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LARGE EDDY SIMULATION OF WALL-BOUNDED AND HEATED CO_2-FLOW IN AN ANNULUS AT SUPERCRITICAL CONDITIONS: FLOW DYNAMICS AND ENTROPY GENERATION

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ABSTRACT

A cryogenic turbulent stream of carbon dioxide at supercritical pressure ($sCO2$) which flows inside a heated concentric annulus is investigated by using a computationally efficient Large Eddy Simulation (LES) technique. The LES approach consists of a low-Mach number formulation combined with a tabulated look-up table method to calculate the thermo-physical properties. It is shown in the present study that such a LES approach is able to predict heat and fluid flow properties accurately under supercritical thermodynamic conditions as testified by comparison with DNS data. Furthermore, distinctive features of turbulent heat and fluid flow dynamics along with entropy generation mechanisms evolving in the heated $sCO2$ annulus flow are examined. Thereby, it turned out that the physics in supercritical annulus flow differs significantly to that found under subcritical conditions. In particular, (1) the flow is locally accelerated near the heated wall due to thermal expansion caused by pseudo-boiling effects, (2) peak values of the turbulent kinetic energy in the vicinity of the heated wall are damped during the pseudo-boiling process due to shear reduction, and (3) entropy is primarily generated in the vicinity of the wall during the pseudo-boiling process, which suggests that especially the design of the wall as well as the thermodynamic operating conditions are of profound importance for efficient use of energy in such heat/flow arrangements.

Introduction

It is well known that once operating a fluid at pressures and temperatures exceeding its critical point, the boundaries between the gas and liquid phases do not exist anymore and consequently surface tension vanishes. To work under such extreme thermodynamic conditions allows to increase the thermal efficiency of processes, to reach higher specific energy conversion rates and/or to enhance heat and mass transport. Supercritical carbon dioxide ($sCO2$) is proven to be a potential working fluid under such operating conditions, and due to its high thermal efficiency and minimal initial cost, it has become the preferred choice for advanced energy systems (Jackson (2013); Cheng *et al.* (2008)), like $sCO2$ heat pumps, supercritical-cooled nuclear reactors, etc., in which the unique thermo-hydraulic characteristics of supercritical fluids have undoubtedly become one of the relevant concerns (Lei *et al.* (2017)).

Since the 1960s, various numerical and experimental studies have been carried out in large devices or in microchannels to understand the heat transfer in $sCO2$ flowing tubes. Review papers are provided by Cabeza *et al.* (2017); Jackson (2013); Cheng *et al.* (2008), among others. Focused especially on numerical investigations, progress in computational resources and RANS modeling software led to an increased amount of contributions in supercritical convection simulations as recently reported by Lei *et al.* (2017); Lisboa *et al.* (2010). However, up to date, these efforts based on RANS modeling do not deliver comprehensively satisfactory results, especially in the case of predicted heat transfer coefficients.

In fact, due to the coupling of strongly varying thermo-physical properties of the fluid and the formation of complex flow structures in heating tubes, the flow and heat transfer in heating or cooling devices working under supercritical thermodynamic conditions feature more complex dynamics along with pseudo-boiling effects which are very difficult to correctly capture using RANS-based models (see in Ries *et al.* (2017*b*,*a*)). Furthermore, there is still no consensus on the effects of various parameters on the convective heat transfer, especially in cases with high heat flux/mass flux ratios (Lei *et al.* (2017)).

