RESEARCH ARTICLE

Zonal PANS: evaluation of different treatments of the RANS-LES interface

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The partially averaged Navier-Stokes (PANS) model, proposed by Girimaji [1], can be used to simulate turbulent flows either as RANS, LES or DNS. Its main parameter is f_k whose physical meaning is the ratio of the modeled to the total turbulent kinetic energy. In RANS $f_k = 1$, in DNS $f_k = 0$ and in LES f_k takes values between zero and one.

Three different ways of prescribing f_k are evaluated for decaying grid turbulence and fully-developed channel flow: $f_k = 0.4$, $f_k = k_{tot}^{3/2}/\varepsilon$ [2] and from its definition $f_k = k/k_{tot}$ where k_{tot} is the sum of the modeled, k , and resolved, k_{res} , turbulent kinetic energy. It is found that the $f_k = 0.4$ gives the best results.

In [3], a method was proposed to include the effect of the gradient of f_k . This approach is used at RANS-LES interface in the present study. Four different interface models are evaluated in fully developed channel flow and embedded LES of channel flow; in both cases, PANS is used as a zonal model with $f_k = 1$ in the URANS region and $f_k = 0.4$ in the LES region. In fully developed channel flow, the RANS-LES interface is parallel to the wall (horizontal) and in embedded LES it is parallel to the inlet (vertical).

The importance of the location of the horizontal interface in fully developed channel flow is also investigated. It is found that the location – and the choice of the treatment at the interface – may be critical at low Reynolds number or if the interface is placed too close to the wall. The reason is that the modeled turbulent shear stress at the interface is large and hence the relative strength of the resolved turbulence is small. In RANS, the turbulent viscosity – and consequently also the modeled Reynolds shear stress – is only weakly dependent on Reynolds number. It is found in the present work that that also applies in the URANS region.

Keywords: LES; PANS; 2G-RANS; Zonal model; Embedded LES; Hybrid RANS-LES; RANS-LES interface condition

1. Introduction

Large Eddy Simulation (LES) is very expensive in wall-bounded flow. To be able to extend LES to high Reynolds number many proposals have been made in the literature to combine LES with unsteady RANS (URANS) near the walls. The first and most common method is Detached Eddy Simulation (DES) [4–6]. Later, other researchers have proposed hybrid LES/RANS [7, 8] and Scale-Adapted Simulations (SAS) [9, 10]; for a review, see [11]. DES and hybrid LES/RANS use the cell size as the SGS length scale. SAS does not use the cell size (except as a limiter) but uses the von Kármán lengthscale instead.

The main object of the methods mentioned above is that they reduce the turbulent viscosity in the LES region. There are three options to achieve this.

- (1) The turbulent viscosity, ν_t , is reduced by modifying its formulation;
- (2) The dissipation term in the equation for the modeled, turbulent kinetic

- energy, k , is increased by decreasing the turbulent lengthscale, or
 (3) the destruction term in the lengthscale equation (ε or ω) is decreased. This
 increases the dissipation term in the k equation as well as decreases the
 turbulent viscosity directly since ε (or ω) appears in the denominator of
 the expression for ν_t .

DES [12] is based on the first option. X-LES [13] and the one-equation hybrid
 LES-RANS [8, 14] use option number two: ν_t is decreased and the dissipation term
 in the k equation is increased. The third option is used in the partially averaged
 Navier-Stokes (PANS) model [1] and the Partially Integrated Transport Model
 (PITM) [15, 16]. PANS is used as a zonal LES-RANS method in the present work
 where RANS is used near the walls and LES is employed further away from the
 walls. We will also use PANS in embedded LES.

Much work has been presented on embedded LES lately. Menter et al. [17] present
 embedded LES of channel flow and the hump flow. They use the SST RANS model
 upstream of the embedded LES interface. Downstream of the interface they use the
 model of Shur et al. [6] which consists of the Smagorinsky model in the LES region
 and a mixing-length model in the RANS region. At the interface, the modeled
 turbulence is converted into resolved turbulence using synthetic turbulence from a
 vortex method [18].

Shur et al. [19] proposed a new recycling method in a interface zone between
 RANS and LES. The RANS and LES zones overlap and identical grids are used in
 the overlap region. Only the fluctuating components are recycled since the mean
 components are available in the entire overlap zone. They evaluated the method
 for flat plate boundary flow and flow over a two-dimensional airfoil.

Poletto et al. [20] made embedded LES of the hump flow. They used Delayed
 Detached Eddy Simulation (DDES) in the entire region (both upstream and down-
 stream of the interface). At the LES interface they added synthetic fluctuations
 from the divergence free synthetic eddy method [21].

Gritskevich et al. [22] used the Improved Delayed Detached Eddy Simulation
 (IDDES) to make embedded LES of the hump flow. They first computed the entire
 flow with 2D RANS. Then they used the RANS solution to prescribe the inlet
 mean velocity profile at the embedded LES interface. The modeled k was taken
 from the RANS solution and ω was computed from k and the grid size. Synthetic
 fluctuations were generated with a synthetic turbulence generator [23].

Shur et al. [24] present embedded LES of the flow over a hump. They used over-
 lapping RANS and IDDES in the embedded interface region. At the interface they
 added synthetic turbulence. They show very good agreement with measurement
 data.

Xiao and Jenny [25] presented a novel method for treating the RANS-LES inter-
 face in hybrid LES-RANS. They solved the RANS and LES equations in the entire
 domain. The RANS mesh in the LES region does not need to be the same as the
 LES mesh and vice versa. Drift forces were added in the overlapping regions.

As mentioned above, the PANS model is in the present work used both as a
 zonal hybrid LES-RANS model. f_k is set to one in the RANS regions, and it is
 set to 0.4 in the LES region. The interface between the RANS and LES regions is
 defined along a grid plane, an approach also chosen in ZDES [26]. As an alternative
 to using a constant f_k in the LES region, f_k can be computed using the cell size
 and the integral length scale, $k_{tot}^{3/2}/\varepsilon$ [2], where k_{tot} is the sum of the resolved
 and the modeled turbulent kinetic energy, i.e. $k_{tot} = k_{res} + k$. The reason why f_k
 is not computed in the present study is that it has been shown that a constant
 $f_k = 0.4$ works well in the LES region [27–30]; it was even shown in [30] that
 using constant $f_k = 0.4$ works better than computing f_k , not to mention that

it is numerically more stable. Section 4 compares three alternatives ($f_k = 0.4$, computing f_k according to the equation above, and computing f_k from its definition k/k_{tot}) for decaying homogeneous grid turbulence and fully developed channel flow. It should be mentioned that Basara et al. [2] have shown that computing f_k works well when using the $k - \varepsilon - \zeta - f$ model.

In [3], a method was proposed to include the effect of the gradient of f_k . The gradient appears because the PANS filtering operation does not commute with the spatial gradient. At RANS-LES interfaces, the spatial gradient of f_k is large. The approach of Girimaji and Wallin [3] is further developed in the present study and it is used at RANS-LES interfaces.

The appearance of the gradient of f_k at RANS-LES interfaces is similar to the method for treating RANS-LES interfaces in Hamba [31]. He shows that when the filter size varies, an additional term appears because the filtering and the spatial gradients do not commute. The divergence of a flux, q_i , for example, will include an additional term

$$\overline{\frac{\partial q_i}{\partial x_i}} = \frac{\partial \bar{q}_i}{\partial x_i} - \frac{\partial \Delta}{\partial x_i} \frac{\partial \bar{q}_i}{\partial \Delta} \quad (1)$$

Chaouat and Schiestel [32] used the approach in [31] to modify their PITM approach. They derived the modified transport equations including commutation terms as in Eq. 1. The gradients of the filter width, Δ , was replaced with gradient of the cut-off wavenumber, κ_c , which appear in the PITM approach. The method proposed by Hamba [31] was recently further developed and evaluated by Davidson [33] at RANS-LES interfaces using the PDH $k - \omega$ model [34].

The modified approach of including the effect of the gradient of f_k is in the present study evaluated in fully developed channel flow and embedded LES of channel flow; in both cases, PANS is used as a zonal model. In fully developed channel flow, the RANS-LES interface is parallel to the wall and in embedded LES it is parallel to the inlet.

When the RANS-LES interface is parallel to the wall, the term including the gradient of f_k across the interface can be both positive and negative (because v' is both positive and negative). This term is included only when it reduces the modeled turbulence. Hence, the term can be seen as a *forcing* term which represents backscatter. It is used to stimulate growth of the resolved turbulence in the LES region adjacent to the RANS region. The present method reduces the gray area problem described in [35].

