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The effect of pressure on transcritical jets: a DNS study

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Abstract

In this study, a state of the art direct numerical simulations (DNS) dataset is employed to investigate the impact of pressure on turbulent, transcritical jets. Although being characterized by the same Reynolds number, transcritical jets at different pressure show some differences. At large scales, as pressure approaches near critical values, a narrower mean pseudo-boiling region is observed as well as a delayed complete mixing of the jet. At small scale, pseudo-boiling is shown to cause, by means of localized high density gradients, a different behavior in the dissipation range of the turbulent kinetic energy spectrum.

1. Introduction

The operating condition of Liquid Rocket Engines (LRE) thrust chambers are characterized by elevated pressures which allow to have compact geometrical size of the devices and high specific impulse. As a consequence, the injection process, which is responsible of mixing and combustion of the propellants can occur under super-critical pressure conditions. Under these severe thermodynamic conditions, the injection temperature of the reactants can be below their pseudo-boiling temperature[3] and thus in a transcritical thermodynamic state. Such conditions lead to significant deviations from the ideal gas behavior,[31] resulting in many challenging experimental and numerical/theoretical issues for the investigation and modeling of LRE-injection.[17]

Transcritical flows have been largely experimentally investigated[4,5,7,16,18,19,25] mainly showing that the overall mixing process is significantly influenced by the thermodynamic non-linearities occurring in the pseudo-boiling temperature range. However, given the extreme thermodynamic conditions encountered by these experiments, the fidelity of the results is still difficult to be assessed.[1] In this context, direct numerical simulations (DNS) represent a fundamental tool for studying transcritical flows since it allows for a systematic statistical description of both large and small scale of the turbulent flow.

In the past years the availability of high performance computing (HPC) has enabled a number of studies based on DNS and thus prompting the generation of relevant DNS datasets. However, due to their thermodynamic complexity, DNS data on transcritical mixing remain scarse and limited to low to moderate Reynolds numbers. Three dimensional, transcritical flow was investigated by Tani et al.[27] in a mixing layer configuration while recent efforts have been devoted to planar jets and in particular to their mixing,[11] turbulent pseudo-boiling[9] and averaging procedure.[12] Round-jets were also investigated in a three dimensional setting by Ries et al.[23] observing that turbulent diffusion dominates the turbulent kinetic energy budget.

In the present contribution, we employ a recently developed DNS dataset[13] in order to investigate the effect of pressure on turbulent, transcritical jets. The direct simulations have been carried out using a reference equation of state (EoS) for nitrogen together with accurate thermodynamic and transport properties. This thermodynamic modeling has been used in conjunction with a high order numerical framework based on the spectral element method (SEM) allowing a proper resolution of the small scale interactions between turbulence and the thermodynamic non-linearities induced by the pseudo-boiling phenomenon. This contribution is organized as follows. Firstly, the dataset and the main flow features are briefly summarized. Secondly, the low-Mach number conditions are assed through a detailed a-posteriori analysis of the numerical results. Finally the impact of pressure on both the mean field and fluctuations of the fluid velocity and density are investigated.

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2. DNS dataset

In this work we use the dataset presented in[13] to which the reader is referred for a comprehensive description. The DNS have been carried out using high-order methods in order to correctly resolve the complex thermodynamic behavior and small scale stratification of transcritical flows. In order to perform such simulations, a low-Mach number version[11] of the massively parallel, spectral element method (SEM)-based CFD code `nek5000`[6] has been used. Thermodynamic and transport properties are evaluated using NIST software `refprop`, which implements a reference EoS for nitrogen developed by Span et al.[26] and transport properties taken from the work of Lemmon and Jacobsen.[14] Such approach is known to increase the overall thermodynamic modeling accuracy compared to the standard approaches employing cubic EoS with two- or three-parameters.[2,8,10]

As a results, the highly non-linear behavior and peculiar characteristics of transcritical fluids in near critical conditions are expected to be correctly captured by the high-order discretization obtained with SEM[21] coupled with the elevated accuracy of `refprop`. In addition, the adoption of a low Mach number approximation has prevent the occurrence of spurious pressure oscillations caused by the transcritical conditions, retaining by construction the mechanical equilibrium of pressure across the pseudo-boiling transition.[15,20,22,24,28–30]

Table 1: Summary of the main physical and computational parameters used for the 4 DNS of transcritical temporally evolving jets at different pressures. The initial jet Reynolds number $Re_{jet} = 3000$ and jet width $H = 2$ mm are kept constant for all the cases.

