the secondary flows in the tube.

Keywords: supercritical carbon dioxide; tube-in-tube heat exchanger; heat transfer coefficient; forced convective heat transfer; buoyancy effect; computational fluid dynamics
Nomenclature

\( a \) constant in the \( \mu_t \) expression of the shear stress transport model, \( a=0.31 \)

\( B \) constant in log-law velocity profile, \( B=5.2 \) for hydraulically smooth walls

\( C_p \) specific heat capacity of fluid, \( J/kg \)

\( d \) inner diameter, \( \text{mm} \)

\( f \) variable related to energy redistribution

\( F_1 \) blending function between the Wilcox \( k-\omega \) model and the standard \( k-\varepsilon \) model

\( F_2 \) auxiliary variable in the \( \mu_t \) expression of the shear stress transport model

\( g_i \) components of the acceleration of gravity, \( i=1, 2, 3, \text{m/s}^2 \)

\( G \) mass flux, \( \text{kg/m}^2\text{s} \)

\( Gr_b \) Grashof number

\( h \) specific enthalpy of fluid, \( \text{m}^2/\text{s}^2 \)

\( k \) turbulence kinetic energy, \( \text{m}^2/\text{s}^2 \)

\( n \) power relating to tube orientation

\( p \) fluid static pressure, \( \text{MPa} \)

\( P_{kb}, P_{\omega b} \) buoyancy production term in the \( k \)-equation and \( \omega \)-equation, respectively, \( \text{J/m}^3 \)

\( Pr \) fluid Prandtl number

\( Pr_t \) turbulent Prandtl number, \( Pr_t=0.9 \)

\( q_w \) water heat flux across the tube wall, \( \text{kW/m}^2 \)

\( Re \) Reynolds number at inlet of the tube

\( Re_b \) Reynolds number based on bulk velocity in the tube

\( Ri \) Richardson number

\( S_{\varepsilon} \) source term of energy equation, \( \text{J/m}^3 \)

\( S_i \) specific body force, \( i=1, 2, 3, \text{m/s}^2 \)

\( t \) time, \( \text{s} \)

\( T \) local temperature of fluid, \( ^\circ\text{C}, \text{K} \)

\( T_0 \) reference temperature of fluid, \( ^\circ\text{C}, \text{K} \)

\( T_1 \) fluid temperature at inlet of the tube, \( ^\circ\text{C}, \text{K} \)

\( T_b \) mean bulk temperature of fluid, \( ^\circ\text{C}, \text{K} \)

\( T_c \) temperature at pseudo critical point of fluid, \( ^\circ\text{C}, \text{K} \)

\( T_{\varepsilon} \) fluid temperature in the first mesh layer, \( ^\circ\text{C}, \text{K} \)

\( T^+ \) dimensionless temperature in the boundary layer

\( T' \) fluctuation of fluid temperature, \( \text{K} \)

\( u_b \) bulk velocity of fluid in the tube, \( \text{m/s} \)

\( u_i, u_j \) Reynolds time-averaged velocity components of fluid in a Cartesian coordinate system, \( i, j=1, 2, 3, \text{m/s} \)
\( u_n \) fluid velocity near wall, m/s
\( u'_t \) turbulent fluctuation velocity of fluid, m/s
\( u_r \) friction velocity of fluid at wall, \( u_r = \sqrt{\tau_w/\rho} \), m/s
\( u_r^{\log}, u_r^{\text{vis}} \) friction velocities at wall by using the solutions in the log-law and sublayer layers
\( U \) mean heat transfer coefficient, W/m²K
\( v^2 \) velocity scale for turbulence transport, m²/s²
\( x_i, x_j \) coordinates of a Cartesian coordinate system, \( i, j = 1, 2, 3, m \)
\( y_n \) distance to the nearest wall from the first mesh layer, m
\( y^+ \) dimensionless wall distance, \( y^+ = \sqrt{\tau_w/\rho} y_n/\nu \)

**Greek**
\( \alpha, \beta_1, \sigma_{\omega_1} \) model constants in the \( \omega \)-equation of the Wilcox \( k-\omega \) model, \( \alpha_1 = 5/9, \beta_1 = 0.075, \sigma_{\omega_1} = 2 \)
\( \alpha_2, \beta_2, \sigma_{\omega_2} \) model constants in the \( \omega \)-equation of the \( \omega \)-transformed standard \( k-\epsilon \) model, \( \alpha_2 = 0.44, \beta_2 = 0.0828, \sigma_{\omega_2} = 1/0.856 \)
\( \alpha_3, \beta_3, e, \sigma_{\omega_3} \) blended model constants in the \( \omega \)-equation of the blended Wilcox \( k-\omega \) and standard \( k-\epsilon \) models, \( \alpha_3 = F_1 \alpha_1 + (1-F_1) \alpha_2, \beta_3 = F_1 \beta_1 + (1-F_1) \beta_2, \sigma_{\omega_3} = F_1 \sigma_{\omega_1} + (1-F_1) \sigma_{\omega_2} \)
\( \beta \) auxiliary variable in dimensionless fluid temperature expression in the boundary layer
\( \beta_k \) model constant in the \( k \)-equation of the Wilcox \( k-\omega \) model and the \( \omega \)-transformed standard \( k-\epsilon \) model, \( \beta_k = 0.09 \)
\( \beta_\nu \) volumetric thermal expansion coefficient of fluid, 1/K
\( \gamma \) magnitude of the strain rate of fluid velocity, 1/s
\( \gamma_{ij} \) strain rate tensor of fluid velocity, 1/s
\( \Gamma \) auxiliary variable dimensionless fluid temperature in boundary layer
\( \epsilon \) dissipation rate of turbulence kinetic energy, m²/s³
\( \zeta_t \) turbulent thermal diffusivity, m²/s
\( \kappa \) von Kármán constant, \( \kappa = 0.41 \)
\( \lambda \) thermal conductivity of fluid, W/m K
\( \mu \) molecular dynamic viscosity of fluid, Pa.s
\( \mu_t \) turbulent eddy viscosity, Pa.s
\( \nu \) molecular kinematic viscosity of fluid, m²/s
\( \xi_1, \xi_2 \) auxiliary variables in the \( F_1 \) expressions
\( \xi_3 \) auxiliary variable in the \( \mu_t \) expression of the shear stress transport model
\( \rho \) density of fluid, kg/m³
\( \rho_0 \) reference density of fluid, kg/m³
\( \sigma_{k1} \) model constant in the \( k \)-equation of the Wilcox \( k-\omega \) model, \( \sigma_{k1} = 2 \)

\( \sigma_{k2} \) model constant in the \( k \)-equation of the standard \( k-\varepsilon \) model, \( \sigma_{k2} = 1 \)

\( \sigma_{k3} \) blended model constant in the \( k \)-equation of the blended Wilcox \( k-\omega \) and standard \( k-\varepsilon \) models, \( \sigma_{k3} = F_1 \sigma_{k1} + \beta_1 (1-F_1) \sigma_{k2} \)

\( \tau_w \) wall shear stress, Pa

\( \omega \) rate of dissipation per unit turbulent kinetic energy, 1/s

\( \omega_1 \) total \( \omega \) near wall, 1/s

\( \omega_{log}, \omega_{vis} \) \( \omega \) values calculated by the solutions in the logarithmic and linear near-wall regions, 1/s

**Subscript**

\( i, j \) index of the Cartesian coordinate system

**Abbreviation**

1D one-dimensional

2D two-dimensional

3D three-dimensional

BLS baseline

CFD computational fluid dynamics

CO\(_2\) carbon dioxide

DNS direct numerical simulation

HX heat exchanger

LES large eddy simulation

MHTC mean heat transfer coefficient

RANS Reynolds-averaged Navier-Stokes equations

RGP real gas property

RNG renormalisation group

SCO\(_2\) supercritical carbon dioxide

SST shear stress transport

std standard deviation
1 Introduction

Cooling is one of the key energy consumers. Cooling consumes up to 14% of the UK’s electricity, and the cooling demand will grow by about three folds the current generating capacity by 2030 in the UK [1]. The recycling of waste cold and the storing of cold energy produced by excess renewable energy power generated at night can be a practical solution to provide low-carbon, zero-emission cooling and power. In this context, a combined cooling and cold storage system using carbon dioxide (CO2) hydrate slurry as both working fluid and storage medium was proposed by us in a granted project. A water-cooled supercritical carbon dioxide (SCO2) heat exchanger (HX) will be used in the system, thus SCO2 heat transfer needs to be enhanced to improve its effectiveness and compactness [2]. The prediction of the thermo-hydraulic performance of heat transfer enhancement under SCO2 flow conditions based on computational fluid dynamics (CFD) will play a key role in SCO2 HX design and optimization. As the first step, the convective heat transfer in a water-cooled experimental SCO2 tube-in-tube HX was investigated by using CFD approach to establish a numerical method and validate heat transfer and fluid flow models under the condition where the thermophysical and transport properties vary significantly with temperature and pressure.

Numerical analysis of turbulent flows of SCO2 with forced convective heat transfer in a tube started in the 1960s. The methods used in the numerical analysis can be classified into five groups: (1) one-dimensional (1D) analytical Reynolds-averaged Navier-Stokes equations (RANS) method, (2) two-dimensional (2D) RANS method, (3) three-dimensional (3D) RANS method; (4) large eddy simulation (LES) method; (5) direct numerical simulation (DNS) method. In the 1D RANS method, SCO2 is considered as a viscous compressible fluid and its steady flow in a tube is axisymmetric, turbulent, and fully developed. As a result, the flow is simplified to a 1D flow in the tube radial direction only, i.e., the continuity, momentum, energy equations are as functions of radius only. In the 2D RANS method, the steady flow of viscous compressible SCO2 is turbulent and axisymmetric, but not fully developed in a tube, thus the variation of fluid velocity and temperature along the tube can be characterized. The finite difference or finite volume approach was employed to solve 2D steady time-averaged compressible Navier-Stokes equations and energy equation as well as turbulence closure model by using in-house computer programs. In the 3D RANS method, the flow of viscous compressible SCO2 is 3D and turbulent with buoyancy effect in a tube. The finite volume method and general CFD software, namely Fluent or CFX, were used. In the LES method, the unsteady, compressible Navier-Stokes equations and energy equation of SCO2 in microchannels were solved with LES turbulence models accounting for turbulence contributions to momentum and thermal energy transport, respectively. For the DNS method, the unsteady, compressible Navier-Stokes equations or its low-Mach-number form and the energy equation of SCO2 in a tube were solved directly by using an in-house computer
program or the open-source finite volume code OpenFOAM without any turbulence closure models.

