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Structure of wall-bounded flows at transcritical conditions

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At transcritical conditions the transition of a fluid from a liquid-like state to a gas-like state occurs continuously, which is associated with significant changes in fluid properties. Therefore boiling in its conventional sense does not exist, and the phase transition at transcritical conditions is known as “pseudo-boiling”. In this work, direct numerical simulations (DNS) of a channel flow at transcritical conditions are conducted in which the bottom and top walls are kept at temperatures below and above the pseudo-boiling temperature, respectively. Over this temperature range, the density changes by a factor of 18 between both walls. Using the DNS data, the usefulness of the semi-local scaling and the Townsend attached eddy hypothesis is examined in the context of flows at transcritical conditions—both models have received much empirical support from previous studies. It is found that while the semi-local scaling works reasonably well near the bottom cooled wall, where the fluid density changes only moderately, the same scaling has only limited success near the top wall. In addition, it is shown that the streamwise velocity structure function follows a logarithmic scaling and the streamwise energy spectrum exhibits an inverse wavenumber scaling, thus providing support to the attached eddy model at transcritical conditions.

Keywords: Transcritical flow, wall modeling, turbulent channel flow, pseudo-boiling, turbulent boundary layer

I. INTRODUCTION

At subcritical pressures, fluids at a liquid state can be unambiguously distinguished from those at the gaseous state. At supercritical pressures, however, a substance can exist partly as liquid and partly as vapor near the critical temperature, and the transition between the two phases becomes continuous. During this process, all fluid properties change dramatically, and the flow exhibits a liquid-like density and a gas-like diffusivity [1, 2]. As an example, Fig. 1 shows the thermo-transport properties of nitrogen across the pseudo-boiling line (a.k.a. Widom line), which is defined by the thermal condition where the specific heat capacity attains its maximum at a given pressure [3, 4]. These conditions are relevant for several engineering applications [5]. Examples are the transcritical injection in diesel engines, gas turbines, and rocket motors, where reactants are injected into chambers at supercritical pressures. These flow configurations conform with the classical jet configurations, and processes of interest are the atomization of the injected reactants and their subsequent combustion (see, e.g., [3, 6, 7] for experimental studies and [8, 9] for numerical investigations). Besides the transcritical injection, in refrigerators, power plants and nuclear reactors, coolants are pressurized to supercritical conditions to prevent the so-called boiling crisis [10, 11]. In this work, we consider wall-bounded flows at transcritical conditions, which are of relevance to regenerative cooling systems in rocket motors, where one of the cryogenic propellants is first used to cool the combustion chamber prior to its injection. Laboratory measurements of wall-bounded turbulence at transcritical conditions are scarce, and most earlier experiments reported only wall heat transfer rates (see, e.g., [12–14]), which, albeit its relevance to engineering systems, provide only limited information about the near-wall turbulence.

Our knowledge of turbulence at transcritical conditions mostly comes from direct numerical simulations (DNS), where turbulent motions at all scales are numerically resolved, and pressure,
FIG. 1. State diagram and thermo-transport properties of nitrogen (critical pressure of 3.40 MPa and critical temperature of 126.2 K) from NIST database [15]. (a) pressure-temperature state diagram with the compressibility factor contours shown in gray and specific heat capacity at constant pressure shown as red contours in units of J/(g·K). The blue solid line is the coexistence line and the blue dashed line is the pseudo-boiling line defined by the peak of specific heat capacity. The black dot represents the critical point; (b) density, specific heat capacity, and dynamic viscosity plotted as a function of temperature at three different pressures, emphasizing the drastic property changes in the pseudo-boiling region.

dynamic viscosity, and heat capacity, etc. are tabulated as a function of temperature and pressure [16, 17]. Here we briefly review recent DNS investigations and relevant findings. In Refs. [18, 19], the authors conducted DNS of annular flows between two simultaneously heated and cooled walls, and it was found that turbulence is attenuated near the hot wall. Considering the channel configuration, it was reported in Ref. [20] that the mean velocity profiles at various flow conditions collapse when using the semi-local scaling (although we note the heat capacity was kept constant in Ref. [20]). In contrast, in Ref. [21], the authors found that the mean velocity may be collapsed using conventional viscous length and velocity scales. In addition to these studies on flows that are fully developed and statistically homogeneous along the streamwise and spanwise (annular) directions, developing thermal boundary layers were studied in Refs. [22, 23].

Although DNS allows us to access full three-dimensional flow field, using it as a design tool for practical engineering problems remains infeasible owing to its computational cost [24], and numer-
ical difficulties associated with representing large density gradients in transcritical flows [25–28]. Such numerical difficulties have limited DNS to transcritical flows with $O(1)$ density change [16–19, 21–23]. However, practical engineering flows involve density changes up to $O(100)$, and computationally efficient modeling tools to support engineering design decisions are desired.

To date, low-cost computational fluid dynamic (CFD) models (e.g. Reynolds-averaged-Navier-Stokes) have not been able to accurately predict the wall heat transfer rates at transcritical and supercritical conditions because of an insufficient description of the near-wall turbulent heat transfer [2]. While efforts have been made to enable wall-modeled large-eddy simulation (WMLES) capabilities for problems involving wall heat transfer [29–32], applications of this cost-efficient tool has so far been limited to ideal-gas flows. By addressing this need, the objective of this work is twofold. First, we extend the recently developed modeling capability for simulating transcritical flows [33] to conduct DNS of transcritical channel flow with $O(10)$ density changes in the flow field. Second, we attempt to use DNS to inform low-cost CFD models by examining commonly employed scaling transformations and physical models for variable-property fluids. Specifically, we examine the semi-local scaling [20, 34–38] and the attached eddy model [39–41].

The remainder of the manuscript is organized as follows. Additional background information is provided in Sect. II. In Sect. III, we present details of the computational setup. In Sect. IV, the DNS results are presented, and conclusions are given in Sect. V.

