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Direct numerical simulation database for supercritical carbon dioxide

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The direct numerical simulation data is provided for pipe flow of supercritical CO_2. During this study, over 45 cases were simulated by means of DNS. This includes heating as well as cooling in the vertical orientation of tube. Table-1 and 2 give an overview of the DNS parameters. For heating, we performed DNS only for upward flow, where the heat transfer peculiarity has been reported earlier. These were conducted with 8 MPa and 8.8 MPa as inlet pressure (P_o), 288 K and 301 K as the inlet temperature (T_0) with 3 different diameters of the pipe. Three different heat fluxes were chosen to depict the low, mid and high heat flux for a given mass flux. For the cooling, all three possibilities (Upward, Downward and Forced i.e. with zero gravity) were simulated for 2 mm diameter pipe at two different pressures and two different heat flux.

Table-1: Simulation parameters for heating cases; Denoted as *"Sr. No.- Flow Direction (Diameter, Pressure, Temperature, Heat Flux)"*

Re_0= 5400 | L_h= 60D | T_0 = 288.15 and 301.15 K | P_0= 8 and 8.8 MPa | G = 30~230 kg/m2s					
1-U(2,8,301,10)	**2-**U(2,8,301,20)	**3-**U(2,8,301,30)	**4-**U(2,8,288,10)	**5-**U(2,8,288,20)	**6-**U(2,8,288,30)
7-U(2,8.8,301,10)	**8-**U(2,8.8,301,20)	**9-**U(2,8.8,301,30)	**10-**U(2,8.8,288,10)	**11-**U(2,8.8,288,20)	**12-**U(2,8.8,288,30)
13-U(5,8,301,5)	**14-**U(5,8,301,10)	**15-**U(5,8,301,20)	**16-**U(5,8,288,5)	**17-**U(5,8,288,10)	**18-**U(5,8,288,20)
19-U(5,8.8,301,5)	**20-**U(5,8.8,301,10)	**21-**U(5,8.8,301,20)	**22-**U(5,8.8,288,5)	**23-**U(5,8.8,288,10)	**24-**U(5,8.8,288,20)
25-U(10,8,301,5)	**26-**U(10,8,301,10)	**27-**U(10,8,301,20)	**28-**U(10,8,288,5)	**29-**U(10,8,288,10)	**30-**U(10,8,288,20)
31-U(10,8.8,301,5)	**32-**U(10,8.8,301,10)	**33-**U(10,8.8,301,20)	**34-**U(10,8.8,288,5)	**35-**U(10,8.8,288,10)	**36-**U(10,8.8,288,20)

Table-2: Simulation parameters for cooling cases; Denoted as *"Sr. No.- Flow Direction (Diameter, Pressure, Temperature, Heat Flux)"*

Re_0= 5400 | L_h= 30D | T_0 = 342.05 K | P_0= 8 and 8.8 MPa | G = 30~230 kg/m^2s					
37-U(2,8,342,-30)	**38-**D(2,8,342,-30)	**39-**F(2,8,342,-30)	**40-**U(2,8,342,-61)	**41-**D(2,8,342,-61)	**42-**F(2,8,342,-61)
43-U(2,8.8,342,-30)	**44-**D(2,8.8,342,-30)	**45-**F(2,8.8,342,-30)	**46-**U(2,8.8,342,-61)	**47-**D(2,8.8,342,-61)	

Throughout these DNSs, we rely on the low-Mach assumption, which is a valid assumption for sCO_2 under normal operating conditions. Following equations 1-3 shows the conservation of mass, momentum, and energy for presented DNS.

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$$\partial_t \rho + \nabla . (\rho u) = 0 \tag{1}$$

$$\partial_t (\rho u) + \nabla . (\rho u u) = -\nabla p + \nabla . (2\mu S) + B_f \tag{2}$$

$$\partial_t (\rho h) + \nabla . (\rho u h) = \nabla . (2\kappa \nabla \mathrm{T}) \tag{3}$$

In equations 1-3, ρ denotes the fluid density, u is the velocity vector, p is the pressure, μ represents the dynamic viscosity, h is the specific enthalpy, κ is the thermal conductivity and T denotes the temperature. The B_f is the body force due to gravity and its value is $[0, 0, \pm\rho g]^T$ and S represents the strain tensor. The thermophysical were implemented by a piecewise spline functions. These properties were derived from REFPROP and error-bound of the derived spline function and the NIST database was within ±1% for all thermophysical properties. Equations 1 to 3 were solved by finite volume method and such discretization schemes were used so that overall code has second-order accuracy in both space and time.