Compared with 1D RANS, 2D RANS, LES and DNS methods, the use of 3D RANS method is a trade-off between accuracy and time-consumption in HX design, hydraulic and thermal performance estimation. Additionally, it is well-known that the 3D RANS method can capture the heat transfer deterioration effect. Therefore, this method is adopted here.

In the 3D RANS method, the standard $k-\varepsilon$ model with low Reynolds number corrections [3] [4] [5], SST model [6] [7] [8] [9] [10], and 4-equation eddy viscosity model of $k-\varepsilon-v^2-f$ [11] as well as turbulent stress tensor (elliptic blending second-moment closure)- $\varepsilon$ model [12] have been examined in SCO2 heat transfer simulations. The standard $k-\varepsilon$ model with the Lam–Bremhorst correction [3] or Abe-Kondoh-Nagano correction [4] [5] leads to the best agreement with the experimental mean heat transfer coefficient (MHTC). The SST model performs better than the realizable $k-\varepsilon$ model with enhanced wall treatment in accuracy and computational efficiency [6]. The SST model is better than the $k-\omega$ model in bulk flow and the $k-\varepsilon$ model in computational accuracy near wall region [7]. There is no comparison between the SST model and the other models [8] [9] [10]. The 4-equation eddy viscosity model of $k-\varepsilon-v^2-f$ model was compared with DNS and the fair agreement in Nusselt number was achieved between the two models [11]. The Reynolds stress spanwise profile and SCO2 MHTC curve predicted by the turbulent stress tensor-$\varepsilon$ model agree better with the measurement than the Reynolds stress models proposed by Shin et al, and Dol et al [12]. A comparison was made among the standard $k-\varepsilon$ model, RNG $k-\varepsilon$ model, $k-\varepsilon$ model with low Reynolds number correction, $k-\omega$ model and SST model in terms of SCO2 MHTC at tube wall, and it was demonstrated that the standard $k-\varepsilon$ model with enhanced wall treatment results in the best agreement with the experimental MHTC [13]. In [14], the standard $k-\varepsilon$ and RNG $k-\varepsilon$ models were compared in terms of both SCO2 MHTC and wall temperature, suggesting the RNG $k-\varepsilon$ model is better than the standard $k-\varepsilon$ model. Obviously, whether the standard $k-\varepsilon$ and RNG $k-\varepsilon$ models are better than the SST model for simulating SCO2 convective heat transfer in the tube-in-tube HX needs to be confirmed further.

In the present article, the convective heat transfer of SCO2 in a water-cooled tube-in-tube HX is investigated based on CFD simulations in ANSYS CFX 2019R2 by using 3D RANS method with the shear stress transport (SST) turbulence model. A complete geometrical model and a sole tube geometrical model for the HX were generated, the forced convective heat transfer of SCO2 in the models are simulated, and the sole tube geometrical model was chosen over the complete geometrical model based on simulation practice. Effects of SCO2 mass flux (200, 400, 600kg/m²s), tube diameter (4, 6mm), inlet pressure (8, 9MPa), wall heat flux (6, 12, 24, 33kW/m²), numerical scheme for advection terms in the SST model equations, conservative and hybrid values of tube wall temperature on the MHTC profiles of SCO2 were
clarified and compared with the MHTC of SCO2 obtained in heat transfer experiments on the HX [15]. The effects of the other turbulence models such as the eddy transport, standard $k$-$\varepsilon$, renormalization group (RNG) $k$-$\varepsilon$, Wilcox $k$-$\omega$, baseline (BLS) $k$-$\omega$ and $\omega$-stress turbulence models in [16] were also investigated. The buoyancy effect was discussed.

Such a detailed CFD study on convective heat transfer of SCO2 in tube-in-tube HXs has not been seen in the literature so far. The article can provide guidelines for the selection of appropriate geometrical models, flow models and numerical schemes as well as the assessment of buoyancy effect for CFD simulations, but also deliver an understanding of the complex SCO2 heat transfer phenomenon in the HX. Particularly, the unique thermophysical and transport property variations and the buoyancy effect in SCO2 heat transfer were considered.

2 Methodology

2.1 The geometrical models

There are several experiments on heat transfer in water-cooled tube-in-tube SCO2 HXs. Unfortunately, most of them cannot be employed to validate SCO2 flow models and numerical methods due to the lack of detailed geometrical parameters and experimental conditions. Thus, the counter-flow tube-in-tube SCO2 HX in [15] has to be chosen in the article. The schematic of the experimental set-up and the axial-cross-sectional view of the tube-in-tube SCO2 HX, geometrical dimensions of the HX, a brief on experimental procedure and the experimental conditions are outlined in Appendix A.

According to the geometrical dimensions of the counter-flow tube-in-tube HX shown in Appendix A, two geometrical models, i.e., complete model, and sole tube model, as shown in Figure 1, were built and examined. Since the HX structure is geometrically symmetric, only half of the HX was employed in the two models. The complete model consists of a 1mm thick inner tube with $15d$ long upstream and downstream extensions, and an annulus with 50mm long, 6mm diameter upstream and downstream branches. The outer surfaces of the annulus and the two extensions are insulated and adiabatic. In this model, both the water temperature at the annulus inlet and the water flow rate were not provided in [15], and thus must be guessed to meet a known constant experimental wall heat flux across the inner tube wall from the hot SCO2 to the cold water in [15] in a SCO2 heat transfer simulation.
Initial CFD simulations proved that the complete geometrical model was considerably time-consuming and succeeded in one case only. It was very difficult to guess a series of correct water flow rates and inlet temperatures for a known wall heat flux in the simulations, and the water inlet temperature could influence the inner wall temperature subsequently the SCO2 MHTC sustainably. Thus, the sole tube model has to be tried then. In the sole tube model, the annulus is removed, and the water-cooling effect on the hot SCO2 is reproduced with a known constant experimental outward heat flux \( q_w \). This model requires SCO2 inlet temperature and pressure only, and the experimental outward heat flux \( q_w \) is imposed as a boundary condition, hence, the computational time of this model is significantly reduced. In the following sections, all the results are obtained by using the sole tube model, but the difference in the heat transfer between the two geometrical models will be analysed in the discussion section late on.

2.2 The fluid flow and heat transfer models

The CFD software ANSYS 2019R2 CFX is employed to conduct SCO2 heat transfer simulations. The SCO2 in CFD simulations is treated as subsonic compressible gas and its thermophysical and transport properties vary with both temperature and pressure. Ten SCO2 thermophysical and transport property constants were calculated by using the REFPROP Version 9.0 program issued by the National Institute of Standards and Technology. Then, the values of these property constants were read into a custom MATLAB program to generate the
real gas property (RGP) table file based on the TASCflow (early version of CFX) RGP format provided in [17]. The file was read in Materials Tab in CFX-Pre by specifying a new material SCO2 and the location and name of the RGP file on the hard drive. Based on the RGP table, the SCO2 thermophysical and transport property constants will be interpolated with local temperature and pressure in the fluid domain during a CFD simulation.

The SCO2 flow and heat transfer models, which are adopted in the paper, include the 3D RANS equations, energy equation and SST turbulence model. The details of these equations and models are present in Appendix B.

2.3 The boundary conditions and initialization

In CFD heat transfer simulations, a couple of boundary conditions and one initialization condition are needed. In CFX, mass flow rate, pressure and temperature cannot be imposed simultaneously at the inlet; as such the pressure and temperature are given at the inlet, and the mass flow rate has to be assigned at the outlet.

In the complete model, the pressure and temperature of SCO2 are imposed, the flow direction option is zero gradient, and the turbulence intensity is 5%, at the inlet of the inner tube. At the outlet of the tube, the flow of SCO2 is subsonic and its mass flow rate is specified based on the prescribed SCO2 mass flux and the cross-section area of the inner tube with the CFX expression language. The walls of the inner tube, two branches and annulus are subject to velocity no-slip condition and symmetrical boundary condition is imposed on the symmetrical plane of the tube, two branches and annulus. The adiabatic condition is applied to the surfaces of the upstream and downstream extensions, and the outside surfaces of the annulus and its two branches. The adiabatic condition is imposed on the outside surfaces of the annulus and branches, a uniform velocity, temperature and 5% turbulence intensity of water at the inlet of one branch, and the zero pressure are implemented at the outlet of the other branch, respectively. The pressure and temperature of water at the inlet, 5% turbulence intensity and \( u_1 = u_2 = 0, \ u_3 = -0.1\text{m/s} \) constant velocities are given to the water fluid domain.

In the sole tube model, the boundary conditions at the inlet and outlet of the inner tube and on the surfaces of the upstream and downstream extensions are the same as those in the complete model. However, a known outward heat flux (negative value) is prescribed at the wall of the inner tube inside the HX. The pressure and temperature of SCO2 at the inlet, 5% turbulence intensity and \( u_1 = u_2 = 0, \ u_3 = 1\text{m/s} \) constant velocities are assigned to the SCO2 fluid domain.

2.4 Examination on mesh size independence

A mesh size independence examination was exercised with the sole tube model for the case: \( p_1 = 8\text{MPa}, \ G = 200\text{kg/m}^2\text{s}, \ q_w = 12\text{kW/m}^2, \) and \( T_1 = 26-65^\circ\text{C}. \) Three meshes, namely Mesh1, Mesh2 and Mesh3 were generated with three mesh sizes in the ANSYS meshing module, and their information is tabulated in Table 1. The pattern of these meshes is identical to the pattern
in the inner tube shown in Figure 7a. Six-node wedge elements (57–75%) are dominant over four-node tetrahedron elements. \( y^+ \) varies with mesh size and SCO2 mean bulk temperature \( T_b \), which is the mean temperature based on the local temperatures at ten axial locations shown in Error! Reference source not found. For Mesh1, Mesh2 and Mesh3, \( y^+ \) is in the ranges of 0.83–2.83, 0.86–2.67 and 0.73–2.19, respectively.