II. BACKGROUND

A. Scaling transformations

For constant-property wall-bounded turbulent flows, the near-wall time-averaged velocity follows the law of the wall [42]

\[
\overline{u^+} = y^+, \quad \text{in the viscous sublayer, } y^+ < 5;
\]

\[
\overline{u^+} = \frac{1}{\kappa} \log(y^+) + B, \quad \text{in the logarithmic region, } 30 \lesssim y^+ \lesssim 0.1\delta;
\]

(1)

where $u$ is the streamwise velocity, $+$ indicates normalization by wall units, $\kappa \approx 0.4$ is the von Kármán constant, $B \approx 5$ is an additive constant, $y$ is the wall-normal coordinate, and $\overline{\cdot}$ indicates ensemble average. The wall units used for normalization are $u_\tau = \sqrt{\tau_w/\rho_w}$ and $\delta_\nu = \nu/\rho_w u_\tau$, where the subscript $w$ indicates quantities evaluated at the wall, $\rho$ is the fluid density, $\mu$ is the dynamic viscosity, $\tau_w$ is the mean wall-shear stress. $y^+ = y/\delta_\nu$, $u^+ = \overline{u}/u_\tau$ represent the viscous scaling. For constant-property flows, $\rho_w = \rho$ is a constant, and $\mu_w = \mu$ is also a constant.

For variable-property flows, both the fluid density and the dynamic viscosity (and other flow properties including heat capacity) are functions of temperature and pressure, leading to additional complexities. For example, the time-averaged velocity does not follow the law of the wall, unless a scaling transformation is applied. One commonly used velocity transformation is the so-called van Driest transformation [43]

\[
\overline{u_{VD}^+} = \int_0^{\overline{u^+}} \left( \frac{\rho}{\rho_w} \right)^{1/2} du^+.
\]

(2)

The intention of this (and other) velocity transformation is for the transformed velocity $\overline{u_{VD}^+}$ to collapse with the incompressible law of the wall as a function of $y^+$ (i.e. Eq. (1)). The van Driest transformation works quite well for boundary-layer flows above adiabatic walls (see, e.g., [44–46]).
However, for flows above non-adiabatic walls, Eq. (2) fails, and the transformation developed in Ref. [35] has been recommended

\[ y_{SL} = \frac{y \sqrt{\tau_w \rho}}{\mu}, \]

\[ u_{TL} = \int_{0}^{u^+} \left( \frac{\rho}{\rho_w} \right)^{1/2} \left[ 1 + \frac{1}{2} \frac{1}{\rho} \frac{d\rho}{dy} y - \frac{1}{\mu} \frac{d\mu}{dy} y \right] du^+, \]

(3)

where the transformed velocity \( u_{TL} \) is expected to follow the law of the wall as a function of \( y_{SL} \) (note \( y_{SL} \) is non-dimensional). In Ref. [35], Eq. (3) was derived by equating the turbulent momentum flux and the viscous stress to their incompressible counterparts. The same transformation was later derived in Ref. [20] using a slightly different approach. While the above transformation has been quite successful [30, 35, 47], it is worth noting that Eq. (3) is not based on first principles, but is a consequence of reasonable assumptions, which may be valid for certain flows but may also prove to be inadequate in other flows. The subscript “SL” in Eq. (3) is the acronym for semi-local.

The starting point of the semi-local scaling [34] is such that a fluid parcel at a wall-normal location \( y_{SL} \) in a variable-property flow subjects to the same large- and small-scale effects as a fluid parcel at a wall-normal location \( y^+ \) in a constant-property flow (given the two flows are at the same friction Reynolds number). Following Ref. [35], the friction Reynolds number of a variable-property flow is defined using the semi-local friction velocity \( u_*^\tau = \sqrt{\tau_w / \rho} \), the boundary layer height (or the half channel height) \( \delta \), and the local kinematic viscosity \( \mu / \rho \).

The semi-local scaling proves to be quite useful. Collapsed Reynolds stresses, pre-multiplied energy-spectra, Kolmogorov length scales, mixing lengths, and eddy viscosities at difference Reynolds numbers were reported in Refs. [20, 36, 37]. However, it is worth noting that the equations of state used in Refs. [20, 36] are not completely realistic. For example, the authors held the specific heat capacity constant. In addition, only moderate density changes were considered in Refs. [20, 36, 37], where STD(\( \rho' / \rho \)) did not exceed 15%. Here fluctuations are denoted using the superscript \( \tau \), and STD(\( \cdot \)) is the standard deviation of the bracketed quantity. Considering that transcritical flows in practical applications often encounter density change of \( O(10 \sim 100) \), it is of interest to test the usefulness of the semi-local scaling in flows with large density variations. Such tests were previously conducted in Ref. [28] for boundary layer flows at transcritical conditions, where deficiencies of the semi-local scaling were observed.

### B. Attached-eddy hypothesis

While the scaling of the time-averaged velocity may be derived using dimensional arguments (see, e.g., [42]), one often needs to resort to more sophisticated models like the attached-eddy hypothesis for scaling predictions of turbulent statistics in wall-bounded flows [39, 41, 48, 49]. The attached eddy hypothesis is comprised of three sub-hypotheses. The first sub-hypothesis states that, at high Reynolds numbers, there exists a range of wall-normal distances, within which range, neither viscous effects nor large-scale effects play a significant role. This wall-normal distance range is also known as the logarithmic range. The second sub-hypothesis states that the sizes of the fluid structures within the logarithmic range scale as their distance from the wall, and these structures are space-filling. These structures are now known as attached eddies. The last sub-hypothesis states that instantaneous velocity fluctuations at a generic location in the flow field result from a superposition of all the eddy-induced velocities at that location. This last sub-hypothesis is a direct consequence of Bio-Savart law. A sketch of the hypothesized boundary-layer structure is shown in Fig. 2(a).
FIG. 2. (a) A sketch of hypothesized boundary layer structure. The attached eddies are space filling. On a vertical plane cut as shown here, the number of eddies doubles as the size halves. An eddy affects the shaded region below it. The velocity at a generic point in the flow field is a result of the additive superposition of all the eddy-induced velocity fields there. (b) A sketch of the additive cascade in wall-bounded flows. The sketch is the same as (a), but we have retained only the hierarchical organization of the attached eddies, schematically indicated by color lines. The two black squares indicate two points in the flow field. For these particular points under consideration (at the same wall-normal height), eddies in blue affect the two points simultaneously, eddies in orange can only affect one of the two points and eddies in gray affect neither of them.