Simulation label	**R2P1**	**R2P2**	**R2P3**	**R2P4**
Reduced pressure p_0/p_{cr}	1.25	1.5	2.0	3.0
Initial mean shear ΔU_{jet} (m/s)	0.089	0.091	0.093	0.098
Reference viscosity ν_{ref} (m/s^2)	$5.95 \cdot 10^{-8}$	$6.05 \cdot 10^{-8}$	$6.22 \cdot 10^{-8}$	$6.50 \cdot 10^{-8}$
Density ratio ρ_{jet}/ρ_{env} (-)	14.82	12.42	9.43	6.45
Max Prandtl number Pr_{max} (-)	5.74	3.47	2.28	1.67
SEM grid $(E_x \times E_y \times Ez)N^3$	291Mill	139Mill	72Mill	46Mill

The DNS configuration used is a temporally evolving, planar jet initially characterized by $Re_{jet} = \Delta UH/\nu_{ref} = 3000$, being ΔU the mean shear, $H = 2$ mm the jet width and ν_{ref} the minimum viscosity across the mixing layers. The configuration and initial conditions are consistent with previous studies[11] and different background pressures are investigated, namely $p_0/p_{cr} = 1.25, 1.5, 2.0, 3.0$ where p_{cr} is the nitrogen critical pressure. The basic parameters are listed in Table 1.

3. Results

3.1 Flowfields overview

Recent studies[11] have shed light on the structural differences in the jet development and mixing between transcritical and supercritical jets. It has been shown that transcritical jets share some similarities with liquid jets in a gaseous environment while supercritical jets closely resemble gas-gas mixing. The DNS data used in this work highlight a different aspect of this, by varying the pressure and keeping the jet temperature in the transcritical range $T_{jet} < T_{pb}$ being T_{pb} the isobaric pseudo-boiling temperature. In fact, as the pressure increases from $p_0/p_{cr} = 1.25$ of the R2P1 case to $p_0/p_{cr} = 3.0$ in the R2P4 case, the pseudo-boiling is smeared over a wider range of temperature and therefore limiting its impact on the jet development. As a result, transcritical jets characterized by elevated reduced pressure, thus far from pseudo-boiling and the ensuing near critical enhancement, will behave similarly to a supercritical jet at a lower pressure.

These considerations are confirmed by Fig. 1 which shows instantaneous temperature field realizations of the 4 four jets of the DNS dataset. In particular, it is of interest to notice the differences between the near critical case R2P1 and the largely supercritical case R2P4.

3.2 Low-Mach number conditions

As previously mentioned the DNS database has been generated using a low-Mach number approach, therefore in this section we assess the low-Mach conditions by means of a-posteriori analysis. In order to asses that the conditions are