Despite the obvious shortcomings of RANS modeling in the case of complex supercritical flows, only very few large eddy simulation (LES) studies of turbulent $sCO2$ heat transfer in wall-bounded flows are reported in the literature. Recently Nabil & Rattner (2018) performed LES of turbulent $sCO2$ heat transfer in microchannels, where a Peng-Robinson equation of state has been used within a LES framework including WALE model (Nicoud & Ducros (1999)) to determine the subgrid-scale viscosity and thermal diffusivity. Regarding LES of supercritical turbulent pipe flow, Wang & Xu (2005) employed a compressible LES approach to study turbulent $sCO2$ pipe flow with constant wall heat flux at a moderate Reynolds number. In their LES study, the authors used the dynamic Smagorisky (Germano (1991); Lilly (1992)) and dynamic Prandtl number approaches (Moin *et al.* (1991); Lilly (1992)) to close the subgrid-scale viscosity and thermal diffusivity, respectively. Thermo-physical properties were calculated in their approach using a tabulated look-up table method generated by the PROPATH database (PROPATH (2001)). Even of great relevance, a wall-bounded and heated $sCO2$ in an annulus has not yet been investigated using LES which are able to advance understanding of supercritical fluid heat transfer in such configurations and subsequently to better support engineering tasks. To validate a suggested LES approach and to use this approach to analyze heat and fluid flow dynamics along with entropy generation mechanisms evolving in a heated $sCO2$ annulus flow represent the objectives of this paper.

The paper is organized as follows. First, the designed LES approach and thermodynamic modeling are introduced. Then, the numerical test case a cryogenic turbulent stream of carbon dioxide at supercritical pressure which flows inside a heated concentric annulus is described. Subsequently, LES results are presented and compared with available direct numerical simulation data from the literature. Finally, some concluding remarks close this paper.

LES approach for supercritical flows

In the present LES approach, a low-Mach number formulation suitable for incompressible Newtonian fluid flow ($Ma < 0.3$) with variable physical properties and Fourier heat transport is employed. For such flow conditions the balance equations of mass, momentum and sensible enthalpy can be formulated as

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}_i}{\partial x_i} = 0, \tag{1}$$

$$\frac{\partial \overline{\rho}\widetilde{u}_i}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}_i\widetilde{u}_j}{\partial x_j} = \frac{\partial \overline{\sigma}_{ij}}{\partial x_j} - \frac{\partial \overline{\rho}\tau_{ij}^{sgs}}{\partial x_j}, \tag{2}$$

$$\frac{\partial \overline{\rho}\widetilde{h}}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}_j\widetilde{h}}{\partial x_j} = -\frac{\partial \overline{q}_j}{\partial x_j} + \overline{\sigma}_{<ij>}\frac{\partial \widetilde{u}_i}{\partial x_j} - \frac{\partial \overline{\rho} q_j^{sgs}}{\partial x_j}, \tag{3}$$

where $\widetilde{(.)}$ are Favre-filtered quantities and $(.)^{sgs}$ denotes subgrid-scale quantities. ρ expresses the mass density, u_i the velocity, σ_{ij} the stress tensor, τ_{ij}^{sgs} the sgs stress tensor, q_j the heat flux vector and q_j^{sgs} the unresolved heat flux. Assuming Navier-Stokes-Fourier fluid as stated above, the stress tensor is modeled as

$$\overline{\sigma}_{ij} = \overline{\sigma}_{<ij>} - \overline{p}\delta_{ij} = \overline{\mu}\left(\frac{\partial \widetilde{u}_i}{\partial x_j} + \frac{\partial \widetilde{u}_j}{\partial x_i} - \frac{2}{3}\frac{\partial \widetilde{u}_k}{\partial x_k}\delta_{ij}\right) - \overline{p}\delta_{ij}, \tag{4}$$

where μ is the molecular viscosity and p is the pressure. The resolved heat flux is expressed by the Fourier's law for incompressible flow as

$$\overline{q}_j = -\overline{\lambda}\frac{\partial \widetilde{T}}{\partial x_j} = -\frac{\overline{\lambda}}{\overline{c_p}}\frac{\partial \widetilde{h}}{\partial x_j}, \tag{5}$$

where λ is the thermal conductivity and c_p the isobaric heat capacity of the fluid.