The attached eddy hypothesis was pioneered by Townsend [50], then extended in Refs. [51–55] by accounting for wake effects, effects of vortex clustering and the mutual exclusion effects of the attached eddies of the same size. However, these earlier works have relied on the use of a few specific wall-attached eddies, and investigations of the scaling implications of the attached eddies were not until quite recent (see, e.g., [40, 48, 56–58]). A notable recent development on the scaling implications of the attached eddy model is the hierarchical random additive process (HRAP) model, where only the assumed hierarchical organization of the wall-attached eddies is retained (see Fig. 2(b)) and the streamwise velocity fluctuation at a generic location in the flow field is modeled as a random additive process

\[ \overline{u' \prime} = \sum_{i=1}^{N_y} a_i, \]  

(4)

where \( a_i \) represents a contribution from an attached eddy of size \( \delta/2^i \), and the number of addends \( N_y \) is obtained by integrating the eddy population density \( P(y) \sim 1/y \) from the location of interest to the boundary layer height

\[ N_y = \int_y^\delta P(y)dy \sim \log(y). \]  

(5)

Squaring and averaging both sides of Eq. (4) leads to the logarithmic scaling of the variance of the streamwise velocity fluctuations

\[ \overline{u'^2} = N_y a^2 = A_1 \log(y) + B_1, \]  

(6)

which scaling was first derived by Townsend [50], and has so far received considerable empirical support [59–61]. Here, \( A_1 \) is the Townsend-Perry constant, and \( B_1 \) is a constant. Next, let us consider two points that are separated by a distance \( r \) in the flow direction. The attached eddies may be grouped into three groups, first, eddies that affect the two points simultaneously (whose height is \( r \lesssim h \lesssim \delta \), and will be referred to as type-I eddies); second, eddies that affect only one of the two points (whose height is \( y \lesssim h \lesssim r \) and will be referred to as type-II eddies); and third,
eddy densities that affect neither of the two points (whose height is \( h \lesssim y \) and will be referred to as type-III eddies). If we take the difference between the two points, only contributions from type-II eddies remain, and we obtain the logarithmic scaling of the second-order structure function

\[
(u'(x, y) - u'(x + r, y))^2 = \left( \sum_{i=N_r}^{N_y} a_i - b_i \right)^2 = 2(N_y - N_r)a^2 = 2A_1 \log(r/y) + B_{1,s},
\]  

(7)

where \( a_i \) and \( b_i \) are addends that contribute to the velocity fluctuations at the two points, and \( B_{1,s} \) is yet another constant. By taking the difference between Eq. (6) and Eq. (7), we have

\[
\frac{u'(x, y)u'(x + r, y)}{u'^2} = u'^2 - 0.5(u'(x, y) - u'(x + r, y))^2 = A_1 \log(\delta/r) + B_{1,c},
\]  

(8)

whose Fourier transformation leads directly to the celebrated wavenumber inverse scaling of the streamwise energy spectra

\[
E_{u'u'} \sim k^{-1},
\]  

(9)

where \( k \) is the streamwise wavenumber and \( B_{1,c} \) is a constant.

Because the above derivation for the scalings in Eqs. (7) to (9) does not rely on any specifically-shaped attached eddy, we conclude that the existence of the logarithmic scalings Eq. (7) and the \( k^{-1} \) scaling are evidence of the presence of a hierarchy of wall-attached eddies as sketched in Fig. 2.

### III. COMPUTATIONAL SETUP

The computational domain is schematically illustrated in Fig. 3. The working fluid is nitrogen, whose critical pressure and critical temperature are \( p_c = 3.40 \) MPa and \( T_c = 126.2 \) K, respectively. The flow is at a bulk pressure of 3.87 MPa, corresponding to a reduced pressure \( \rho_r = p/p_c \) of 1.14. The flow is confined between two isothermal walls, which are kept at \( T_{w,b} = 100 \) K and \( T_{w,t} = 300 \) K, where \( T \) is the temperature, and the subscripts ‘b’ and ‘t’ denote ‘bottom’ and ‘top’, respectively. The reduced temperature \( (T_r = T/T_c) \) is 0.79 at the bottom cooled wall and 2.38 at the top heated wall. The periodic channel is of size \( L_x \times 2L_y \times L_z \) with \( L_x/L_y = 2\pi, L_z/L_y = 4\pi/3 \) and half-channel height of \( L_y = 0.09 \) mm, where \( x, y, \) and \( z \) are the streamwise, wall-normal and spanwise directions, respectively. The wall-normal coordinate extends from \( y = -L_y \) to \( y = L_y \). A constant mass flow rate is enforced and the bulk velocity, defined as \( \bar{u}_0 = \int \rho u dV/\int \rho dV \), is 27.3 m/s, where the integration is over the entire channel, and \( u \) is the streamwise velocity. The size of the computational domain is typical for channel-flow calculations and was proved to be sufficient for capturing the wall-normal statistics [62].