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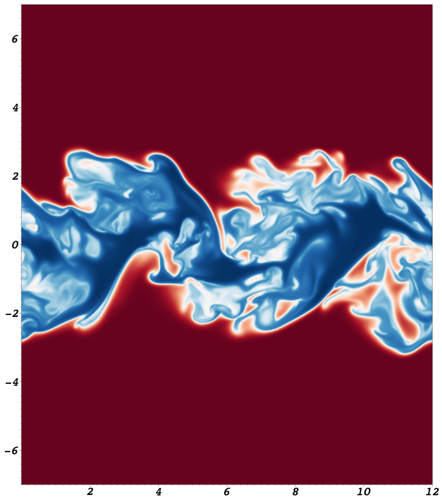
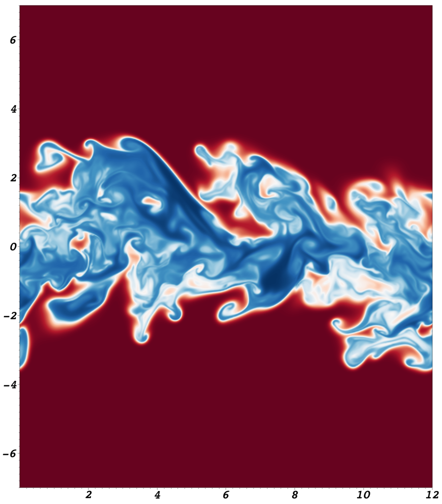
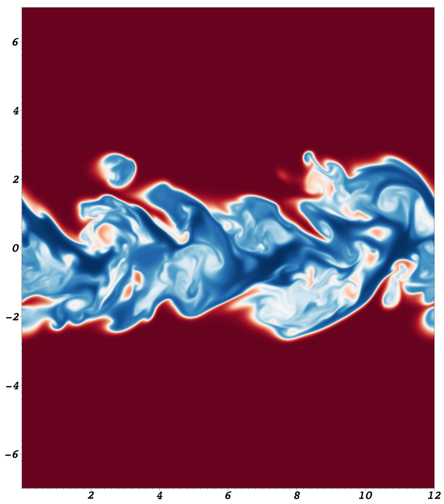


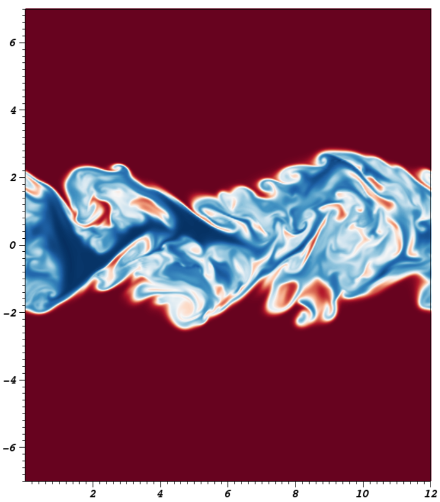
(a) p_0/p_{cr}=1.25, R2P1



(b) p_0/p_{cr}=1.50, R2P2



(c) p_0/p_{cr}=2.00, R2P3



(d) p_0/p_{cr}=3.00, R2P4

Figure 1: Instantaneous temperature field visualization of the DNS database using a spanwise cut of the 3D domain. The color coding varies from blue (T = 120 K) to dark red (T = 300 K).

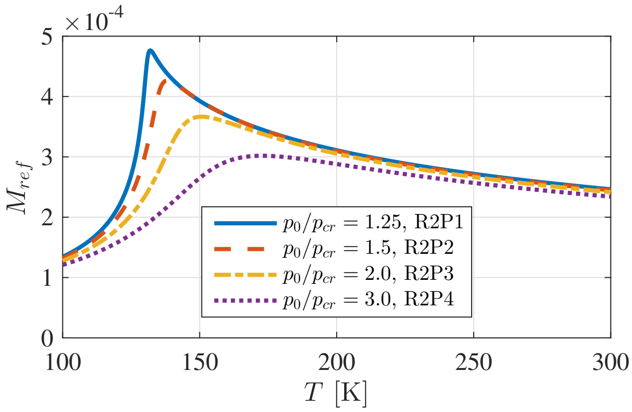


Figure 2: Reference Mach number as a function of temperature.

