

Numerical Analysis of Flow and Heat Transfer Characteristics of CO₂ at Vapour and Supercritical Phases in Micro-Channels

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Abstract. Supercritical carbon dioxide (CO₂) has special thermal properties with better heat transfer and flow characteristics. Due to this reason, supercritical CO₂ is being used recently in air-condition and refrigeration systems to replace non environmental friendly refrigerants. Even though many researches have been done, there are not many literatures for heat transfer and flow characteristics of supercritical CO₂. Therefore, the main purpose of this study is to develop flow and heat transfer CFD models on two different phases; vapour and supercritical of CO₂ to investigate the heat transfer characteristics and pressure drop in micro-channels. CO₂ is considered to be in different phases with different flow pressures but at same temperature. For the simulation, the CO₂ flow was assumed to be turbulent, non-isothermal and Newtonian. The numerical results for both phases are compared. From the numerical analysis, for both vapour and supercritical phases, the heat energy from CO₂ gas transferred to water to attain thermal equilibrium. The temperature of CO₂ at vapour phase decreased 1.78% compared to supercritical phase, which decreased for 0.56% from the inlet temperature. There was a drastic increase of 72% for average Nu when the phase changed from vapour to supercritical. The average Nu decreased rapidly about 41% after total pressure of 9.0 MPa. Pressure drop (ΔP) increased together with Reynolds number (Re) for vapour and supercritical phases. When the phase changed from vapour to supercritical, ΔP was increased about 26%. The results obtained from this study can provide information for further investigations on supercritical CO₂.

1 Introduction

Carbon dioxide (CO₂) gas, which has zero ozone depleting potential (ODP) and zero effective global warming potential (GWP) was reintroduced as an environmental friendly gas, and used as working fluid in refrigerators and air conditioning systems. Moreover, there are a few advantages of using CO₂, such as it is non-toxic and safe to humans, abundant and non-combustible. As the supercritical CO₂ reaches near to its critical point, the physical properties shows extremely rapid variations with a change in temperature and pressure, which makes it as the most important characteristics [1]. The current refrigerants, such as chlorofluorocarbons (CFCs) and hydro chlorofluorocarbons (HCFCs), which are being used in air conditioning and refrigeration systems, have high ozone depletion and effective global warming potentials. Hence, CO₂ can be the ideal replacement for these non-environmental friendly refrigerants with the thermo-fluid properties and appropriate design, at supercritical phase.

Furthermore, the density and dynamic viscosity of CO₂ at supercritical phase undergo a significant, which is almost vertical within a very narrow temperature range while the enthalpy undergoes a sharp increase near the critical point [2]. As the temperature of supercritical CO₂ was increased in near-critical region, the pressure drop

and heat transfer coefficient are increased too [3]. At larger Reynolds number, heat transfer coefficient increased as the heat transfer rate increased [4]. Therefore, to understand the underlying physics, an appropriate implementation of fluid flow and heat transfer correlation is the systems are needed. Even though a few researches had performed studies and investigation on cooling heat transfer and flow of supercritical CO₂ in micro-channels, it still could not solve this issue. The thermophysical properties and variables of supercritical CO₂ are obtained from NIST Refrigerants Database REFPROP [5]. The density (ρ), thermal conductivity (λ), viscosity (μ) and specific heat (C_p) of supercritical CO₂ vary with different pressures along increased temperature [6].

Many researchers have studied the flow and heat transfer characteristics of supercritical CO₂ by using numerical and experimental methods. The geometry often used for mathematical model is the circular tube-in-tube heat exchanger, where supercritical CO₂ flow in the inner tube and water flow in the annular space [7]. Most numerical analysis are done by using Renormalization Group (RNG) k - ϵ and Low-Reynolds number (LRN) k - ϵ models as the turbulence model with ANSYS FLUENT CFD codes [8-11]. Besides, the flow domains are divided into two; CO₂ and water for cooling process [12, 13].

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The main purpose of this study is to develop flow and heat transfer mathematical models for CO₂ at vapour and supercritical phases in micro-channels, and to compare both phases to prove which phase is the best for heat transfer and flow characteristics of CO₂. This study is expected to provide better knowledge on reducing the ozone depletion effect and global warming potentials by replacing the existing non-environmental friendly refrigerant with supercritical CO₂.