The governing equations for the description of transcritical flows are the conservation of mass, momentum and total energy, taking the following form

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (10a)
\]

\[
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + p \mathbf{I}) = \nabla \cdot \mathbf{\tau} + \mathbf{f}, \quad (10b)
\]

\[
\frac{\partial (\rho E)}{\partial t} + \nabla \cdot [\mathbf{u}(\rho E + p)] = \nabla \cdot (\mathbf{\tau} \cdot \mathbf{u}) - \nabla \cdot \mathbf{q} + \mathbf{u} \cdot \mathbf{f}, \quad (10c)
\]

where \( \mathbf{u} \) is the velocity vector, \( p \) is the pressure, \( \mathbf{f} \) is the body force and \( E \) is the specific total energy. The viscous stress tensor and heat flux are

\[
\mathbf{\tau} = \mu \left[ \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right] - \frac{2}{3} \mu (\nabla \cdot \mathbf{u}) \mathbf{I},
\]  

(11a)

\[
\mathbf{q} = -\lambda \nabla T,
\]  

(11b)
where $\lambda$ is the thermal conductivity. The specific total energy is related to the specific internal energy, $e$, and the specific kinetic energy as follows

$$E = e + \frac{1}{2} u \cdot u. \quad (12)$$

The body force, $f$, is applied along the streamwise direction to impose a pre-specified flow rate [63]. The system is closed with a constitutive equation, for which the Peng-Robinson (PR) cubic equation of state (EoS) [64, 65] is used

$$p = \frac{RT}{v - b} - \frac{a \alpha}{v^2 + 2bv - b^2}, \quad (13)$$

where $R$ is the gas constant, $v = 1/\rho$ is the specific volume, and the parameters $a$, $b$ and $\alpha$ account for effects of intermolecular forces and excluded volume,

$$a = 0.457236 \frac{R^2 T_c^2}{p_c}, \quad (14a)$$

$$b = 0.077796 \frac{RT_c}{p_c}, \quad (14b)$$

$$\alpha = \left[ 1 + c \left( 1 - \sqrt{\frac{T}{T_c}} \right) \right]^2. \quad (14c)$$

The coefficient $c$, appearing in Eq. (14c), is

$$c = 0.37464 + 1.54226 \omega - 0.26992 \omega^2, \quad (15)$$

where $\omega = 0.04$ is the acentric factor of nitrogen. Procedures for evaluating thermodynamic quantities such as internal energy, specific heat capacity and partial enthalpy using the PR EoS are described in detail in Refs. [27, 33, 66].

The finite-volume compressible code CharLES$^x$ is used in this study. This code has been extensively used for turbulent-flow calculations (see, e.g., [27, 67, 68]). Here we only briefly summarize the main features of the code, and further details can be found in Refs. [33, 69], and references therein. The flux reconstruction uses a central scheme where fourth-order accuracy is obtained on
uniform meshes. A sensor-based hybrid central-ENO scheme is used to capture flows with large density gradients and to minimize the numerical dissipation while stabilizing the simulation. For regions where the density ratio between the reconstructed face value and the neighboring cells exceeds 25%, a second-order ENO reconstruction is used on the left- and right-biased face values, followed by an HLLC Riemann flux computation. An entropy-stable double-flux model, developed for transcritical flows [33], is employed to prevent spurious pressure oscillations and to ensure the physical realizability of numerical solutions. A Strang-splitting scheme [70] is employed to separate the convection operator from the remaining operators of the system. A strong stability preserving third-order Runge-Kutta scheme [71] is used for time integration. Equation (13) is used as the state equation, and the molecular transport properties, including the dynamic viscosity and the thermal conductivity, are evaluated according to Chung’s model for high-pressure fluids [72, 73].

For the present study, a structured grid is used, and the mesh is of size \( N_x \times N_y \times N_z = 384 \times 256 \times 384 \), with uniform grid spacings in the streamwise and spanwise directions. The near-wall flow is dominated by the momentum-carrying motions, and therefore, the near-wall grid resolution is often evaluated in terms of wall units, i.e. \( u_\tau \) and \( \mu_w / \rho_w / u_\tau \). The grid resolutions are \( \Delta x^+ = 7.0 \), \( \Delta y_{\text{min}}^+ = 0.29 \), \( \Delta y_{\text{max}}^+ = 6.7 \), \( \Delta z^+ = 4.7 \) based on the wall units at the bottom cooled wall, and \( \Delta x^+ = 4.8 \), \( \Delta y_{\text{min}}^+ = 0.20 \), \( \Delta y_{\text{max}}^+ = 4.6 \), \( \Delta z^+ = 3.2 \) based on the wall units at the top hot wall.

The friction Reynolds number \( Re_\tau = L_\tau \rho u_\tau / \mu_w \) is \( Re_{\tau, b} = 430 \) and \( Re_{\tau, t} = 300 \) based on wall units at the bottom and top walls, respectively. DNS of incompressible channel flows typically require grid resolutions \( \Delta x^+ \approx 10 \), \( \Delta y_{\text{min}}^+ \approx 0.5 \), \( \Delta y_{\text{max}}^+ \approx 10 \), \( \Delta z^+ \approx 10 \) [61, 62, 74]. Considering additional physics in a numerical simulation often requires higher resolution, and therefore a finer grid may be needed for channels at transcritical conditions. A grid convergence study was conducted in Ref. [28] for wall-bounded transcritical flows, showing grid independent first- and second-order statistics for grid resolutions \( \Delta x^+ = \Delta z^+ \lesssim 7.3 \), \( \Delta y^+ \lesssim 0.2 \sim 7.3 \), using a code that has similar numerics. Following Ref. [28] and being conservative, we have used a slightly finer grid for the transcritical flow calculation here. Since the present work considers high density ratios, a separate grid convergence study is performed to ensure that statistical flow properties of interest are converged. Results from this study are presented in Appendix B. Near the center of the channel, flow motions are dominated by energy-transferring motions. There, the grid resolution is better evaluated in terms of the Kolmogorov length scale \( \eta_u = ((\overline{\rho u^2}) \bar{\rho})^{1/4} \), where \( \epsilon \) is the dissipation rate. The grid resolution in terms of the Kolmogorov length scale is \( \Delta x = 4.6 \eta_u \), \( \Delta z = 3 \eta_u \), \( \Delta y = 4.3 \eta_u \) at the center of the channel, and grid resolution in terms of the thermal Kolmogorov length scale \( \eta_T = \eta_u / \sqrt{Pr^*} \), where \( Pr^* = \tau_c \bar{\rho} / \lambda \) is the local Prandtl number, and is shown in Fig. 6(b) as a function of the wall-normal coordinate) is \( \Delta x = 11 \eta_T \), \( \Delta z = 11 \eta_T \), and \( \Delta y = 7.8 \eta_T \). A similar resolution was employed in Ref. [38]. The flow is well resolved and the ENO scheme is active on less than 0.06% of the cell faces. Simulations are advanced in time at a unity acoustic CFL number. After the flow reaches a statistically stationary state, we average across the homogeneous directions and over six flow-through times to obtain fully converged statistics, where one flow-through is defined as \( t_f = L_x / \tilde{u}_0 \).