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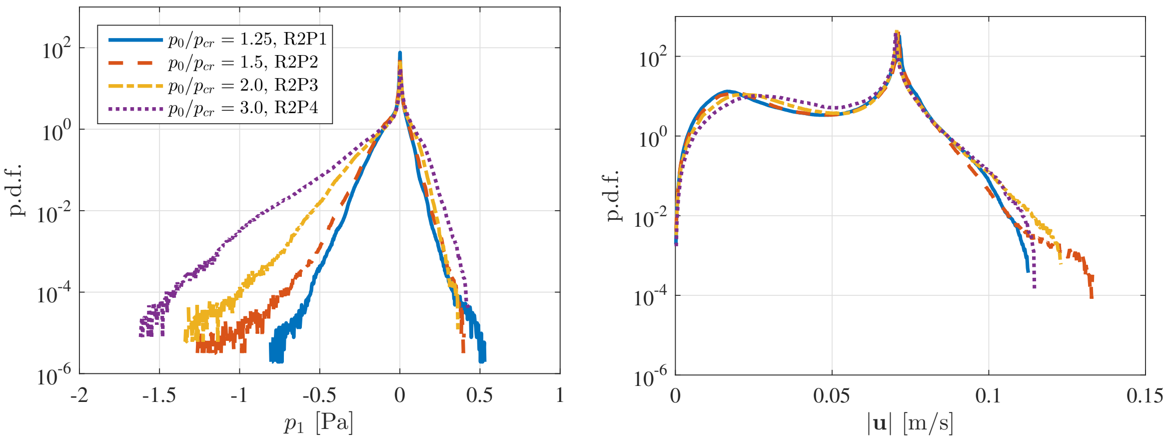

(a) Hydrodynamic pressure (b) Velocity magnitude

Figure 3: Probability density functions of hydrodynamic pressure and velocity magnitude at the reference time.

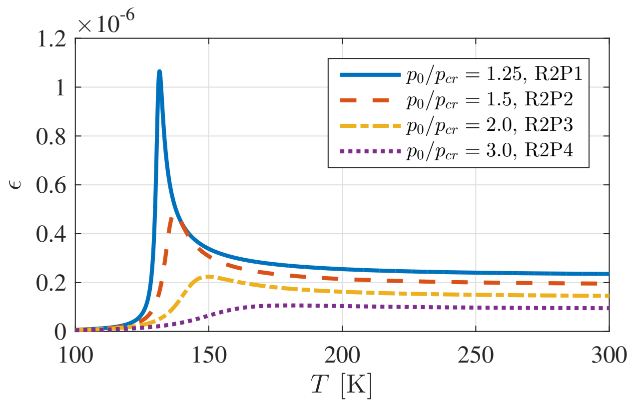

Figure 4: Error in the evaluation of density due to local hydrodynamic pressure variations.

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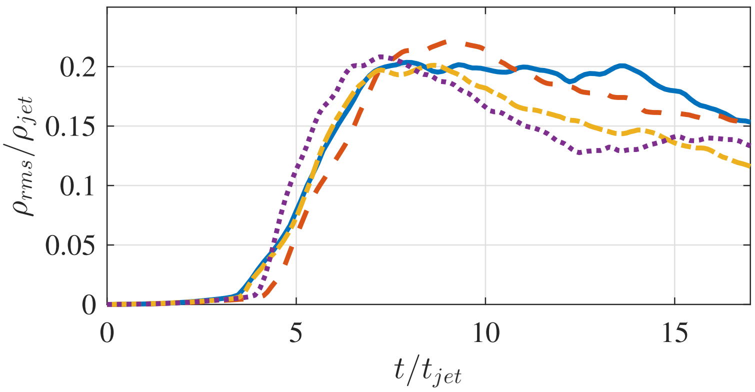

Figure 5: Density rms normalized by the cold jet density as a function of time for the present study.

effectively low-Mach, i.e. negligible effect of local hydrodynamic pressure variations on the density, we can define a reference Mach number as $M_{ref} = \Delta U/a$ based on the velocity difference between the jet and the environment and on the speed of sound at p_0 as shown in Fig. 2. Note that local velocities greater than ΔU are hardly experienced in any of the four simulations as clearly observable in panel (b) of Fig. 3 in which the p.d.f. of the velocity magnitude is shown. As a result, we can consider the definition of M_{ref} amply conservative.