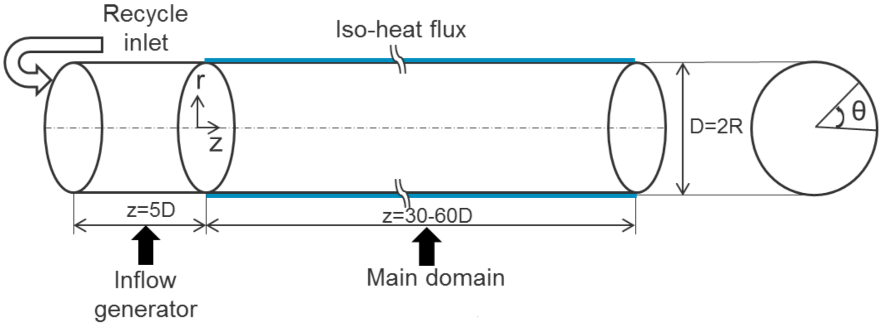

Figure 1: Computational domain for the DNS

The simulation domain consists of a tube of 2-10 mm diameter with a total length of 35 to 65 diameters as depicted in Fig. 1. In the main domain, the no-slip boundary condition is imposed at the wall while a convective outflow boundary condition is implemented for the velocity and other variables at the outlet. The distinction between upward and downward flow is made by changing the direction of gravity in the momentum equation while the distinction between forced and mixed convection is made by omitting or including the gravity term in the momentum equation. The cylindrical pipe is filled with the structured hexahedral mesh. Typically, DNS requires a huge amount of computational resource which resolves all the small-scale motions. Therefore, the grid resolution is reduced to 70×120×1500 for the main domain from the past work. From the grid independence study, we found that mean statistics (wall temperature and wall shear stress) have a negligible effect compared with very fine resolution (refer Appendix-B).

<u>Please cite/refer following work, if you use this data:</u>

- X. Chu, E. Laurien, Direct Numerical Simulation of Heated Turbulent Pipe Flow at Supercritical Pressure, ASME Journal of Nuclear Engineering and Radiation Science 2 (3) (2016).

- S. Pandey, X. Chu, E. Laurien, Investigation of in-tube cooling of carbon dioxide at supercritical pressure by means of direct numerical simulation, International Journal of Heat and Mass Transfer, 114 (2017), 944–957.

