

Heat Transfer Performance of Heated Upward Turbulent Supercritical CO₂ Flow in a Microchannel: A Numerical Study

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1. Introduction and Background

Many advanced engineering systems, including microelectronic devices [1], require state-of-the-art high heat flux thermal management technologies. Conventional subcritical single-phase liquid or two-phase boiling cooling methods may not be capable of managing anticipated heat flux levels of such emerging equipment. Supercritical carbon dioxide (sCO₂) heat transfer has been used in industrial applications since the 1960s [2]. However, supercritical transport behavior has only been experimentally investigated for narrow working ranges. Prior empirical studies with sCO₂ [3,4] have focused on large diameter circular tubes ($4.08 < D < 22.7$ mm) with uniformly heated surface at low heat fluxes ($0.05 < q'' < 330$ W cm⁻²). Various observations on heat transfer enhancement or deterioration due to buoyancy effects, pseudo-boiling, channel orientation, range of heat/mass flux, flow acceleration, etc. have been reported for supercritical fluids. Only one experimental study with limited working range exists for microscale diameter ranges ($D_H < 1$ mm) [5]. Thus, the goal of this work is to investigate the underlying supercritical transport phenomenon at microscale. Supercritical convection simulations relied on Reynolds-Averaged (RANS) turbulence modeling approaches in the 1990s and 2000s, and were focused on moderate heat flux (< 100 W cm⁻²) water and CO₂ flows in 2-D large hydraulic diameter vertical tubes and rod bundles. Therefore, they were not able to capture unsteady supercritical effects such as intrinsic pulsations [6] and mixed forced and free convection (*i.e.*, pseudo-boiling phenomenon). To address these limitations, some investigations adopted 3D unsteady turbulence resolving approaches [7]. So far, the only available computational work on microscale supercritical heat transfer has been performed by Asinari [8], using $k - \epsilon$ RANS modeling, which cannot capture unsteady 3D turbulent flow effects.

In the present investigation, high resolution large eddy simulations (LES) of sCO₂ vertical upward flows in microchannels are performed at high mass fluxes ($G = 1000$ kg m⁻²s⁻¹) and moderate heat fluxes ($q'' = 1.6 - 8.7$ W cm⁻²), and flow inlet temperature in the range of $T_{in} = 20 - 100$ °C to predict sCO₂ heat transfer coefficients inside and outside pseudocritical region. Results are compared with our prior computational study of horizontal microchannels at similar thermophysical conditions [9] to determine the effect of channel orientation on possible enhancement or deterioration of heat transfer. Results are also compared with available empirical supercritical heat transfer correlations of [5,10] to assess their applicability at these working conditions. This study represents the initial set of simulation cases in a comprehensive numerical investigation that will later include higher heat fluxes

2. Simulation Approach

In this study, a single vertical microchannel test section of $750 \mu\text{m} \times 737 \mu\text{m}$ cross section, and 5 mm length represents the simulation geometry (Fig. 1). The channel is uniformly heated from all four sides with constant temperature. The governing continuity, momentum, and energy equations are listed as follows for velocity (u), pressure (p), and enthalpy (h) fields.

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0 \quad (1)$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j u_i) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}[(\mu + \mu_{SGS})\frac{\partial u_i}{\partial x_j}] + \rho g_i \quad (2)$$

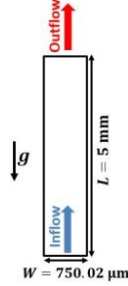


Fig. 1 – Schematic side-view of the simulation geometry

$$\frac{\partial(\rho h)}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i h) = \frac{\partial}{\partial x_j}[(\alpha + \alpha_{SGS})\frac{\partial h_i}{\partial x_j}] \quad (3)$$

In the above formulation, μ_{SGS} and α_{SGS} represent the LES turbulence model contributions to momentum and thermal energy transport, respectively. Fluid thermophysical properties (ρ, c_p, μ, k) are calculated at each time step, using either explicit formulations (*i.e.*, Peng-Robinson equation of state [11]) for sCO₂ density, or accurate curve fits (*i.e.*, for specific heat (c_p), dynamic viscosity (μ), and Prandtl number (Pr) based on data from [12,13]) for the studied reduced pressure of $P_r = 1.1$. A velocity-pressure-enthalpy coupled unsteady compressible flow solver in OpenFOAM v1612+ [14] is employed (*buoyantPimpleFoam*). The wall-adapting local eddy-viscosity (WALE) LES model [15] is adopted to model subgrid-scale eddy (SGS) viscosity and diffusivity. Second and third order discretization schemes were used for time and space discretization. The mesh structure for all the simulation cases was configured such that first-cell $y^+ = 0.26$, which was found to be sufficient for LES heat transfer studies at comparable high Prandtl numbers [16]. The cell lengths are uniform in the flow direction. All the channel walls were specified with constant temperature boundary conditions. The inflow temperature field was specified with a time-averaged turbulent law of the wall profile, while an advective temperature boundary condition was imposed at the outflow. Inlet velocity, turbulent diffusivity α_t , and turbulent eddy viscosity ν_t profiles were mapped from 4 mm downstream to achieve quasi-fully developed turbulent flow structures. For all the walls, no-slip velocity and *fixed-zero-flux* pressure boundary conditions were used. A *0-gradient velocity boundary condition* was selected for the outflow patch. Finally, fixed-value pressure inlet and outlet boundary conditions were imposed to the computational domain to ensure the target mass flux of ~ 1000 kg m⁻² s⁻¹.