By using the low-Mach number assumption, the pressure p is further divided into a thermodynamic p^{th} and a mechanical p^{dyn} part. The density variations caused by the mechanical part are neglected. In this way, in contrast to a fully compressible formulation, pressure and density are formally decoupled by defining the density and all thermo-physical properties through constitutive equations expressed in terms of local temperature T and constant thermodynamic pressure p^{th}. Only the mechanical pressure part appears in the momentum equation. In terms of this, constitutive relations for ρ, μ, λ, c_p and h are required as function of local temperature and thermodynamic pressure, whereby it is essential to consider the non-ideal gas behavior of the fluid flow under supercritical conditions. This is often not an easy task in CFD, since accurate constitutive relations for supercritical conditions are usually computationally expensive and most often not applicable for all kind of substances. For these reasons, many researchers employed tabulated look-up table methods to evaluate the thermo-physical properties of the supercritical fluids during the simulation (see e.g. Kawai (2019); Bae *et al.* (2005*a*)), which is also applied in this work. Thereby, in the present low-Mach number approach, thermodynamic and fluid transport properties are first tabulated in a database for a given constant thermodynamic pressure p^{th} as a function of temperature T. Then, thermo-physical properties are evaluated locally during the simulation by means of linear interpolation.

In order to close the LES momentum and enthalpy equations, the unknown subrgrid-scale stress tensor τ_{ij}^{sgs} and the unresolved heat flux vector q_j^{sgs} have to be related to the resolved velocity and enthalpy fields, respectively. Regarding the modeling of subgrid-scale momentum transport, the wall-adapting linear eddy-viscosity model (WALE) proposed by Nicoud & Ducros (1999) is applied in this work in order to reproduce the correct flow behavior at solid walls. In terms of turbulent heat flux, the commonly used linear thermal diffusivity model with a constant subgrid-scale Prandtl number of $Pr_{sgs} = 1$ is applied.

The final LES equations are numerically solved using a merged PISO-SIMPLE algorithm (Issa (1985); Patankar & Spalding (1972)). This approach was added to the open-Source software OpenFOAM 2.4.0 and applied with a second order differencing scheme for all spatial derivatives, expect the enthalpy fluxes that are discretized by means of a second order minmod scheme (Roe (1986)) in order to ensure total variation diminishing of the solution. Regarding temporal discretization, second order backward integration is used for all time derivatives. Further details on the present numerical approach can be found in Ries *et al.* (2017*b*).

Numerical Test case

The numerical approach described in the previous section is used to perform LES of heated carbon dioxide flow at supercritical conditions in an annulus at $Re_b = 8900$ (based on the inlet bulk velocity and hydraulic diameter). An illustration of the annulus flow configuration is presented in figure 1, where an isometric view of half the annulus geometry (top) and a view along the flow direction x (bottom) are shown. δ denotes the channel half width of the concentric annulus, which is selected as $\delta = 0.5mm$ according to the reference DNS study of Bae *et al.* (2008).

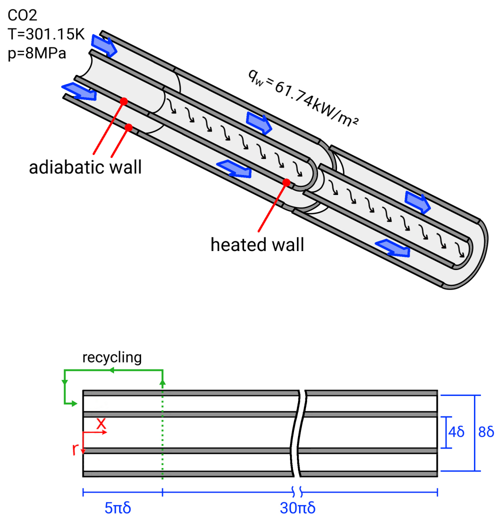
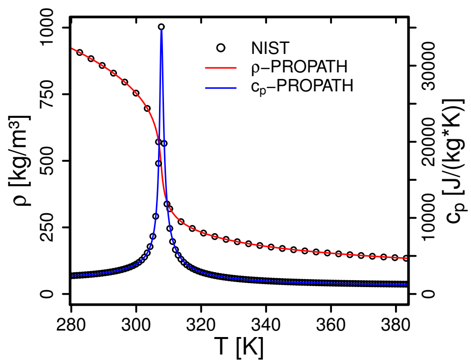


Figure 1: Schematic of the turbulent heated annulus flow at supercritical pressure. (top) isometric view; (bottom) view along x-axis.