ACKNOWLEDGEMENTS

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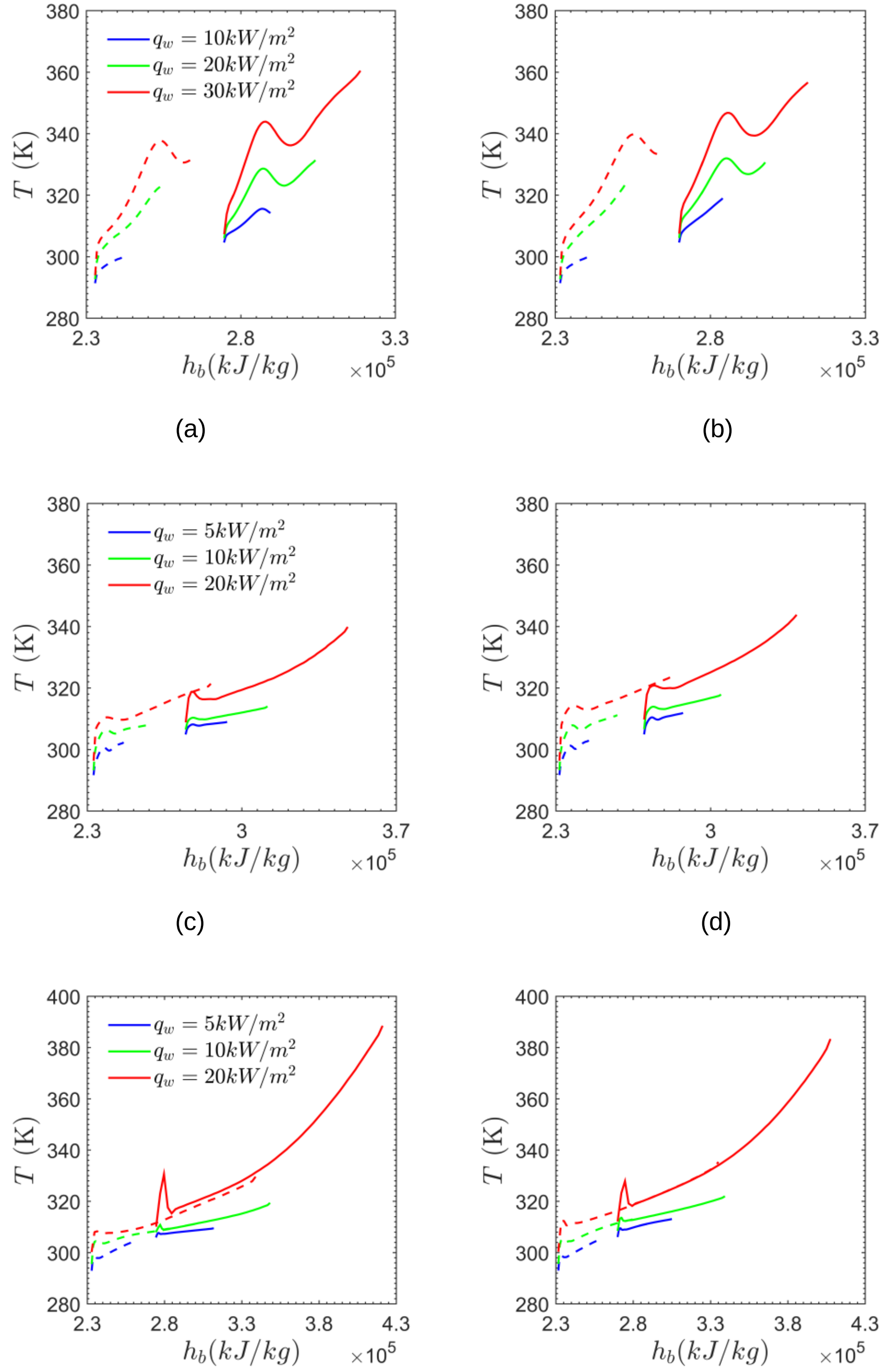
APPENDIX-A: Graphical representation of data

