On thermodynamic small scales in transcritical turbulent jets

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Nomenclature

C_p	=	constant pressure heat capacity, [J/kgK]
E_{1D}	=	one-dimensional turbulence energy spectrum, [m^3/s^2]
h	=	enthalpy [J/kg]
p	=	pressure, [Pa]
Pr	=	Prandtl number, [-]
Re	=	Reynolds number, [-]
T	=	temperature, [K]
δ	=	layer thickness, [m]
ν	=	kinematic viscosity, [m^2]
ρ	=	density, [kg/m^3]
ξ	=	mixing variable, [-]
χ	=	scalar dissipation rate, [s^{-1}]

Subscripts

env	=	environment
jet	=	jet
pb	=	pseudo-boiling
ref	=	reference
$+$	=	gas-like
$-$	=	liquid-like

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I. Introduction

Transcritical thermodynamic conditions are of relevance for many aerospace applications, such as the injection and active cooling systems of high performance liquid rocket engines. These conditions are explored when reactants are injected at subcritical temperature into chambers at supercritical pressures. During transcritical mixing all fluid properties change dramatically as the fluid *pseudo-boils*, hence it transitions from a liquid-like to a gas-like state across a region of large non-linearities of thermodynamic and transport properties [1]. This transition is marked by the pseudo-boiling (PB) or Widom line, defined by the thermal condition where the specific-heat capacity attains its maximum at a given pressure [2]. In addition, as the pressure increases, the PB phenomenon is less evident and the thermodynamic non-linearities gets smeared out on a wider temperature range and eventually become negligible at extremely elevated pressures.

In the context of high-pressure and non-ideal gas flows, direct numerical simulations (DNS) is emerging as a fundamental tool to both investigate and model small scale flow features in such extreme thermodynamic conditions. The development of reliable datasets, models as well as physical insights is a key aspect for many present and future applications as recently described by Oefelein [3]. Recently an increasing effort has been devoted to the complex behavior of multi-species mixing under supercritical conditions, see [4–6] among others. However, DNS data of flows under transcritical conditions remain limited due to the extremely challenging conditions that PB poses in a turbulent environment. In fact, many studies have been limited to simulate a binary mixing layer behind an injector lip under high-Reynolds conditions only in a two-dimensional setting [7, 8]. On the other hand, three dimensional configurations have been simulated to address physical [9] as well as modeling [10, 11] considerations although limited to low Reynolds numbers.

In order to bridge this gap, moderate Reynolds number have been explored under the low-Mach number approximation in a three dimensional setting by Ries et al. [12] confirming that under transcritical conditions the budget of turbulent kinetic energy is governed by turbulent diffusion. They also employed the same simulation to investigate entropy production as well as turbulent heat transfer anisotropy [13]. Moderate Reynolds number flows have been also recently explored to investigate the effect of pressure on the large scale, low-Mach number jet dynamics and small-scale velocity features [14]. It has been confirmed that under transcritical conditions the so-called *solid wall effect*, investigated in the absence of pseudo-boiling in [15, 16] and discussed under such conditions in [17], decrease its effectiveness as pressure increases and moves far from the critical pressure. As a result, it was found that the length of the liquid-like dense core decreases with an increasing pressure and constant jet Reynolds number. In the context of the present work, such DNS dataset [14] featuring four jets at the same Reynolds number and developed under the low-Mach number approximation, provides a solid basis for the investigation of small scales features of thermodynamic properties under transcritical conditions in a turbulent flow.

In this note, using data from transcritical jets at moderate Reynolds number, we introduce concept and scalings. Firstly the existence of sub-Kolmogorov scales, expected due to the elevated Prandtl number, is assessed by evaluating the Batchelor scale and by investigating the enthalpy fluctuations spectra. Secondly a complete characterization of the range of scales at play is given using conditional averages of thermodynamic properties gradients consistently evaluated at the boundaries of the pseudo-boiling phenomenon.