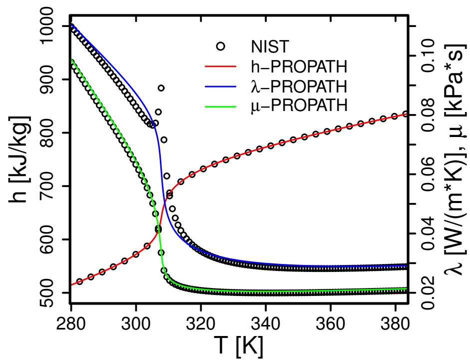
In the test case, a cryogenic fully-developed turbulent stream of carbon dioxide at supercritical pressure ($T = 301.15K < T_{crit}$, $p = p^{th} = 8MPa > p_{crit}$, $Re_b = 8900$) flows inside a concentric annulus with an inner-to-outer wall radius ratio of $r_i/r_o = 0.5$ and an hydraulic diameter of $D_h = 4\delta = 2mm$. After an entrance length of $5\pi\delta$ with adiabatic walls, the stream of carbon dioxide is heated up at the inner wall of the concentric annulus with a constant wall heat flux of $q_w = 61.74kW/m^2$. Due to the resulting temperature conditions $T_\infty < T_{crit} < T_w$, carbon dioxide cross its critical temperature within the thin boundary layer of the turbulent annulus flow and pseudo-boiling takes place. Thereby the density among other thermo-physical properties undergo a transition from a liquid-like to a vapor-like character while the fluid is subject to a strong acceleration in flow direction at the same time.

The computational domain applied in the LES study has a total length of $35\pi\delta$ and a height of 2δ. In accordance with the DNS of Bae *et al.* (2008), only one quarter sector of the fully cross section is considered for model evaluation. By doing so one could argue that the flow structures in the flow core as well as in the near-wall region are not captured correctly. However, about five circumferential integral length scales are resolved within the quarter sector of the fully cross section, while based on Shannon-Niquist theorem only two circumferential integral length scale are required. In order to perform a grid sensitivity analysis of LES results, three different block-structured numerical grids with 851760, 1752408 and 3412578 control volumes are employed in the validation study. The numerical grids are refined in the near-wall regions to ensure that the small turbulence scales and steep gradients of thermodynamic properties in the vicinity of the wall are fully resolved.

To be consistent with the DNS study, the thermodynamic database for the look-up table is generated by the computer program PROPATH (2001). A comparison of the generated thermodynamic table with reference data from NIST (2018) is provided in figure 2.



(a)



(b)

Figure 2: Comparison of the generated thermodynamic database from PROPATH (2001) with reference data from NIST (2018). (a) mass density ρ and isobaric heat capacity c_p; (b) specific sensible enthalpy h, thermal conductivity λ and molecular viscosity μ.

Apparently in figure 2, values of mass density, isobaric heat capacity and specific enthalpy generated by means of PROPATH (2001) are in excellent agreement with the reference dataset from NIST (2018). However, discrepancies appear in the case of predicted transport properties especially in the case of thermal conductivity. These discrepancies are most notable where the thermo-physical properties undergo a transition from liquid- to vapor-like character ($300K < T < 315K$) as well as at the region of dense fluid properties ($T < 300K$). Notwithstanding these discrepancies, the PROPATH (2001) database is used in the present study for the sake of consistency with the reference DNS study of Bae *et al.* (2008).

Regarding the boundary conditions, no-slip condition is set at the walls for each velocity component and zero Neumann condition for the mechanical pressure. At the heated wall, a constant heat flux condition is imposed as $q_w = \frac{\lambda}{c_p}\frac{\partial h}{\partial r}\big|_{r=2\delta} = 61.74kW/m^2$ and a zero temperature gradient condition is specified at the unheated walls. In order to obtain realistic inflow turbulence, the velocity field is extracted for each time step at the $x = 5\pi\delta$ plane downstream of the inlet and used to prescribe the velocity field at the inflow plane. At the outlet, a convective boundary condition is utilized for the velocity to maintain the overall mass conservation, while the kinematic pressure is set to a constant value. Periodic boundary conditions are used in the circumferential direction.