Table 1: The information about the meshes employed in CFD simulations of SCO2

<table>
<thead>
<tr>
<th>Geometrical model</th>
<th>Sole tube model</th>
<th>Complete model</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mesh name</td>
<td>Mesh1</td>
<td>Mesh2</td>
</tr>
<tr>
<td>Element size(mm)</td>
<td>0.45</td>
<td>0.4</td>
</tr>
<tr>
<td>Nodes</td>
<td>469,305</td>
<td>773,564</td>
</tr>
<tr>
<td>Elements</td>
<td>Total 1,154,802</td>
<td>1,812,034</td>
</tr>
<tr>
<td></td>
<td>Hex8 0(%)</td>
<td>0(%)</td>
</tr>
<tr>
<td></td>
<td>Tet4 450,262(39%)</td>
<td>565,474(31%)</td>
</tr>
<tr>
<td></td>
<td>Wed6 704,540(61%)</td>
<td>1,246,560(66%)</td>
</tr>
<tr>
<td>Element quality</td>
<td>0.356±0.3790</td>
<td>0.234±0.3457</td>
</tr>
<tr>
<td>Aspect ratio</td>
<td>20.55±26.07</td>
<td>22.73±23.46</td>
</tr>
<tr>
<td>Skewness</td>
<td>0.1420±0.1286</td>
<td>0.1147±0.1205</td>
</tr>
<tr>
<td>Orthogonal quality</td>
<td>0.8540±0.1270</td>
<td>0.8828±0.1198</td>
</tr>
<tr>
<td>First layer height(mm)</td>
<td>0.0055</td>
<td>0.005</td>
</tr>
<tr>
<td>Number of layers</td>
<td>10</td>
<td>14</td>
</tr>
<tr>
<td>Growth rate</td>
<td>1.2</td>
<td>1.2</td>
</tr>
<tr>
<td>( y^+ )</td>
<td>0.83–2.83</td>
<td>0.86–2.67</td>
</tr>
</tbody>
</table>

The MHTCs between the SCO2 and the inner tube wall predicted with Mesh1, Mesh2 and Mesh3, are indicated in Figure 2a as a function of \( T_b \). The MHTC is calculated by using a known wall heat flux \( q_w \), mean wall temperature \( T_w \), which is the mean of temperature at ten axial locations shown in Figure A.1, and SCO2 mean bulk temperature \( T_b \) in terms of the following expression:

\[
U = \frac{q_w}{T_b-T_w}
\]

In Figure 2a, the pseudocritical point of SCO2 at 8MPa occurs at \( T_c=34.5°C \) [15]. Both the predicted and measured MHTCs are in the maximum values at 35.1°C, which is slightly higher than the pseudocritical point \( T_c \), then reduce precipitously away from that point, especially in the range \( T_b<T_c \). Additionally, the coefficients vary considerably in the \( T_b<T_c \) range with mesh size.
The relationship of the Reynolds number at the inner tube inlet with SC2 mean bulk temperature is plotted in Figure 2b. The Reynolds number varies more significantly with mesh size on the left-hand side of the pseudocritical point than on the right-hand side of the point. This may be attributed to the sharp increase in the SOC2 dynamic viscosity, thermal conductivity and density with decreasing temperature as shown in Figure 2d.

Likewise, the predicted mean Prandtl number with Mesh1, Mesh2 and Mesh3 agrees well with each other except on the left-hand side of the pseudocritical point. Further, the maximum predicted Prandtl number emerges at $T_c=34.5^\circ C$ for all three meshes.

Based on Figure 2a, the MHTCs predicted with three meshes all agree with the experimental data [15] on the right-hand side of the pseudocritical point, but the MHTC in
Mesh2 agrees better with the measurement in comparison with those in Mesh1 and Mesh3. Thus, Mesh2 is adopted in CFD heat transfer simulations in the present study.

In Mesh2, the peak MHTC is 4.26 times larger than the MHTC at $T_b=26^\circ$. Based on the mean Prandtl number, which is the ratio of momentum diffusivity (kinematic viscosity) to thermal diffusivity of SCO2, shown in Figure 2c, the peak Prandtl number is 4.32 times higher than the number at $T_b=26^\circ$. Hence, the peak MHTC is caused by the peak Prandtl number. In the experiment [15], the ratio of the peak MHTC to the MHTC at $T_b=26^\circ$ is about 3.0. This value is smaller than the theoretical value of 4.26.

3 Results

3.1 Effects of turbulence model

The Wilcox $k$-$\omega$ and standard $k$-$\varepsilon$ two-equation turbulence models in 3D RANS methods are often applied in simulations of SCO2 convective heat transfer [3] [13] [14], thus they were examined at two mass fluxes. The scalable log-law wall function [16] was used to the $k$-$\varepsilon$ two-equation model but the Automatic Near-Wall Treatment expressed by Eqs. (B.12) and (B.13) is adopted in the Wilcox $k$-$\omega$ model. In Mesh2, the two turbulence models were employed under the same flow conditions, the predicted SCO2 MHTCs are plotted as a function of the SCO2 mean bulk temperature in Figure 3. The errors in MHTC between the CFD prediction and the experimental data are tabulated in Table 2. The SST model results in the smallest error in the MHTC among the three turbulence models.

![Figure 3](image-url) The SCO2 MHTCs predicted with SST, $k$-$\omega$ and $k$-$\varepsilon$ two-equation turbulence models at two mass fluxes $G=200, 400\, \text{kg/m}^2\text{s}$, (a)$G=200\, \text{kg/m}^2\text{s}$, (b)$G=400\, \text{kg/m}^2\text{s}$, Exp-the experimental data from [15]
Table 2 The errors of MHTC predicted with three turbulence models in CFD simulations against the experimental data

<table>
<thead>
<tr>
<th>Inner diameter, (d) (mm)</th>
<th>Inlet pressure, (p_1) (MPa)</th>
<th>Wall heat flux, (q_w) (kW/m²)</th>
<th>Mass flux, (G) (kg/m² s)</th>
<th>Model</th>
<th>Error in MHTC (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>200</td>
<td></td>
<td>max</td>
</tr>
<tr>
<td>6</td>
<td>8</td>
<td>12</td>
<td>200</td>
<td>(k-\omega)</td>
<td>61.9</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>200</td>
<td>(k-\varepsilon)</td>
<td>11.9</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>200</td>
<td>SST</td>
<td>33.6</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>400</td>
<td>(k-\omega)</td>
<td>53.8</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>400</td>
<td>(k-\varepsilon)</td>
<td>9.9</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>400</td>
<td>SST</td>
<td>36.6</td>
</tr>
</tbody>
</table>

The error in MHTC is defined as \(100 \times \frac{\text{prediction} - \text{experiment}}{\text{experiment}}\), max—maximum error, min—minimum error, mean—mean error, std—standard deviation of error.

At two mass fluxes, the \(k-\varepsilon\) model gives a fairly good prediction on the left-hand side of the pseudocritical point, but an underpredicted MHTC on the right-hand side of the point. Contrarily, the \(k-\omega\) model provides a decent prediction of MHTC on the right-hand side of the point, but an overprediction on the left-hand side of the point. The \(k-\omega\) model overpredicts the MHTC at the pseudocritical point but the \(k-\varepsilon\) model underestimates it. Obviously, the \(k-\omega\) model is more suitable to SCO2 flows at large mass flux and high inlet temperature, i.e., high Reynolds number, while the \(k-\varepsilon\) model is more applicable to SCO2 flows at small mass flux and low inlet temperature, i.e., low Reynolds number. In comparison with the \(k-\omega\) and \(k-\varepsilon\) models, the SST model produces even better MHTCs against the measurements at both mass fluxes.

Additional four turbulence models, including the eddy transport, renormalisation group (RNG) \(k-\varepsilon\), baseline (BSL) \(k-\omega\), and \(\omega\)-stress models, which are not popular as the \(k-\varepsilon\), \(k-\omega\) and SST models, were attempted to simulate the SCO2 convective heat transfer only in three inlet temperatures herein. The MHTCs predicted with these models are listed in Table 3 at 42.5 (right of \(T_c\)), 36 (near \(T_c\)) and 30°C (left of \(T_c\)) inlet temperatures, respectively. The results given by the standard \(k-\varepsilon\), Wilcox \(k-\omega\) and SST models are presented in the table, too. It is demonstrated that the MHTCs predicted by the eddy transport, standard \(k-\varepsilon\) and RNG \(k-\varepsilon\) models are very similar in the same inlet temperature and mass flux, and the MHTC produced by the RNG \(k-\varepsilon\) model is the lowest in the three models.
Table 3: The MHTCs predicted with seven turbulence models at 42.5, 36 and 30°C inlet temperatures

<table>
<thead>
<tr>
<th>Model</th>
<th>Eddy transport</th>
<th>$k$-$\varepsilon$</th>
<th>Wilcox $k$-$\omega$</th>
<th>Blended $k$-$\omega$ and $k$-$\varepsilon$</th>
<th>$\omega$-stress</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Standard</td>
<td>RNG</td>
<td>Automatic near Wall Treatment (blended linear-law and log-law)</td>
<td></td>
</tr>
<tr>
<td>Wall function</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Right of $T_c$ - 42.5°C</td>
<td>1936.7</td>
<td>1895.1</td>
<td>1721.2</td>
<td>3211.1</td>
</tr>
<tr>
<td></td>
<td>Near $T_c$ - 36°C</td>
<td>4366.8</td>
<td>4464.3</td>
<td>3907.5</td>
<td>7604.6</td>
</tr>
<tr>
<td></td>
<td>Left of $T_c$ - 30°C</td>
<td>1499.3</td>
<td>1604.1</td>
<td>1411.9</td>
<td>1915.7</td>
</tr>
</tbody>
</table>

Likewise, the MHTCs estimated by the Wilcox $k$-$\omega$, BSL $k$-$\omega$, SST and $\omega$-stress models are close to each other in magnitude in the same inlet temperature and mass flux. Particularly, the MHTCs predicted by the SST model are the smallest among these four models. This effect possibly could be attributed to the eddy viscosity suppressed by Eq. (20). Based on Figure 3, the MHTCs produced by the SST model are the closest to the experimental observations, thereby, the SST model should be adopted in SCO2 heat transfer simulations.