II. DNS dataset

A recently developed DNS dataset is employed which consists in four iso-Reynolds, temporally evolving, nitrogen jets characterized by a different pressure [14]. The initial jet Reynolds number $Re_{jet} = \Delta U H/\nu_{\rm ref} = 3000$ and jet width $H = 2$ mm are kept constant while the mean shear ΔU is adjusted for each case to keep the Re_{jet} constant since $\nu_{\rm ref}$ changes with pressure. Note that, despite the limited physical size of the domain, the simulations falls well inside the continuum regime and the low-Mach number conditions of the jets leads to a rather similar and small convective Mach number of $\sim 9 \cdot 10^{-5}$. Recalling that the critical pressure of nitrogen is $p_{cr} = 3.39$ MPa, the pressure values explored by the dataset spans from near-critical up to largely supercritical $p_0/p_{cr} = 1.25, 1.5, 2.0, 3.0$ named respectively case R2P1, R2P2, R2P3 and R2P4. All the jets mix under transcritical thermodynamic conditions where the cold jet temperature T_{jet} is lower than the pseudo-boiling temperature T_{pb} while the warm environment $T_{env} > T_{pb}$.

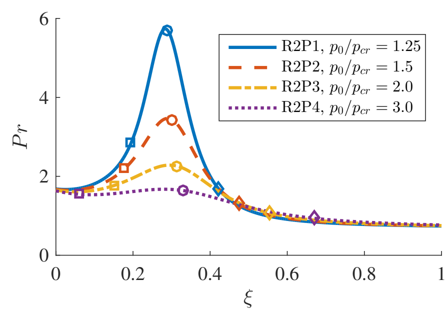


Figure 1: Prandtl number as a function of the non-dimensional enthalpy while symbols represent for each pressure case ξ_{pb} (circles), ξ^- (squares) and ξ^+ (diamonds).

Figure 1 shows the Prandtl number Pr, for the conditions encountered in the four pressure cases, as a function of the mixing variable ξ, a dimensionless enthalpy defined as $\xi = (h - h_{jet})/(h_{env} - h_{jet})$. As pressure increases, the peak Pr located in the PB region is smeared out, as evident for the R2P4 case. In fact, as discussed by Banuti [2], for pressure values close to $p_0/p_{cr} = 3.0$ pseudo-boiling effects become negligible so the R2P4 case can be considered the reference case for the present investigation. Figure 1 also displays the thermodynamic location of PB ξ_{pb} and the boundaries of this non-linear isobaric transition from a liquid-like reference state $\xi^- < \xi_{pb}$ to a gas-like state $\xi^+ > \xi_{pb}$ [2]. Such definition will be used throughout the paper as done in [14, 18].

The described dataset was generated using a low-Mach number approximation of the governing equations which allows an efficient use of high-fidelity real fluid equation of state (EoS) and transport properties [10,19] directly taken from the reference software *refprop* [20] which features a substantial higher fidelity compared to two- or more parameters cubic EoS [11, 21–23]. The simulation have been performed by means of a modified [19,24], EoS independent, variable density version of *nek5000* [25] which is a massively parallel code based on the spectral element method (SEM) [26] and recently used for many state of the art DNS, see [27] among others. As discussed in [18] this framework is particularly tailored for the investigation of transcritical mixing small scale features since it combines spectral accuracy as well as high-fidelity thermodynamic and transport modeling.