In order to avoid uncertainties caused by the initial solution, three flows through the domain are simulated before averaging is started. In addition, results from the coarse grid are used to initialize the velocity and enthalpy fields of the subsequent finer grids.

Results

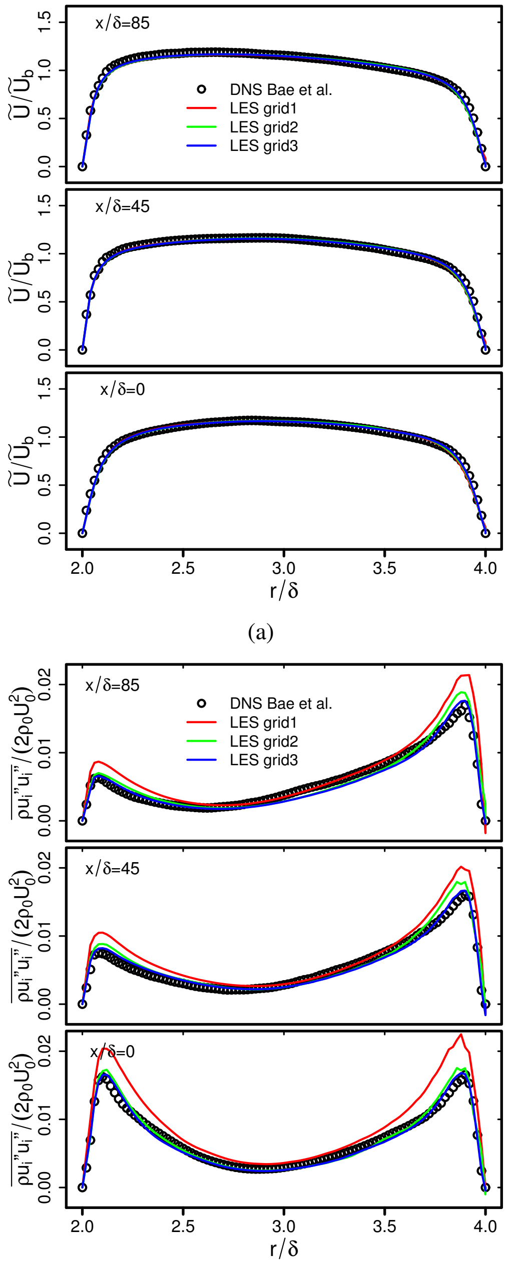
First the heat and fluid flow dynamics of the *sCO2* annulus flow is analyzed. In this context the applicability and accuracy of the present LES approach are evaluated. Then, irreversibilities evolving in such a flow arrangement is examined by using entropy generation analysis.

Heat and fluid flow dynamics

To start with the features of the flow field, figure 3 shows the evolution of (a) mean axial velocity and (b) turbulent kinetic energy profiles at various locations downstream ($x/\delta = 0, 45, 85$). Mean velocity profiles are normalized using the local bulk velocity U_b while profiles of the turbulent kinetic energy are normalized by means of the density ρ_0 and velocity U_0 at the inflow. The DNS data of Bae *et al.* (2005*b*, 2008) are utilized to evaluate the LES results.

Regarding mean velocity profiles, it can be clearly observed in figure 3 (a), that the flow is locally accelerated near the heated wall, due to thermal expansion caused by pseudo-boiling effects. This leads to asymmetric velocity profiles as the flow progresses downstream. Thereby, peak values of turbulent kinetic energy in the vicinity of the heated wall are damped (see figure 3 (b)), leading to a flow laminarization in this region. Both, asymmetric velocity profiles and damping of turbulent kinetic energy in the vicinity of the heated wall are well retrieved by the LES. This behavior is observed almost for all grid resolutions under consideration.