2 Mathematical formulations

2.1 Governing equations

In this study, the flow field is assumed to be incompressible, steady, non-isothermal and two-dimensional (2D) flow. Therefore, the governing equations for the continuity, momentum and energy can be expressed as [14]:

Continuity equation for incompressible flow:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \quad (1)$$

$$\vec{\nabla} \cdot \vec{V} = 0 \quad (2)$$

where u, v and w are velocity components in the x, y and z directions, respectively, and $\vec{\nabla}$ is divergence operator.

Momentum equation:

$$\rho \frac{D\vec{V}}{Dt} = \rho \left[\frac{\partial \vec{V}}{\partial t} + (\vec{V} \cdot \vec{\nabla})\vec{V} \right] = -\vec{\nabla}P + \rho\vec{g} + \mu\nabla^2\vec{V} \quad (3)$$

where ρ is density of the fluid (kg/m³), V is velocity vector of the fluid (m/s), t is time (seconds), g is gravitational acceleration (m/s²) and μ in the fluid viscosity (kg/m.s)

Conservation of energy equation:

$$\begin{aligned} \rho \frac{DE}{Dt} = & \frac{\partial(u\sigma_{xx})}{\partial x} + \frac{\partial(v\sigma_{yy})}{\partial y} + \frac{\partial(w\sigma_{zz})}{\partial z} \\ & + \frac{\partial(u\tau_{yx})}{\partial y} + \frac{\partial(v\tau_{zx})}{\partial z} + \frac{\partial(v\tau_{xy})}{\partial x} + \frac{\partial(v\tau_{zy})}{\partial z} \\ & + \frac{\partial(w\tau_{xz})}{\partial x} + \frac{\partial(w\tau_{yz})}{\partial y} - \frac{\partial q_x}{\partial x} - \frac{\partial q_y}{\partial y} - \frac{\partial q_z}{\partial z} \end{aligned} \quad (4)$$

where σ is stress and τ is shear stress.

2.2 Pressure drop equations

Pressure drop (ΔP) takes place due to pressure loss in a system due to friction in the system. The ΔP equation represents the relationship between friction factor, length to diameter of tube ratio, and density and velocity of the fluid [14]. The general equation of ΔP is:

$$\Delta P = f \cdot \frac{L}{D} \cdot \frac{\rho V^2}{2} \quad (5)$$

where ΔP is pressure drop (MPa): f is friction factor, L is length the tube (m) and D is diameter of the tube (m).

Meanwhile, Reynolds number also is calculated with following formula:

$$Re = \frac{\rho V D}{\mu} \quad (6)$$

where Re is Reynolds number and ρ is density of the fluid (kg/m³). The friction factor for equation (1) will be calculated with Reynolds number obtained from equation (6). For laminar flow, the friction factor was:

$$f = \frac{64}{Re} \quad (7)$$

Meanwhile, for turbulent flow, Colebrook equation was used to calculate friction factor:

$$\frac{1}{\sqrt{f}} = -2.0 \log \left(\frac{\varepsilon D}{3.7} + \frac{2.51}{Re \sqrt{f}} \right) \quad (8)$$

where ε is pipe roughness.

2.2 Heat transfer rate equations

Convective heat transfer rate (\dot{Q}_{conv}) is the amount of heat transferred per unit time. The rate of convection heat transfer was expressed by Newton's Law of Cooling [15]:

$$\dot{Q}_{conv} = hA_S(T_S - T_\infty) \quad (9)$$

where \dot{Q}_{conv} is convection heat transfer rate (W), h is convection heat transfer coefficient (W/m²°C), A_S is heat transfer surface area (m²), T_S is temperature of surface (°C) and T_∞ is temperature of the fluid sufficiently far from the surface (°C).

Besides, Nusselt number (Nu) was calculated using the following equation:

$$Nu = \frac{hL_C}{\lambda} \quad (10)$$

where λ is thermal conductivity (W/m.K) and L_c is characteristics length (m).

3 Numerical analysis

3.1 Computational domain

The flow domain of CO₂ and water was designed in Design Modeler software. It was designed according to the tube-in-tube heat exchanger concept. The diameter of the inner tube was measured from the smallest tube available in market and the cooling length was the minimum value obtained from previous studies. The model was designed in 2D, as shown in Figure 1. The pipe-in-pipe flow domain was designed with the dimensions stated in Table 1. The 2D model is the half of the whole tube-in-tube heat exchanger.