IV. RESULTS

In this section, DNS results are presented. In order to validate the double-flux formulation, we also performed an additional calculation of a channel flow at a bulk pressure of 4.0 MPa and both walls are set to an equal and constant temperature of 300 K; results of this calculation are discussed in Appendix A. We will also use the results of this calculation for comparison purposes.
A. Mean flow

We start our discussion by examining the mean flow. Figure 4 shows the Favre- and Reynolds-averaged velocity and temperature as a function of the wall-normal coordinate. Here Reynolds average is used as a conventional ensemble average, which is denoted as $\bar{\phi}$, and the Favre average is defined as $\tilde{\phi} = \rho \phi / \rho$. From Fig. 4, $u \approx \tilde{u}$ and $T \approx \tilde{T}$.

Figure 4(a) shows an asymmetric velocity profile, with the momentum boundary layer near the top heated wall being thinner than that near the bottom cooled wall. The wall-normal coordinate at which $u$ attains its maximum is defined as $y_\delta$, which takes the value of 0.56$L_y$ (see dashed line). The top and bottom wall boundary layer heights are thus determined by taking the difference between $y_\delta$ and the $y$-coordinate of the two walls. Instead of using $y_\delta$, one can also use the height at which $\tilde{u}'\tilde{v}' = 0$, which yields essentially the same wall-normal coordinate. The same asymmetry is found in the temperature profile. Moreover, we notice that the temperature in the bulk of the channel is fairly close to the pseudo-boiling temperature, $T_{pb} = 128.7$ K.

Next, we examine the thermal properties. Figure 5 shows ensemble-averaged values of density ($\rho$), compressibility factor ($Z$), Mach number ($M$), dynamic viscosity ($\mu$) and heat conductivity ($\lambda$) as a function of mean temperature $\overline{T}$ and the wall-normal coordinate. Near the top heated wall, the fluid can be approximated as ideal gas ($Z$ approaches unity). The density and compressibility change drastically over a few degrees of Kelvin near the pseudo-boiling temperature $T_{pb}$. Because $\overline{T}$ is close to the pseudo-boiling temperature $T_{pb}$ in the bulk region, the wall-normal gradients of these quantities in the bulk region are comparably moderate. Density, dynamic viscosity and heat conductivity change appreciably near the two walls as a function of the wall-normal distance. Last, the Mach number is everywhere below 0.16, so that this configuration corresponds to the low-speed flow regime.

Figure 6 shows the mean heat capacity and Prandtl number as a function of the wall-normal coordinate. Because of turbulent mixing, the time-averaged specific heat capacity $\overline{c_p}$ shows a much moderate peak than the specific heat capacity computed using the averaged temperature and density (see also Ref. [36]). The temporally averaged Prandtl number is nearly the same as $\overline{c_p} \overline{\mu} / \overline{\lambda}$.
FIG. 5. Ensemble-averaged density ($\rho$), compressibility factor ($Z$), Mach number ($M$), dynamic viscosity ($\mu$) and heat conductivity ($\lambda$) as (a) a function of the normalized mean temperature and (b) a function of the wall-normal coordinate. Density, dynamic viscosity and heat conductivity are normalized by their respective values at the bottom wall.

FIG. 6. (a) Ensemble-averaged heat capacity and the heat capacity computed using ensemble averaged temperature and density as a function of the wall-normal coordinate. (b) Ensemble-averaged local Prandtl number and $\tau_p \mu/\lambda$ as a function of the wall-normal coordinate.

B. Instantaneous flow field

Next we examine the instantaneous flow field and discuss statistical results pertaining to the near-wall structure. Figure 7 shows instantaneous isosurfaces of $\rho = \{60, 100, 200\}$ kg/m$^3$. The fluid density is 44 kg/m$^3$ and 785 kg/m$^3$ at the top and bottom walls, respectively. Figure 7(a)-(c) are at increasing distances from the bottom cooled wall. Footprints of A-vortices can be discerned in Fig. 7(a). Further into the bulk region, at $\rho = 100$ kg/m$^3$, the near-wall vortices break down, leading to turbulent spots among comparably quiescent regions [75]. At $\rho = 200$ kg/m$^3$, the isosurface becomes highly corrugated, indicating strong mixing. We also note that the density and the velocity in this particular flow are well correlated, and there is barely any variation in the coloring of each isosurface.

Figure 8 shows instantaneous contours of reduced pressure, temperature, fluid density and streamwise velocity on a $z$–$y$ plane. The pressure fluctuates 0.5% around the reduce pressure of $p_r = 1.14$. Violent density fluctuations can be seen in Fig. 8(c), with intrusions of high-density fluid into fluid of lower density and vice versa. However, at this moment, the exact mechanisms
FIG. 7. Isosurfaces of constant density, colored by streamwise velocity. (a) $\rho = 60 \text{ kg/m}^3 \ (y_s/L_y = 0.98)$, (b) $\rho = 100 \text{ kg/m}^3 \ (y_s/L_y = 0.9)$ and (c) $\rho = 200 \text{ kg/m}^3 \ (y_s/L_y = 0.6)$. The fluid density at top and bottom walls is 44 kg/m$^3$ and 785 kg/m$^3$, respectively; $y_s$ denotes the mean location of the isosurface of density.
FIG. 8. Instantaneous contours on an $z-y$ plane for (a) reduced pressure, (b) temperature (the black line indicates $T/T_{pb} = 1$), (c) density ($\rho_0$ is the volume-averaged bulk density), and (d) streamwise velocity.