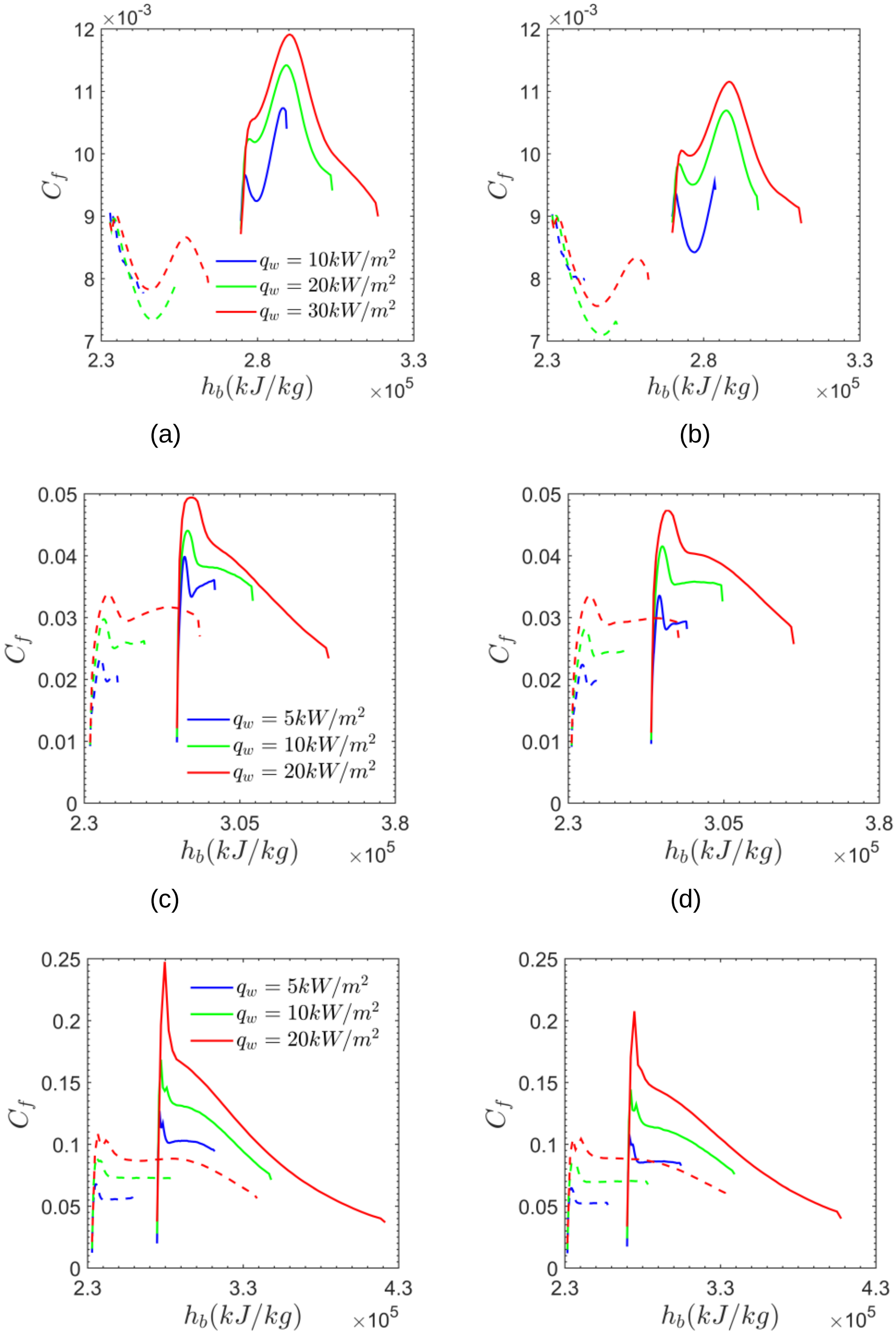


(a) (b)

(c) (d)

(e) (f)

Figure A.1: Variation of wall temperature; (a, b): *D*= 2mm, (c, d): *D*= 5 mm, and (e, f): *D*= 10 mm; first column= 8 MPa and second column 8.8 MPa; Dashed lines: T_0=288 K, solid lines: T_0=301 K (Case 1-36)



(a) (b)

(c) (d)

(e) (f)

Figure A.2: Variation of skin friction coefficient; (a, b): *D*= 2mm, (c, d): *D*= 5 mm, and (e, f): *D*= 10 mm; first column= 8 MPa and second column 8.8 MPa; Dashed lines: T_0=288 K, solid lines: T_0=301 K (Case 1-36)

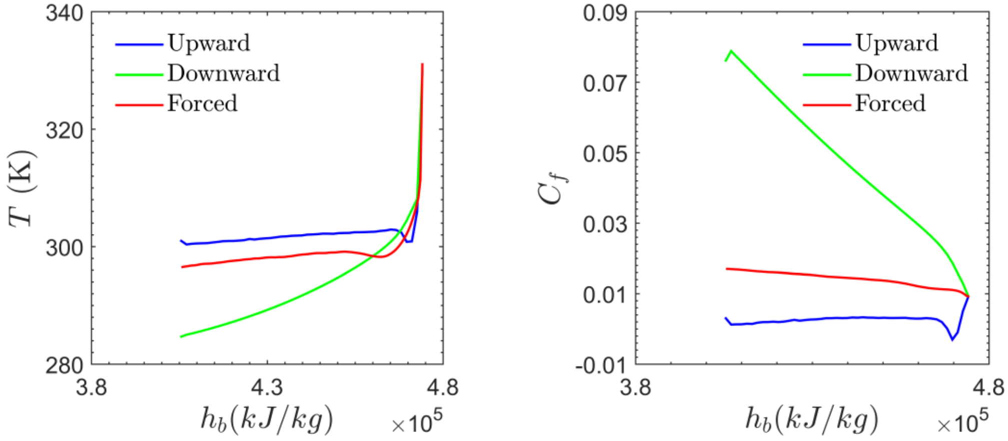


Figure A.3: Variation of: (a): wall temperature, (b): skin friction coefficient; *D*= 2 mm, P_0= 8 MPa, T_0= 342 K, *q*=-30.87 kW/m^2; Note: direction is right to left due to cooling (Case 37-39)