The hydrodynamic (or perturbation) pressure p_1 can be denoted as $p_1(x,t) = p(x,t) - p_0(t)$, where $p(x,t)$ is the pressure field and $p_0(t)$ the uniform background pressure, which is constant in the open domain considered. Such hydrodynamic pressure is an $O(M^2)$ deviation from the background pressure so that $p_1/p_0 = O(M^2)$. Panel (a) of Fig. 3 displays the pdfs of the computed p_1, showing the extremely limited range of hydrodynamic pressures as expected from the low Mach numbers at play. Indeed, a reference pressure disturbance can be estimated as $\delta p \approx p_0 \max(M^2_{ref})$, based on the maximum reference Mach number. We obtain for R2P1 case $\delta p \approx 0.964 \cdot 10^{-5}$ bar, for R2P2 case $\delta p \approx 0.927 \cdot 10^{-5}$ bar, for R2P3 case $\delta p \approx 0.9125 \cdot 10^{-5}$ bar and for R2P4 case $\delta p \approx 0.928 \cdot 10^{-5}$ bar. These pressure perturbations are largely insufficient to influence the property evaluation in any significant way, so that $\phi(h; p_0) \approx \phi(h; p_0 \pm \delta p)$. In order to confirm this consideration, we can define an error in the density evaluation as a function of h, or equivalently of T, as $\epsilon(h) = |\rho(h; p_0) - \rho(h; p_0 \pm \delta p)|/\rho(h; p_0))$. By using this definition we obtain, maximum error for each case as follows: $\max(\epsilon(h)) \sim 1.065 \cdot 10^{-6}$ for case R2P1, $\max(\epsilon(h)) \sim 0.485 \cdot 10^{-6}$ for case R2P2, $\max(\epsilon(h)) \sim 0.224 \cdot 10^{-6}$ for case R2P3 and $\max(\epsilon(h)) \sim 0.107 \cdot 10^{-6}$ for case R2P4. Such error is shown in Fig. 4 as a function of T for the four pressure considered where is clearly observable that its value is on the order of 10^{-6} confirming its negligibility. Although negligible, it of interest to notice that the major discrepancies can be observed at near-critical pressure and in the pseudo-boiling region.

Finally, it is important to remark that the configuration and parameters have been intentionally chosen in order to achieve extremely small Ma numbers. Indeed, considering the definition of the Reynolds number, $Re_{jet} = \Delta U H/\nu_{ref}$, while the viscosity is fixed by the thermodynamic conditions, ΔU and H can be chosen such that Ma is sufficiently low (e.g. $Ma << 0.3$ being 0.3 the classical low-Mach threshold) and the simulation will scale accordingly. In particular, lower Ma numbers can be obtained by lowering ΔU and increasing H since the speed of sound a, similarly to ν, is determined only by the thermodynamic conditions.

3.3 Jet evolution

As mentioned in the introduction of the manuscript, DNS data of transcritical shear flows are quite limited. Similar cases in the literature are our previous works of transcritical jets[11] and the recent work by Ries et al.[23] The latter study, however, is devoted to a round jet at $Re \sim 5000$ and, therefore not directly comparable to the presented dataset. However, a as shown in Fig. 5 similar trends are qualitatively observable for the transcritical jets investigated in the present study. In particular, after the jet breakup and the generation of three dimensional transitional turbulence, as pressure increases the density fluctuations tend to decrease. In fact, only under near-critical conditions the density fluctuations profile remain rather flat after the jet jet break-up around $t/t_{jet} \sim 7$.

The overall behavior of the jets, previously described using instantaneous realizations of temperature (see Fig. 1), is here discussed using Reynolds averages of the streamwise velocity component as shown in Fig. 6. In such figure the pseudo-boiling region is evidenced by means of characteristic temperature isolines[9] highlighting that, as the pressure increases, the jet's averaged liquid-like core is pseudo-boiled faster. In fact, the largely supercritical case R2P4 show