Table 1. Dimensions of flow domain.

Parameter	m
Inner tube height (H_i)	0.0025
Outer tube height (H_o)	0.01
Cooling length (L)	1

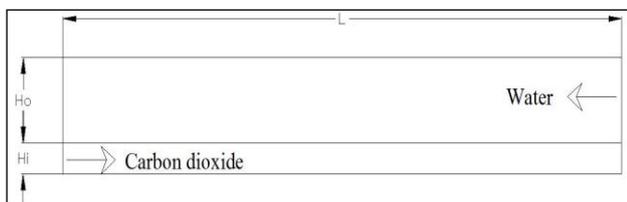


Figure 1. 2D pipe-in-pipe heat exchange design in Design Modeler.

As mentioned above, the fluids used for the numerical analysis are water as the cooling fluid and CO₂ as the main fluid. Since the thermophysical properties of water are at room temperature, the details are available in ANSYS FLUENT material database. However, the thermophysical properties of CO₂ available in ANSYS FLUENT database are only at room temperature. Therefore, the thermophysical process of CO₂ at vapor and supercritical were obtained from National Institute of Standards and Technology (NIST) web book [6]. The density, thermal conductivity, viscosity and specific heat of supercritical CO₂ vary with different pressures along the increased temperature. The thermophysical properties of CO₂ in both vapour and supercritical phases from 3.5 MPa to 10.0 MPa pressures respectively with 313 K inlet temperature are obtained, and are tabulated in Table 2.

3.2 Meshing

The mesh size is setup to be fine. Meanwhile, the mesh size at the interface between inner tube and annular part

was setup to be finer to obtain accurate heat transfer data between CO₂ and water. Moreover, mesh independent test was conducted to make sure that the numerical analysis results were same for all mesh sizes at 3.5 MPa pressure only. The inlet and outlet faces for CO₂ and water, interfaces, symmetries and walls were renamed. For both vapour and supercritical phases' models, the number of meshes used is same, which are 15,000 elements.

Table 2. Thermophysical properties of CO₂ [6].

Pressure, P (MPa)	Density, ρ (kg/m ³)	Thermal conductivity, λ (W/m.K)	Viscosity, μ (Pa.s)	Specific heat, C_p (J/g.K)
3.5	70.871	0.020268	1.6298x10 ⁻⁵	1.1735
4.0	83.758	0.020901	1.6494 x10 ⁻⁵	1.2527
5.0	113.05	0.022622	1.7029 x10 ⁻⁵	1.4697
6.0	149.26	0.025392	1.7860 x10 ⁻⁵	1.8335
7.5	231.53	0.034950	2.0452 x10 ⁻⁵	3.3553
8.0	277.90	0.042376	2.2345 x10 ⁻⁵	4.9501
9.0	485.50	0.070590	3.4806 x10 ⁻⁵	12.833
10.0	628.61	0.071410	4.7825 x10 ⁻⁵	5.6575

3.3 Boundary conditions

For this study, the CO₂ was assumed as incompressible flow for both vapour and supercritical phases. The CO₂ and water flow in the inner tube and outer tube respectively. The parameters, which were used in the numerical analysis, are tabulate in Table 3.

Table 3. Boundary conditions.

Boundaries	Variables	Vapour phase	Supercritical phase
CO ₂ inlet	Pressure-inlet with constant temperature	3.5 MPa	7.5 MPa
CO ₂ outlet	Constant	313 K	313 K
Water inlet	Velocity-inlet with constant temperature	10 m/s	10 m/s

4 Results and discussions

The heat transfer and pressure drop are obtained from dynamic pressure, velocity, temperature, Nusselt number and Reynolds number data from the numerical analysis. These data are analysed and compared. The convective

heat transfer coefficients, Nusselt number, Reynolds number and pressure drop are recorded, and calculated.

4.1 Heat transfer

The temperature of CO₂ for both vapour and supercritical phases decreased along the 1 m tube, as shown in Figure 2. The temperature of CO₂ is constant up to 0.2 m and started reducing subsequently. However, the temperature of CO₂ at vapour phase decreased 1.78% compared to supercritical phase, which decreased for 0.56% from the inlet temperature. This is because the tube length was not enough for CO₂ at supercritical phase to transfer heat energy to attain thermal equilibrium at high total pressure. For vapour phase, due to low total pressure, it attained thermal equilibrium faster.