III. Results

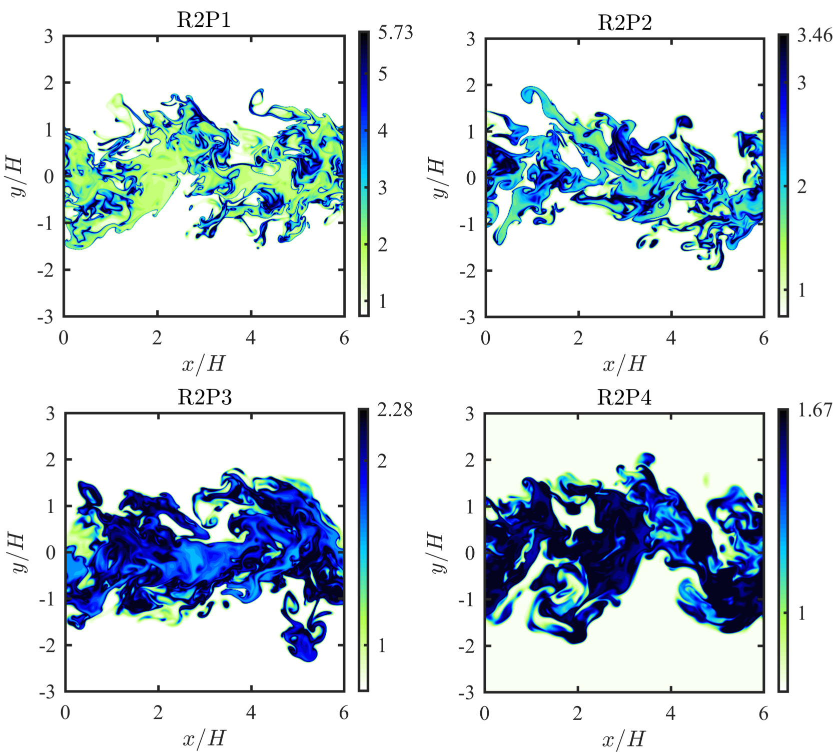


Figure 2: Spanwise cuts of Pr fields of the four DNS cases. The fields are color coded from a common value of $Pr^{min} = 0.75$ (white) to the maximum Pr (black) of each case.

Transcritical conditions in a turbulent flow can lead to the formation of peculiar flow patterns as clearly displayed by Fig. 2 which shows a spanwise cut of the Pr fields for the four temporal jets. All the cases, the other results throughout the paper, are presented at the end of the simulation, hence $t/t_{jet} = 16$ where $t_{jet} = H/\Delta U$ is the jet time unit. In the near critical case R2P1 the formation of a wide range of scales is evident comprising two main features: long and strained regions in which high-Pr number values occur in very thin layers, thick regions of high-Pr number occurring at the boundaries of warm pockets deeply entrained in the cold jet core. The latter regions have been demonstrated to be responsible of negative dilatation rates in transcritical, $Pr \neq 1$, turbulent jets [18]. In the higher pressure cases, observing from R2P2 to R2P4, the formation of thin layers and small scale features become less evident. In addition, the jets boundary or turbulent non-turbulent interface (TNTI), appear less corrugated compared to R2P1. In fact, in particular for the R2P1 case, the TNTI, shows the formation of secondary Kelvin Helmholtz instabilities due to the high density gradient across the PB. A similar behavior has been observed, in conjunction with a forward turbulent kinetic energy cascade, in a reference 2D shear layer behind a splitter plate [7].

In $Pr > 1$ flows a sub-Kolmogorov scale, denoted as Batchelor scale η_B [28, 29], is in principle to be expected. Such scale is usually expressed as $\eta_B = \eta_K Pr^{-1/2}$, where η_K is the Kolmogorov scale, in constant propriety flows. Under transcritical conditions, the Prandtl number explore a wide range of values as discussed when presenting Fig. 1. Describing the DNS database in [14], the adequacy of the employed resolution was investigated using a conservative estimate for Batchelor scale, in this case representing the smallest scales of the thermal mixing, as $\eta_B = \eta_K Pr_{max}^{-1/2}$ where Pr_{max} is the maximum Prandtl number of each pressure case. It has also been assessed that η_K values calculated from the DNS are consistent with experimental measurements at the same moderate Re_{jet} [30]. Similar considerations were used in previous transcritical DNS [9], while more recent works [12, 13] have used only η_K to assess their grid resolution. Note that scalar transport that occurs at scales smaller than the η_K has been also observed in supercritical, high-density, multi species flows [31].