3.2 Effects of inlet pressure

Since the thermophysical and transport properties of SCO2 relate to both temperature and pressure, e.g., specific heat capacity at constant pressure $C_p$, as shown in Figure 4a, the inlet pressure can affect MHTC in the tube-in-tube HX. The effect of SCO2 inlet pressure on the MHTC is demonstrated in Figure 4b under the condition of $G=400$kg/m²s, $q_w=12$kW/m² and $d=6$mm tube inner diameter. Because the pseudocritical point moves to a higher temperature and the corresponding specific heat capacity decreases as the inlet pressure increases, the $\Lambda$-shaped MHTC curve moves to a higher temperature range and becomes blunter with the increasing inlet pressure. The predicted MHTC curves agree well with the experimental data and reflect their variation with inlet pressure precisely. For instance, the maximum, minimum, mean, and standard deviation of the error in MHTC against the experimental data are 12.2%, -13.6%, 0.6% and 7.3% at $p_1=9$MPa, compared with 36.6%, -2.4%, 9.7% and 11.1% at $p_1=8$MPa.
Figure 4  The MHTCs of CO2 at the inlet pressures of 8 and 9MPa, respectively, but the CO2 mass flux G=400kg/m²s, wall heat flux q_w=12kW/m², and tube diameter d=6mm remain unchanged, (a) CO2 specific heat capacity-temperature curves at constant pressure, (b) CO2 MHTC-mean bulk temperature curve, the experimental data after [15]

At the pseudocritical points, the heat capacity is decreased by 56.6% when the inlet pressure increases from 8MPa to 9MPa. Comparably, the peak MHTC decreases by 40.5% in the CFD simulation, and 38.2% in the experiment. This fact suggests that the specific heat capacity is responsible for the Λ-shaped MHTC curve and its varying trend with the mean bulk temperature of CO2.

### 3.3 Effects of mass flux and wall heat flux

The effect of CO2 mass flux on MHTC is demonstrated in Figure 5a. If the tube diameter, inlet pressure and inlet temperature are given, then the Reynolds number of CO2 ascends or descends as the mass flux of CO2 increases or decreases. Usually, the heat transfer coefficient will rise or decline with increased or decreased Reynolds number. As a result, the MHTC should rise or decline with increased or decreased mass flux. This trend is clearly indicated in the figure.
The effect of wall heat flux on SCO2 MHTC is presented in Figure 5b and c at a given SCO2 mass flux of $G=200\text{kg/m}^2\text{s}$. The wall heat flux is primarily determined by the temperature difference across the inner tube wall. The SCO2 MHTC is in a Λ-shaped curve at the wall heat fluxes of 6, 12, 24 and 33kW/m² against the mean bulk temperature. However, the peak coefficient declines, and two legs rise with increasing wall heat flux. Both the predicted and the measured MHTCs reflect this property. The errors of the MHTC predicted against the experimental data are listed in Table 4. The agreement in the MHTCs between prediction and measurement is quite good when the wall heat fluxes are at 12, 24 and 33kW/m². The largest error in the MHTC is found at and near the pseudocritical point at the wall heat flux of 6kW/m².
Table 4: The errors of MHTC between CFD prediction and experimental data under various conditions

<table>
<thead>
<tr>
<th>HX model</th>
<th>$d$ (mm)</th>
<th>$p_1$ (MPa)</th>
<th>$G$ (kg/m²s)</th>
<th>$q_w$ (kW/m²)</th>
<th>Order of advection scheme</th>
<th>Option in CFX-Post</th>
<th>Buoyancy</th>
<th>Error in MHTC (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>max</td>
</tr>
<tr>
<td>Solo tube</td>
<td>6</td>
<td>9</td>
<td>12</td>
<td>1</td>
<td>Con</td>
<td>No</td>
<td></td>
<td>12.2</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>8</td>
<td>200</td>
<td></td>
<td>1st</td>
<td>Con</td>
<td>No</td>
<td>35.5</td>
</tr>
<tr>
<td></td>
<td>12</td>
<td></td>
<td>1</td>
<td>Con</td>
<td>No</td>
<td></td>
<td>33.6</td>
<td>-9.6</td>
</tr>
<tr>
<td></td>
<td>24</td>
<td></td>
<td>1</td>
<td>Con</td>
<td>No</td>
<td></td>
<td>22.9</td>
<td>-11.5</td>
</tr>
<tr>
<td></td>
<td>33</td>
<td></td>
<td>1</td>
<td>Con</td>
<td>No</td>
<td></td>
<td>17.8</td>
<td>-13.9</td>
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<td></td>
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<td>1</td>
<td>Hybrid</td>
<td>No</td>
<td></td>
<td>4.4</td>
<td>-32.0</td>
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<td></td>
<td></td>
<td>2</td>
<td>Hybrid</td>
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<td></td>
<td>24.9</td>
<td>-12.3</td>
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<td></td>
<td></td>
<td></td>
<td>1</td>
<td>Con</td>
<td>Yes</td>
<td></td>
<td>50.6</td>
<td>-3.8</td>
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<td></td>
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<td>Hybrid</td>
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<td>11.7</td>
<td>-15.7</td>
</tr>
<tr>
<td>Complete</td>
<td>6</td>
<td>8</td>
<td>200</td>
<td></td>
<td>1st</td>
<td>Con</td>
<td>No</td>
<td>53.0</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>9</td>
<td>600</td>
<td></td>
<td>12</td>
<td>1st</td>
<td>Con</td>
<td></td>
</tr>
</tbody>
</table>

The error in MHTC is defined as $(\text{prediction-experiment}) \times 100\% / \text{experiment}$, Con-conservative value in CFX-Post, hybrid-hybrid values in CFX-Post, max-maximum error, min-minimum error, mean-mean error, std-standard deviation of error, the order of advection scheme is for the advection terms in the equations of the SST model.

3.4 Effects of tube inner diameter

Usually, the MHTC at the wall in a tube with a small inner diameter is higher than in a tube with a big inner diameter at the same Reynolds number. The Reynolds number of SO2 flowing in a tube is defined as

$$Re_b = \frac{u_b \rho_b}{\mu_b}, \quad u_b = \frac{G \pi d^2}{\rho_b} = \frac{G}{\rho_b}$$

(2)

where $\rho_b$ is the bulk density of SO2, $\mu_b$ is the bulk dynamic viscosity of SO2, $u_b$ is the bulk velocity of SO2 in the tube. Based on mass flux $G$ and viscosity $\mu_b$, SO2 Reynolds number in a tube is expressed by

$$Re_b = \frac{Gd}{\mu_b}$$

(3)

The MHTCs in the tubes with 4mm and 6mm inner diameters are plotted as a function of SO2 mean bulk temperature in Figure 6. In the figure, $Gd$ is identical for the two tubes, as a result, at the same fluid mean bulk temperature, the fluids in the two tubes have an identical Reynolds number. Clearly, the MHTC in the tube with a small diameter is higher than in the tube with a big diameter at the same mean bulk temperature. The trend of the predicted MHTC agrees well with the experimental data, see Table 4 for the errors.
Figure 6  The MHTCs in two tubes with 4mm and 6mm inner diameters are plotted as a function of SCO2 mean bulk temperature, symbol-experimental data in [15], line-CFD prediction

3.5 Effects of geometrical model

Initially, CFD heat transfer simulations were performed on the complete geometrical model as shown in Figure 1a. In a simulation, besides the SCO2 mass flux, inlet pressure and temperature, the inlet temperature and flow rate of the cooling water must be provided to meet a known experimental wall heat flux between the SCO2 and the cooling water. Since there is no information about the inlet temperature and flow rate of the cooling water in [15], it is extremely hard and time-consuming to provide the correct inlet temperature and flow rate of the cooling water for a known wall heat flux in [15] so as to match the experimental MHTCs. Therefore, just one case was performed successfully, and the corresponding MHTCs are illustrated in Figure 7, where the partial view of the mesh is shown, too. The information on the mesh (i.e., Mesh4) is listed in Table 1. Since the $y^+$ values are comparable to the Mesh2, a check on mesh size independence is not exercised.
In comparison with the MHTC from the sole tube geometrical model, the MHTC based on the complete geometrical model agrees well with the experimental data on the right-hand side of the pseudocritical point, but poorly on the left-hand side of the point. As shown in Table 4, even though the minimum error of MHTC against the experimental data is quite small (-1.8%), the maximum and mean errors are as large as 53.0% and 18.0%, respectively. This suggests that the guessed water flow rate and inlet temperature which have met the experimental wall heat flux may not be those experienced in the experiment. For this reason, the complete geometrical model has to be abandoned.

The temperature contours of the SCO2 flow in the two geometrical models are demonstrated in Figure 8 under the same thermal and flow conditions: \( G=200\text{kg/m}^2\text{s}, q_w=12\text{kW/m}^2, p_1=8\text{MPa} \) and \( T_1=30, 65^\circ\text{C} \). The SCO2 temperature contours in the complete model are remarkably similar to those in the sole tube model in the same inlet temperature, pressure and mass flux. However, the profile of the core hot flow in the former is longer and narrower than in the latter model, especially at \( T_1=30^\circ\text{C} \). This might be caused by the lower inlet temperature of water assumed.
Figure 8 The temperature contours of the SCO2 flow predicted based on the complete geometrical and sole tube models at the same SCO2 thermal and flow conditions: $G=200\text{kg/m}^2\text{s}$, $q_w=12\text{kW/m}^2$, $p_1=8\text{MPa}$, $T_1=30, 65^\circ\text{C}$

4 Discussion

A series of CFD simulations of convective heat transfer in the experimental counter-flow tube-in-tube HX in [15] was performed when SCO2 was cooled by a stream of water. First, the most suitable turbulence model and mesh size were identified. The influences of SCO2 inlet pressure, mass flux, wall heat flux and geometrical model of the HX on the MHTC curve were then examined and compared with the experimental data of the MHTC in [15]. These comparisons are more extensive and complete than those in the literature. Similar work has not been seen in the literature as well.