The paper is organized as follows. The next section describes the equations and the interface models. The following section describes the numerical method. Then there is a section comparing three different ways of treating f_k , followed by a section which presents and discusses the results. The final section presents the conclusions.

136 2. The PANS Model

137 The low-Reynolds number partially averaged Navier-Stokes (LRN PANS) turbu-
138 lence model reads [27]

$$\begin{aligned}
 \frac{Dk}{Dt} &= \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_{ku}} \right) \frac{\partial k}{\partial x_j} \right] + P_k + P_{k_{tr}} - \varepsilon \\
 \frac{D\varepsilon}{Dt} &= \frac{\partial}{\partial x_j} \left[\left(\nu + \frac{\nu_t}{\sigma_{\varepsilon u}} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{\varepsilon 1} P_k \frac{\varepsilon}{k} - C_{\varepsilon 2}^* \frac{\varepsilon^2}{k} \\
 \nu_t &= C_\mu f_\mu \frac{k^2}{\varepsilon}, P_k = 2\nu_t \bar{s}_{ij} \bar{s}_{ij}, \bar{s}_{ij} = \frac{1}{2} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \\
 C_{\varepsilon 2}^* &= C_{\varepsilon 1} + \frac{f_k}{f_\varepsilon} (C_{\varepsilon 2} f_2 - C_{\varepsilon 1}), \sigma_{ku} \equiv \sigma_k \frac{f_k^2}{f_\varepsilon}, \sigma_{\varepsilon u} \equiv \sigma_\varepsilon \frac{f_k^2}{f_\varepsilon} \\
 \sigma_k &= 1.4, \sigma_\varepsilon = 1.4, C_{\varepsilon 1} = 1.5, C_{\varepsilon 2} = 1.9, C_\mu = 0.09, f_\varepsilon = 1
 \end{aligned} \tag{2}$$

139 where $D/Dt = \partial/\partial t + \bar{u}_j \partial/\partial x_j$ denotes the material derivative. The damping
140 functions are defined as

$$\begin{aligned}
 f_2 &= \left[1 - \exp \left(- \frac{y^*}{3.1} \right) \right]^2 \left\{ 1 - 0.3 \exp \left[- \left(\frac{R_t}{6.5} \right)^2 \right] \right\} \\
 f_\mu &= \left[1 - \exp \left(- \frac{y^*}{14} \right) \right]^2 \left\{ 1 + \frac{5}{R_t^{3/4}} \exp \left[- \left(\frac{R_t}{200} \right)^2 \right] \right\} \\
 R_t &= \frac{k^2}{\nu \varepsilon}, \quad y^* = \frac{U_\varepsilon y}{\nu}, \quad U_\varepsilon = (\varepsilon \nu)^{1/4}
 \end{aligned} \tag{3}$$

141 The term $P_{k_{tr}}$ in Eq. 2 is an additional term which is non-zero in the interface
142 region because $Df_k/Dt \neq 0$. The function f_ε , the ratio of the modeled to the total
143 dissipation, is set to one since the turbulent Reynolds number is high. f_k is set to
144 1 in the RANS region and to 0.4 in the LES region (in Section 4 it may also be
145 computed in the LES region).

146 It was shown in [30] that the k and ε equations in the LES region are in local
147 equilibrium, i.e.

$$\langle P_k \rangle - \langle \varepsilon \rangle = 0 \tag{4}$$

148

$$\left\langle C_{\varepsilon 1} \frac{\varepsilon}{k} P_k \right\rangle - \left\langle C_{\varepsilon 2}^* \frac{\varepsilon^2}{k} \right\rangle = 0 \tag{5}$$

149 ($\langle \cdot \rangle$ denotes averaging in all homogeneous directions, i.e. t, z and, in fully developed
150 channel flow, also x). It seems that Eqs. 4 and 5 cannot both be satisfied since
151 $C_{\varepsilon 1} \neq C_{\varepsilon 2}^*$; indeed, the equations are not satisfied instantaneously for which the
152 convective terms play an important role. Equation 5 is satisfied but

$$C_{\varepsilon 1} \frac{\langle \varepsilon \rangle}{\langle k \rangle} \langle P_k \rangle - C_{\varepsilon 2}^* \frac{\langle \varepsilon^2 \rangle}{\langle k \rangle} \neq 0. \tag{6}$$

153 Equations 4 and 5 are both satisfied because the correlation between ε, k^{-1} and
154 P_k (left side of Eq. 5) is stronger than that between ε^2 and k^{-1} (right side). The

155 correlation between the quantities on the left side is larger than that on the right
 156 side because $C_{\varepsilon 2}^* > C_{\varepsilon 1}$. For more detail, see [30].

157 2.1. The Interface Condition

158 The commutation error in PANS was recently addressed in [3]. In PANS, the equa-
 159 tion for the modeled turbulent kinetic energy, k , is derived by multiplying the
 160 k_{tot} equation ($k_{tot} = k_{res} + k$) by f_k . The convective term in the k equation with
 161 constant f_k is then obtained as

$$f_k \frac{Dk_{tot}}{Dt} = \frac{D(f_k k_{tot})}{Dt} = \frac{Dk}{Dt} \quad (7)$$

162 where

$$f_k = \frac{k}{k_{tot}}. \quad (8)$$

163 Now, if f_k varies in space, we get instead

$$f_k \frac{Dk_{tot}}{Dt} = \frac{D(f_k k_{tot})}{Dt} - k_{tot} \frac{Df_k}{Dt} = \frac{Dk}{Dt} - k_{tot} \frac{Df_k}{Dt} \quad (9)$$

164 Since f_k in the present work is constant in time, $Df_k/Dt = \bar{u}_i \partial f_k / \partial x_i$. The second
 165 term on the right side of Eq. 9 is the commutation term; it represents (excluding
 166 the minus sign) energy transfer from resolved to modeled turbulence. It can be
 167 written (on the right side of the k equation)

$$k_{tot} \frac{Df_k}{Dt} = (k + k_{res}) \frac{Df_k}{Dt} = k \frac{Df_k}{Dt} + \frac{\langle \bar{u}_i' \bar{u}_i' \rangle}{2} \frac{Df_k}{Dt} \quad (10)$$

168 The commutation term in the k_{res} equation is the same but with opposite sign, i.e.

$$-k \frac{Df_k}{Dt} - \frac{\langle \bar{u}_i' \bar{u}_i' \rangle}{2} \frac{Df_k}{Dt} \quad (11)$$

169 The question is now which term should be added to the momentum equations
 170 to get the commutation term in the k_{res} equation. We start by the second term in
 171 Eq. 11. This term can be represented by the source term

$$S_i^1 = -\frac{1}{2} \bar{u}_i' \frac{Df_k}{Dt} \quad (12)$$

172 in the momentum equation. To show that this term corresponds to the commuta-
 173 tion term in Eq. 11, consider the momentum equation for the fluctuating velocity,
 174 $\bar{u}_i'$. Multiplying S_i^1 by $\bar{u}_i' = \bar{u}_i - \langle \bar{u}_i \rangle$ and time-averaging gives the source term in
 175 the k_{res} equation as

$$-\left\langle (\bar{u}_i - \langle \bar{u}_i \rangle) \frac{1}{2} \bar{u}_i' \frac{Df_k}{Dt} \right\rangle = -\left\langle \frac{1}{2} \bar{u}_i' \bar{u}_i' \frac{Df_k}{Dt} \right\rangle = -\frac{1}{2} \langle \bar{u}_i' \bar{u}_i' \rangle \frac{Df_k}{Dt} \quad (13)$$

176 Equation 13 is equal to the time average of the second term in Eq. 11 as it should.

Figure 1. Fully developed channel flow. The URANS and the LES regions.

Figure 2. Embedded LES. Vertical thick line shows the interface at $x_I = 0.95$. f_k varies linearly in the gray area (width x_{tr}) from 1 to 0.4. $\delta = 1$.

177 A term corresponding to the first term in Eq. 11 can be added as a source term
 178 in the momentum equation as

$$S_i^2 = -\frac{\langle k \rangle \bar{u}_i'}{\langle \bar{u}_m' \bar{u}_m' \rangle} \frac{Df_k}{Dt} \quad (14)$$

179 Multiplying S_i^2 by $\bar{u}_i'$ and time averaging gives

$$-\frac{\langle k \rangle \langle \bar{u}_i' \bar{u}_i' \rangle}{\langle \bar{u}_m' \bar{u}_m' \rangle} \frac{Df_k}{Dt} \simeq -\langle k \rangle \frac{Df_k}{Dt} \quad (15)$$

180 where we assume that the correlation between k and $\bar{u}_i'$ is weak. Equation 15 is
 181 equal to the time average of the first term in Eq. 11 as it should.