In the present work, the Batchelor scale is evaluated, similarly to η_K, using directly the definition, following [32], as $\eta_B = (\widetilde{\epsilon}/\widetilde{\nu}\widetilde{D}^2)^{1/4}$ where $\widetilde{\cdot}$ denote Favre averages, employed in order to ensure consistency in a variable density context as discussed in [32] while ϵ is the momentum dissipation rate and $\widetilde{D}$ is the Favre-averaged thermal diffusivity.

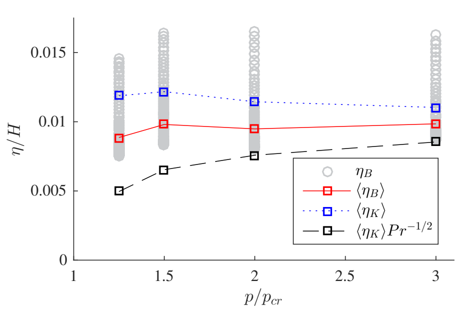
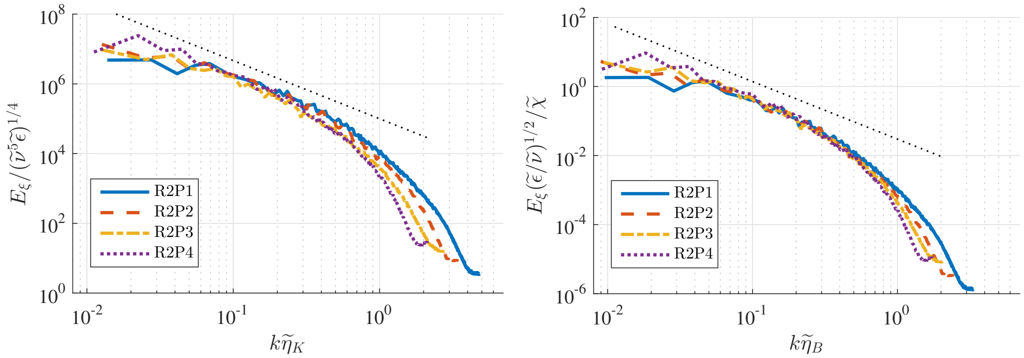


Figure 3: Averaged turbulence small scales as functions of the reduced pressure.

In the temporal jet configuration employed η_K and η_B, are function of the inhomogeneous direction y and averaged values along such direction, $\langle \eta_K \rangle$ and $\langle \eta_B \rangle$ are employed. Figure 3 shows the averaged smallest scale of the flow for each of the four pressure cases together with the simplified, constant properties, definition of the Batchelor scale $\langle \eta_K \rangle Pr_{max}^{-1/2}$. It can be observed that $\langle \eta_B \rangle$ slightly increases with pressure, while $\langle \eta_K \rangle Pr_{max}^{-1/2}$ show, a more pronounced dependence on pressure. As a result the estimate for Batchelor scale $\eta_B = \eta_K Pr_{max}^{-1/2}$ is clearly lower than both the averaged and y-dependent η_B. This suggests that following such estimation for the fulfillment of DNS grid requirements could be excessively conservative. It can be also observed that, although being characterized by the same Re_{jet}, the average value of the Kolmogorov scale is also depending to some extent on pressure. In fact, the reduced impact of the solid wall effect in the largely supercritical case R2P4 allows the creation of slightly smaller velocity small-scale.



(a) (b)

Figure 4: One dimensional streamwise scalar fluctuations spectra scaled using Kolmogorov units (a) and Batchelor units (b), dashed line represent the $-5/3$ slope.