Frankly, a couple of in issues, such as mesh size independence, numerical scheme, CFD result extraction method and buoyancy effect are important to SCO2 convective heat transfer
simulations, and there are a few limitations in the paper. These issues will be discussed in the following sections.

4.1 An explanation of mesh size independence

In Section 2.4 the mesh size independence is achieved on the right-hand side of the pseudocritical point, and the MHTC still varies with the mean bulk temperature on the left-hand side of the point and at the point itself. This phenomenon will be explained here. The MHTC is associated with the heat transfer coefficient in the laminar/viscous sublayer at the wall. Eq. (B.13) was employed in CFX to model the heat transfer in the viscous sublayer analytically. Based on the equation the heat transfer coefficient \( q_w/(T_w - T_n) \) across the layer is expressed as

\[
\begin{align*}
\frac{q_w}{T_w - T_n} &= \frac{\rho C_p u_T}{T^+}, \\
T^+ &= Pr y^+ e^{-\Gamma} + [0.1\ln(y^+) + \beta] e^{-1/\Gamma}, \\
\Gamma &= \frac{0.01(Pr y^+)^4}{1+5Pr y^+}, \\
Pr &= \frac{\mu C_p}{\rho}, \\
\beta &= \left(3.85Pr^{1/3} - 1.3\right) + 0.1\ln(Pr)
\end{align*}
\]

(4)

where the Prandtl number \( Pr \), the density \( \rho \), specific heat capacity at constant pressure \( C_p \) and wall shear stress \( \tau_w \) of SCO2 are extracted from a CFD result simulated, the dimensionless velocity in the viscous sublayer \( u_T \) is equal to \( \sqrt{\tau_w/\rho} \), i.e., \( u_T = \sqrt{\tau_w/\rho} \) yields. The heat transfer coefficient \( q_w/(T_w - T_n) \) at three typical inlet temperatures \( T_i = 26, 36, 65^\circ C \), and the inlet pressure \( p_i = 8MPa \), mass flux \( G = 200kg/m^2s \), wall heat flux \( q_w = 12kW/m^2 \) were calculated with Eq. (4), and plotted in Figure 9 after being normalized with the maximum \( q_w/(T_w - T_n) \) values based on \( u_T = 1.78, 2.89, 5.25cm/s, Pr = 2.60, 10.8, 1.36, C_p = 3211.8, 23995, 2069.8J/kg K \).

Figure 9 The normalized heat transfer coefficient across the viscous sublayer versus \( y^+ \) under the conditions: \( T_i = 26, 36, 65^\circ C, p_i = 8MPa, G = 200kg/m^2s, \) and \( q_w = 12kW/m^2 \)
The shape of the normalized \( q_w / (T_w - T_n) \) curve at \( T_1 = 26^\circ C \) is similar to that at \( T_1 = 65^\circ C \), but different from that at \( T_1 = 36^\circ C \). The change in mesh size can result in a variation in normalized \( q_w / (T_w - T_n) \) on the curve. Obviously, when the mesh size changes from Mesh1 to Mesh3, the largest variation in the normalized \( q_w / (T_w - T_n) \) is found at \( T_1 = 36^\circ C \), the moderate variation occurs at \( T_1 = 26^\circ C \), while the smallest variation is observed at \( T_1 = 65^\circ C \). This variation trend of the normalized \( q_w / (T_w - T_n) \) seems to be responsible for the MHTC curves in Mesh1, Mesh2 and Mesh3 shown in Figure 2a.

Additionally, the \( y^+ \) values in the three meshes at \( T_1 = 26, 36^\circ C \) are in the regions with a steeper slope in the normalized \( q_w / (T_w - T_n) \) curves. However, the \( y^+ \) values in the meshes at \( T_1 = 65^\circ C \) are located in the range with a flatter slope. The mesh size at \( T_1 = 26, 36^\circ C \) should be altered to allow the corresponding \( y^+ \) values to be moved into a region with a smaller slope in the normalized \( q_w / (T_w - T_n) \) curves. In this case, the mesh size independence will reach on the left-hand side of the pseudocritical point and the point itself. This fact suggests that the different mesh sizes should be adopted for the different inlet temperatures in SCO2 heat transfer simulations. Note that the mesh size independence was explored and achieved at the single inlet temperature of 330K (≈57°C) in terms of local heat transfer coefficient in [3] rather than in a range of inlet temperatures in terms of MHTC in the present paper.

### 4.2 The maximum MHTC point

The maximum MHTC of SCO2 occurs at a higher mean bulk temperature than the pseudocritical point, as shown in Figure 2a for the given inlet pressure of 8MPa. This phenomenon has been observed when SCO2 was cooled in a tube-in-tube HX [18]. The reason for this effect is attributed to uneven temperature profile in a cross-section of the tube and the wall temperature is the lowest in the cross-section [18]. The CFD simulations do prove that the uneven temperature profile exists, see Figure 8. As the pressure rises, the SCO2 specific heat capacity at the pseudocritical point is not much larger than those at the other temperatures, as illustrated in Figure 4a, therefore, this phenomenon is less dominant when the inlet pressure is higher than 8MPa.

### 4.3 Effect of conservative and hybrid values of wall temperature

The MHTC of SCO2 has been overpredicted at the pseudocritical point and in its nearby regions, as shown in Figure 2 to Figure 7. The same phenomenon has been observed in the MHTC predicted with the SST model [6] [7] [8] [9] [10]. This might be resulted from the difference between the mean temperature at the tube wall and the mean bulk temperature of SCO2. Fluid flow variables such as velocity, temperature, pressure, and density are defined and solved in control volumes in the ANSYS CFX solver. As default, i.e., **conservative option** in CFX-Post, a flow variable at a mesh node at the wall is calculated by averaging the variable in its surrounding control volumes without any interpolation from the variables in
internal control volumes to that at a node on the boundary. The velocity calculated in this way is non-zero for the no-slip velocity boundary. Fortunately, the hybrid option is provided in CFX-Post, where the variable is interpolated from the variables in internal control volumes, and the velocity at a wall keeps zero for the no-slip velocity condition.

The MHTC shown in the foregoing figures (Figure 2–Figure 7) is based on the mean wall temperature calculated with the conservative option, which is called the conservation value. For comparison, the MHTC calculated with the hybrid option, which is known as the hybrid value, is illustrated in Figure 10 with two cases: (1) \( q_w=12\text{kW/m}^2 \), (2) \( q_w=33\text{kW/m}^2 \), while \( G=200\text{kg/m}^2\text{s}, \ d=6\text{mm}, \) and \( p_1=8\text{MPa} \) remain unchanged. The MHTC, i.e., \( U \), is calculated with known wall heat flux \( q_w \) and the difference in the mean temperature \( T_b-T_w \) by using Eq. (1). Note that \( T_b \) and \( T_w \) are obtained from CFD simulations, but only the values of \( T_w \) depend on the hybrid or conservative option.

Since \( q_w \) is constant in each case, the \( U \) is proportional to the mean temperature difference \((T_b - T_w)\) inversely. The values of \((T_b - T_w)\) are minimum when the conservative option is held somewhere near the pseudocritical point. Therefore, a small change in \((T_b - T_w)\) can result in a significant increase in \( U \) there. This effect should be responsible for the overprediction in \( U \). The overprediction disappears when the hybrid option is chosen due to the raised \((T_b - T_w)\). However, the \( U \) curve moves down, and a significant error in the \( U \) occurs on the left-hand side of the pseudocritical point.

4.4 Effect of advection scheme in SST model

The numerical discretisation scheme of the advection terms in the SST model influences the MHTC of SCO2 significantly. In ANSYS CFX, two discretisation schemes are

![Figure 10](image-url)
provided: one is 2nd-order high-resolution scheme, and the other is 1st-order upwind scheme. The high-resolution (2nd-order) scheme was imposed on the advection terms in RANS equations. However, the high-resolution scheme and the 1st-order scheme have been tried for the advection terms in the SST model. The MHTCs predicted with the high-resolution scheme are illustrated in Figure 11 under the conditions: \( p_1=8\text{MPa}, \ G=200\text{kg/m}^2\text{s} \) and \( q_w=33\text{kg/m}^2\). The MHTC predicted with the 2nd-order scheme and the wall temperature of the hybrid values overlaps the coefficient predicted with the 1st-order scheme and the wall temperature of conservative values in the ranges \( T_b<35\degree\text{C} \) and \( T_b>40\degree\text{C} \). In the range near the pseudocritical point, however, the coefficient predicted with the 2nd-order scheme is above the coefficient predicted with the 1st-order scheme. The 2nd-order scheme intensifies the overprediction in the coefficient in the range near the point. The errors in the MHTC in Table 4 reflect this feature, too.

The predicted MHTCs with the two schemes are illustrated in Table 5 at \( G=200\text{kg/m}^2\text{s}, \ p_1=8\text{MPa}, \ q_w=12\text{kJ/m}^2\text{s} \) and \( T_1=42.5, \ 36, \ 30\degree\text{C} \), respectively. The 2nd-order scheme can raise the MHTC by (11-28)%, dependent on the mean bulk temperature of SCO2, especially at the pseudocritical point and on the left-hand side of the \( \Lambda \)-shaped MHTC curve. As a result, it slightly improves the agreement between the prediction and the measurement on the left-hand side of the \( \Lambda \)-shaped curve but makes it worse on the right-hand side of the curve. The high-resolution scheme for the advection terms in the SST model can increase \( y^+ \) and wall shear stress values. In this regard, the 1st-order scheme for the advection terms in the SST model was adopted in CFD simulations of SCO2 heat transfer here.

