A novel approach to accurately model heat transfer to supercritical fluids

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1   Abstract

We propose to solve the standard turbulence models on their semi-locally scaled form to considerably increase their accuracy for predicting turbulent heat transfer to supercritical fluids. Many previous studies have shown that current turbulence models are incapable to provide reasonable result for heat transfer calculations [1], which leaves heat exchanger manufactures to rely on empirical correlations in their design process. Using simulations that are based on first principles, i.e. simulations that completely resolve turbulence without using turbulence models, we gained fundamental knowledge on turbulent heat transfer to supercritical fluids [14, 19] that allowed us to considerably improve turbulence models.

2   Introduction

Research in the field of supercritical heat transfer has been active since the fifties to support the thermal design of fossil fueled power plants operating at supercritical pressures. The interest in this field regained momentum in the nineties [21] owing to its potential to improve the thermal efficiency in modern nuclear power plants. Several experiments were conducted during this period using water or CO_2 flowing in heated vertical tubes at supercritical pressures to collect data for heat transfer distributions and wall temperatures. Most of the experiments were conducted in the turbulent regime with high Reynolds numbers. Results from these experiments, especially in upward flows, showed peculiar features of turbulent heat transfer to supercritical fluids such as heat transfer enhancement and deterioration [1]. Peculiar characteristics of heat transfer were often observed when the bulk temperature (T_b) was less than the pseudo-critical temperature (T_{pc}) and the wall temperature (T_w) was higher than the pseudo-critical temperature, namely $T_b < T_{pc} < T_w$. Relevant for the compression process of the supercritical $CO2$ power cycle [26]. Several comprehensive reviews on heat transfer to supercritical fluids have been published by [20, 6, 10, 9, 22, 21, 3] and more recently by [27].

More recently, detailed numerical simulations (direct numerical simulations, DNS) have been performed to study heat transfer to supercritical fluids in turbulent pipe flows by [1, 14]. However, these accurate simulations are limited to simple geometries and low Reynolds numbers. Because of this fact, turbulence models rely on a limited number of accurate data, and their development is

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moreover hampered by the lack of knowledge on how turbulence is affected by strong variations of thermophysical properties, e.g. in the supercritical region. Since all turbulence models have been developed for incompressible flows, several extensions have been proposed in the past by [7, 23, 28] to include compressible effects, but their predictive capability for flows with strong thermophysical property variations is still low.

In this work we propose to use turbulence models in their semi-locally scaled form to properly account for thermo-physical variations. The starting point of the derivation is the semi-locally scaled (SLS) turbulent kinetic energy (TKE) equation, which was derived by Pecnik and Patel [19]. The derivation is based on analytic scaling laws and is therefore applicable, as we will discuss later in this paper, to many eddy viscosity models. The results of the models are then compared to DNS data for a fully developed turbulent channel flow with varying thermo-physical properties [16], and a heated turbulent pipe flow with CO_2 at super-critical pressure [14].

3   SLS turbulence modelling

The semi-local scaling (SLS) as proposed by Huang *et al.* [8], is based on the wall shear stress τ_w and local mean quantities of density ρ and viscosity μ to account for changes in viscous scales due to mean variations in thermophysical properties. The main purpose of the semi-local scaling was to collapse turbulence statistics for compressible flows at high Mach numbers with turbulence statistic for incompressible flows. The semi-locally scaled friction velocity and viscous length scales are defined as, $u_\tau^\star = \sqrt{\tau_w / \langle \rho^* \rangle}$ and $\delta_v^\star = \langle \mu^* \rangle / \langle \rho^* \rangle u_\tau^\star$, respectively, where $\langle \cdot \rangle$ indicated Reynolds averaging. Accordingly, the semi-local wall distance can be defined as

$$y^\star = y/\delta_v^\star,$$

and the semi-local Reynolds number as,

$$Re_\tau^\star = \frac{u_\tau^\star \langle \rho^* \rangle h^*}{\langle \mu^* \rangle} = \sqrt{\frac{\langle \rho^* \rangle}{\rho^*_w}} \frac{\mu^*_w}{\langle \mu^* \rangle} Re_\tau, \tag{1}$$

where $Re_\tau = u_\tau \rho^*_w h^* / \mu^*_w$, is the friction Reynolds number and $u_\tau = \sqrt{\tau_w / \rho^*_w}$, is the friction velocity, both based on viscous wall units. Given the scaling based on wall units and semi-local units, any flow variable can be non-dimensionalized as outlined in table 1.