The evaluated scales are now employed to scale the spectra of the non-dimensional enthalpy fluctuations E_ξ. The 1D spectra are calculated following [14, 32] on the jet centerline along the streamwise direction x and scaled in both Kolmogorov and Batchelor units. Figure 4(b) shows remarkable collapsing of E_ξ is obtained by using Favre-averaged Batchelor units, compared to Kolmogorov units of Fig. 4(a). The spectra follow, in the limited range of scales of the present dataset, the inertial scaling of $\sim k^{-5/3}$. Contrary to the results presented by Ries et al. [13], where a narrow $\sim k^{-1}$ region has been observed for the temperature fluctuations spectrum, for the present data such region is absent or too narrow to be observed in the spectra. Although a direct comparison cannot be easily made, such region is expected to be present at higher Re and higher Pr_{max}.

The findings of Fig. 4(b) are a peculiar behavior of transcritical flows since, in other variable-density contexts, such as non-premixed combustion, when Favre-averaged quantities are employed the mixing variable (i.e. mixture fraction) spectral behavior is rather similar to that of turbulence energy spectrum [33]. In addition, the difference between reacting and non reacting flows is usually taken out completely by using Favre-averaging [32]. In the present cases, although being characterized by density jumps on the same order of flames ($\rho_{jet}/\rho_{env} \sim 10$), the thermodynamic non-linearities in the PB region promote a more complex behavior of scalar fluctuations spectra.

It is now of interest to estimate the mean value of the interface thickness in order to better characterize the scales induced by PB. The PB diffuse interface actively interacts with turbulence which in turns induce stretching and curvature effects [18]. The thickness of an interface for the generic scalar variable ϕ, can be estimated as the inverse of the normalized magnitude of the scalar gradient $\Delta\phi/|\nabla\phi|$ at each space-time location [34]. In order to statistically compare the 4 cases of the dataset, the mean thickness of a generic ϕ layer is defined taking the averages of $\Delta\phi/|\nabla\phi|$ conditioned to a particular ξ^* iso-surface as $\delta^*_\phi = \overline{\Delta\phi/|\nabla\phi||_{\xi^*}}$.

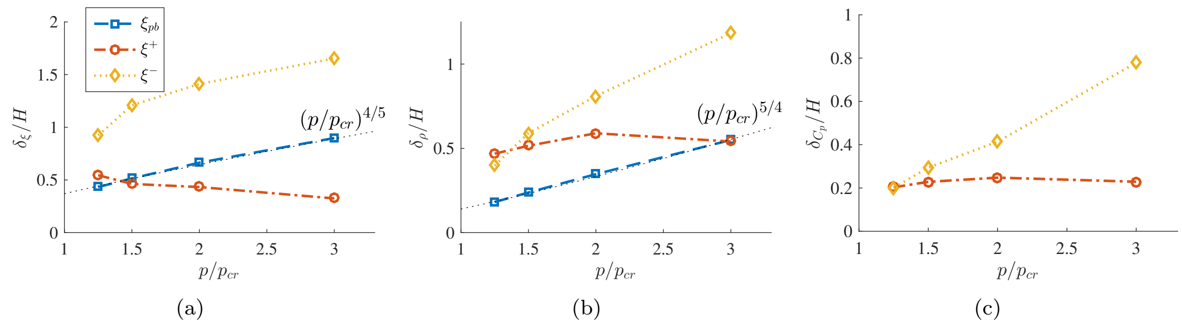


Figure 5: Mean thickness of the ξ (a), ρ (b) and C_p (c) layers conditioned to the reference ξ^+ gas-like, ξ_{pb} pseudo-boiling and ξ^- and liquid-like iso-surfaces plotted as functions of reduced pressure values p/p_{cr}.