Next, the stream-wise turbulent heat fluxes obtained from the LES simulations are compared with DNS results at a stream-wise location of $x/\delta = 60$ in figure 4. Similar results are obtained at other locations and therefore not shown here. Turbulent axial heat fluxes are non-dimensionalized by the wall heat flux q_w.



(a)

(b)

Figure 3: Predicted radial profiles of (a) mean axial velocity and (b) turbulent kinetic energy at $x/\delta = 0, 25, 45, 65, 85$. Comparison of LES results with DNS data of Bae *et al.* (2005*b*, 2008).

As expected, axial turbulent heat fluxes are very high at the heated wall, peak in its vicinity and decrease rapidly away from it. Thereby, peak values of $\overline{\rho u_x'' h''}$ increase downstream. The physics of turbulent heat transfer are well retrieved by the LES. The observed results are very close to the DNS data with slight influence of the spatial resolution.

To close the evaluation study and analysis of distinctive heat and fluid flow features in the sCO_2 annulus flow, the distributions of predicted local Nusselt numbers along the heated inner wall of the annulus flow are compared with DNS in figure 5. Thereby the local Nusselt number is calculated as $Nu = h_i D_h/\lambda_0$, where h_i is the convective heat transfer coefficient at the heated wall.

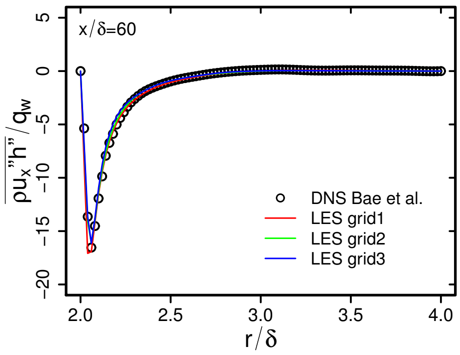


Figure 4: Comparison of axial turbulent heat fluxes with DNS results of Bae *et al.* (2008, 2005*b*) at $x/\delta = 60$. Values are normalized by the wall heat flux q_w.

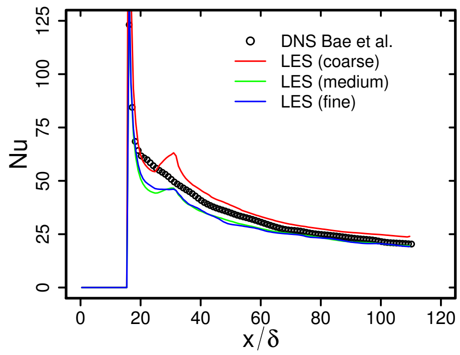


Figure 5: Distributions of local Nusselt number along the heated inner wall. Comparison of LES predictions with DNS data of Bae *et al.* (2008, 2005*b*).

As it can be seen in figure 5, the distributions of local Nusselt number show similar trend to the reference DNS dataset. However, discrepancies in the Nusselt number occur in the range of $20 < x/\delta < 60$. Following the error analysis procedure described in Ries *et al.* (2018), it appears that the normalized mean absolute error (nMAE) between LES and DNS is $nMAE \sim 13\%$ within the range of $20 < x/\delta < 60$ for the medium grid resolution. Further downstream ($x/\delta > 60$), this error metrics decreases significantly to $nMAE \sim 3\%$. However, the relatively high value of $nMAE$ at $20 < x/\delta < 60$ remains unclear since it can not be attributed to the limitations of spatial resolution due to a similar $nMAE$ value obtained for the finer grid resolution. Nevertheless, the overall physics are well reproduced by the LES. Thus, it can be concluded that the designed LES approach is appropriate to describe turbulent wall-bounded flows with heat transport and variable thermo-physical properties under supercritical thermodynamic conditions, suggesting its applicability for further numerical investigations such as entropy generation analysis as presented next.