FIG. 9. Instantaneous contours of the streamwise velocity fluctuations at (a) $y_{SL} = 80$ from the bottom wall and (b) $y_{SL} = 80$ from the top wall. The velocity fluctuations are normalized using the friction velocity at the respective wall.

that lead to these violent density fluctuations in the near-wall region is not entirely clear. Also, it is apparent from Fig. 8(d) that the momentum boundary layer is significantly thinner near the top heated wall.

Figure 9 shows instantaneous contours of streamwise velocity fluctuations at a distance $y_{SL} = 80$ (defined in Eq. (3)) from the bottom cooled wall and the top heated wall. We make one observation. Fluid structures at the same semi-local-scaled distance $y_{SL}$ from the two walls are qualitatively different—near the bottom cooled wall, elongated low-speed streaks span the entire streamwise extent of the computational domain (Fig. 9(a)), whereas the streaks near the top heated wall (Fig. 9(d)) are often shorter.

This difference is evidenced in Fig. 10, showing the two non-zero invariants of the anisotropic tensor $b_{ij}$, where $b_{ij} = \frac{u_i' u_j'}{u_k' u_k'} - \frac{\delta_{ij}}{3}$ is the normalized deviatoric part of the Reynolds stress tensor. Defining $b_{ij} = \frac{u_i'' u_j''}{u_k'' u_k''} - \frac{\delta_{ij}}{3}$ leads to similar results and are not shown here for brevity.
Following Ref. [76], the two invariants of $b_{ij}$ are $\eta = \sqrt{1/6 \, b_{ij}b_{ji}}$ and $\xi = (1/6 \, b_{ij}b_{jk}b_{ki})^{1/3}$. The third invariant is $b_{ii} = 0$. Figure 10 shows $\eta$ as a function of $\xi$ for $b_{ij}$ near both walls and for $b_{ij}$ in a low-speed constant-property channel flow at $Re_\tau = 390$. The bounding triangle in Fig. 10 is known as the Lumley triangle, where $\eta = 0$, $\xi = 0$ corresponds to isotropic turbulence, $P_2 = (\eta, \xi) = (1/3, 1/3)$ corresponds to one-component turbulence and the other points on the triangle represent two-component and axis-symmetric turbulence. $P_1$ is at $(\eta, \xi) = (-1/6, 1/6)$. The wall-normal distance increases from $P_1$ to $P_2$ and from $P_2$ to the origin. $\eta = \xi$, i.e. points joining $P_2$ and the origin, represents the limiting state of axis-symmetric expansion. $\xi = 0$ represents the limiting state of plane-strain turbulence. Compared to low-speed constant-property wall-bounded flows, where the Reynolds stresses are mainly axis-symmetric, flows at transcritical conditions yield stress tensors that deviate appreciably from an axis-symmetric description, especially near the top heated wall, where the turbulence is at a state slightly away from the limiting state of axis-symmetric expansion.

C. Semi-local scaling

Figure 11 shows the semi-local wall-normal distance scaling as a function of $y^+$ near the two walls. The friction Reynolds numbers, defined based on semi-local quantities, are higher than the Reynolds numbers defined based on wall quantities.

Figure 12 shows the Kolmogorov length scale as a function of $y_{SL}$. To correctly measure the Kolmogorov length, one needs to resolve the energy spectra. If the simulation is under-resolved, the energy spectra will usually increase towards the grid cutoff. The spectra will be shown later in Fig. 17, confirming that the the energy spectra are well-resolved. Measurements from constant-property flows at various Reynolds numbers are included for comparison. The Kolmogorov scales near the two walls do not collapse as a function of $y_{SL}$, and they do not collapse with their constant-property counterparts at similar Reynolds number. This is in direct contrast with Ref. [20], where (nearly) perfect data collapse was reported among different variable-property flows at different (but similar) Reynolds numbers. In Fig. 12, only $\eta_{u,b}(y_{SL,b})$ agrees with the experimental results in Ref. [77].
Figure 11. $y_{SL} = y/\sqrt{\tau w_0/\mu}$ as a function of $y^+$ near the two walls. $y_{SL} = y^+$ for constant-property boundary-layer flows, and is included for comparison. $y_b$ is the distance from the bottom wall, and $0 < y_b < y_\delta + L_y$. $y_t$ is the distance from the top wall and $0 < y_t < L_y - y_\delta$.

Figure 12. Kolmogorov length scale $\eta_u$ and $\eta_T = \eta_u/\sqrt{Pr}$ as a function of $y_{SL}$. $Re^*_\tau = \delta \sqrt{\tau w_0(y = \delta)/\mu(y = \delta)}$ is the friction Reynolds number defined based on semi-local quantities at a distance $y = \delta$ from the wall. $\delta$ is an outer length scale and is $L_y + y_\delta$ for the boundary layer near the bottom wall and is $L_y - y_\delta$ for the boundary layer near the top wall. Results near the bottom cooled wall are shown as solid lines and results near the top heated wall are shown as dashed lines. $\eta_u$ and $\eta_T$ are shown in different colors. EXP are experimental results reported in Ref. [77] for two constant-property boundary layers at $Re_\tau = 2800$ and $Re_\tau = 19000$. Patel16 are DNS results reported in Ref. [20] for a constant-property channel at $Re_\tau = 395$.

Figure 13 shows $\bar{u}_{V,D}^+$ and $\bar{u}_T^+$ as a function of $y^+$, and $\bar{u}_{TL}^+$ as a function of $y_{SL}$. The van Driest transformation works reasonably well near both walls despite the non-adiabatic walls. $\bar{u}_{TL}^+$ collapses reasonably well with the law of the wall near the bottom cooled wall, but the scaling shows deficiencies near the top heated wall.