![Figure 11](image-url)  
*Figure 11 The comparison of the MHTCs predicted between 2nd-order (high resolution) and 1st-order schemes for the advection terms in the SST model under the conditions: \( p_1=8\text{MPa}, \ G=200\text{kg/m}^2\text{s} \) and \( q_w=33\text{kJ/m}^2\), the experimental data from [15]*

The predicted MHTCs with the two schemes are illustrated in Table 5 at \( G=200\text{kg/m}^2\text{s}, \ p_1=8\text{MPa}, \ q_w=12\text{kJ/m}^2\text{s} \) and \( T_1=42.5, \ 36, \ 30\degree\text{C} \), respectively. The 2nd-order scheme can raise the MHTC by (11-28)%, dependent on the mean bulk temperature of SCO2, especially at the pseudocritical point and on the left-hand side of the \( \Lambda \)-shaped MHTC curve. As a result, it slightly improves the agreement between the prediction and the measurement on the left-hand side of the \( \Lambda \)-shaped curve but makes it worse on the right-hand side of the curve. The high-resolution scheme for the advection terms in the SST model can increase \( y^+ \) and wall shear stress values. In this regard, the 1st-order scheme for the advection terms in the SST model was adopted in CFD simulations of SCO2 heat transfer here.
Table 5 The effect of discretisation scheme of advection terms in the SST model on MHTC at 
$G=200\text{kg/m}^2\text{s}$, $p_i=8\text{MPa}$, $q_w=12\text{kW/m}^2$ and $T_i=42.5, 36, 30^\circ\text{C}$

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<thead>
<tr>
<th>$U$ (W/m$^2$K)</th>
<th>1$^{st}$-order</th>
<th>2$^{nd}$-order</th>
<th>Increment (%)</th>
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<td>Right of $T_c=42.5^\circ\text{C}$</td>
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<td>2952.0</td>
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<td>5319.1</td>
<td>6779.7</td>
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<tr>
<td>Left of $T_c=30^\circ\text{C}$</td>
<td>1268.2</td>
<td>1560.9</td>
<td>23.1</td>
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</table>

4.5 Buoyancy Effect

Like CO2 flowing in vertical miniature tubes [19] [14], mini or normal size tubes [18] [20] [21] [22], or an inclined tube [11] [23], there exists buoyancy effect that non-uniformity of CO2 density can significantly influence on the primary flow, turbulence fields, and heat transfer effectiveness in a horizontal tube [4] [24] when the CO2 is heated or cooled. The CO2 heat transfer in vertical tubes with buoyancy effect was modelled analytically [25] [26] and investigated numerically based on CFD [27] [28] [8] [9] [29]. The buoyancy effect can impair CO2 heat transfer effectiveness, resulting in heat transfer deterioration in all these arrangements except CO2 downward flows. The impaired heat transfer or heat transfer deterioration relates to suppressed or reduced turbulence production near the wall.

The Nusselt number of CO2 with buoyancy effect can be correlated to a buoyancy parameter $Gr_b/Re_b^n$, where $Gr_b$ and $Re_b$ are the Grashof number and Reynolds number of CO2 in a tube, $n$ is a constant, depending on the tube orientation [30], and for a horizontal tube, $n=2$ [19], $Gr_b/Re_b^n$ called Richardson number $Ri$. When CO2 in a tube is cooled with a stream of water outside the tube, the Grashof number $Gr_b$ is expressed as:

$$Gr_b = \frac{(\rho_w-\rho_b)\rho_b d^2}{\rho_w^2}$$  \hspace{1cm} (5)

where $\rho_w$ is the density of CO2 at the tube wall, $g$ is the acceleration of gravity, $g=9.81\text{m/s}^2$, $u_b$ is calculated from CO2 mass flux and tube diameter with the following expression:

$$Ri = \frac{Gr_b}{Re_b^n} = \frac{(\rho_w-\rho_b)g d}{\rho_b u_b^n}$$  \hspace{1cm} (6)

Replacing $u_b$ in Eq.(6) with the expression in Eq.(2), $Ri$ arrives at the following expression:

$$Ri = \frac{(\rho_w-\rho_b)\rho_b d}{g^2}$$  \hspace{1cm} (7)

The Richardson number $Ri$ relates explicitly to $G$, $d$, $\rho_b$ and $\rho_w$. Specially, $\rho_b$ and $\rho_w$ depend on the inlet pressure and temperature of CO2, and wall heat flux. Usually, a large wall heat flux can lead to a significant difference $\rho_w-\rho_b$, and a low inlet temperature and a high inlet pressure will result in a large $\rho_b$. Thus, a large wall heat flux, low inlet temperature, high inlet pressure, big tube diameter and small mass flux will raise $Ri$ value to intensify the
buoyancy effect on the heat transfer behaviour of SCO2. The Ri of SCO2 is plotted in Figure 12 as a function of SCO2 mean bulk temperature $T_b$ for four cases selected from Table A.1.

At the fixed $d$, $p_1$, $G$ and $q_w$, the $Ri$ of SCO2 varies with mean bulk temperature $T_b$, and arrives at a peak near the pseudocritical point. At the same $T_b$, the $Ri$ changes from one case to another but in the range of 0.0014-0.23. The heat transfer regime of SCO2 in a cooled horizontal tube depends on the Richardson number. Theoretically, when $Ri$ < 0.001, the natural heat transfer induced by the buoyancy effect can be negligible [19] and the SCO2 heat transfer is purely forced convective heat transfer. When $Ri$ > 0.01, the buoyancy effect will play a part in SCO2 heat transfer in a cooled horizontal tube [3]. When $0.1 < Ri < 10$, the SCO2 heat transfer in the tube is mixed convection of natural convection and forced convection [4] [5]. Based on these criteria for SCO2 heat transfer in a cooled horizontal tube, the heat transfer in four cases shown in Figure 12 should be mixed convection and the buoyancy effect should be considered in CFD simulations of SCO2 heat transfer.

![Figure 12](image)

*Figure 12* The Richardson number $Ri$ is plotted as a function of SCO2 mean bulk temperature $T_b$ under different tube diameters, SCO2 inlet pressures, mass fluxes and wall heat fluxes

Based on the figure, the buoyancy effect is the strongest in the case: $d$=6mm, $p_1$=8MPa, $G$=200kg/m$^2$s and $q_w$=33kW/m$^2$. CFD Simulations of the case were launched when the buoyancy effect was taken into account and the predicted MHTC is shown in Figure 13a. The Boussinesq approximation was implemented, and the reference condition of the buoyancy effect is at the critical point. Thus, the SCO2 density $\rho$ and specific body force $S_i$ in Eq.(11) are expressed as

$$\rho = \rho_0 - \beta_v \rho_0 (T - T_0), S_i = g_i$$

(8)
where \( \rho_0 \) and \( T_0 \) are the reference density and temperature of SCO2 at the critical point, \( \beta_v \) is the volumetric thermal expansion coefficient of SCO2, \( g_i \) are the components of the acceleration of gravity. Because the coordinate \( x_2 \) of the coordinate system of the flow domain is downward, see Figure 1, \( g_1 = g_3 = 0, g_2 = 9.81 \text{m/s}^2 \) are held. Since the inlet temperature of SCO2 is low in CFD simulations, the viscous dissipation has a negligible contribution to the buoyancy effect and the viscous dissipation to the effect was disabled.

In the figure, the buoyancy effect can raise the MHTC by using downward secondary flow near the tube wall. Additionally, when the wall temperature is calculated by means of conservative values, the MHTC increases significantly. Although the agreement between the prediction and the observation is improved on the left branch of the \( \Lambda \)-shaped curve, the agreement on the right-hand side is poorer. If the hybrid option is employed to calculate the wall temperature, the MHTC with buoyancy effect exhibits pretty good agreement with the experimental one, the corresponding errors are demonstrated in Table 4.

In Figure 13b, a secondary flow starts to be induced after the SCO2 flows into the segment where there is an outward heat flux applied at the wall in the tube-in-tube HX. The SCO2 fluid elements with a lighter density at the bottom stream upwards to near the central vertical plane until the top, then go down along the tube wall until the bottom to finish a cycle. Such a cycle is repeated until the SCO2 is out of the segment. Since the SCO2 fluid elements are carried by the primary flow downstream, the secondary flow moves in the tube in a spiral pattern. Since the secondary flow brings the core hot fluid to the wall and results in long flow paths, the SCO2 heat transfer is enhanced. The well-known heat transfer deterioration does not exist in the horizontal tube-in-tube HX under SCO2 flow conditions.

In Figure 13c, the temperature contour of SCO2 in the cross-sections of the tube develops into nonuniform profiles gradually from the inlet to the outlet, and the low-temperature zone with increased size downstream is located in the region near the bottom of the tube, exhibiting a thermal stratification effect. As shown in Figure 13d, the low-velocity zone also accumulates in the area near the bottom of the tube and expands from the inlet to the outlet. Obviously, the temperature and velocity profiles are no longer symmetrical about the horizontal plane through the centre line of the tube due to the buoyancy effect. If the effect is not taken into account in the CFD simulation the temperature (Figure 8) or velocity will be symmetrical about the centre line. The flow patterns, velocity and temperature contours shown in Figure 13 are consistent with those presented in [5].
Figure 13 The MHTC curves (a), the secondary flow near the tube wall (b), temperature contour (c) and velocity contour (d) predicted when the buoyancy effect is considered in the case: \( d=6\text{mm}, p_1=8\text{MPa}, G=200\text{kg/m}^2\text{s} \) and \( q_w=33\text{kW/m}^2 \), the experimental data after [15], in (b), \( T_1=35\text{°C} \)

4.6 Limitations

In the CFD simulations, a single-phase flow model is adopted. In this circumstance, the SCO2 is still treated as a gas in ANSYS CFX even though a few input conditions in the CFD simulations enters into the liquid state, shown in Figure 14. This fact may affect the accuracy of MHTC prediction, but it needs further confirmation with other flow models. Ideally, two-phase flow models, which include a mixture of liquid CO2 and vapour CO2 as well as a thermodynamic phase-change model, should be employed at least on the left-hand side of the Λ-shaped MHTC curve. The state of CO2 is determined by the phase-change model based on
known CO2 pressure and temperature and bubble nucleation as well as the other thermophysical and transport property constants.