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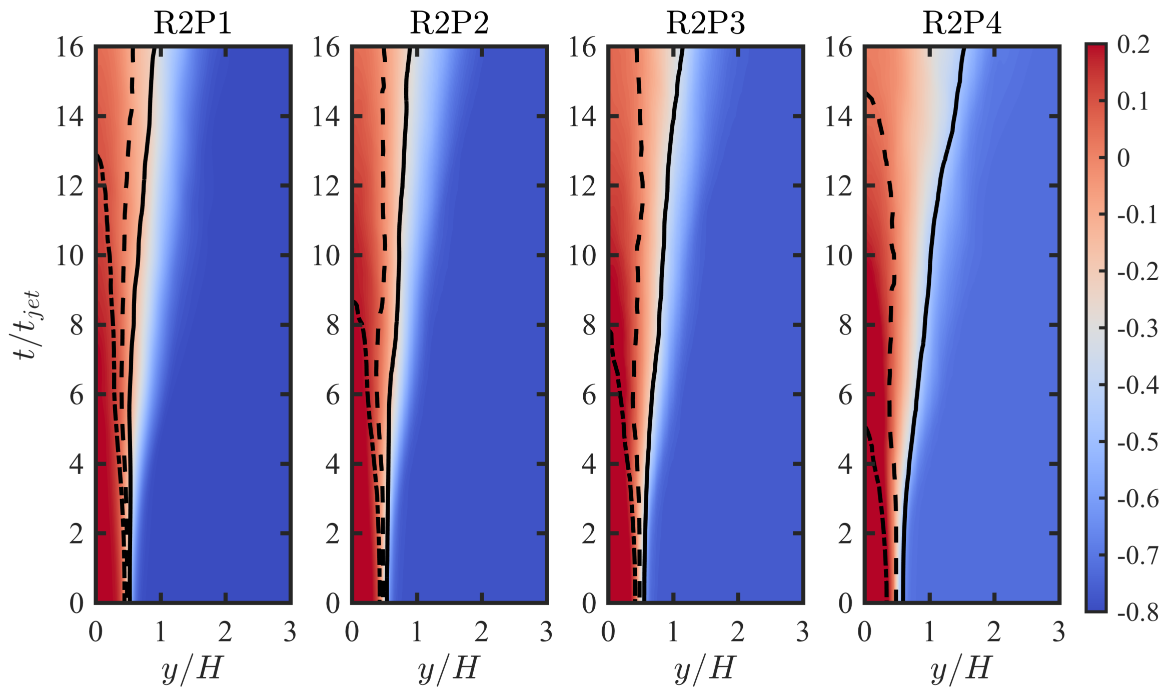

Figure 6: Reynolds averages of the streamwise velocity component with superimposed isolines of temperature evidencing the pseudo-boiling region namely $\overline{T}^{-}$ (dashed dotted line), $\overline{T}_{pb}$ (dashed line) and $\overline{T}^{+}$ (continuos line) as defined in.[9]

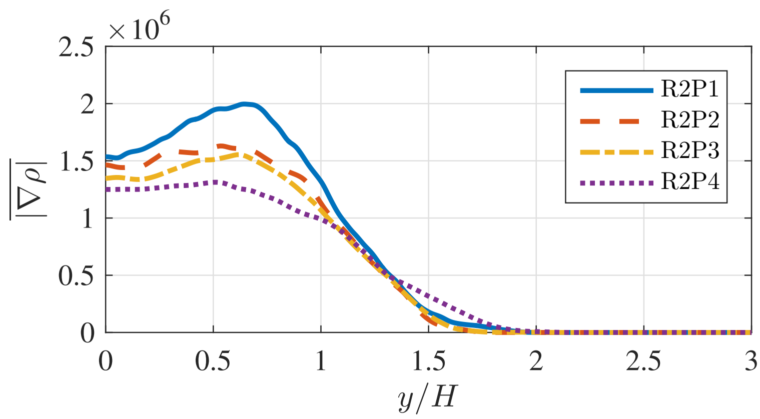

Figure 7: Density rms normalized by the cold jet density as a function of time for the present study (temporally evolving jet, panel a) and as a function of axial distance (spatially evolving jet, panel b) for the work of Ries et al.[23]

