Computational appraisal of the thermalhydraulic characteristics of supercritical carbon dioxide in heated mini-channel for HVAC applications

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Abstract. Over last couple of decades, supercritical fluid has found enhanced applications in numerous commercial sectors, encompassing aerospace, chemical, fast reactors, fusion reactors and renewable energy. Supercritical fluid is of major interest to the thermal engineers, primarily owing to its superior heat transport characteristics around the pseudocritical temperature. Supercritical carbon dioxide has particularly been identified as the next-generation coolant in power industry, due to its low critical temperature and reasonable critical pressure. The heating, ventilation and air-conditioning sector has also seen increasing popularity of supercritical CO$_2$ with the phasing out of the conventional halocarbons, as it has zero ozone depletion potential and substantially smaller global warming potential. While decent volume of literature is available regarding the application of supercritical CO$_2$ in macrochannel, thermalhydraulics of supercritical CO$_2$ in minichannel lacks comprehensive investigation, and the present work attempts to fill that specific void through a computational appraisal of a heated horizontal minichannel of 2 mm inner diameter. Systematic simulations have been performed to explore the role of the wall heat flux ranging from 30–50 kW/m$^2$, operating pressure ranging from 8–9 MPa, inlet temperature ranging from 295–315 K and buoyancy parameter on the thermalhydraulic characteristics of supercritical CO$_2$. The Reynolds number in the present simulation ranges from 10000-17000. This article is aimed to explore the phenomena of heat transfer deterioration in horizontal minichannel subjected to uniform wall heat flux. It is observed that increase in wall heat flux leads to lower area-averaged heat transfer coefficient. The results show an early heat transfer deterioration on top half surface whereas, normal heat transfer is observed on bottom half surface. Heat flux has significant effect on heat transfer deterioration and higher heat flux leads to reduction in peak value of heat transfer coefficient. At higher inlet temperature heat transfer coefficient decreases and peak of heat transfer coefficient shifted in the upstream direction. Also, peak of heat transfer coefficient vanishes for inlet temperature higher than pseudocritical temperature due to non-significant variation in thermophysical properties at higher temperature. Stratification of temperature, velocity and density is observed along the channel due to local buoyancy produced by non-linear thermophysical property variation of supercritical CO$_2$. 
1. Introduction
Due to environmental risk such as global warming potential and ozone depletion potential associated with conventional refrigerants such as chlorofluorocarbon (CFC) and hydrofluorocarbon (HCFC), use of these refrigerants are gradually phasing out. Supercritical carbon dioxide has shown a high potential in HVAC sector due to its zero ODP and substantially smaller GWP. Also, having relatively high working pressure reduces the compressor volume as compressor volume is approximately inversely proportional to the suction pressure.

In recent years, supercritical fluids thermal properties have attracted researchers due to necessity of substitute refrigerants and high intensity heat and mass transportation in power industry. Dang and Hihara [1] studied thermal behavior of supercritical CO₂ subjected to cooling condition and reported that heat transfer coefficient value and pressure drop across channel increases as the value of mass flux was increased. Song et al. [2] studied flow and thermal behavior of sCO₂ in vertical channel and observed that larger diameter channel is more susceptible to heat transfer deterioration because of buoyancy effect. Bourke et al. [3] investigated flow and heat transfer behavior of sCO₂ in vertical circular channel and an unstable buoyant effect was observed for relatively lower value of mass flux and moderate value of heat flux boundary conditions. Xiang et al. [4] and Chu et al. [5] reported heat transfer behaviors of supercritical carbon dioxide in a horizontal channel subjected to cooling condition. The result showed that heat transfer coefficient is higher at lower half surface, temperature stratification and secondary flow was observed because of buoyancy effect. Also, asymmetric radial velocity and turbulent kinetic energy profiles were observed due to buoyancy effect. Similar observation was reported by Cao et al. [6].

It is evident that there exists a significant gap in the research on heat transfer behavior of horizontal minichannel under heating condition and most of the reported literature concern flow and thermal behavior of vertical channel subjected under cooling condition. Also, heat transfer performance of channel with horizontal orientation subjected to uniform wall heating can significantly differ due to imposed boundary condition. Therefore, present study is aimed to reduce the gap by numerical investigation of convective heat transfer behavior of supercritical pressure carbon dioxide in a horizontal minichannel having inner diameter of 2 mm under heating condition for different heat flux, static operating pressure and inlet temperature.

2. Physical model and Numerical methods

2.1. Basic physical domain and boundary conditions
In this article the flow and thermal behavior of sCO₂ in minichannel having inner diameter 2 mm and length 840 mm is considered. The physical domain consists of an adiabatic section of length 240 mm and heated section of length 600 mm as shown in Fig. 1. Mass flux boundary condition at the inlet, adiabatic wall condition at the adiabatic section, uniform wall heat flux at the heated section and pressure outlet at the outlet is used. The gravity force acts along the negative y-axis.

![Fig. 1. Schematic of computational domain](image-url)
2.2. Governing equations
The steady state, three dimensional governing equations for supercritical fluids in a rectangular coordinate system are as follows:

- **mass equation:**
  \[ \frac{\partial}{\partial x_i} (\rho u_i) = 0 \]

- **Navier-Stokes equations:**
  \[ \frac{\partial}{\partial x_j} (\rho u_i u_j) = \frac{\partial}{\partial x_j} \left[ \mu_{\text{eff}} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu_{\text{eff}} \frac{\partial u_k}{\partial x_k} \right] - \frac{\partial p_i}{\partial x_i} + \rho g_i \]

- **Energy equation:**
  \[ \frac{\partial}{\partial x_i} \left( \rho u_i c_p T \right) = \frac{\partial}{\partial x_i} \left( \lambda \frac{\partial T}{\partial x_i} \right) + \phi \]

2.3. Numerical methods
The model equations are discretised using finite volume approach with pressure-implicit with splitting of operators (PISO) is chosen for pressure and velocity coupling. The pressure, momentum and energy equation terms are discretized using second-order upwind scheme and PREssure Staggering Option (PRESTO) scheme, respectively. The SST \( \kappa-\omega \) turbulence model is used to capture turbulent behavior. The nonlinear thermophysical properties of \( \text{sCO}_2 \), NIST Standard Reference Database 23 (REFPROP) version 9 is referred, which provides relatively precise properties.