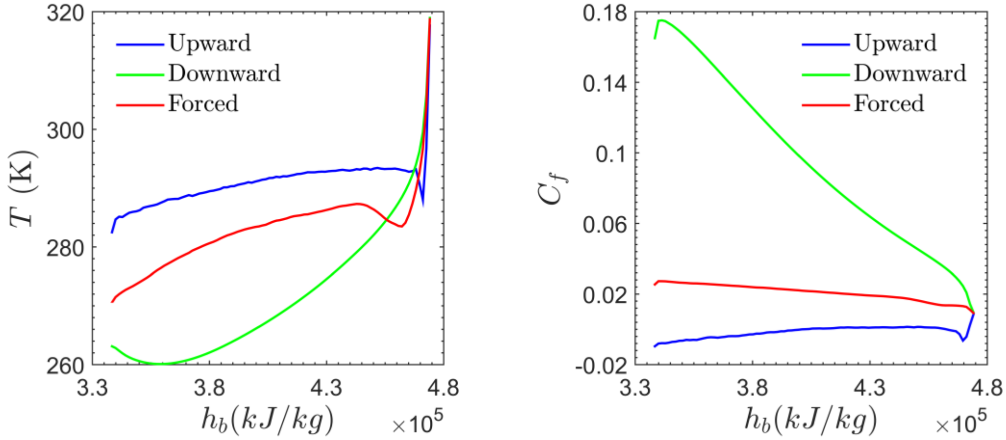


Figure A.4: Variation of: (a): wall temperature, (b): skin friction coefficient; *D*= 2 mm, P_0= 8 MPa, T_i= 342 K, *q*=-61.74 kW/m^2; Note: direction is right to left due to cooling (Case 40-42)

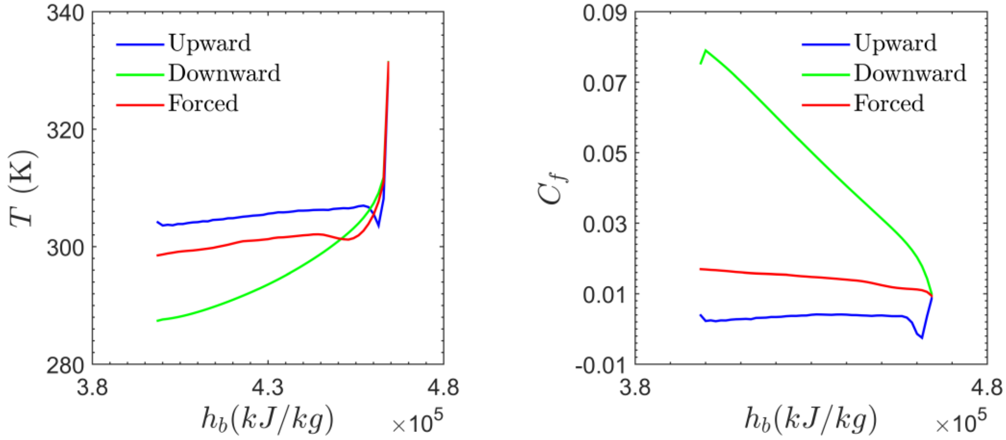


Figure A.5: Variation of: (a): wall temperature, (b): skin friction coefficient; *D*= 2 mm, P_0= 8.8 MPa, T_i= 342 K, *q*=-30.87 kW/m^2; Note: direction is right to left due to cooling (Case 43-45)