3. Results and Discussion

Following the approach of [9], a mesh convergence study was successfully performed for a representative vertical channel case with reduced pressure of $P_r = 1.1$, mass flux $G = 1000$ kg m⁻² s⁻¹ ($Re_{D,H} = 25,360$), and inlet temperature $T_{in} = 34.9$ °C. It was observed that the empirical rate of convergence for average wall heat flux is greater than second order. Mid-plane instantaneous velocity and temperature fields from this case (Table 1, case 3) are shown in Fig. 2, below. Five simulation test cases were evaluated in this study (Table 1). Following the suggested method of [17], the results of three mesh levels were used to calculate Richardson-extrapolated value for average wall heat flux. These extrapolated values are compared with available supercritical heat transfer correlations for vertical channel in the

literature [5,10] as well as the numerical results of our prior work on horizontal channel orientation [9] (Table 2). Out of the two available empirical correlations in the literature which are applicable to vertical channel flow [5,10], only the model of Liao and Zhao [5] was developed using microchannel supercritical heat transfer data (tube diameter of $d = 0.7 - 2.16$ mm). The predictions of this model for the cases 2 and 3, *i.e.*, operating near pseudocritical temperature ($T_{pc} = 35.25^\circ\text{C}$), shows a close agreement with maximum deviation of $\pm 21\%$ (Table 2). This observation suggest that scale dependent mixed convection and boundary layer effects are quite important in this region. For the cases 1-4, the correlation of [10] also yields a close agreement compared to our simulation heat fluxes with a range of maximum deviation from $\pm 9\%$ to $\pm 28\%$. However, Jackson and Hall [10] have used data from various resources to develop their suggested correlation without reporting its applicability range or the size of tube diameter(s). It should be noted that for case 5 at which sCO_2 is outside of the pseudocritical region and its behavior is similar to a gaseous fluid, the heat flux predictions of both correlations deviate from our result by more than $\pm 50\%$. For this case, the prediction of Gnielinski [18] for turbulent channel flow heat transfer ($q''_{\text{Gen}} = 74,100 \text{ W m}^{-2}$), which was not specifically proposed for a supercritical fluid, yields a good agreement of $\pm 18\%$.

Table 1. Specifications of selected simulation test cases.

Case #	Re_{in}	$T_{\text{in}} [^\circ\text{C}]$	$T_{\text{wall}} [^\circ\text{C}]$	$q''_{\text{avg,VU}} [\text{W m}^{-2}]$
1	11,840	20.1	26.2	$35,660 \pm 11,230$
2	15,110	29.9	32.4	$22,800 \pm 260$
3	25,360	34.9	35.7	$15,990 \pm 2,210$
4	37,470	69.9	84.7	$66,100 \pm 11,830$
5	35,870	99.9	116.7	$87,290 \pm 19,660$

Table 2. Comparison of the simulation results against predictions from supercritical correlations and horizontal microchannel simulation results

Case #	$q''_{\text{avg,VU}} [\text{W m}^{-2}]$	$q''_{\text{avg,H}} [\text{W m}^{-2}]$ [9]	$q'' [\text{W m}^{-2}]$ [10]	$q''_{\text{LZ}} [\text{W m}^{-2}]$ [5]
1	$36,700 \pm 11,200$	$35,700 \pm 11,000$	46,080	59,570
2	$22,800 \pm 260$	$22,400 \pm 7,300$	24,840	28,570
3	$16,000 \pm 2,200$	$17,150 \pm 60$	22,210	19,780
4	$66,100 \pm 11,800$	$69,800 \pm 16,100$	56,860	46,870
5	$87,300 \pm 19,700$	$88,900 \pm 20,900$	57,660	44,840

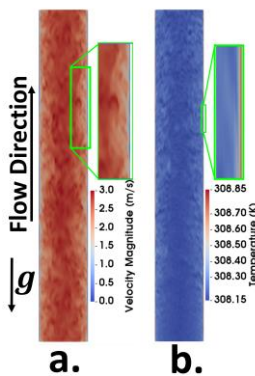


Fig. 2 – Simulation results for convergence test case (case 3). **a.** Cross-section velocity magnitude, with magnified view of pseudo-boiling phenomenon near right wall. **b.** Cross-section temperature field with detail view of thermal boundary layer (5% of channel near right wall)

Finally, it is observed that the simulation heat fluxes for vertical upward flow and horizontal flow [9] only deviate by $\pm 8\%$. This might be explained using an approximate analysis by [10], which suggested that if the ratio of mean Grashof number to flow Reynolds number is $Gr_m/Re^{2.7} < 10^{-5}$ (valid for all the cases in this study), the heat flux deterioration in upward flow due to buoyancy effects (partial laminarization of the flow), is negligible.