182 In [3], the second term on the right side of Eq. 9 is represented by introducing an
 183 additional turbulent viscosity, ν_{tr} , in a diffusion term in the momentum equation
 184 as

$$\frac{\partial}{\partial x_j} (\nu_{tr} \bar{s}_{ij}), \quad \bar{s}_{ij} = \frac{1}{2} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \quad (16)$$

185 where

$$\nu_{tr} = \frac{P_{k_{tr}}}{|\bar{s}|^2}. \quad (17)$$

186 The term, $P_{k_{tr}}$, is computed as

$$P_{k_{tr}} = k_{tot} \frac{Df_k}{Dt} \quad (18)$$

Figure 3. Control volume, P , in the LES region adjacent to the interface.

187 $P_{k_{tr}}$ is an additional production term in the k equation, see Eq. 2. In [3], $P_{k_{tr}}$ is
 188 re-written using Eq. 8 as

$$P_{k_{tr}} = \frac{k}{f_k} \frac{Df_k}{Dt} \quad (19)$$

189 2.2. Modeling the Interface

190 The gradient of f_k across a RANS-LES interface gives rise to an additional term in
 191 the momentum equations and the k equation. In the present work, these terms are
 192 included only when the flow goes from a RANS region to an LES region. The effect
 193 of these terms will reduce k and act as a forcing term in the momentum equations.
 194 Four different models are investigated.

195 2.2.1. Interface Model 1

196 This is based on the approach suggested in [3]. The additional turbulent viscosity,
 197 ν_{tr} , gives an additional production term, $P_{k_{tr}}$, in the k equation, see Eq. 19. Since
 198 we are interested in stimulating resolved turbulence in the LES region adjacent to
 199 the RANS region, only negative values of ν_{tr} are included. A negative ν_{tr} means
 200 physically transfer of kinetic energy from modeled to resolved. It is found that the
 201 magnitude of the positive values of ν_{tr} is actually larger than the magnitude of
 202 the negative ones, which means that $\langle \nu_{tr} \rangle > 0$. The negative values correspond
 203 to $Df_k/Dt < 0$ (see Eqs. 17, 18 and 19), i.e. when a fluid particle in a RANS
 204 region passes the interface into an adjacent LES region. However, ν_{tr} takes such
 205 large (negative) values that $\nu_t + \nu_{tr} < 0$. To stabilize the simulations, it was found
 206 necessary to introduce a limit $\nu_t + \nu_{tr} > 0$ in the diffusion term in the momentum
 207 equation. No such limit is used in the k equation, and hence $P_k + P_{k_{tr}}$ is allowed
 208 to go negative.

209 2.2.2. Interface Model 2

210 This model is identical to Model 1 except that Eq. 18 is used instead of Eq. 19.
 211 k_{tot} in Eq. 18 is defined as

$$k_{tot} = k + \frac{1}{2} \langle \bar{u}_i' \bar{u}_i' \rangle_{r.a} \quad (20)$$

where subscript *r.a.* denotes running average. Is is averaged in all homogeneous directions including time (note that time is not a homogeneous direction in decaying grid turbulence, see Section 4.1). Since k_{tot} is mostly larger than k/f_k [30], this approach will give a larger magnitude of the (negative) production than Model 1. It will be seen that this modification is of utmost importance.

2.2.3. Interface Model 3

The right side of Eq. 10 is added to the k equation, but only when the flow goes from a RANS region to an LES region (i.e. $Df_k/Dt < 0$), i.e.

$$P_{k_{tr}} = k_{tot} \min \left(\frac{Df_k}{Dt}, 0 \right) \quad (21)$$

where k_{tot} is computed as in Eq. 20. The production term $P_{k_{tr}} < 0$ which means that it reduces k as it should. The sum of the S_i^1 and S_i^2 terms (see Eqs. 12 and 14) in the momentum equations read

$$S_i = - \min \left(\frac{Df_k}{Dt}, 0 \right) \left(0.5 + \frac{\langle k \rangle}{\langle \bar{u}'_m \bar{u}'_m \rangle_{r.a.}} \right) \bar{u}'_i \quad (22)$$

Since $Df_k/Dt < 0$, the source S_i has the same sign as $\bar{u}'_i$; this means that the source enhances the resolved turbulence as it should.

It may be noted that Df_k/Dt in Eq. 21 assumes the correct (i.e. negative) sign irrespectively of the orientation of the RANS-LES interface. Consider, for example, the RANS-LES interfaces at the lower and upper wall in fully-developed channel flow (Fig. 1). For these interfaces, the gradient of f_k in Eq. 21 reads $\bar{v} \partial f_k / \partial y$. When a fluid particles at the lower interface goes from the RANS region to the LES region, $\bar{v} > 0$ and $\partial f_k / \partial y < 0$ so that $\bar{v} \partial f_k / \partial y < 0$ as intended. Also for the upper interface we get $\bar{v} \partial f_k / \partial y < 0$ since $\bar{v} < 0$ and $\partial f_k / \partial y > 0$. For non-cartesian grids the material derivative, $Df_k/Dt < 0$, has to be formulated in local grid coordinates.

It is however found that the forcing often becomes too strong when S_i is added to the momentum equation. The effect of adding or neglecting S_i in the momentum equations is evaluated in Section 5.

The differences between Model 3 and 2 are that

- When $S_i = 0$, no explicit modification is made in the momentum equation in Model 3 (recall that $-\nu < \nu_{tr} < 0$ is used in the momentum equation in Models 1 and 2).
- Model 2 (and Model 1) may need regularization in case $|\bar{s}| \rightarrow 0$ in the denominator of ν_{tr} in Eq. 18. No such regularization, however, is used in the present work. It can be argued that the commutation term in Model 3 is introduced in a more physical way compared to Models 1 and 2 where artificially negative viscosities are used.

2.2.4. Interface Model 4

This interface model was developed in [30] for horizontal interfaces. The modeled turbulent kinetic energy in the LES region adjacent to the interface is reduced by setting the usual convection and diffusion fluxes of k at the interface to zero. New fluxes are introduced in which the interface condition is set to $k_{int} = f_k k_{RANS}$ ($f_k = 0.4$), where k_{RANS} is the k value in the cell located in the URANS region adjacent to the interface. No modification is made for the convection and diffusion of ε across the interface. The implementation is presented in some detail below.

We write the discretized equation in the y direction (see Figs. 1 and 3) as [36]

$$a_P k_P = a_N k_N + a_S k_S + S_U, \quad a_P = a_S + a_N - S_P$$

where a_S and a_N include to the convection and diffusion through the south and north face, respectively, and S_U and $S_P k_P$ include the production and the dissipation term, respectively. For a cell in the LES region adjacent to the interface (cell P), a_S is set to zero, setting the usual convection and diffusion fluxes to zero. New fluxes, including f_k , are incorporated in additional source terms as

$$\begin{aligned} S_U &= (C_s + D_s) f_k k_S, \quad S_P = -(C_s + D_s) \\ C_s &= \max(\bar{v}_s A_s, 0), \quad D_s = \frac{\mu_{tot} A_s}{\Delta y} \end{aligned} \quad (23)$$

where C_s and D_s denote convection (first-order upwind) and diffusion, respectively, through the south face, and A_s is the south area of the cell. As can be seen, the k_S is multiplied by f_k and hence the new convective flux is a factor f_k smaller than the original one. Also the diffusion flux is smaller; it is $D_s(f_k k_S - k_P)$ compared with the original flux $D_s(k_S - k_P)$.

The treatment of the k equation for a vertical interface (the embedded interface in the channel flow) is exactly the same as for a horizontal interface. The difference is that an interface condition is needed also for the ε equation which reads [28]

$$\varepsilon_I = C_\mu^{3/4} \frac{k_I^{3/2}}{\ell_{sgs}}, \quad \Delta = V^{1/3}, \quad C_S = 0.1, \quad \ell_{sgs} = C_S \Delta \quad (24)$$

where subscript I denotes inlet or interface; V is the volume of the cell. The sensitivity to the value of the Smagorinsky coefficient, C_S , was investigated in [30] and was found to be weak.

3. Mean flow equations and numerical method

The momentum equations with an added turbulent viscosity reads

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial \bar{u}_j \bar{u}_i}{\partial x_j} = \delta_{1i} - \frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left((\nu + \nu_t) \frac{\partial \bar{u}_i}{\partial x_j} \right) + S_i \quad (25)$$

where the first term on the right side is the driving pressure gradient in the stream-wise direction, which is used only in the fully-developed channel flow simulations. The last term on the right side is the additional source term in Model 3, see Eq. 22. The effect of this term is shown in Figs. 15 and 25.