Next, we examine the Reynolds stresses. In Fig. 14, we show $R'_{ij} = \rho T'_{ij}/\tau_w$ and $R'_{ij} = u'_i u'_j / u'^2_\tau$ as functions of $y_{SL}$, where $i, j = 1, 2, 3$ denote the three Cartesian directions. $R'_{ij} \approx R''_{ij}$. $R'_{11}$ do not collapse as a function of $y_{SL}$ near the two walls. This is probably expected considering that the two boundary layers near the two walls are at fairly different Reynolds numbers. The peak values in $R'_{11}$ fall below their incompressible counterparts. Nevertheless, reasonable agreements of
FIG. 13. Mean velocity profiles as a function of wall-normal distance near (a) the bottom cooled wall and (b) the top heated wall. VD, van Driest transformation; TL, transformation by Trettel & Larsson [35]. The law of the wall corresponds to the established log-scaling $u^+ = \log(y^+)/\kappa + B$. $\kappa = 0.38$, $B = 5.2$ for the solid gray line. The viscous scaling $u^+ = y^+$ is also included for comparison.

FIG. 14. (a) $R''_{ij}$ and (b) $R'_ij$ as a function of $y_{SL}$. Different components are color-coded, and we use different line types to differentiate between the statistics near the bottom wall and the statistics near the top wall. $R''_{ij}$ in (a) are shown using thin lines and $R'_ij$ in (b) are shown using bold lines. We have shown only data in the near-wall regions. Results of incompressible flows at $Re_\tau = 395$ and $Re_\tau = 2000$ are included for comparison. The solid black line indicates the expected scaling of $u'^{+2}$ at high Reynolds numbers, $1.26\log(\delta/y) + 2.0$.

$R''_{11}$ with their incompressible counterparts at matched Reynolds numbers are found slightly away from the wall. Aside from $R''_{11}$, other components do seem to collapse.

Last, we examine the eddy viscosity. Eddy viscosity may be computed as follows in the logarithmic region, where molecular viscosity is negligible

$$\mu_{t,\text{log}} = \frac{\tau_w}{d\bar{u}/dy}.\quad (16)$$

We may estimate $d\bar{u}/dy$ using the velocity transformations

$$\frac{d\bar{u}}{dy} = \frac{d\bar{u}}{dU} \frac{dU}{dy} \frac{dY}{dy},\quad (17)$$

where $U$ and $Y$ are the transformed velocity and wall-normal distance. Both the van Driest transformation and the transformation proposed in Ref. [35] lead to

$$\mu_{t,\text{log}} = \sqrt{\rho\tau_w} \kappa y\quad (18)$$
away from the wall. In the near-wall region, Eq. (18) is often used with a damping function \( D \)

\[
\mu_t = D \mu_{t, \log},
\]

where \( D = 0 \) at the wall and \( D \) approaches 1 away from the wall in the logarithmic region. For constant-property flows, the van Driest damping function works quite well (see, e.g., [78])

\[
D_{VD}(y^+) = \left[1 - \exp\left(-\frac{y^+}{A^+}\right)\right]^2,
\]

where \( A^+ = 17 \). In Fig. 15, we show the computed damping functions as functions of \( y_{SL} \) and \( y^+ \). The van Driest damping function is included for comparison. Near the bottom cooled wall, the eddy viscosity approaches \( \mu_{t, \log} \) away from the wall (where \( D \approx 1 \)). Near the top heated wall, the semi-local scaling does not provide a very good prediction of the eddy viscosity in the logarithmic region, where \( D \) is found to be smaller than unity from \( y_b \) to \( y = L_y \). Both \( y^+ \) scaling and the semi-local scaling collapse data at the two walls; however, the computed damping functions collapse well with the van Driest damping only as a function of \( y_{SL} \).

D. Attached eddy hypothesis

The presence of wall-attached eddies in the near-wall region may be examined by considering statistics including the velocity energy spectra and the velocity structure functions. The structure functions following the logarithmic scaling as in Eq. (7) and the velocity energy spectra following the \( k^{-1} \) scaling as in Eq. (9) are direct evidence of the presence of the wall-attached eddies.

Figure 16 shows \( \Delta u'^2 = (u'(x + r, y) - u'(x, y))^2 \) as a function of the two-point displacement in the streamwise direction at various wall-normal locations near the bottom cooled wall and the top heated wall. Results of \( \Delta u'^2 \) are similar and are not shown here for brevity. Results from a constant-property boundary-layer flow at \( Re_{\tau} = 395 \) are included for comparison. \( \Delta u'^2 \) at the same \( y^+ \) distance from the two walls are distinctly different. Better data collapse is found when using the semi-local scaling. However, \( \Delta u'^2 \) at different \( y_{SL} \) locations only collapse as a function of \( r_x/y \) near the bottom cooled wall. Near the top heated wall, the semi-local scaling fails to collapse the velocity structure functions at different \( y_{SL} \) locations as a function of \( r/y \). In addition to data collapse, the velocity structure function near the bottom-cooled wall follows the same logarithmic
scaling as its constant-property counterpart, suggesting the presence of the same wall-attached eddies near the bottom cooled wall.

Figure 17 shows streamwise energy spectra as a function of the streamwise wave number at a few wall-normal distances from the bottom cooled wall and the top heated wall. It is worth noting that the DNS calculation has only a limited streamwise extent, i.e., $L_x = 2\pi\delta$, therefore some large scales are not resolved. However, according to the investigation in Ref. [62], the energy spectra of the resolved scales can be correctly captured. The data collapses near the bottom cooled wall at large scales, but the semi-local scaling fails at collapsing data near the top heated wall. The streamwise energy spectra exhibit power-law-like scaling $k^m$ across an extended range of scales with the scaling exponent only slightly smaller than $-1$, suggesting the presence of attached eddies near both walls.
FIG. 18. Probability density function of the density at several wall-normal distances from (a) the bottom wall and (b) the top wall. The fluid density at top and bottom walls is 44 kg/m$^3$ and 785 kg/m$^3$, respectively. The volume-averaged bulk density is 365 kg/m$^3$.