Instead of using the semi-local scaling as a tool to collapse turbulence statistics for flows with different Mach numbers, Pecnik and Patel [19] extended the use of the SLS to derive an alternative form of the TKE equation for wall-bounded flows with strong variations in thermophysical properties properties. The derived SLS TKE equation then reveals that effects of property variations on turbulence can be characterized by gradients of the semi-local Reynolds number $Re_\tau^\star$ only, and that the additional compressible terms in the TKE equation, such as the solenoidal dissipation, pressure -work, -diffusion and -dilatation, have a minor effect on the change in near-wall turbulence [8, 19]. The SLS TKE reads,

$$t_\tau^\star \frac{\partial \hat{\rho}\hat{k}}{\partial t^*} + \frac{\partial \hat{\rho}\hat{k}\hat{u}_j}{\partial \hat{x}_j} = \hat{P}_k - \hat{\rho}\hat{\varepsilon} + \frac{\partial}{\partial \hat{x}_j} \left[\left(\frac{\hat{\mu}}{Re_\tau^\star} + \frac{\hat{\mu}_t}{\sigma_k} \right) \frac{\partial \hat{k}}{\partial \hat{x}_j} \right], \tag{2}$$

with P_k as the turbulent production and $t_\tau^\star = h^*/u_\tau^\star$. Note, for a fully developed turbulent channel flow the turbulent production can be written as $P_k = \mu_t \left(\partial u / \partial y \right)^2$. If the equation above is used to determine the turbulent shear stress using the Boussinesq approximation, it was shown that the

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Table 1: Comparison of local ϕ and semi-local $\hat{\phi}$ scaling for most relevant quantities. The superscript $*$ denotes dimensional quantities. The subscript 0 indicates a reference condition, most commonly the value at the wall is chosen, denoted by w. h^* is the characteristic length of the flow geometry.

Quantity		Local scaling		Semi-local scaling	Units
Length	$x_i^* =$	$x_i h^*$	$=$	$\hat{x}_i h^*$	$[m]$
Velocity	$u^* =$	$u u_{\tau,0}$	$=$	$\hat{u} u_\tau^\star$	$[m/s]$
Pressure	$p^* =$	$p \rho^*_0 u_{\tau,0}^2$	$=$	$\hat{p} \langle \rho^* \rangle u_\tau^{\star 2}$	$[(kg\ m/s^2)/m^2]$
Density	$\rho^* =$	$\rho \rho^*_0$	$=$	$\hat{\rho} \langle \rho^* \rangle$	$[kg/m^3]$
Dynamic viscosity	$\mu^* =$	$\mu \mu_0^*$	$=$	$\hat{\mu} \langle \mu^* \rangle$	$[kg/(m\ s)]$
Eddy viscosity	$\mu_t^* =$	$\mu_t \rho^*_0 h^* u_{\tau,0}$	$=$	$\hat{\mu}_t \langle \rho^* \rangle h^* u_\tau^\star$	$[kg/(m\ s)]$
Turbulent kinetic energy	$k^* =$	$k u_{\tau,0}^2$	$=$	$\hat{k} u_\tau^{\star 2}$	$[m^2/s^2]$
Turbulent dissipation	$\varepsilon^* =$	$\varepsilon u_{\tau,0}^3/h^*$	$=$	$\hat{\varepsilon} u_\tau^{\star 3}/h^*$	$[m^2/s^3]$
Specific turbulent dissipation	$\omega^* =$	$\omega u_{\tau,0}/h^*$	$=$	$\hat{\omega} u_\tau^\star/h^*$	$[1/s]$
Wall distance	$y^* =$	$y^+ h^*/Re_\tau$	$=$	$y^\star h^*/Re_\tau^\star$	$[m]$

model ($v^2 - f$ model [4]) results significantly improve – if compared to DNS – for turbulent channel flows with strong variations in density and viscosity.

In this work we investigate if other eddy viscosity turbulence models can be used in their semi-locally scaled form as well to improve their predictive capability for flows with large property variations. We chose five models

- an algebraic model developed by Cess in 1958 [2],
- the one-equation model of Spalart-Allmaras (SA) [24],
- the low Reynolds number k-ε model of Myong and Kasagi (MK) [13],
- Menter's shear stress transport (SST) model [12],
- and the four-equations $v^2 - f$ model [4].