An incompressible, finite volume code is used [7]. The numerical procedure is based on an implicit, fractional step technique with a multigrid pressure Poisson solver and a non-staggered grid arrangement. For the momentum equations, second-order central differencing is used for the fully developed channel flow. For the embedded channel flow, we use the second-order upwind [37] scheme in the RANS region upstream of the interface and second-order central differencing in the LES region downstream of the interface. The Crank-Nicolson scheme is used in the time domain and the first-order hybrid central/upwind scheme is used in space for solving the k and ε equations.

Figure 4. DHIT, decaying turbulence. — : 32^3 ; - - : 64^3 ; - · - : 128^3 .

278 4. Should f_k be constant or should it be computed?

279 The physical meaning of f_k is the ratio of modeled to total turbulent kinetic energy,
 280 see Eq. 8. Hence it is expected that it should be smaller when the grid is refined.
 281 One way to compute f_k is as proposed by [2]

$$f_k = C_\mu^{-1/2} \left(\frac{\Delta}{L_t} \right)^{2/3}, \quad L_t = \frac{k_{tot}^{3/2}}{\varepsilon}, \quad \Delta = (\Delta V)^{1/3} \quad (26)$$

282 Kenjeres and Hanjalic [38] have made a slightly different proposal which reads

$$f_k = \frac{\Delta}{L_t} \quad (27)$$

283 This expression was found to give far too small f_k and hence the formula in Eq. 26
 284 was chosen for evaluation.

285 Since the running average of k_{tot} is computed in Model 2 and 3, the option of
 286 computing f_k from its definition is also evaluated, i.e.

$$f_k = \frac{k}{k_{tot}} \quad (28)$$

287 where k_{tot} is computed using the running average (see Eq. 20); the instantaneous
 288 value of k is used.

289 In this section we evaluate the difference between computing f_k from Eq. 26 or
 290 Eq. 28, or using constant $f_k = 0.4$ in the LES regions. For comparison, the results
 291 using the Dynamic Smagorinsky model [39, 40] are also included in Section 4.1.

Figure 5. DHIT, computed f_k . — : 32^3 ; - - : 64^3 ; - · - : 128^3 . Figure 6. DHIT, turbulent viscosity. — : 32^3 ; - - : 64^3 ; - · - : 128^3 .

292 4.1. Decaying homogeneous isotropic turbulence

293 The first test case is decaying homogeneous isotropic turbulence (DHIT). The
 294 computational domain is a cubic box with side length 2π . Three different meshes
 295 have been employed: 32^3 , 64^3 and 128^3 cells. Periodic boundary conditions are
 296 prescribed at all boundaries.

297 The predictions are compared with experiments [41]. We have made the exper-
 298 imental data nondimensional using the characteristic scales, $u_{ref} = (1.5u_{rms,0})^{1/2}$
 299 and $L_{ref} = 11M_g/(2\pi)$, where $u_{rms,0}$ denotes the initial measured RMS fluctua-
 300 tion and M_g is the mesh size of the turbulence generating grid in the experiments.
 301 The turbulence spectra in the experiments were measured at three downstream
 302 locations corresponding to the times $tU_0/M_g = 42, 98$ and 171 . The corresponding
 303 non-dimensional times in the simulations are $0, 0.87$ and 2 , respectively.

304 The initial velocity is obtained by inverse Fourier transformation using the mea-
 305 sured spectrum at $tU_0/M_g = 42$. The initial velocity field is generated by a widely
 306 used computer program from the group of Prof. Strelets in St. Petersburg. Initial

Figure 7. DHIT, Energy spectra. — : $f_k = 0.4$; - - : computed f_k , Eq. 26; - - : Dynamic model; ··· : computed $f_k = k/k_{tot}$, Eq. 28; ∇ : $t = 0.87$; $\circ$: $t = 2$;

Figure 8. DHIT, SGS dissipation, $\varepsilon_{sgs} = -\tau_{ij} \frac{\partial \bar{u}_i'}{\partial x_j}$ (τ_{ij} denotes the SGS stress tensor). — : 32^3 ; - - : 64^3 ; ··· : 128^3 .

boundary conditions for the turbulent quantities are set as in [27], i.e. $k = f_k k_{res}$ ($f_k = 0.4$) and $\varepsilon = C_\mu^{3/4} k^{3/2} / \ell_{sgs}$ with the SGS length scale, ℓ_{sgs} , taken from the

Smagorinsky model as $\ell_{sgs} = C_s \Delta$ ($C_s = 0.1$).

Figure 4 presents the decay of resolved turbulence versus time. The predictions are compared with two experimental data at $t = 0.87$ and 2. The decay is initially stronger when f_k is computed from Eq. 26 compared to $f_k = 0.4$ but at the last measurement station ($t = 2$) the two approaches give similar resolved turbulence. Computing f_k from Eq. 28 gives a more consistent behaviour compared to Eq. 26: the decay rate increases smoothly when the grid is refined. The decay with DNS (no model) with the 128^3 mesh is also included in Fig. 4c; DNS gives, as expected, a slightly slower decay than when computing f_k from Eq. 28. The predicted decay by the Dynamic model is in slightly better agreement with experiments than all PANS models. Figure 5 explains the strong decay with the 32^3 mesh when f_k is computed using Eq. 26: the reason is that the computed f_k is close to one. As expected, the finer mesh, the smaller f_k . For the 128^3 mesh, Eq. 26 gives $f_k \simeq 0.4$. Computing f_k from Eq. 28 gives much smaller f_k than Eq. 26.

Figure 6 presents the turbulent viscosities. Considering the f_k in Fig. 5, it is consistent that f_k from Eq. 26 gives much larger turbulent viscosity than when using Eq. 28 (with $f_k = 0.4$ between the two). f_k from Eq. 28 gives even a smaller viscosity than the Dynamic model on all three meshes. Furthermore, when using Eq. 26 the turbulent viscosity increases with time, especially so for the coarse mesh. In RANS, the turbulent kinetic energy and its dissipation decay as $k \propto t^{-5/4}$ and $\varepsilon \propto t^{-9/4}$, respectively, so that $\nu_t \propto t^{-1/4}$, i.e. the turbulent viscosity decreases with time. We expect that the turbulent viscosity should decrease with time also in LES; this is the case for both the Dynamic model, constant f_k and using Eq. 28 (Figs. 6a,c,d), but not when computing f_k from Eq. 26 (Fig. 6b).

Figure 7 shows the energy spectra for the four models on the three meshes and DNS on the fine mesh. On the coarse mesh, computing f_k from Eq. 26 gives slightly better agreement with experiments than $f_k = 0.4$, but on the other two meshes, $f_k = 0.4$ gives better – or much better – agreement. Comparing $f_k = 0.4$ with using Eq. 28, we find that the latter model gives too small a decay at high wavenumbers. The PANS simulations in Fig. 7 can be summarized as follows: f_k from Eq. 26 gives too large a decay at high wavenumbers, f_k from Eq. 28 too small a decay, and $f_k = 0.4$ in between the two. This is consistent with the turbulent viscosities in Fig. 6. The spectra using the Dynamic model give better agreement with experiments than all the PANS models.

For the fine mesh, the spectrum using Eq. 28 gives good agreement with experiments. The PANS model is supposed to behave as DNS when f_k becomes small. f_k is indeed small for the finest mesh, see Fig. 5b. It is therefore interesting to make a comparison between f_k from Eq. 28 and DNS, see Fig. 7d. It can be seen that DNS gives reasonable spectra, but the increase at high wavenumbers reveals – as expected – that the dissipation is insufficient, i.e. the mesh is too coarse for DNS. Nevertheless, comparison between Figs. 7c and 7d shows that the PANS simulations using Eq. 28 and DNS are fairly similar; an even finer mesh would probably increase the similarity. Using Eq. 26, the similarity with DNS is much smaller (cf. Figs. 7b and 7d) and the reason is that the predicted f_k is much larger than when using Eq. 28. However, if the mesh is strongly refined, it is expected that the PANS results using Eq. 26 will be similar to DNS since it is expected that the mesh refinement will make f_k go towards zero (the mesh refinements from 32^3 to 128^3 does indeed reduce f_k , see in Fig. 5a).

Finally we plot the SGS dissipation, see Fig. 8. This quantity dissipates resolved turbulent kinetic energy. According to the theory, the cut-off is located in the $-5/3$ region. Hence, when the grid is refined/coarsened and the location of cut-off moves in wavenumber space, the SGS dissipation should in theory not change.

Figure 9. Fully developed channel flow. $Re_\tau = 8000$. Model 4 is used at the interface. Thick vertical line show the location of the RANS-LES interface. — : 32^3 ; - - : 64^3 ; - · - : 128^3 ; + : $U^+ = \ln(y^+)/0.4 + 5.2$.