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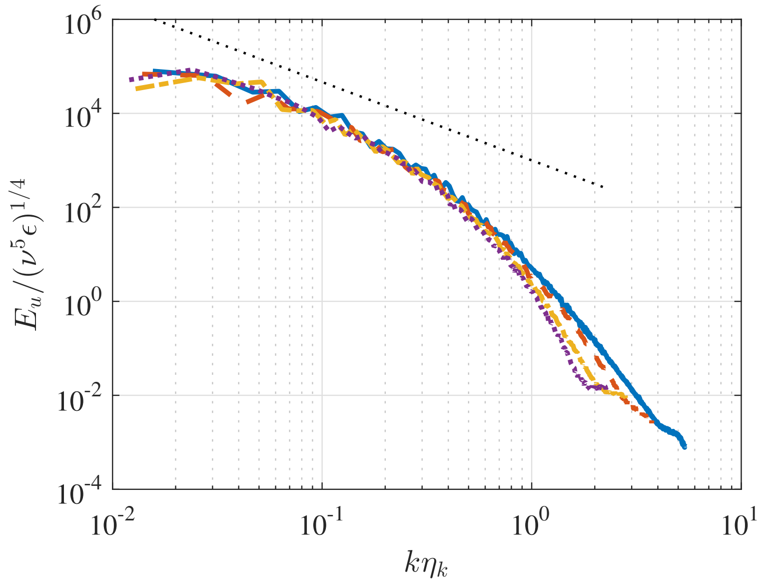

Figure 8: Auto-spectra of the streamwise velocity component scaled using Kolmogorov units calculated at $t/t_{jet} = 12$ and $y/H = 0$. The black dashed line represents the classical $-5/3$ slope. The line legend follows from the previous plots of the manuscript.

the shortest liquid-like jet core while R2P1 the longer one. This behavior can be directly attributed to the so called *solid-wall* effect, which is caused by the elevated density stratification in transcritical flows at near critical conditions[32] such as those encountered by the R2P1 simulation.[13] The density stratification modify the development of large scale Kelvin-Helmholtz instability (KH) altering the mixing layers dynamics, reducing the velocity fluctuations in the crosswise direction and amplifying the fluctuations in the streamwise direction.

Figure 7 shows the averaged magnitude of the density gradient for the 4 jets considered at $t/t_{jet} = 12$, the same reference time investigated in.[13] In the mixing layer region, the entity of such gradient increases as the pressure approaches near critical conditions confirming the previous observations. Moreover it can be seen as a direct impact of pseudo-boiling on the mean field and on the large scale of the motion. Conversely, at small scale pseudo-boiling is expected to influence the dissipative scales by means of the baroclinic vorticity generation. The latter phenomena is caused by the high density gradients regions, which are thin interfaces that effectively act as localized sources of vorticity. This behavior is further confirmed by the one dimensional auto-spectra of the streamwise component of the fluid velocity as shown in Fig. 8. In fact, in the dissipative range some discrepancies between the iso-Reynolds jets at different pressure can be observed even if a consistent scaling using Kolmogorov units has been applied. In particular, different slopes at small scales are present although the auto-spectra have been calculated at the same time instant and crosswise location.

4. Conclusion

A recently developed DNS dataset[13] has been used in the present contribution to investigate the effect of pressure on turbulent, transcritical jets. The data have been obtained using high fidelity thermodynamic modeling in conjunction with a high order numerical framework based on the spectral element method (SEM). This results in a proper resolution of the small scale interactions between turbulence and the thermodynamic non-linearities induced by the pseudo-boiling phenomenon.

The impact of pressure on the main flow features have been discussed by inspecting the instantaneous realizations of the temperature fields. It has been assessed that transcritical jets characterized by elevated reduced pressure will behave similarly to supercritical jets at a lower pressure. Pressure effects have been also discussed in terms of its effect on the low-Mach number conditions of the flow. A detailed analysis has shown that all the 4 jets of the employed database are effectively under low-mach number conditions and thus the local hydrodynamic pressure has a negligible effect on the thermodynamic properties evaluation. Finally, the effect of pressure at both large and small scale of the flow is investigated. At large scale, it has been shown that, as pressure approaches near critical conditions (see R2P1 case) the averaged pseudo-boiling region remain narrower delaying the complete mixing of the jet. On the other hand,

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at small scale different slopes of the streamwise velocity autospectra in the dissipation range has been observed and attributed to the local density gradients caused by pseudo-boiling.

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