In order to change a model into its semi-locally scaled form, it is necessary to set $\rho = 1$, replace μ by $1/Re_\tau^\star$, replace ∂u in P_k by $\partial u^{vD} = \sqrt{\langle \rho^* \rangle / \rho_w^*}\, \partial(\{u^*\}/u_\tau)$, and, if a model makes use of y^+ and/or Re_τ, replace them by $y^\star$ and $Re_\tau^\star$, respectively [19]. Where, $\{\cdot\}$ indicated Favre averaging.

4 Test cases

In order to test the proposed modifications, a fully developed channel flow for a fluid with varying thermo-physical properties similar to those of CO_2 and a heated turbulent pipe flow with a fluid undergoing heat transfer at super-critical pressure are investigated. Tables 2 and 3 describe the test cases simulated in this study for the channel and the pipe flow, respectively.

4.1 Fully developed channel flow

The Favre-averaged Navier-Stokes equations, written in Cartesian coordinates, are used to simulate a fully developed channel flow. The conservation equations for streamwise momentum and energy are solved in non-dimensional form, normalized by values at the channel wall, and are given as,

$$0 = \langle \rho \rangle \langle f_x \rangle + \frac{\partial}{\partial y}\left(\frac{\langle \mu \rangle}{Re_\tau} \frac{\partial \{u\}}{\partial y} \right) - \langle \rho u'' v'' \rangle, \tag{3}$$

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Table 2: Test case investigated for the fully developed channel flow: $CRe_\tau^\star$ - refers to a variable property case with a fluid whose density and viscosity are proportional to $1/T$ and $\sqrt{1/T}$, respectively, such that $Re_\tau^\star$ remains constant across the channel. The DNS data were taken from Patel *et al.* 2016 [18]. $Re_{\tau w}^\star$ and $Re_{\tau c}^\star$ refer to the value of the semi-local Reynolds number at the wall and center of the channel, respectively, while Φ refers to the volumetric heat source.

Case	ρ/ρ_w	μ/μ_w	$Re_{\tau w}^\star$	$Re_{\tau c}^\star$	Φ
Constant $Re_\tau^\star$ $(CRe_\tau^\star)$	$(T/T_w)^{-1}$	$(T/T_w)^{-0.5}$	395	395	95

Table 3: Test cases investigated. A flow with forced convection flow and an upward flow with high buoyancy are considered. The DNS was taken from Nemati *et al.* [14]. The forced convection and the mixed flow are named case A and case C in [14], respectively. $Re_{\tau w}$ is the Reynolds number based on the friction velocity at the pipe inlet, while Q refers to the dimensionless wall heating.

Case	Type	Flow direction	Re_τ	Ri	Q
A	Forced	-	360	0.0	2.4
C	Mixed	Upward	360	-79.67	2.4

$$0 = \frac{1}{Re_\tau Pr_w} \left[\Phi + \frac{\partial}{\partial y} \left(\lambda \frac{\partial \{T\}}{\partial y} \right) \right] + \left\langle \rho v'' H'' \right\rangle, \tag{4}$$

where H, T, and λ are the locally scaled enthalpy, temperature and thermal conductivity, respectively, all normalized with wall quantities. The wall Prandtl number is defined as $Pr_w = \mu_w^* Cp_w^* / \lambda_w^*$, where Cp^* is the isobaric heat capacity. The flow is driven by an external body force, $\langle \rho \rangle \langle f_x \rangle$, which is 1 for the normalized momentum equation. The temperature at both channel walls is maintained constant and the uniform volumetric heat source is increasing the temperature within the channel, such that also density and viscosity change. The Reynolds shear stress and turbulent heat flux, are modelled using the Boussinesq approximation: $-\langle \rho u'' v'' \rangle \approx \mu_t \partial \{u\}/\partial y$ and the gradient diffusion hypothesis $\langle \rho v'' H'' \rangle \approx Cp \, \mu_t / Pr_t \partial \{T\}/\partial y$, respectively. The turbulent Prandtl number is assumed constant as $Pr_t = 1$ [17]. As the normalized conservation equations are solved, the semi-locally scaled eddy viscosity $\hat{\mu}_t$, which is provided by the turbulence model, has to be transformed to the conventionally scaled form μ_t, see table 1.