361 This means we would like our model to dissipate the same amount of turbulence
 362 as we refine/coarsen the mesh. In other words, the SGS model should be *grid-*
 363 *independent*. As seen in Fig. 8, the constant f_k does a fairly good job in keeping
 364 ε_{sgs} constant as the grid is coarsened. Computing f_k from Eqs. 26 and 28 both
 365 give a larger spread in ε_{sgs} when refining the grid; the Dynamics model gives a
 366 ε_{sgs} as grid-independent ε_{sgs} as $f_k = 0.4$. It may be noted that for the fine mesh,
 367 ε_{sgs} using f_k from Eq. 28 goes to zero for $t > 2.1$; the reason is the small f_k , see
 368 Fig. 5b.

369 Often, we take it for granted that the turbulent viscosity should increase when
 370 the grid is coarsened. But in order to keep ε_{sgs} constant when the grid is coarsened,
 371 the finite volume method must respond in an appropriate manner and reduce the
 372 resolved velocity gradients, $\partial \bar{u}_i' / \partial x_j$ so that ε_{sgs} stays constant (for wavenumbers
 373 in the $-5/3$ region $\partial \bar{u}_i' / \partial x_j \propto \Delta^{-2/3}$ and, since $\varepsilon_{sgs} \propto \Delta^0$, ν_t must be proportional
 374 to $\Delta^{4/3}$). When coarsening the grid, the key question is neither that the viscosity
 375 should increase nor that the resolved velocity gradients should decrease, but that
 376 the product of the modeled, turbulent stresses and the velocity gradient, $\varepsilon_{sgs} =$
 377 $-\tau_{ij} \partial \bar{u}_i' / \partial x_j$, should stay constant.

378 4.2. Fully developed channel flow at $Re_\tau = 8000$

379 The Reynolds number is defined as $Re_\tau = u_\tau \delta / \nu$ where δ denotes half channel
 380 height. The streamwise, wall-normal and spanwise directions are denoted by x , y
 381 and z , respectively. The size of the domain is $x_{max} = 3.2$, $y_{max} = 2$ and $z_{max} = 1.6$.
 382 The mesh has 32×32 , 64×64 or 128×128 cells in the $x - z$ planes. Details of the
 383 grids are given in Table 1. The location of the interface is $y^+ \simeq 500$. f_k is set to one
 384 in the RANS regions near the walls, see Fig. 1. In the LES region f_k is either set to
 385 0.4 or it is computed from Eqs. 26 or 28. Model 4 (see Section 2.2.4) is used at the

Figure 10. Fully developed channel flow. $Re_\tau = 8000$. Model 4 is used at the interface. — : 32^3 ; - - : 64^3 ; - · - : 128^3 .

Figure 11. Fully developed channel flow. Computed f_k . $Re_\tau = 8000$. Model 4 is used at the interface. — : 32^3 ; - - : 64^3 ; - · - : 128^3 .

Figure 12. Fully developed channel flow. $Re_\tau = 8000$. Total, turbulent kinetic energy. Model 4 is used at the interface. — : 32^3 ; - - : 64^3 ; - · - : 128^3 ; ○: DNS at $Re_\tau = 4200$ [42].

Re_τ	Δy^+	Δx^+	Δz^+	N_y	f_y
2 000	2.0 – 230	200	100	80	1.13
4 000	2.2 – 520	400	200	80	1.15
8 000	1.5 – 1 050	800	400	96	1.15

Table 1. Grids. Fully developed channel flow. f_y denotes geometric stretching.

RANS-LES interfaces. A running average is used when computing k_{tot} (Eq. 20) in the definition of f_k . Since the simulations are always started from results obtained from earlier simulation (using, for example, another interface model), the running average is always started from the first timestep. The same procedure is used when Model 2 and 3 are used in the next section. The sensitivity to running averaging for k_{tot} is evaluated in Section 5.

Figures 9, 11, 10 and 12 present the velocity profiles, the turbulent viscosities, the computed f_k and the total, turbulent kinetic energy. As can be seen, when computing f_k from Eq. 26 on the coarse mesh it attains values close to one. The result is a poorly predicted velocity profile, very large viscosities ($\langle \nu_t \rangle_{max}/\nu \simeq 415$, not shown) in the LES region; furthermore, the resolved turbulence is zero in the entire domain. The predictions on the fine mesh are not very good either. The velocity profile near the center on the fine mesh of the channel is somewhat overpredicted (Fig. 9b); it seems that the turbulent viscosity gets too small in the LES region, see Fig. 10b. Computing f_k from Eq. 28 gives accurate results for the coarse grid; this is probably rather fortuitous because the turbulence viscosity is essentially zero in the LES region for all three meshes. On the medium and the fine mesh, Eq. 28 predicts very poor velocity profile; the reason is the small f_k (Fig. 11b) and consequently a very small turbulent viscosity (Fig. 10b).

The results using Eq. 26 on the coarse grid may seem somewhat surprising: we get $f_k \simeq 1$ (Fig. 11a) in the entire region, but yet the solution does not correspond to a RANS solution as expected. The reason is the interface term (Model 4), which decreases the turbulent viscosity near the RANS-LES interface, see Fig. 10b. Without interface term, we get a steady RANS solution as expected (not shown). This is also the case when using Eq. 28: without the interface term the flow gives a steady RANS solution as it should (not shown).

Contrary to computing f_k from Eqs. 26 or 28, using $f_k = 0.4$ in the LES region gives velocity profiles which are in good agreement with the log-law. It may be noted that the turbulent viscosity stays constant as the grid is refined; the turbulent viscosity is *grid-independent*. This is probably a big advantage when using the model in flow with complex geometries where the cell size may vary strongly. The total, turbulent kinetic energy agrees fairly well with DNS on $Re_\tau = 4\,200$ for all three meshes, however it is somewhat overpredicted in the RANS region.

5. Results

In the previous section it was found that a constant $f_k = 0.4$ in the LES region is superior compared with computing f_k from Eqs. 26 or 28. In the literature, there are several proposals on how to compute f_k . The proposals by Basara et al. [2] and Kenjeres and Hanjalic [38] are given in Eqs. 26 and Eq. 27, respectively. Other formulations are proposed by Girimaji and Abdol-Hamid [44] who compute it as $3(\Delta_{min}/L_t)^{2/3}$ where Δ_{min} is the smallest grid cell size and $L_t = (k + k_{res})^{3/2}/\varepsilon$. Foroutan and Yavuzkurt [45] derives an expression from the energy spectrum which

Figure 13. Fully developed channel flow. $N_k = 32$. $Re_\tau = 4000$. $---$: Model 1. $---$: Model 2. $---$: Model 3, $S_i = 0$; $\bullet$: no interface model.

Figure 14. Fully developed channel flow. $Re_\tau = 8000$. For legend, see Fig. 13.

$$f_k = 1 - \left[\frac{(\Lambda/\Delta)^{2/3}}{0.23 + (\Lambda/\Delta)^{2/3}} \right]^{9/2} \quad (29)$$

Figure 15. Fully developed channel flow. $Re_\tau = 8000$. Model 3. $S_i \neq 0$. $\bullet$: the location of the computational cell centers. Thick vertical line show the location of the RANS-LES interface.

Figure 16. Fully developed channel flow. $Re_\tau = 2000$. --- : Model 1. --- : Model 2. --- : Model 3, $S_i = 0$; --- : Model 4.

Figure 17. Fully developed channel flow. Model 4. $Re_\tau = 2000$ (lower lines), $Re_\tau = 4000$ (middle lines), and $Re_\tau = 8000$ (upper lines). Vertical dashed thick lines show the location of the interfaces. --- : $y_{interface}^+ = 250$; --- : $y_{interface}^+ = 500$; --- : $y_{interface}^+ = 1000$; --- : 1D RANS using AKN model [43].

Figure 18. Fully developed channel flow. $Re_\tau = 2000$, $y_{interface}^+ = 250$. Resolved (upper lines) and viscous plus modeled (lower) shear stresses. For legend, see Fig. 16.

It may that Eq. 26 – or any other formulation – could be better calibrated, but that is out of the scope of the present work. In this section we will evaluate the four interface models presented in Section 2.2 in two flows, fully developed channel flows (at different Reynolds numbers) and embedded LES. In the LES region we set $f_k = 0.4$.

5.1. Fully Developed Channel Flow

Simulations at different Reynolds numbers are made, $Re_\tau = 2000$, $Re_\tau = 4000$ and $Re_\tau = 8000$. The size of the domain is $x_{max} = 3.2$, $y_{max} = 2$ and $z_{max} = 1.6$. The mesh has 32×32 cells in the $x - z$ planes. A simulation with twice as large domain in the $x - z$ plane ($x_{max} = 6.4$ and $z_{max} = 3.2$) with 64×64 cells was also made for $Re_\tau = 4000$, and identical results were obtained as for the smaller domain. Details of the grids are given in Table 1. The location of the interface is

440 $y^+ \simeq 500$.