E. Density variation

It was shown in the previous section that the semi-local scaling works reasonably well near the bottom cooled wall, but it shows deficiencies near the top heated wall, in contrast with earlier works by Patel and co-authors. Compared to earlier calculations [36], the present DNS employs a real-gas state equation, which allows the specific heat capacity to change as a function of temperature and pressure. In addition, much more drastic mean density variation and instantaneous density fluctuations are found in the present calculation near the top heated wall. Because the semi-local scaling works quite well near the bottom cooled wall, and the specific heat capacity peaks between $y = -L_y$ and $y = y_δ$ (see Fig. 6), it is unlikely the failure of the semi-local scaling near the top heated wall is because of a non-constant $c_p$. Moreover, because the flow near the top heated wall is better resolved than the flow near the bottom cooled wall (see discussion in Sect. III), it is also unlikely that the grid resolution is the culprit. It seems that the semi-local scaling fails near the top heated wall because of the strong density variations there. To support this hypothesis, we quantify the density fluctuations in the flow field. Figure 18 shows the probability density function (p.d.f.) of the fluid density at several wall-normal heights, and Fig. 19 shows the standard deviation, skewness and kurtosis of the density fluctuations as a function of $y_{SL}$. Density fluctuations near both walls are highly skewed towards the density of the fluid at the other wall, indicating strong mixing (see Fig. 18). The most violent density fluctuations are found near $y = y_δ$, which corresponds to a wall-normal distance of $y_t^+ = 200$ from the top wall. STD($ρ′/ρ$) barely exceeds 10% near the bottom wall and in flows considered in Ref. [36], whereas STD($ρ′/ρ$) ≈ 35% near the top heated wall. In addition, the density fluctuations are highly super-Gaussian near the top heated wall, whereas the skewness and kurtosis of the density fluctuation near the bottom wall are not very far from being Gaussian.

V. CONCLUSIONS

In this work, DNS calculations of a channel flow at transcritical conditions are conducted. A temperature difference of 200 K is considered between the two isothermal walls for nitrogen at a bulk pressure only slightly higher than the critical pressure. The density changes by a factor of 18 in the flow field (a factor of three near the bottom cooled wall and a factor of six near the top heated wall). The fluid temperature changes drastically near the two walls, however, in the bulk region, $\bar{T} \approx T_{pb}$. As a result of heating, the boundary layer is thinner near the top heated wall. The
semi-local scaling is found to be quite useful near the bottom cooled wall, where the mean density variation is moderate. However, the same scaling is shown to have limited success near the top heated wall, where violent density fluctuations are found. Hence, the semi-local scaling is generally useful for real fluids at transcritical conditions as long as density fluctuations are moderate. In particular, results from the present study indicate that the semi-local scaling would be most useful for flows where \( \text{STD}(\rho')/\bar{\rho} \lesssim 40\% \).

We have also examined the presence of attached eddies in flows at transcritical conditions. Despite the limited Reynolds numbers, a logarithmic scaling is found in streamwise structure functions and we have provided evidence for the presence of a \( k^{-1} \) scaling in the energy spectra, suggesting the presence of attached eddies at transcritical conditions.

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Appendix A: A validation case

We present a validation case of a channel flow at an operating condition that is not affected by transcritical transition, thereby enabling a comparison with DNS benchmark calculations. For this, we consider nitrogen between two isothermal walls kept at $T_w = 300$ K ($T_r = 2.38$) at a bulk pressure of $p_0 = 4.0$ MPa ($p_r = 1.18$). The Mach number is $M < 0.2$ so that the flow can be considered as incompressible. We drive the fluid in the streamwise direction by a constant mass flow rate and the resulting friction Reynolds number is $Re_f \approx 390$. A grid of size $N_x \times N_y \times N_z = 256 \times 256 \times 256$ is used and the grid resolution is $\Delta x^+ \approx 9.6$, $\Delta y^+_{\min} = 0.60$, $\Delta y^+_{\max} = 4.8$, $\Delta z^+ = 6.4$, which is the same as Moser et al. [74]. In Fig. 20 we compare the current calculation with the DNS by Moser et al. [74] at a similar Reynolds number $Re_f = 395$. Since we only consider first and second order statistics in this work, we compare only the mean velocity and the second-order Reynolds stresses with previous DNS. Good agreement between these results is observed.

Appendix B: Grid convergence

We confirm that the grid used in the main text qualifies for DNS. Grid convergence studies have been done in, e.g., Ref. [28], for flows at transcritical conditions, and the purpose of this appendix is to confirm that the conclusions drawn in Ref. [28] are also valid for density ratios considered in the current study. We refer to the grid in the main text as the “regular grid”. In addition, a “coarse grid” calculation and a “fine grid” calculation are performed for the same flow at $N_x \times N_y \times N_z = 272 \times 182 \times 272$ and $N_x \times N_y \times N_z = 543 \times 356 \times 543$, respectively. Table I shows the averaged wall-shear stresses and the wall heat transfer rates at both walls. The values are normalized using the corresponding values of the regular grid calculation for direct comparison. A difference within 3% is found between the two grids and the regular grid. Figure 21 show the mean velocity and the mean temperature profiles as functions of the wall-normal coordinate. Figure 22 shows comparisons of density, compressibility factor, Mach number, viscosity and heat conductivity as a function of the mean temperature. Figure 23 (a) shows the second-order statistics, and Fig. 23 (b) shows the $y$-coordinate normalized using the Kolmogorov length scale. There is no significant difference between different grids, and adequate grid convergence is found between all grids.

In conclusion, the flow is well resolved if a near-wall resolution of $\Delta x^+ \approx \Delta z^+ \lesssim 7$, $\Delta y^+ \lesssim 0.2$
FIG. 21. Profiles of (a) mean velocity and (b) mean temperature as a function of the wall-normal coordinate. The symbols are shown every five grid points for better visualization.

FIG. 22. Density, compressibility factor, Mach number, viscosity and heat conductivity as a function of mean temperature. Symbols are plotted the same way as in Fig. 21. Different quantities are color-coded.

FIG. 23. (a) Mean velocity profiles as a function of the wall-normal coordinate. Symbols are plotted the same way as in Fig. 21. (b) y coordinate normalized using the local Kolmogorov length.
TABLE I. Averaged wall-shear stresses and wall heat transfer rates at both walls. The values are normalized using the corresponding values of the regular grid calculation.

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to 7 is used. The same conclusion may also be found in Ref. [28].