The result for all turbulence models are now compared with the results obtained by DNS, see figure 1. In all of the resulting plots, the DNS data are plotted using symbols, while the model results are depicted with lines. The results for the velocity are reported in terms of the u/u_{max}, figure 1(a), and $u^\star$, figure 1(b), whereby u_{max} is the maximum DNS velocity and $u^\star = \int_0^{u^{vD}} \left[1 + (y/Re_\tau^\star) \partial Re_\tau^\star / \partial y \right] \partial u^{vD}$ is the universal transformation as given in Patel *et al.* [18]. The Reynolds shear stresses are shown in figure 1(c). The modification clearly improves the performance of the turbulence models for flows with strong variations on the thermo-physical properties. For both profiles of $u^\star$ and $\{u'' v''\}/u_\tau^2$, a good collapse is seen with the DNS data for most of the turbulence models solved in semi-local form, outperforming the conventional models.

4.2 Supercritical carbon dioxide flow in a pipe

The Favre-averaged Navier-Stokes equations, written in cylindrical coordinates, are solved to investigate the heated turbulent pipe flow with a fluid undergoing heat transfer at super-critical pressure. The governing equations for momentum, in radial and streamwise direction, and the energy can be expressed in non-dimensional form, assuming a two-dimensional axis-symmetric flow, without time
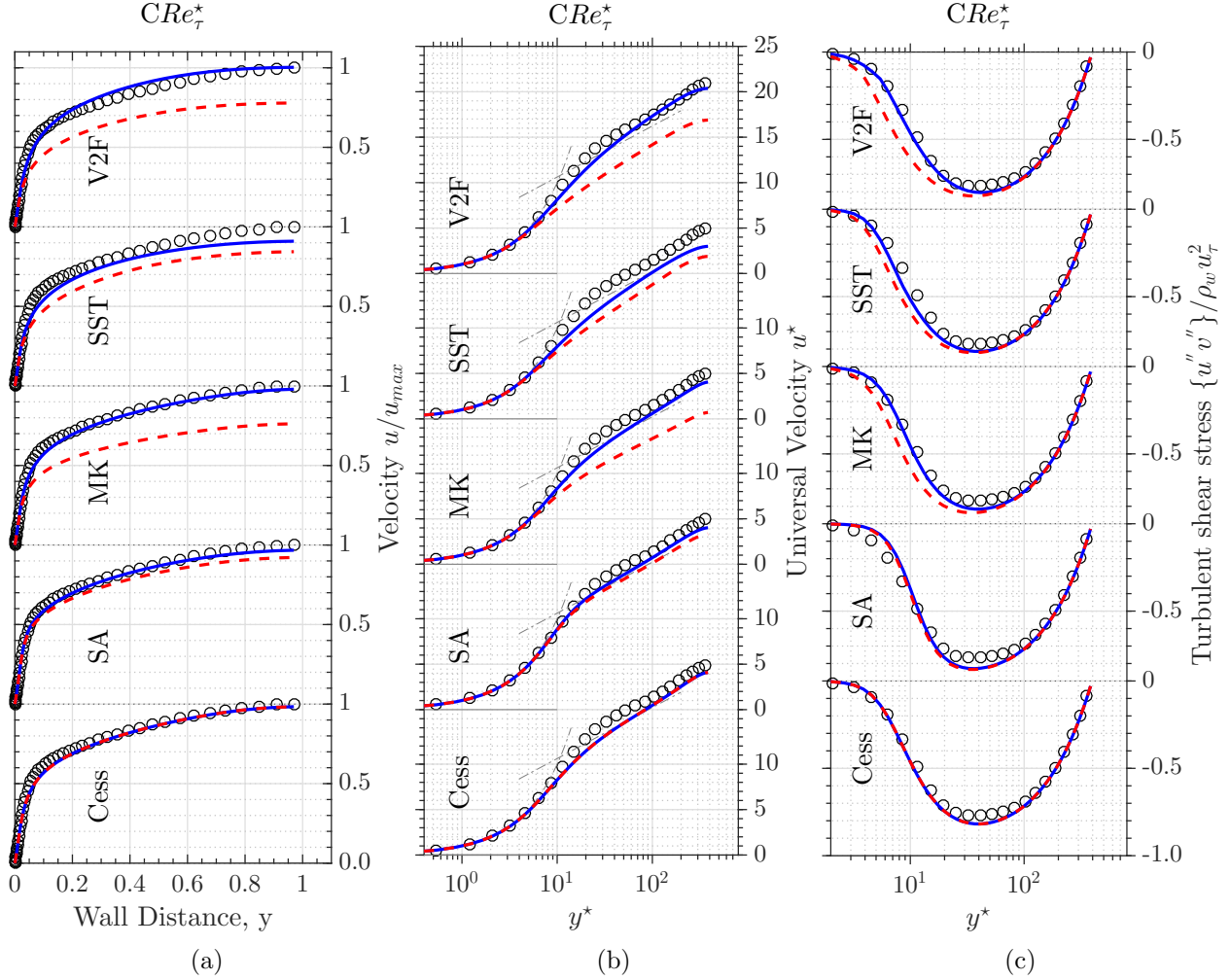
Figure 1: Fully developed turbulent channel flow results, DNS in symbols compared to conventional (dashed red line) and current study (solid blue line) turbulence model for five turbulence models: Cess, Spalart Allmaras, Myong and Kasagi, Menter's shear stress transport and Durban's $v'^2 - f$. (a) Mean velocity by maximum DNS velocity u/u_{max} with respect to the wall-normal distance y, (b) Universal velocity transformation $u^\star$ with respect to the semi-locally scaled wall normal distance $y^\star$, and (c) Semi-locally scaled Reynolds stress $\{u''v''\}/u_\tau^2$ with respect to the semi-locally scaled wall normal distance $y^\star$. The grey dashed line in b) respresent $u^\star = y^\star$ and $u^\star = 1/\kappa \ ln(y^\star) + C^\star$ in the viscous sublayer and log-law region, respectively, where $\kappa = 0.41$ and $C^\star = 5.5$.