441 5.1.1. $Re_\tau = 4000$

442 Figure 13 presents the velocity profiles, the turbulent viscosities, the production
443 terms in the k equation and the shear stresses. The vertical thick dashed lines show
444 the location of the interface. The momentum source in Model 3, S_i (see Eq. 22) is
445 set to zero. Model 2 and 3 give a velocity profile in good agreement with the log-law.
446 Model 1 does not sufficiently reduce the turbulent viscosity in the LES region and
447 the result is that the turbulent viscosity is much too large but somewhat smaller
448 than “no interface model”.

449 With Model 2, the magnitude of the additional turbulent viscosity, ν_{tr} , near the
450 interface in Fig. 13b is actually larger than ν_t , which makes their sum, $\nu_t + \nu_{tr}$,
451 go negative. Recall that in the momentum equations $\nu_t + \nu_{tr}$ is not allowed to go
452 negative; it is negative only in $P_{k_{tr}}$, see Section 2.2.1. As a consequence of the large,
453 negative ν_{tr} , $P_k + P_{k_{tr}} < 0$ at the interface, see Eq. 13c. The production terms in
454 Model 2 and 3 are very similar, which is expected since ν_{tr} in Model 2 is defined
455 from $P_{k_{tr}}$, see Eqs. 17 and 19. The shear stresses in Fig. 13d show that without
456 interface condition the flow goes steady. The reason is that the turbulent viscosity
457 in the LES region is too large because there is no commutation term to reduce k .
458 Note that to enhance the readability of Fig. 13d, the viscous and modeled shear
459 stresses are plotted with negative sign. Recall that the total shear stress, τ_{tot} , will
460 always – irrespectively of model – obey the linear law

$$\tau_{tot} = 1 - y, \quad \tau_{tot} = \tau_{12}^\nu + \tau_{12} - \langle \bar{u}'\bar{v}' \rangle = \langle (\nu + \nu_t) \frac{\partial \bar{u}}{\partial y} - \bar{u}'\bar{v}' \rangle \quad (30)$$

461 With Model 1 the flow is neither in RANS mode nor in LES mode, but it ends
462 up in being in the middle (modeled and resolved stresses are both rather large),
463 which is a most unfortunate condition for a hybrid LES-RANS model. The stresses
464 predicted by Models 2 and 3 are virtually identical.

465 The turbulent viscosity is too large with Model 1 (Fig. 13b). If f_k is reduced
466 to 0.3, the turbulent viscosity is reduced (not shown) because the gradient of f_k
467 across the interface increases; furthermore, a smaller f_k gives a smaller turbulent
468 viscosity in the LES region which promotes growth of resolved turbulence. With
469 $f_k = 0.3$, Model 1 gives a velocity profile that is almost identical to that of Model
470 2; the maximum streamwise fluctuation, $\langle \bar{u}'\bar{u}' \rangle_{max}$, is 10% larger with Model 1.
471 If f_k is reduced to 0.3 also in Model 2 (not shown), the prediction with the two
472 models are even closer to each other ($\langle \bar{u}'\bar{u}' \rangle_{max}$ is a couple of percent larger with
473 $f_k = 0.3$ compared to $f_k = 0.4$).

474 5.1.2. $Re_\tau = 8000$

475 Figure 14 shows the same quantities as Fig. 13, but now for $Re_\tau = 8000$. Again,
476 Models 2 and 3 give good velocity profiles. Model 1 and the “no interface condition”
477 give rather good velocity profiles although the velocity is somewhat too high in the
478 LES region. The reason for the larger velocity levels is seen in Fig. 14b which
479 presents the turbulent viscosities. The “no interface model” does not manage to
480 reduce ν_t in the LES region; also Model 1 is much less efficient in reducing ν_t
481 than are Models 2 and 3. This is also clearly seen in the shear stresses (Fig. 14d)
482 which show that the transition from RANS to LES is fastest for Models 2 and
483 3; the transition is much slower for Model 1 and for “no interface condition”.
484 The production of k becomes negative for Models 2 and 3 as for $Re_\tau = 4000$. It
485 can be noted that the magnitude of the negative production at the interface for
486 both $Re_\tau = 4000$ (Fig. 13c) and $Re_\tau = 8000$ (Fig. 14c) is slightly larger with

Model 2 than Model 3. The reason is probably that Model 2 reduces the turbulent viscosity in the momentum equations by ν_{tr} (but its magnitude is not allowed to exceed ν , i.e. $\nu_{tr} > \nu$ when $\nu_{tr} < 0$) which slightly reduces the damping of the resolved fluctuation which in turn increases the fluctuating velocity gradients and the magnitude of P_k . It could be noted that if f_k is reduced to 0.3, Model 1 gives virtually identical velocity profile and resolved stresses as Model 2.

Figure 15 presents results where the momentum source S_i (Eq. 22) has been activated. It can be seen that the predicted velocity profile is slightly worse than without momentum source term (Fig. 14a). The source terms in the momentum equation are – as is $P_{k_{tr}}$ – very large; recall that the driving pressure gradient (the first term on the right side of Eq. 25) is one. It may at first seem somewhat surprising that the source term S_i is non-zero since it includes the time average of a resolved fluctuation which should be zero, i.e. $\langle u'_i \rangle = 0$. The reason is that S_i , at the lower RANS-LES interface for example, is added only when $Df_k/Dt = \bar{v}\partial f_k/\partial x_2 < 0$, i.e. when $\bar{v} > 0$ (recall that at the lower RANS-LES interface $\partial f_k/\partial x_2 < 0$); the average of the samples of $\bar{u}'_i$ when $\bar{v} > 0$ is not zero.

It may be noted that the magnitude of the resolved shear stress near the RANS-LES interface exceeds one (see Fig. 15d) and hence it is larger than the wall shear stress. This seems to violate Eq. 30. However, when $S_1 \neq 0$, the right side of Eq. 30 includes also the integral of S_1 , i.e. the global force balance reads

$$2\delta x_{max} z_{max} - 2\tau_w x_{max} z_{max} + \int_V S_1 dx dy dz = 0 \quad (31)$$

where the first term is the driving pressure gradient (the first term on the right side of Eq. 25). Since $S_1 < 0$, see Fig. 15b, the wall shear stress, τ_w , is reduced when S_1 is added and this explains why the magnitude of the resolved shear (scaled with τ_w) exceeds one.

5.1.3. $Re_\tau = 2000$

Figure 16 presents the same quantities as Fig. 13, but now for $Re_\tau = 2000$. The results of Model 4 are included here; it was shown in [30] that this interface model gives good results for $Re_\tau = 4000$ and 8000. Model 4 predicts a good velocity profile also for this Reynolds number. However, Models 1, 2 and 3 fail; they all give a steady RANS solution. The reason is that the interface conditions do not manage to decrease the modeled turbulent kinetic energy – and hence not the turbulent viscosity – on the LES side of the interface. Obviously it is more difficult for the flow to switch from RANS to LES at $Re_\tau = 2000$. The same effect is seen if the mesh in the wall-parallel plane is refined to 64×64 cells (not shown). One difference between the $Re_\tau = 2000$ and the higher Reynolds numbers is that in the former case the resolved stress is much smaller at the interface.

5.1.4. Failure of Models 1–3

In order to find the reason for this failure of Models 1–3, the sensitivity to the location of the interface was investigated. Figure 17 presents the velocities, turbulent viscosities and the shear stresses using Model 4 for $Re_\tau = 2000$, 4000 and 8000 for different locations of the interface. The velocity profiles are well predicted for all cases except for $Re_\tau = 8000$ and $y_{interface}^+ = 250$. Note that the turbulent viscosities are plotted using outer scaling (i.e. they are scaled with friction velocity, u_τ , and half channel width, δ) contrary to Figs. 13, 14 and 16 where inner scaling is used (i.e. scaled by ν). The results from a one-dimensional RANS simulation using the AKN model [43] (i.e. PANS with $f_k = 1$) are also included. When plotted versus y^+ , the RANS turbulent viscosity is virtually independent of Reynolds number and

Figure 19. Embedded LES. Channel flow. Added synthetic Reynolds stresses at the vertical RANS-LES interface.

hence all the green dotted lines in Fig. 17c collapse. Actually this is also the case for the PANS simulations when the interface is defined in outer scaling (i.e. in y): in Fig. 17b, the turbulent viscosity in the URANS region for

- $\{Re_\tau = 2000, y_{interface}^+ = 250\}$, and $\{Re_\tau = 4000, y_{interface}^+ = 500\}$ and $\{Re_\tau = 8000, y_{interface}^+ = 1000\}$ (i.e. $y = 0.125$)
- $\{Re_\tau = 2000, y_{interface}^+ = 500\}$, and $\{Re_\tau = 4000, y_{interface}^+ = 1000\}$ (i.e. $y = 0.25$)
- $\{Re_\tau = 4000, y_{interface}^+ = 250\}$, and $\{Re_\tau = 8000, y_{interface}^+ = 500\}$ (i.e. $y = 0.0625$)

are very similar. As a result, this applies also for the viscous plus modeled shear stresses, see Fig. 17d. It is interesting to note that the viscosity in the RANS region in the PANS simulations is much smaller than that in the 1D RANS simulation. The reason is, as noted in [30], that low modeled k values are transported from the LES region into the RANS region near the lower wall when $v' < 0$ (ε in the LES region in the two simulations are very similar [30]).