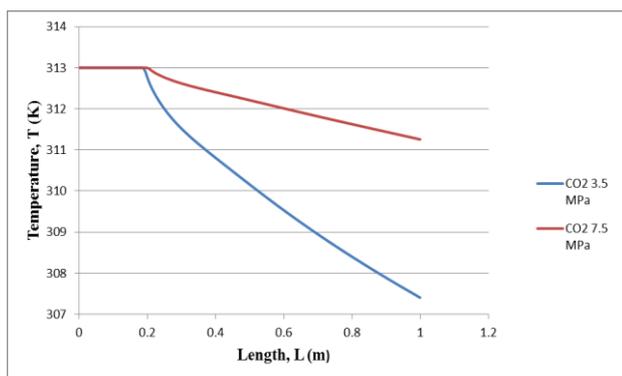


Figure 2. Temperature versus length of carbon dioxide and water for both vapour and supercritical phases.

In Figure 3, the average Nusselt number (Nu) for CO₂ for both vapour and supercritical phases were varying according to total pressures. At vapour phases, Nu of CO₂ increased slowly as the total pressure increased from 3.5 MPa to 6.0 MPa. Meanwhile, at supercritical phase, average Nu also increased together with the total pressure from 7.5 MPa to 9.0 MPa. There was a drastic increase of 72% for average Nu when the phase changed from vapour to supercritical. However, after 9.0 MPa total pressure, average Nu decreased rapidly for 41% because the tube length is not enough to transfer the thermal energy from CO₂ to water.

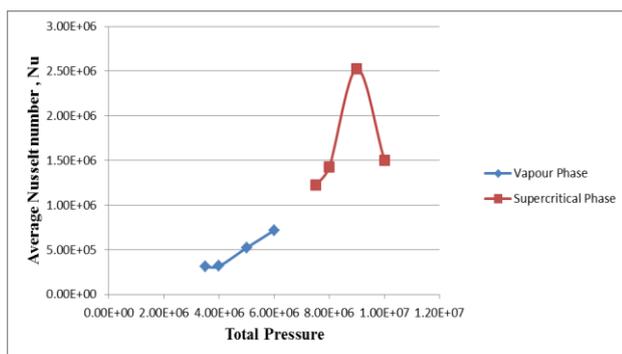


Figure 3. Average Nusselt number (Nu) versus total pressure for both vapour and supercritical pressure phases.

Besides, as shown in Figure 4, the temperature changes of CO₂ along the tube at supercritical pressures were decreasing. The temperature of CO₂ decreased linearly for all supercritical pressure. At total pressure of 7.5 MPa, 8.0 MPa, 9.0 MPa and 10.0 MPa, the temperature decreased 0.56%, 0.4%, 0.44% and 0.53%, respectively from the inlet temperature. At 7.5 MPa, which is closer to critical pressure, the amount of heat loss is highest. Increase on pressure made the heat transfer coefficient decreased closely at pseudocritical temperature [16]. As the total pressure increased from critical pressure, the heat transfer rate reduced. Besides, the length of the tube is not enough for supercritical CO₂ to heat up the water.

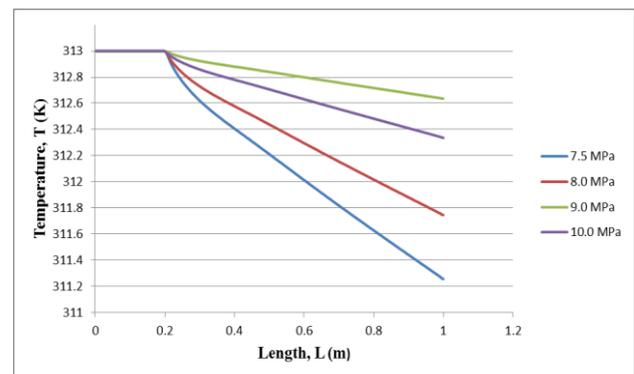


Figure 4. Temperature versus length of CO₂ at supercritical pressures.