derivative as:

$$\frac{\partial \langle \rho \rangle \{u\}^2}{\partial x} + \frac{1}{r} \frac{\partial r \langle \rho \rangle \{u\}\{u_r\}}{\partial r} = -\frac{\partial \langle p \rangle}{\partial x} + \langle \rho \rangle \, Ri_x$$
$$+ \frac{\partial}{\partial x}\left[\left(\frac{\langle \mu \rangle}{Re_\tau} + \mu_t\right)\left(2\frac{\partial \{u\}}{\partial x} - \frac{2}{3}\nabla \cdot \{\mathbf{u}\}\right)\right] + \frac{1}{r}\frac{\partial}{\partial r}\left[r\left(\frac{\langle \mu \rangle}{Re_\tau} + \mu_t\right)\left(\frac{\partial \{u\}}{\partial r} + \frac{\partial \{u_r\}}{\partial x}\right)\right] \tag{5}$$

$$\frac{1}{r}\left[\frac{\partial r \langle \rho \rangle \{u\}\{u_r\}}{\partial x} + \frac{\partial r \langle \rho \rangle \{u_r\}^2}{\partial r}\right] = -\frac{\partial \langle p \rangle}{\partial r} + \frac{1}{r}\frac{\partial}{\partial r}\left[r\left(\frac{\langle \mu \rangle}{Re_\tau} + \mu_t\right)\left(2\frac{\partial \{u_r\}}{\partial r} - \frac{2}{3}\nabla \cdot \{\mathbf{u}\}\right)\right]$$
$$+ \frac{\partial}{\partial x}\left[\left(\frac{\langle \mu \rangle}{Re_\tau} + \mu_t\right)\left(\frac{\partial \{u\}}{\partial r} + \frac{\partial \{u_r\}}{\partial x}\right)\right] - \frac{1}{r}\left(\frac{\langle \mu \rangle}{Re_\tau} + \mu_t\right)\left(\frac{2\{u_r\}}{r} - \frac{2}{3}\nabla \cdot \{\mathbf{u}\}\right) \tag{6}$$

$$\frac{\partial \langle \rho \rangle \{H\}\{u\}}{\partial x} + \frac{1}{r}\frac{\partial r \langle \rho \rangle \{H\}\{u_r\}}{\partial r} = \frac{1}{r}\left[\frac{\partial}{\partial r}r\left(\frac{\langle \lambda \rangle}{Re_\tau Pr} + \frac{\mu_t}{Pr_t}\right)\frac{\partial \{H\}}{\partial r}\right]$$
$$+ \left[\frac{\partial}{\partial x}\left(\frac{\langle \lambda \rangle}{Re_\tau Pr} + \frac{\mu_t}{Pr_t}\right)\frac{\partial \{H\}}{\partial x}\right] \tag{7}$$