Entropy generation analysis

After analyzing heat and fluid flow dynamics occurring in the *sCO2* annulus flow and establishing the applicability of the present LES approach, entropy generation analysis is performed next in order to identify and quantify irreversibilities in such flow arrangements. Thermodynamic irreversibilities in thermo-fluid systems manifests itself as a loss of degree of freedom in the description of the material behavior, as well as the turbulence structure of the flow in the fluid (Sadiki & Hutter (2000)). Based on the second law of thermodynamics, such irreversibilities cause a degradation of available energy into internal energy in the working fluid leading to an increase of entropy in the system, which is called entropy generation, and are responsible for the reduction of thermodynamic efficiency of a system (Keenan (1951); Bejan (1995)). In the present work, entropy generation analysis in the framework of LES is performed using the approach proposed by Ries *et al.* (2019), which allows calculation of local entropy generation rates including the effect of unresolved subgrid-scale irreversibilities in a simple post-processing step.

Figure 6 shows the predicted evolution of Favre-averaged entropy production rates due to viscous dissipation Π_v and heat conduction Π_q at various locations in the vicinity of the heated wall.

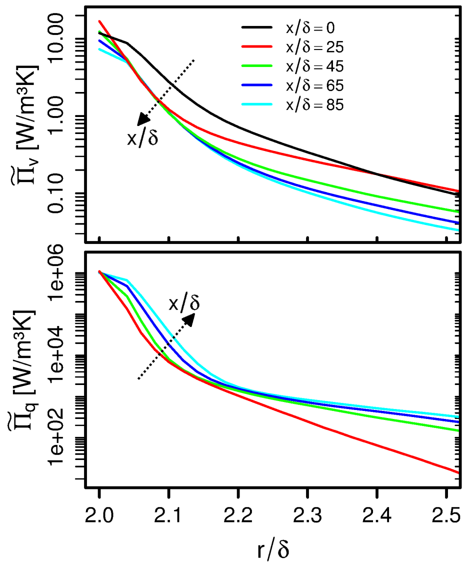


Figure 6: Favre-averaged entropy production rates by viscous dissipation Π_v and heat conduction Π_q at various locations in the vicinity of the heated wall.

It can be clearly seen in figure 6 that both, entropy production by viscous dissipation Π_v and heat conduction Π_q, are predominantly limited to the near wall region, due to steep velocity and temperature gradients. Thereby, it is interesting to observe that Π_v decreases as the flow progresses downstream, which can be directly attributed to a shear reduction process induced by pseudo-boiling effects. This shear reduction leads to a damping of peak values of turbulent kinetic energy in the vicinity of the wall and finally to a laminarization of the flow. In contrast, Π_q increases with increasing x/δ because of additional mixing and steepen temperature gradient induced by the state transition of the fluid from liquid- to gas-like character. Furthermore, it can be observed in figure 6 that entropy is primarily generated by heat transfer and pseudo-boiling effects rather than viscous dissipation. This suggests that especially the thermodynamic operating conditions are of profound importance for effective use of energy in such heat/flow arrangements.

Conclusion

Large eddy simulation of a cryogenic fully-developed turbulent stream of carbon dioxide at supercritical pressure that flows inside a heated concentric annulus was conducted. Thereby, a low Mach-number formulation for the flow field combined with a look-up table method to calculate thermo-physical properties were applied in order to analyze heat and fluid flow dynamics along with entropy generation mechanisms in such flows.

Some important conclusions from this study concerning LES modeling strategies, heat and fluid flow dynamics, and entropy generation mechanisms for flows under supercritical conditions can be outlined as follows:

- A low Mach-number formulation for the flow field combined with a look-up table method to calculate thermo-physical properties proved to be a promising approach for LES of wall-bounded and heated flows at supercritical thermodynamic conditions and low Mach-numbers as testified by comparison with DNS data.
- It turned out that the heat and fluid flow dynamics in supercritical heated annulus flow differs significantly from that found under subcritical conditions. The fluid is locally accelerated near the heated wall due to thermal expansion, while at the same time shear is reduced and peak values of turbulent kinetic energy are damped.
- Using second law analysis it appears that in particular the heated wall acts as a strong source of irreversibilities. Thereby, entropy production by heat conduction overwhelms viscous dissipation effects. This suggests that especially the design of the heated wall as well as the thermodynamic operating conditions are of profound importance for efficient use of energy in such heat/flow arrangements.

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