Now we need to address the question why Models 1-3 fail at $Re_\tau = 2000$. The interface location was moved away from the wall to $y_{interface}^+ \simeq 1000$, but the same results were obtained (not shown). Next, the interface location was moved closer to the wall, to $y_{interface}^+ \simeq 250$. Model 1-3 still fail to predict a good velocity profile (not shown). It was mentioned above that the reason for the poor prediction of the velocity profile at $Re_\tau = 2000$ could be that the resolved shear stress is too low at the interface, and that the low level of resolved turbulence in the interface region would make the transition from RANS mode to LES mode difficult. However, this theory does not hold when we look at the resolved shear stresses at the interface in Fig. 18 which for $Re_\tau = 2000$ are as large or larger than those at $Re_\tau = 8000$ for which good velocity profiles are obtained, see Fig. 14. The reason for the poor prediction at $Re_\tau = 2000$ is that the turbulent viscosity (in outer scaling) – and consequently the modeled shear stress – is much larger than at the higher Reynolds number, see Figure 17b-d. Because of this, Models 1-3 do not manage to sufficiently decrease ν_t in the LES region adjacent to the interface. Large modeled shear stresses at the interface (Fig. 17d) are also the reason for the somewhat poorly predicted velocity profiles (Fig. 17a) – using Model 4 – at $Re_\tau = 4000$ and 8000 with the interface is located at $y^+ = 250$.

Figure 20. Embedded LES. Friction velocity and turbulent viscosity ($\nu_{tot} = \nu + \nu_t + \nu_{tr}$). Model 2. Black, thick, vertical dashed lines show the location of the interface. $\cdots$: $x_{tr} = 1$; $\cdots$: $x_{tr} = 0.5$; $\cdots$: $x_{tr} = 0$, see Fig. 13.

Figure 21. Embedded LES. Model 2. Running average (Eq. 20) in a computational cell at $(x/\delta, z/\delta) = (2.42, 0.8)$. $\cdots$: $y/\delta = 0.014$; $\cdots$: $y/\delta = 0.065$; $\cdots$: $y/\delta = 0.24$; $\cdots$: $y/\delta = 0.83$; $\circ$: every 20th time step.

5.2. Embedded LES of Channel Flow

The Reynolds number is $Re_\tau = u_\tau \delta / \nu = 950$. The domain size is $12.8 \times 2 \times 1.6$ in the streamwise (x), wall-normal (y) and spanwise direction (z), see Fig. 2. The mesh has $256 \times 80 \times 64$ cells. A geometrical stretching of 1.13 in the y direction is used from the walls to the center.

Anisotropic synthetic fluctuations are superimposed to the mean flow profiles at the inlet. The methodology used in [28, 47] is somewhat extended and involves the following steps.

- (1) A pre-cursor 1D RANS simulation is made using the AKN model [43] (i.e. PANS with $f_k = 1$)

Figure 22. Embedded LES. $x = 5.9$. $Re_\tau = 950$. $x_{tr} = 0.5$. $\bullet$: Model 1; $\bullet$: Model 2; $\bullet$: Model 3, $S_i = 0$; $\bullet$: Model 4; $\bullet$: DNS of fully developed flow [46].

- (2) The Reynolds stress tensor is computed using the EARS model [48].
- (3) The Reynolds stress tensor is used as input for generating the anisotropic synthetic fluctuations.
- (4) Since the method of synthetic turbulence fluctuations assumes homogeneous turbulence, we can only use the Reynolds stress tensor in one point. We need to choose a relevant location for the Reynolds stress tensor. In boundary layer flow, the turbulent shear stress is the single most important stress component. Hence, the Reynolds stress tensor is taken at the location where the magnitude of the turbulent shear stress is largest.
- (5) Finally, the synthetic fluctuations are scaled with

$$\left(|\overline{u'v'}| / |\overline{u'v'}|_{max} \right)_{RANS}^{1/2} \quad (32)$$

which is taken from the 1D RANS simulation.

In order to introduce a time correlation, the inlet fluctuations, $\mathcal{U}'$, are computed

Figure 23. Embedded LES. $Re_\tau = 950$. $x_{tr} = 0$. $\nu_{tot} = \nu + \nu_t + \nu_{tr}$. For legend, see Fig. 22.

Figure 24. Embedded LES. $Re_\tau = 950$. $x_{tr} = 0$. Production in the plane in the LES region adjacent to the interface. $\cdots$: $P_k + P_{k_{tr}}$, Model 1. $\cdots$: $P_k + P_{k_{tr}}$, Model 2. $\cdots$: $P_{k_{tr}}$, Model 3, $S_i = 0$; $\cdots$: P_k , Model 4; $\circ$: P_k in RANS region, $x = 0.12$.

$$\mathcal{U}'_m = a\mathcal{U}'_{m-1} + b\mathcal{U}'_m \quad (33)$$

Figure 25. Embedded LES. $x = 5.9$. $Re_\tau = 950$. $x_{tr} = 0$. — : Model 3. $S_i \neq 0$ (see Eq. 22); - - : no interface model; $\circ$: DNS of fully developed flow [46].

where m is the current time step. Constant a is related to the integral time scale, $\mathcal{T}$, as

$$a = \exp(-\Delta t/\mathcal{T}) \quad (34)$$

where Δt is the computational time step and $b = (1 - a^2)^{1/2}$. Constant b is given by the requirement that $\langle \mathcal{U}^2 \rangle = \langle u'^2 \rangle$. Equation 33 introduces a time correlation with an integral timescale $\mathcal{T}$ which is taken as $\mathcal{T} = \mathcal{L}/U_b$ ($\mathcal{L} = 0.15\delta$) using Taylor's hypothesis, where U_b and $\mathcal{L}$ denote the inlet bulk velocity and the integral length scale, respectively.

The inlet mean velocities are set as $V_{in} = W_{in} = 0$ and [49]

$$U_{in}^+ = \begin{cases} y^+ & y^+ \leq 5 \\ -3.05 + 5 \ln(y^+) & 5 < y^+ < 30 \\ \frac{1}{0.4} \ln(y^+) + 5.2 & y^+ \geq 30 \end{cases} \quad (35)$$

The time-averaged interface fluctuations and the two-point correlation of w' are shown in Fig. 19. It can be noted in Fig. 19 that the sign of the shear stress changes at the centerline. This was achieved by simply switching the sign of the wall-normal synthetic fluctuation, v' , for $y > 1$. It can be seen that the variation of all the synthetic stresses across the channel follow the form of the eddy-viscosity shear stress (which is more or less identical to the EARSM shear stress). The reason is that Eq. 32 was used to scale all fluctuations. As a consequence, the synthetic normal stresses agree with the EARSM stresses at the location where the EARSM shear stress has its maximum. When creating the synthetic turbulent interface fluctuations, the integral length scale was set to 0.15δ . Figure 19b shows that the two-point correlation of the generated fluctuations agrees well with this value. A Matlab file to generate the synthetic fluctuations can be downloaded at [50].

610 RANS is used upstream of the interface ($f_k = 1$) and LES is used downstream of it
 611 ($f_k = 0.4$) and in the transition region of length x_{tr} (see Fig. 2), f_k varies linearly
 612 between 1 and 0.4. Models 1-4 are used at the vertical interface.