where u_r is the radial velocity component, $\nabla \cdot \{\mathbf{u}\}$ is the divergence of the velocity vector in cylindrical coordinates, and $Ri = g_x h/u_\tau{}^2$ is the Richardson number that takes into account the buoyancy effects with g_x the gravitational acceleration. Moreover, the turbulence models are solved in cylindrical coordinates with buoyancy production G_k in the k-, ε- and ω-equation. In order to estimate the thermo-physical properties of the supercritical CO_2, a multi-parameter equation of state (Kunz and Wagner [11]) is used. The relations between the viscosity and thermal conductivity are given by Fenghour *et al.* [5] and Vesovic *et al.* [25], respectively.

The simulation of the super-critical fluid in the heated pipe consists of two parts. First, a fully developed pipe flow with periodic inlet and outlet boundaries, and no heat transfer from the wall is used to generate the inflow for the developing simulation. Later, a developing pipe flow uniformly heated from the wall is simulated. Two cases are considered, which are reported in table 3. For all the simulations of the supercritical CO_2 flow in a pipe, the inflow conditions correspond to $p_0 = 80 \; bar$ and $T_0 = 301 \; K$. Therefore by heating the pipe, the pseudo-critical conditions are achieved. In the supercritical the transport properties such as the density, viscosity and thermal conductivity show strong gradients.

Figures 2 and 3 show the comparison of the temperature along the pipe wall between DNS (Nemati *et al.* [15]) and the different turbulence models, solved in their conventional and semi-locally scaled form, respectively. For the case of forced convection (figure 2), while for the SA, MK and V2F models, the results for the wall temperature improve, it can be seen that the SST model shows the best agreement with DNS if it is solved in its conventional form. The largest improvement using the semi-locally scaled model is achieved with the V2F model, whereas the conventional V2F significantly over-predicts the wall temperature. In general, it can be seen that using the semi-locally scaled form of the turbulence models, all results are more consistent.

For the case with high buoyancy, shown in figure 3 ($Ri = -79.67$), the flow experiences both heat transfer deterioration and recovery according to the DNS data. The heat transfer deterioration can be noticed by the increase of wall temperature at the beginning of the heated pipe ($x/L < 20$), while afterwards the wall temperature decreases, indicating a better heat transfer and thus a heat transfer recovery. The deterioration and recovery are estimated by the turbulence models with and without modifications. However an over-prediction of the wall temperature is seen in all cases. Moreover, the V2F strongly over emphasises the heat transfer deterioration and recovery. For this specific case, the SLS versions of SA, V2F, and MK are closer to the DNS data. The most likely reason for over predicted wall temperatures using the turbulence model is the crude approximation
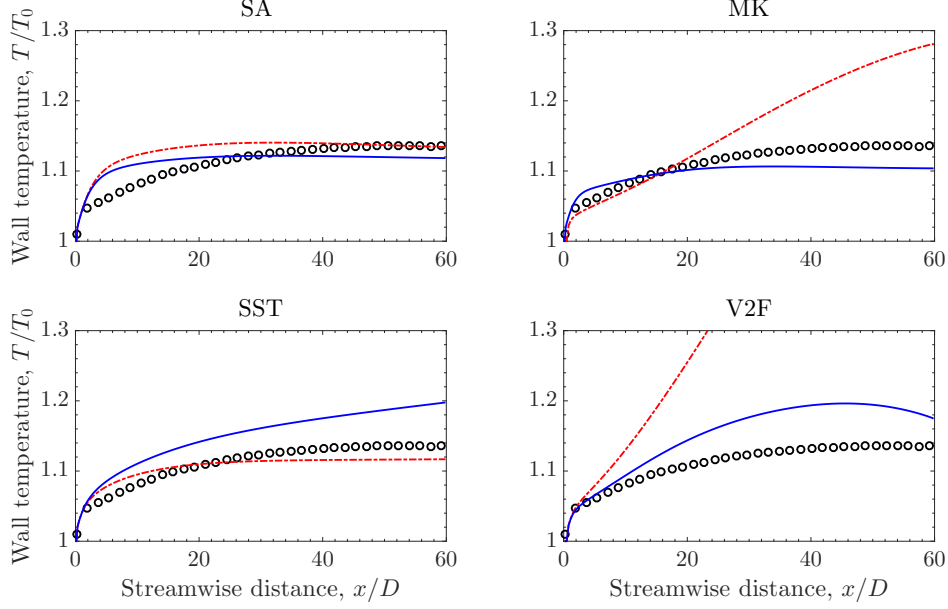
Figure 2: Case A: Wall temperature with respect to the streamwise distance for a heated pipe flow with CO_2 at supercritical pressure under forced convection. DNS results in symbols compared to conventional (dashed red line) and current study (solid blue line) turbulence model for four turbulence models: Spalart Allmaras, Myong and Kasagi, Menter's shear stress transport and Durban's $v'^2 - f$.