Figure 14  The SCO2 pressure-temperature chart and SCO2 input conditions in the CFD simulations

In the CFD simulations, a constant wall heat flux was applied to the tube wall. This wall heat flux is not the true heat flux across the tube wall but an equivalent one to the uneven wall heat flux calculated by using 1D conductive heat transfer formulas. Accordingly, the SCO2 bulk temperature and tube wall temperature predicted by CFD simulations were averaged to obtain an MHTC. The agreement between the predicted and the measured MHTCs makes sense in 1D conductive heat transfer only. A comparison of variable heat transfer coefficients in a tube-in-tube HX requires further experimental data associated with wall temperature longitudinal profile, cooling water flow rate, inlet and outlet temperatures. A very recent experimental work provides quite useful information about cooling water inlet and outlet temperatures to validate forced convective heat transfer simulations in a tube-in-tube heat exchanger by employing complete geometrical models [31].

In Eq. (12), the turbulent Prandtl number $Pr_t$ is selected to be 0.9 as usual based on the Reynolds analogy where the similarity between turbulent transport of momentum and that of heat is postulated. This hypothesis leads to the Reynolds-averaged fluctuating terms $\overline{u'_iT'}$ in the energy equation is proportional to the time-averaged temperature gradients $\partial T/\partial x_i$ with a constant:

$$\overline{u'_iT'} = -\zeta_t \frac{\partial T}{\partial x_i}, \quad \zeta_t = \frac{\mu_t}{\rho Pr_t}$$

where $u'_i$ are the fluctuation of fluid velocity components $u_i$, $T'$ is fluctuation of fluid temperature, $\zeta_t$ is turbulent thermal diffusivity. $Pr_t$ profile in the region of $y^+ < 6$ can influence heat transfer coefficient and wall temperature. To achieve better agreement with
experimental data a number of empirical correlations of $Pr_t$ have been proposed for fully developed turbulent of water or air in a pipe [32] [33] [34] [35] [36] [37] [38]. For forced convective heat transfer associated with SCO2, it is possible that the overproduction in heat transfer coefficient near the pseudocritical point is due to the $Pr_t$ profile across a boundary layer [39]. In this context, a few empirical $Pr_t$ profiles have been developed in the literature [39] [40] [41] [42]. In the present paper, $Pr_t = 0.9$ was used in all CFD simulations. Nevertheless, other variable $Pr_t$ profiles are worth being attempted in SCO2 heat transfer in tube-in-tube HXs in the future.

5 Conclusion

Two geometrical models of an experimental counter-flow tube-in-tube heat exchanger, i.e., complete model and sole tube model, were generated. Then the forced convective heat transfer of SCO2 flowing the heat exchanger was simulated by using the 3D RANS method with SST turbulence model in ANSYS CFX. It was shown that the sole tube geometrical model is viable for CFD heat transfer simulations when the known wall heat transfer flux across the wall between SCO2 and cooling water is given. Except near the pseudocritical point, the mean heat transfer coefficient of SCO2 flows based on the SST model demonstrates better agreement with the experimental data than the other turbulence models. Also, the effects of inlet pressure, mass flux, tube diameter and wall heat flux on the SCO2 mean heat transfer coefficient predicted with the adopted flow models and numerical methods are found similar to those obtained in experiments.

Furthermore, the numerical discretisation scheme of the advection terms in the SST model and conservative and hybrid values in CFX-Post for the wall temperature have a strong influence on the mean heat transfer coefficient. The 1st-order scheme and the wall temperature of conservative values can lead to a better prediction in the mean heat transfer coefficient. The mean heat transfer coefficient predicted with the 2nd-order (high resolution) scheme and the wall temperature of hybrid values in CFX-Post is similar to that obtained with the 1st-order scheme and the wall temperature of conservative values. In addition, the Richardson number for assessing the buoyancy effect in forced convective heat transfer in a horizontal tube is in a range of 0.0014-0.23 among the cases studied. In the case with the largest Richardson number, the buoyancy effect makes a dominant contribution to the mean heat transfer coefficient. In this context, the 1st-order scheme and the wall temperature in terms of hybrid values can improve the accuracy of prediction in mean heat transfer coefficient because of the spiral secondary flows induced by the variable density of SCO2 across the tube cross-section under the action of acceleration of gravity.

Acknowledgment
The authors would like to acknowledge the financial support provided by the Engineering and Physical Sciences Research Council (EPSRC) in the UK [grant numbers EP/T022701/1, EP/P028829/1, EP/V042033/1], and the European Commission [grant number 01007976]. Prof Zhibin Yu and Dr Yi Wang provided language editing and proof reading.

Appendix A The Selected Existing Experiment

The schematic of the experimental set-up and the axial-cross-sectional view of the SCO2 counter-flow tube-in-tube HX in [15] are illustrated in Fig. A.1a. The gear pump delivers liquid CO2 to the heater where the CO2 is heated and turns into SCO2. It then enters the test section, and the tube-in-tube HX, and is cooled by water flowing outside the wall of the inner (hot) tube. The cooled SCO2 is discharged from the exchanger and returns to the pump through a cooler.

The test section is a 500mm long horizontal counter-flow tube-in-tube HX. The hot SCO2 flows in the inner tube with 1mm thickness and 6mm inner diameter from the left to the right. A stream of water runs in the annulus between the outer tube (12mm inner diameter) and the inner tube from the right to the left. The flowing water takes heat away from the hot SCO2, and outward heat flux is generated across the wall of the inner tube during this process.
The SCO2 pressure and temperature were measured at both the inlet and outlet of the inner tube; likewise, the water temperature was measured at both the inlet and outlet of the annulus. The SCO2 mass flow rate was measured but the cooling water flow rate was overlooked. The temperature at the outside wall of the inner tube was measured at ten points evenly distributed as shown Fig. A.1b. The inside wall temperature of the inner tube at the 10 locations were calculated from the corresponding outside wall temperature by using 1D conductive heat transfer equations. The mean wall temperature was the arithmetic mean of the ten estimated inside wall temperatures. The SCO2 mean bulk temperature in the inner tube was the arithmetic mean of the measured SCO2 temperatures at the inlet and outlet of the inner tube. The respective experimental conditions in [15] are listed in Table A.1, and will be used in the CFD simulations in the paper.

Table A.1 The cases studied in the SCO2 flow and heat transfer simulations

<table>
<thead>
<tr>
<th>Inner diameter, (d) (mm)</th>
<th>Mass flux, (G) (kg/m² s)</th>
<th>Wall heat flux, (q_w) (kW/m²)</th>
<th>Inlet pressure, (p_i) (MPa)</th>
<th>Inlet temperature, (T_1) (℃)</th>
</tr>
</thead>
<tbody>
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<td>4</td>
<td>800</td>
<td>12</td>
<td>9</td>
<td>23.5-65</td>
</tr>
<tr>
<td>6</td>
<td>200</td>
<td>12</td>
<td>6</td>
<td>26-65</td>
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<td></td>
<td></td>
<td>24</td>
<td>8</td>
<td></td>
</tr>
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<td></td>
<td>33</td>
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<td></td>
</tr>
<tr>
<td>400</td>
<td>12</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Appendix B The Flow and Heat Transfer Models

For subsonic, compressible SCO2, the 3D RANS equations and energy equation with eddy viscosity of turbulence models are written as [16]

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0 \quad \text{(B.1)}
\]

\[
\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial}{\partial x_i}(p + \frac{2}{3} \rho k) + \frac{\partial}{\partial x_j}\left[(\mu + \mu_t)\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + \rho S_i \quad \text{(B.2)}
\]

\[
\frac{\partial}{\partial t}\left(\rho \left(h + \frac{1}{2} u_i u_i + k\right)\right) - \frac{\partial}{\partial x_j}\left[\rho u_j \left(h + \frac{1}{2} u_i u_i + k\right)\right] = \frac{\partial}{\partial x_j}\left(\frac{\lambda}{\rho} \frac{\partial T}{\partial x_j} + \frac{\mu_t}{\rho_t} \frac{\partial h}{\partial x_j}\right) + S_E \quad \text{(B.3)}
\]

where \(\rho\) is the density of SCO2, \(t\) is time, \(u_i\) and \(u_j\) are the Reynolds time-averaged velocity of SCO2 in the coordinate \(x_i\) and \(x_j\) directions, respectively; \(i\) and \(j\) are the coordinate index, \(i, j = 1, 2, 3; p\) is the pressure of SCO2, \(k\) is the turbulence kinetic energy, \(k = \frac{1}{2} \overline{u_i'^2}\), \(u_i'\) is turbulent fluctuation velocity of SCO2, \(\mu\) is laminar dynamic viscosity of SCO2, \(\mu_t\) is turbulent eddy viscosity, \(S_i\) is the specific body force, \(S_i = 0\) is held here, \(h\) is the enthalpy of SCO2, \(\lambda\) is the thermal conductivity of SCO2, \(T\) is the temperature of SCO2, \(Pr_t\) is the turbulent Prandtl number, \(Pr_t = 0.9\), \(S_E\) is the source term of energy, \(S_E = 0\) here; \(\rho, \mu\) and \(\lambda\) are given by the RGP table.

CFD heat transfer simulations of SCO2 require to resolve the viscous sublayer in a boundary layer to achieve correct heat transfer coefficient and wall temperature. Initially, additional low-Reynolds number models for the viscous sublayer were used based on the standard \(k - \varepsilon\) model [43] [44] [45] [3] [4] with very fine mesh near the wall, i.e. \(y^+ = \sqrt{\frac{\tau_w}{\mu} \frac{\gamma_n}{\nu} \leq 2}\), \(\tau_w\) is the shear stress at the wall, \(\gamma_n\) is the distance to the nearest wall from the first mesh layer, \(\nu\) is the kinematic viscosity of SCO2, \(\nu = \mu / \rho\).