From the numerical analysis, for both vapour and supercritical phases, the heat energy from CO₂ gas transferred to water to attain thermal equilibrium, as shown is Figures 2 and 4. The thermal energy from CO₂, which was at 313 K temperature, was transferred to water, which was at 300 K. It was proved that as the total pressure increased, the heat transfer coefficient decreased [3], which is same with the situation in this study. Moreover, for supercritical phase, the tube length was not enough for the heat energy from CO₂ to be transferred fully to water. The tube length should be increased to obtained better results on heat transfer.

4.2 Pressure drop

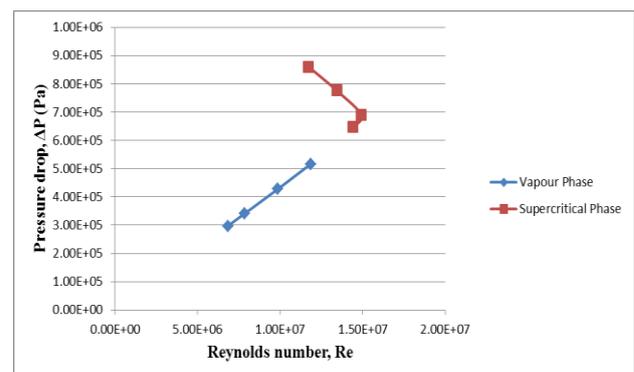


Figure 5. Pressure drop versus Reynolds number of CO₂ at both vapour and supercritical phases.

The dynamic pressure and velocity were analyzed, and compared for both vapour and supercritical phases along the 1 m cooling length. For all total pressures, the dynamic pressure and velocity were directly proportional to each other. As the total pressure of CO₂ flowing in the tube decreased due to heat loss to water, the velocity of CO₂ increased along the tube.

Moreover, the pressure drop, ΔP of CO₂ was calculated from the dynamic pressure data from the numerical analysis. The ΔP increased linearly as the total pressure of increased from 3.5 MPa to 10.0 MPa. As shown in Figure 5, the ΔP increased together with Re for vapour phase, as the pressure is approaching the critical point. When the phase changed from vapour to supercritical, ΔP increased about 26%. For supercritical phase, the ΔP increased along with Re up to 8.0 MPa. Even though the ΔP increased after 8.0 MPa, the value of Re keep decreasing up to 10.0 MPa. Hence, the pressure drop of CO₂ at both vapour and supercritical phases do increased as it was proven. The decrease in Re is due to drastic increase in density and viscosity of CO₂ at total pressure from 8 MPa to 10 MPa. C.H. Son and S.J. Park [17] investigated that variation in the density of CO₂ resulted to decrease in ΔP with increased inlet pressure of gas cooler at supercritical phase, which is against the results in Figure 5.

5 Conclusion

In this study, the mathematical models to investigate the flow and heat transfer characteristics of CO₂ at vapour and supercritical phases in micro-channels were developed. The flow domain of CO₂ and water was designed in 2D by using Design Modeler software, according to the pipe-in-pipe heat exchanger concept, with length of 1000 mm. The thermophysical properties of CO₂ in both vapour and supercritical phases from 3.5 MPa to 10.0 MPa pressures respectively with 313 K inlet temperature were obtained from NIST. The temperature of water was 300 K at velocity of 10 m/s.

From the numerical analysis, for both vapour and supercritical phases, the heat energy from CO₂ gas transferred to water to attain thermal equilibrium. The temperature of CO₂ at vapour phase decreased 1.78% compared to supercritical phase, which decreased for 0.56% from the inlet temperature. According to average Nusselt number (Nu), the heat transfer rate of CO₂ increased as the total pressure is increased. It was proved that as the total pressure increased, the heat transfer coefficient decreased, which is same with the situation in this study. There was a drastic increase of 72% for average Nu when the phase changed from vapour to supercritical. However, after 9.0 MPa total pressure, average Nu decreased rapidly for 41% because the tube length is not enough to transfer the thermal energy from CO₂ to water.

Pressure drop (ΔP) increased together with Reynolds number (Re) for vapour and supercritical phases. When the phase changed from vapour to supercritical, ΔP increased about 26%. There is a rapid

heat transfer between CO₂ and water at low pressure compared to high pressure. The results obtained from this study can provide information for further investigations on supercritical CO₂

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