of the buoyancy production term (G_k). The buoyancy production term we used for the turbulence models is calibrated for a fluid that obeys the ideal gas law. In order to improve the model results, it is thus necessary to develop better models for the buoyancy production term that is based on DNS of supercritical fluid flows.

5   Conclusion

Solving the turbulent transport equations in semi-local scaled form make turbulence models more reliable for wall bounded flows with strong gradients in the thermo-physical properties. The methodology is based on the semi-local scaling of the turbulent transport equations, which has shown excellent agreement with DNS data in previous work. Even though, the semi-locally scaled turbulent equations do not take into account common compressibility terms, such as; pressure work term and pressure dilation, the compressibility effects are taken into account by the semi-locally scaled variables. In general, the semi-locally scaled turbulence models result in a better agreement with the DNS data in terms of the velocity profile and the heat transfer for the investigated cases herein. Interestingly, the original Spalart-Allmaras model, the one equation turbulence model originally developed for external flow, gives the most reliable results, if compared to other standard models, for the variable property cases investigated herein. However, we recommend to use Myong and Kasagi's low Reynolds number model with the method of this study for supercritical CO_2 application as it is a simple model, if compared to the SST and V2F model, and a better approximation of the buoyancy production G_k can be found in literature, the SA has no k-equation and therefore no buoyancy production term.
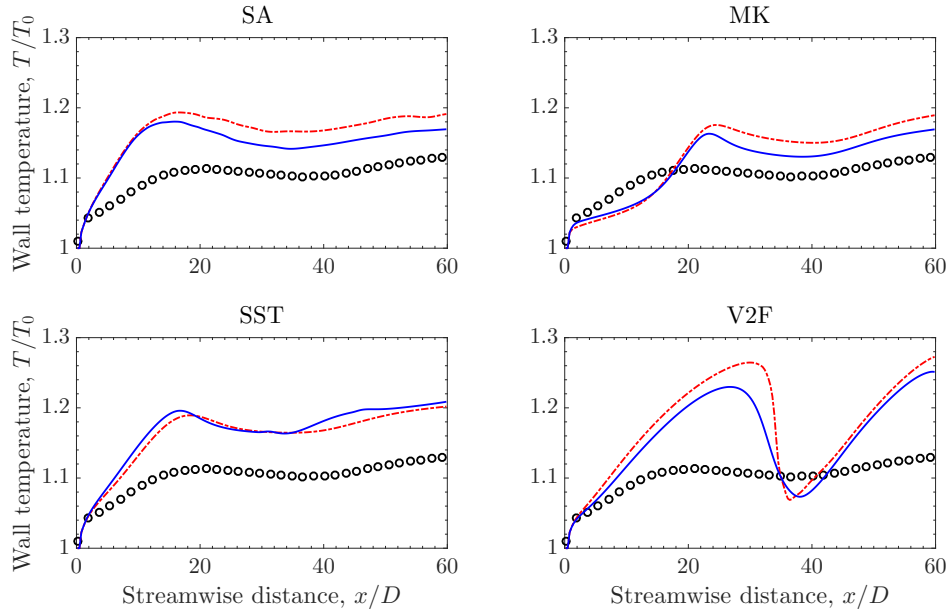
Figure 3: Case C: Wall temperature with respect to the streamwise distance for a heated pipe flow with CO_2 at supercritical pressure under mixed flow and upward flow with average buoyancy $Ri = -79.67$. DNS results in symbols compared to conventional (dashed red line) and current study (solid blue line) turbulence model for four turbulence models: Spalart Allmaras, Myong and Kasagi, Menter's shear stress transport and Durban's $v'^2 - f$.

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