4. Conclusions

This investigation explored the effect of microchannel orientation

on heat transfer performance of sCO_2 . Main findings of this work include:

1. For cases 2 and 3, which are closest to T_{pc} , the predictions of [5] using microchannel experimental, data yields a maximum deviation of $\pm 21\%$.
2. The correlation of [10] also provides good agreement (*max. dev. of $\pm 9\%$ to $\pm 28\%$*) for the cases 1-4.
3. The prediction of turbulent channel flow correlation of [18] yields the closest agreement for case 5, far from T_{pc} .
4. Since $Gr_m/Re^{2.7} < 10^{-5}$ for all the cases, buoyancy-induced degradation of heat transfer is negligible at these conditions.

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References

- [1] Lin, S., Sefiane, K., and Christy, J. R. E., 2002, "Prospects of confined flow boiling in thermal management of microsystems," *Appl. Therm. Eng.*, **22**(7), pp. 825–837.
- [2] Pioro, I. L., and Duffey, R. B., 2007, "Heat Transfer and Hydraulic Resistance at Supercritical Pressures in Power Engineering Applications," ASME.
- [3] Krasnoshchekov, E. A., and Protopopov, V. S., 1966, "Experimental study of heat exchange in carbon dioxide in the supercritical range at high temperature drops (Heat transfer in turbulent carbon dioxide pipeflow at supercritical region)," *High Temp.*, **4**, pp. 375–382.
- [4] Tanaka, H., Nishiwaki, N., and Hirata, M., 1967, "Turbulent heat transfer to supercritical carbon dioxide," *Semi-International Symposium, JSME, Tokyo*.
- [5] Liao, S. M., and Zhao, T. S., 2002, "An experimental investigation of convection heat transfer to supercritical carbon dioxide in miniature tubes," *Int. J. Heat Mass Transf.*, **45**(25), pp. 5025–5034.
- [6] Bishop, A. A., Sandberg, R. O., and Tong, L. S., 1964, Forced-convection heat transfer to water at near-critical temperatures and supercritical pressures, Westinghouse Electric Corp., Pittsburgh, Pa. Atomic Power Div.
- [7] Bae, J. H., Yoo, J. Y., and Choi, H., 2005, "Direct numerical simulation of turbulent supercritical flows with heat transfer," *Phys. Fluids*, **17**(10).
- [8] Asinari, P., 2005, "Numerical prediction of turbulent convective heat transfer in mini/micro channels for carbon dioxide at supercritical pressure," *Int. J. Heat Mass Transf.*, **48**(18), pp. 3864–3879.
- [9] Nabil, M., and Rattner, A. S., 2018, "LES simulation of turbulent supercritical CO2 heat transfer in microchannels," *Proceedings of the 6th International Supercritical CO2 Power Cycles Symposium, Pittsburgh, Pennsylvania, USA*.
- [10] Jackson, J. D., and Hall, W. B., 1979, "Forced convection heat transfer to fluids at supercritical pressure," *Turbul. Forced Convect. Channels Bundles Theory Appl. to Heat Exch. Nucl. React.*, pp. 563–611.
- [11] Peng, D.-Y., and Robinson, D. B., 1976, "A new two-constant equation of state," *Ind. Eng. Chem. Fundam.*, **15**(1), pp. 59–64.
- [12] Fenghour, A., Wakeham, W. A., and Vesovic, V., 1998, "The viscosity of carbon dioxide," *J. Phys. Chem. Ref. Data*, **27**(1), pp. 31–44.
- [13] Vesovic, V., Wakeham, W. A., Olchoway, G. A., Sengers, J. V., Watson, J. T. R., and Millat, J., 1990, "The transport properties of carbon dioxide," *J. Phys. Chem. Ref. data*, **19**(3), pp. 763–808.
- [14] OpenCFD Ltd., 2016, "OpenFOAM v1612+."
- [15] Ducros, F., Nicoud, F., and Poinot, T., 1998, "Wall-adapting local eddy-viscosity models for simulations in complex geometries," *Numer. Methods Fluid Dyn. VI*, pp. 293–299.
- [16] Dong, Y. H., Lu, X. Y., and Zhuang, L. X., 2002, "An investigation of the Prandtl number effect on turbulent heat transfer in channel flows by large eddy simulation," *Acta Mech.*, **159**, pp. 39–51.
- [17] Celik, I. B., Ghia, U., Roache, P. J., Freitas, C. J., Coleman, H., and Raad, P. E., 2008, "Procedure for Estimation and Reporting of Uncertainty Due to Discretization in CFD Applications," *J. Fluids Eng.*, **130**(7), p. 78001.
- [18] Gnielinski, V., 1976, "New equations for heat and mass transfer in turbulent pipe and channel flow," *Int. Chem. Eng.*, **16**(2), pp. 359–368.