2.4 Grid independent test and validation: In the present study, non-uniform mesh is used with refined grid near the wall to ensure flow characteristics are precisely resolved. Inflation method with first layer thickness of 0.002 mm and 9 layers are used to make sure \( y^+ \) value is less than 1. To ensure mesh independency of the final solution, four different grid size is used to study grid sensitivity. The values of fluid bulk temperature at the outlet and pressure drop across the channel is shown in Table. As increasing the number of cells from mesh 3 to mesh 4 yields less than 0.5% variation in fluid bulk temperature and less than 5% variation in pressure drop, therefore, mesh 3 is chosen in present study considering simulation time and precision. The comparison of present simulation heat transfer coefficient with experimental result (Dang & Hihara) is shown in Fig. 2 and the graph shows reasonable agreement with the experimental data.

| Grid    | Grid 1 | Grid 2  | Grid 3  | Grid 4  |
|---------|--------|---------|---------|---------|
| Number of cells | 167265 | 339486  | 482616  | 874324  |
| Bulk Temperature (K) | 309.08 | 311.18  | 313.14  | 314.68  |
| Pressure Drop (kPa)  | 1.548  | 1.763   | 1.895   | 1.983   |
Fig. 2. Comparison of present simulation with experimental data

Fig. 3. Wall temperature variation along channel length

3. Results and discussions

3.1. Heat flux effect analysis
The variation of wall temperature and heat transfer coefficient at different heat flux is shown in Fig. 3 and Fig. 4(a), respectively. For \( q = 30 \text{ kW/m}^2 \), the wall temperature variation is almost linear on both top half and bottom half surface whereas, for \( q = 40 \text{ kW/m}^2 \) and \( q = 50 \text{ kW/m}^2 \), wall temperature gradually increases in axial direction. Average temperature at the top half surface is relatively higher than the bottom half surface. The area-averaged heat transfer coefficient variation is depicted in Fig. 4(a). At higher value of heat flux, magnitude of heat transfer coefficient decreases and peak of heat transfer coefficient shifted in the upstream direction. Also, minima in the heat transfer is observed at the top half surface.

Fig. 4. Variation of heat transfer coefficient (a) along channel length (b) with normalized bulk temperature

3.2. Operating pressure effect on heat transfer
The heat transfer coefficient variation at different operating pressure at top half surface is depicted in Fig. 4(b). For \( T_b < T_{pc} \), higher operating pressure leads to lower heat transfer coefficient and there is a considerable drop in peak at smaller heat flux and for \( T_b > T_{pc} \), slightly higher heat transfer coefficient is observed at higher operating pressure. The drop in peak is due to lower value of specific heat at higher operating pressure.

3.3. Effect of fluid inlet temperature
Heat transfer variation due to different fluid inlet temperature is depicted in Fig. 5(a). As inlet temperature increases, heat transfer coefficient magnitude decreases because isobaric specific heat and
thermal conductivity decreases with inlet temperature. With increase in inlet peak value of heat transfer shifted towards upstream direction. Also, as inlet temperature becomes much higher than pseudocritical temperature, peak in heat transfer coefficient vanishes because thermophysical properties variation far away from pseudocritical point becomes less significant and value of specific heat decreases.

Fig. 5. (a) Effect of inlet temperature on HTC (b) Variation of buoyancy parameter along channel length

3.4. Temperature and flow field development and buoyancy analysis
Development of temperature and flow field is depicted in Fig. 6(a) and Fig. 6(b), respectively. Flow stratification can be seen in temperature contours due to variation of thermophysical properties near the channel wall. The velocity vector depicts natural circulation induced by buoyancy and velocity magnitude is higher in core region whereas, formation of boundary layer reduced velocity magnitude near the channel wall. Buoyancy criteria proposed by Jackson et al. [7] is used to study buoyancy effect. The variation of buoyancy parameter along axial direction is shown in Fig. 5(b). It is evident from figure that effect of buoyancy is significant all along the channel length. The wall heat flux has relatively less effect on buoyancy parameter both near the heated section inlet and near the outlet.

Fig. 6. Development of (a) temperature field (b) velocity vector along channel cross-section for
4. Conclusion
In the present study thermalhydraulic characteristics of supercritical CO$_2$ is studied using parametric simulations. The heat transfer behaviour of supercritical carbon dioxide is significantly affected by the heat flux value and fluid inlet temperature. The wall temperature has an earlier peak on top half surface which indicates heat transfer deterioration whereas, no heat transfer deterioration is observed on bottom half surface. Before the pseudocritical point, with increasing operating pressure lower heat transfer coefficient is observed. Whereas, after the pseudocritical point, slightly higher heat transfer coefficient is reported at higher operating pressure. At higher inlet temperature heat transfer coefficient decreases and peak value of heat transfer coefficient shifted towards upstream direction. When inlet temperature becomes higher than pseudocritical temperature, peak value of heat transfer coefficient vanishes due to non-significant property variation at higher temperature. Therefore, it can be suggested that heat flux and inlet temperature has similar effect on thermal characteristics of supercritical carbon dioxide flowing inside a horizontal minichannel. Flow stratification is observed due to thermophysical variation and velocity vector shows a buoyancy induced local circulation.

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