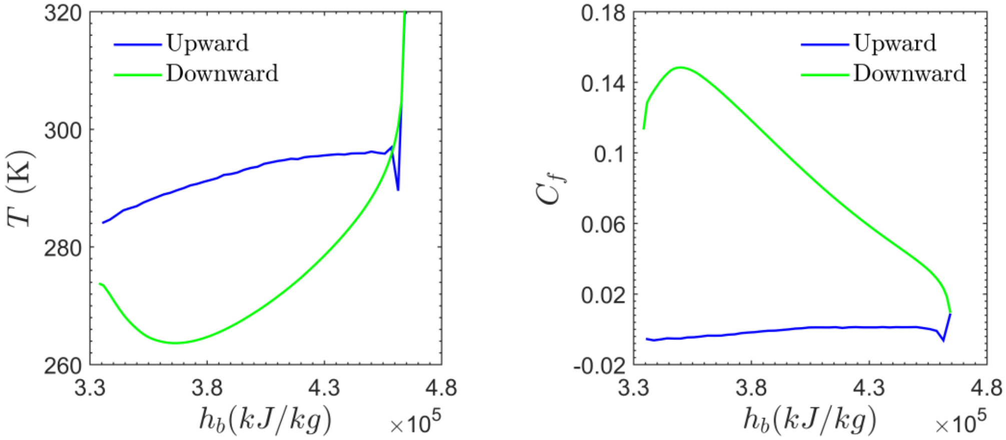


Figure A.6: Variation of: (a): wall temperature, (b): skin friction coefficient; D= 2 mm, P_0= 8.8 MPa, T_i= 342 K, q=-61.74 kW/m^2; Note: direction is right to left due to cooling (Case 46-47)

<u>APPENDIX-B</u>: Grid Independence results

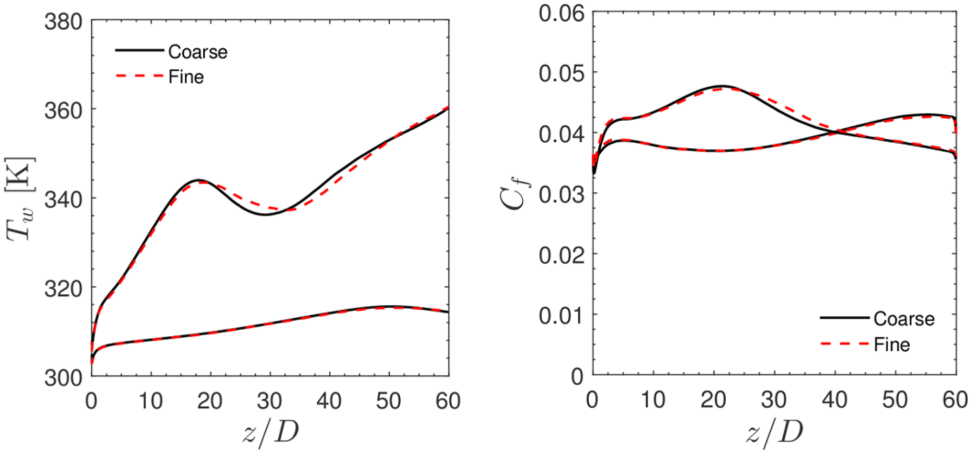


Figure A.7: Variation of; (a): wall temperature, (b): skin friction coefficient for case-1 and case-3

APPENDIX-C:

Following articles contain the detailed analysis of these data or related to this work:

- X. Chu, E. Laurien, Direct Numerical Simulation of Heated Turbulent Pipe Flow at Supercritical Pressure, ASME Journal of Nuclear Engineering and Radiation Science 2 (3) (2016)

- S. Pandey, X. Chu, E. Laurien, Investigation of in-tube cooling of carbon dioxide at supercritical pressure by means of direct numerical simulation, International Journal of Heat and Mass Transfer, 114 (2017)

- X. Chu, E. Laurien, Flow stratification in the horizontal pipe with heated supercritical CO2, The Journal of Supercritical Fluids, Vol. 116 (2016)

- X. Chu, E. Laurien, D. McEligot, Flow relaminarization of Strongly Heated Air Flow in a Pipe, International Journal of Heat and Mass Transfer Vol. 101 (2016)