Figure 5 shows the mean thickness δ of ξ, ρ and C_p layers conditioned to the reference ξ^+ gas-like, ξ_{pb} pseudo-boiling and ξ^- and liquid-like iso-surfaces as functions of reduced pressure values p/p_{cr}. Note that those representative ξ values are changing as the pressure increases, as shown in Fig. 2. In particular, ξ^- is sensibly decreasing from R2P1 to R2P4 approaching the limit value $\xi = 0$ of the cold jet core. Therefore the values of δ conditioned to ξ^-, will result, for the moderate Reynolds number at play, in relatively large thicknesses. Observing Fig. 5 and moving from R2P1 ($p/p_{cr} = 1.25$) to R2P4 ($p/p_{cr} = 3.0$), δ_ξ increases with pressure when conditioned to ξ_{pb} and ξ^-, conversely when conditioned to the gas-like iso-surface ξ^+, it only slightly decreases with p/p_{cr}. It is also observed that the ξ layer at the PB iso-surface scales with reduced pressure as $\delta^{pb}_\xi \sim (p/p_{cr})^{4/5}$. Comparing δ_ξ and δ_ρ, they show similar trends as the gas-like side which is mainly governed by turbulent motion and less influenced by PB. However, the ρ layers are systematically thinner than the ξ ones. As a result, the density layer conditioned to the PB-isosurface scale more than linearly with the reduced pressure $\delta^{pb}_\rho \sim (p/p_{cr})^{5/4}$. Clearly, this is yet another PB effect which induce a largely non-linear relation between ρ and ξ. If a linear or weakly non-linear relation would have been present the same pressure scaling would have been shown.

Finally, the thicknesses of the C_p interface are shown in Fig. 5(c) where only results conditioned to ξ^+ and ξ^- are shown since $C_p(\xi)$ is non monotonic. This implies that, for each pressure, the layer thickness is estimated at ξ^+ taking $\Delta Cp = C_p(\xi_{pb}) - C_p(\xi^+)$ and at ξ^- taking $\Delta Cp = C_p(\xi_{pb}) - C_p(\xi^-)$ where $C_p(\xi_{pb})$ is the highest value possible due to PB definition [2]. Observing Fig. 5(c) it is easily noticeable that $\delta^+_{C_p}$ and $\delta^-_{C_p}$ converge to a rather similar value as pressure decreases. Observing the entire dataset, the layer thicknesses calculated in the gas-like region ξ^+ are consistently thinner than those calculated in the cold liquid core at ξ^-. This happens firstly because C_p is highly non-linear as well as non-symmetric with respect to ξ_{pb}, and secondly because the turbulent perturbations that strain the iso-surfaces are more intense in the gas-like region due to lower density. This point is an other ramification of the solid-wall effect, discussed for the same DNS dataset in [14], as the high density of the core dampens the turbulent fluctuations and reduce the straining effect that leads to thin layers. In fact, as $\delta^-_{C_p}$ remain essentially constant with pressure, the gas-like regions of the jets are governed by the turbulent motion while a marginal role is played by PB.

IV. Conclusion

The effect of pressure on the thermodynamic scales in turbulent jets under transcritical condition has been investigated by means of DNS. It is found that the scalar fluctuations spectra are properly scaled using Batchelor units based on Favre-averaged quantities. The Batchelor scale can be therefore considered to be the proper small scale unit to described turbulent mixing under transcritical conditions. This scale is shown to be less sensitive to the background pressure, with respect to the constant property assumptions based on Pr_{max}.The thicknesses of pseudo-boiling (PB) stratification have been calculated using conditional averages of the thermodynamic gradients on the temperature iso-surfaces that represents the boundaries of PB. In particular, the mean ξ layers, conditioned to the PB iso-surface, scales less than linearly with the reduced pressure as $\sim (p/p_{cr})^{4/5}$. Conversely the density layers scales as $\sim (p/p_{cr})^{5/4}$ while C_P layers, are observed to be barely affected by pressure at the gas-like boundary of PB. Finally it is worth mentioning that the present results have been obtained investigating transcritical jets at moderate Reynolds number, therefore future research effort will be devoted to investigate such small scale features and scalings at higher Reynolds number and increasingly relevance for aerospace applications.

Acknowledgment

The author acknowledge CINECA for HPC resources under Iscra-B Grant DNS-LS and Francesco Creta for the many useful discussions.

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