613 We start by investigating the effect of the length of the transition region. Fig-
 614 ure 20 presents the turbulent viscosities for three different transition lengths,
 615 $x_{tr} = 0$, 0.5 and $x_{tr} = 1$. Model 2 is used at the interface. A large x_{tr} means
 616 that the gradient Df_k/Dt in Eq. 9 is small but that it is active over a large re-
 617 gion. We see immediately in Figure 20a that $x_{tr} = 1$ is too large. The skin friction
 618 does not go back to its target value of one downstream of the interface because the
 619 resolved turbulence is much too small (not shown). Reducing x_{tr} to 0.5 gives an im-
 620 provement but the transition region is still too long. $x_{tr} = 0$ (no transition region,
 621 f_k goes from 1 to 0.4 abruptly) gives good friction velocities; the fully-developed
 622 values of $u_\tau \simeq 0.95$ is reached at $x \simeq 10$, i.e. nine half channel widths downstream
 623 of the interface. The reason why the friction velocity does not reach the target
 624 value of one is that the resolution is somewhat too coarse (or the Reynolds num-
 625 ber too high) so that the velocity profile for fully-developed PANS does not agree
 626 with the inlet log-law profile in Eq. 35 (see Fig. 11a in [27]). When the inlet mean
 627 velocity instead is taken from fully-developed flow on the same mesh using PANS
 628 (with $f_k = 0.4$), the friction velocity goes to one as expected, see green dotted line
 629 in Fig. 20a.

630 Figures 20b and c show that the turbulent viscosity takes negative values for all
 631 transition region lengths, which gives negative production in the k equation; the
 632 smaller the transition region, the larger the magnitude of the negative viscosity.
 633 With no transition region ($x_{tr} = 0$), it can be seen that the magnitude of ν_{tot} gets
 634 very large downstream of the interface ($|\nu_{tot}|/\nu > 550$). Despite the large negative
 635 viscosities adjacent to the RANS-LES interface, they rapidly get back to positive
 636 values as seen in Fig. 20c which show the turbulent viscosities five cells downstream
 637 of the interface. Since $x_{tr} = 0$ is found to give best results above, this choice is
 638 used when presenting the results in more detail below.

639 In Models 2 and 3 a running average is used for computing k_{tot} , see Eq. 20.
 640 The running average is applied at the start of the simulations. Figure 21 shows
 641 how fast the running average converges. The inlet conditions are used as initial
 642 conditions in the entire computational domain. Figure 21a shows that the running
 643 average converges fairly well within 0.1 time units. One test was also made where
 644 the running average was made only in time, not in the spanwise direction. In this
 645 case, ν_{tr} in Eq. 17 was set to zero during the first 10 time steps in order to get
 646 some reasonable value of k_{tot} in Eq. 20. Figure 21b shows the convergence of the
 647 running average, and as can be seen it converges fairly quickly but slightly slower
 648 than in Fig. 21a. The predicted results (not shown) using the two different running
 649 averages in Figs. 21a and 21b are identical.

650 Figures 22 and 23 present velocity profiles, resolved turbulence, friction velocity
 651 and turbulent viscosity. The momentum source, S_i (Eq. 22), is set to zero. First, it
 652 can be seen that with Model 1, too small a part of the resolved turbulence survives
 653 in the LES region because it is killed by the large turbulent viscosity. The friction
 654 velocity (Fig. 23a) is the most critical parameter. Models 2-4 give very similar u_τ
 655 for $x > 5$ and reach their fully developed values at $x \simeq 10$. The velocity profile
 656 and resolved turbulence are also fairly well predicted at $x = 5.9$ (i.e. five half
 657 channel widths downstream the interface), see Fig. 22. In the case of Model 1, the
 658 resolved turbulence further downstream ($x \gg 6.4$) will probably first be completely
 659 killed and then the flow will eventually go into RANS mode. With Models 2-4, the
 660 resolved turbulence at the interface increases strongly (Fig. 23b) thanks to the
 661 added non-isotropic fluctuations, but also thanks to interface conditions of Models

2-4 which succeed in drastically decreasing the modeled turbulent kinetic energy and thereby the turbulent viscosity, see Fig. 23c. For Model 1 and 2, the reduction in the turbulent viscosity is clearly seen in Fig. 23d. Model 2 gives a much larger magnitude in negative viscosity than Model 1 and as a consequence the turbulent viscosity for Model 2 is zero for $y < 0.8$ at $x = 5.9$, see Fig. 23e.

For the fully developed channel flow at $Re_\tau = 4000$, it was found that when f_k was reduced to 0.3 using Model 1 (see Section 5.1.1), the predictions were found to be very similar to those of Model 2. When f_k is reduced to 0.3 for this flow with Model 1, the results improves somewhat (not shown), but they are still considerably poorer compared with Model 2. The skinfriction reaches a value of 0.9 near the outlet of the domain (cf. Fig. 23b) and the peak of the resolved shear stress is approximately 0.5 (cf. Fig. 22e) near the outlet of the domain. The reason is that the turbulent viscosity at $x = 5.9$ is reduced only by a factor of two compared to $f_k = 0.4$ (cf. Fig. 23d).

The production of k in the LES region adjacent to the RANS-LES interface is shown in Fig. 24. As for the fully-developed channel flow, it is found that the productions by the interface models, $P_{k_{tr}}$, are very large and negative for Models 2 and 3. These large negative productions ensure the strong decrease in turbulent viscosity across the RANS-LES interface, see Fig. 23d, which in turn facilitates the rapid increase in resolved turbulence downstream of the interface, see Fig. 23b.

Figure 25 presents results using Model 3 with the momentum source term, S_i , see Eq. 22. Comparing with Fig. 22 we can see that the momentum source has a similar influence as for fully-developed flow: the resolved turbulence is slightly stronger. The predicted friction is as a consequence increased and somewhat closer to the target value of one.

Figure 25 includes also results when no interface model is used at all. When comparing with the results when using an interface model (Figs. 22), the differences are clear: without interface model, the turbulent viscosity is not reduced on the LES side of the interface and the consequence is that almost all resolved turbulence is killed. If the domain in Fig. 25 were made larger in the streamwise direction, the flow would surely return to steady RANS further downstream.

6. Conclusions

Simulations using Zonal PANS are made where $f_k = 1$ in the URANS regions and $f_k = 0.4$ in the LES regions. There is a strong gradient of f_k across the RANS-LES interface. Recently a modification of the PANS model was proposed by Girimaji and Wallin [3] where they take the gradient of f_k into account. This approach is used at the RANS-LES interfaces and it is further developed and evaluated in the present work. Four different treatments of the interface are evaluated, one is the approach proposed in [3] (called Model 1). Models 2 and 3 are modifications of Model 1 and Model 4 is the approach presented in [30]. The beauty of Models 1-3 is that they do not depend on any constants or tuning; they use the gradient of f_k across the interface. The advantage of Model 3 is that it – unlike Models 1 and 2 – does not involve any unphysical negative viscosities and does not require any regularization. The disadvantage of Model 4 is that it depends on how the modeled k and ε are treated at the interface. The four models are evaluated in fully developed channel flow and embedded LES in channel flow.

Before evaluating the different interface models, the paper evaluates different ways to prescribe f_k . Two different ways of computing f_k (Eqs. 26 and 28) and in the third option a constant f_k is used ($f_k = 0.4$). The three different options are evaluated for decaying grid turbulence and fully developed channel flow and it is

found that the best option is to use a constant $f_k = 0.4$.

Model 1 does not give good results. Its effect is too weak and the model does not sufficiently decrease the turbulent viscosity on the LES side of the interface. For fully developed channel flow, it works well if f_k is reduced to 0.3. For embedded LES, a reduction of f_k to 0.3 in Model 1 improves the predictions but Model 1 still performs much worse than Model 2.

Models 2 and 3 give mostly good results and virtually identical results. Model 3 includes an additional production term, $P_{k_{tr}}$ and a source term in the momentum equations, S_i (Eq. 22); it is found that it is preferable to set $S_i = 0$. To make Models 1 and 2 numerically stable, the additional turbulent viscosity, ν_{tr} , from the models must be positive in the momentum equations. In the production term in the k equation ν_{tr} is permitted to go negative. The magnitude of the negative added production, $P_{k_{tr}}$, in Models 2 and 3 is much larger than the ordinary P_k in RANS. This is the key to the success: $P_{k_{tr}}$ is large and negative in the LES region adjacent to the interface which reduces k and thereby the turbulent viscosity. Models 2 and 3 fail for the fully developed flow at the lowest Reynolds number ($Re_\tau = 2000$); they both give steady RANS results. Model 4 works well for all flows.

In fully developed channel flow using RANS, the turbulent viscosity, and hence the modeled Reynolds shear stress, is virtually independent of the Reynolds number. Using Zonal PANS, it is found that this also applies for the turbulent viscosity and the modeled Reynolds shear stress in the URANS region.

The conclusion is that interface Model 4 works best and that Models 2 and 3 fail in one flow (fully developed channel flow at $Re_\tau = 2000$). The disadvantage of Model 4 is that it depends on the prescribed boundary conditions of k and ε at the RANS-LES interface.

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