Further, the Wilcox \(k - \omega\) turbulence model was applied to SCO2 heat transfer simulations [13]. The Wilcox \(k - \omega\) model employs a wall function in which the friction velocities and \(\omega\) values for the sublayer and the turbulence dominated log-law layer are analytically blended [46]. As a result, a low-Reynolds number model is not needed, and the simulated results are less dependent on \(y^+\) values. The turbulent eddy viscosity, however, is overpredicted because the transport of the turbulent shear stress is not considered, and the predicted heat transfer coefficients do not agree with the observations well [13].

Recently, the SST turbulence model has played an increasingly important role in SCO2 heat transfer simulations [6] [7] [8] [9] [10]. The SST model is a blended version of the Wilcox \(k - \omega\) model and the standard \(k - \varepsilon\) model. In the SST model, the flow near the wall is handled by the Wilcox \(k - \omega\) model, but the core flow is simulated by the standard \(k - \varepsilon\) model. Taking into account the transport of the shear stress, the overprediction of turbulent eddy viscosity is suppressed in the Wilcox \(k - \omega\) model [46]. The Wilcox \(k - \omega\) model is expressed as [16]
\[ \frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_j} (\rho u_j k) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_{k1}} \right) \frac{\partial k}{\partial x_j} \right] + P_k - \beta_k \rho k \omega + P_{kb} \]  \hspace{1cm} (B.4)

\[ \frac{\partial}{\partial t} (\rho \omega) + \frac{\partial}{\partial x_j} (\rho u_j \omega) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_{k1}} \right) \frac{\partial \omega}{\partial x_j} \right] + \frac{\alpha_1}{\nu_t} P_k - \beta_1 \rho k \omega^2 + P_{ob} \]  \hspace{1cm} (B.5)

where \( \sigma_{k1} \), \( \beta_k \), \( \alpha_1 \) and \( \beta_1 \) are the model constants, \( \sigma_{k1} = \sigma_{\omega1} = 2 \), \( \alpha_1 = 5/9 \), \( \beta_k = 0.09 \), \( \beta_1 = 0.075 \); \( P_{kb} \) and \( P_{ob} \) are the buoyancy production term in the \( k \)-equation and \( \omega \)-equation, respectively; since the SC02 inlet temperature is low, the two production terms are ignored.

The \( \omega \)-transformed standard \( k-\epsilon \) model is written as:

\[ \frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_j} (\rho u_j k) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_{k2}} \right) \frac{\partial k}{\partial x_j} \right] + P_k - \beta_k \rho k \omega + P_{kb} \]  \hspace{1cm} (B.6)

\[ \frac{\partial}{\partial t} (\rho \omega) + \frac{\partial}{\partial x_j} (\rho u_j \omega) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_{\omega2}} \right) \frac{\partial \omega}{\partial x_j} \right] + \frac{\alpha_2}{\nu_t} P_k - \beta_2 \rho k \omega^2 + \frac{2p}{\sigma_{\omega2}} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} + P_{ob} \]  \hspace{1cm} (B.7)

where \( \sigma_{k2} \), \( \sigma_{\omega2} \), \( \alpha_2 \) and \( \beta_2 \) are the model constants, \( \sigma_{k2} = 1 \), \( \sigma_{\omega2} = 10/8.56 \), \( \alpha_2 = 0.44 \), \( \beta_2 = 0.0828 \).

Introducing a blending function \( F_1 \) and combining Eq.(B.4) and (B.6), Eq.(B.5) and (B.7) in the manner such as \( F_1 \times \text{Eq.}(B.4)+(1-F_1) \times \text{Eq.}(B.6) \) and \( F_1 \times \text{Eq.}(B.5)+(1-F_1) \times \text{Eq.}(B.7) \), respectively, then a blended \( k-\omega \) model is achieved as:

\[ \frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_j} (\rho u_j k) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_{k3}} \right) \frac{\partial k}{\partial x_j} \right] + P_k - \beta_k \rho k \omega + P_{kb} \]  \hspace{1cm} (B.8)

\[ \frac{\partial}{\partial t} (\rho \omega) + \frac{\partial}{\partial x_j} (\rho u_j \omega) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_{\omega3}} \right) \frac{\partial \omega}{\partial x_j} \right] + \frac{\alpha_3}{\nu_t} P_k - \beta_3 \rho k \omega^2 + (1-F_1) \frac{2p}{\sigma_{\omega2}} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} + P_{ob} \]  \hspace{1cm} (B.9)

where \( \sigma_{k3} \), \( \sigma_{\omega3} \), \( \alpha_3 \) and \( \beta_3 \) are the blended model constants, expressed as \( \sigma_{k3} = F_1 \sigma_{k1} + \beta_1 (1-F_1) \sigma_{k2} \), \( \sigma_{\omega3} = F_1 \sigma_{\omega1} + (1-F_1) \sigma_{\omega2} \), \( \alpha_3 = F_1 \alpha_1 + (1-F_1) \alpha_2 \), and \( \beta_3 = F_1 \beta_1 + (1-F_1) \beta_2 \); \( F_1 \) is a blending function between the Wilcox \( k-\omega \) model and the standard \( k-\epsilon \) model, especially, \( F_1 = 1 \) at the wall, \( F_1 = 0 \) in the core flow, and \( 0 < F_1 < 1 \) between the wall and the core flow. A specific expression for \( F_1 \) is written as [16] [46]:

\[ F_1 = \tanh(\xi_1), \xi_1 = \min \left( \max \left( \frac{\sqrt{\nu}}{\beta_k \omega \gamma_n}, \frac{500 \nu}{\xi_2 \sigma_{\omega2} \gamma^2} \right), \frac{4 \rho k}{\xi_1} \right), \xi_2 = \max \left( \frac{2p}{\sigma_{\omega2}} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}, 1.0 \times 10^{-10} \right) \]  \hspace{1cm} (B.10)

where \( \gamma_n \) is the distance to the nearest wall.

In ANSYS CFX, the model expressed by Eqs. (B.8)-(B.10) is called the baseline (BLS) \( k-\omega \) model [16]. This model usually overpredicts the turbulent eddy-viscosity. To take the SST into account, the eddy-viscosity should be limited in some way. In [46], a mathematical expression was proposed to help address the overprediction of the eddy-viscosity, which reads as:

\[ \mu_t = \min \left( \frac{\rho k}{\omega}, \frac{a \rho k}{S \nu_2} \right), \gamma = \sqrt{2y_\gamma y_\gamma}, y_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), F_2 = \tanh(\xi_3), \xi_3 = \max \left( \frac{2\sqrt{\nu}}{\beta_k \omega \gamma_n}, \frac{500 \nu}{\gamma^2} \right) \]  \hspace{1cm} (B.11)

where \( a \) is model constant, \( a = 0.31 \), \( \gamma \) is the magnitude of the strain rate and \( y_{ij} \) represents the strain rate tensor; \( F_2 \) and \( \xi_3 \) are auxiliary variables. In ANSYS CFX, the model composed by
Eqs. (B.7)-(B.10) is the SST model. Note that the SST is not considered explicitly but implicitly by limiting the eddy-viscosity in the model.

In the SST model, the low-Reynolds number model for the viscous sublayer is replaced with a blended wall function, which is called as the Automatic Near-Wall Treatment in ANSYS CFX. It is a function of $y^+ (=u_\tau y_n/\mu)$, where $u_\tau$ denotes the friction velocity of SCO2 at the wall. Based on the solutions in the linear and the logarithmic near-wall regions, the blended wall function is focused on both $\omega$ and $u_\tau$, and written as [46]:

$$
\begin{align*}
\omega_1 &= \sqrt{\omega_{vis}^2 + \omega_{log}^2}, \quad \omega_{vis} = \frac{6\nu}{\beta y^2}, \quad \omega_{log} = \frac{u_\tau}{a_{v_k}} \\
u_t &= \left(4 (u_{t_{vis}})^4 + (u_{t_{log}})^4\right)^{1/4}, \quad u_{t_{vis}} = \frac{u_1}{y^+}, \quad u_{t_{log}} = \frac{u_n}{2\ln(y^+)+B}
\end{align*}
$$

(B.12)

where $\omega_{vis}$ and $\omega_{log}$ are the $\omega$ values calculated by the solutions in the linear and the logarithmic near-wall regions, $\omega_1$ is the total $\omega$ near wall, $u_{t_{vis}}$ and $u_{t_{log}}$ are the friction velocities at a wall by using the solutions in the sublayer and log-law layers, $u_n$ is the fluid velocity near the wall, $B$ is a constant, $B=5.2$ for hydraulically smooth walls, $u_\tau$ is the resultant friction velocity at the wall, and related to the wall shear stress with $\tau_w = \rho u_\tau^2$; $\kappa$ is the von Kármán constant, $\kappa=0.41$. The fluxes in the momentum equation and the $k$-equation at wall are detailed in [16].

In the sublayer and log-law regions, the following empirical expression in [47] is employed in CFX to determine the dimensionless temperature in convective heat transfer presented in [46]:

$$
\begin{align*}
T^+ &= Pr y^+ e^{-\Gamma} + [0.1\ln(y^+)] e^{-1/\Gamma}, \quad \Gamma = \frac{0.01(Pr y^+)^{4}}{1+5Pr^3y^+} \\
q_w &= \frac{\rho C_p u_t}{y^+} (T_w - T_n), \quad Pr = \frac{\mu C_p}{\lambda}, \quad \beta = (3.85 Pr^{1/3} - 1.3) + 0.1 \ln(Pr)
\end{align*}
$$

(B.13)

where $\Gamma$ is the auxiliary variable of $Pr$ and $y^+$, $q_w$ is the wall heat flux, $C_p$ is the specific heat capacity of SCO2, $T^+$ is the dimensionless temperature in the boundary layer, $T_w$ is the wall temperature, $T_n$ is the SCO2 temperature in the first mesh layer, $\beta$ is an auxiliary variable of the model, $Pr$ is the SCO2 Prandtl number; the SCO2 property constants, $\rho, \mu, C_p$ and $\lambda$ should be the local values in the first mesh layer. Based on Eqs. (B.12) and (B.13), the flow and heat transfer variables at the wall such as shear stress, wall temperature or heat flux can be calculated.

References


