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1 **A dual-mesh hybrid RANS-LES simulation of the buoyant**
2 **flow in a differentially heated square cavity with an improved**
3 **resolution criterion**

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15 **Keywords:** Hybrid RANS/LES, Buoyant flow, Differentially heated cavity, LES resolution, OpenFOAM

16 **Highlights:**

- A hybrid RANS/LES simulation of a $Ra = 10^{11}$ square cavity flow was run using OpenFOAM.
- The new criterion distinguishes between the viscous sublayer and the laminar core.
- The new criterion leads to sustained turbulence levels in the dual-mesh simulation.

1 **Abstract**

2 In this work, the dual-mesh hybrid RANS-LES approach was applied for the first time to a natural convection
3 flow, namely a high Rayleigh number differentially heated square cavity flow. This approach involves running an
4 unsteady Reynolds Averaged Navier-Stokes (RANS) simulation and a coarse Large Eddy Simulation (LES)
5 simultaneously using two different grids that overlap each other (typically, a highly wall-refined grid is used for
6 the RANS, whereas a more homogenous and isotropic mesh is used for the LES). The two simulations correct
7 each other using a switching criterion that determines the driving and the driven simulations at every point in
8 space. It is demonstrated that the flow unsteadiness and the coexistence of laminar and turbulent regions in the
9 square cavity complicate the task of choosing a suitable switching criterion. Accordingly, a new criterion based
10 on comparing the turbulence lengthscales to the grid size was developed to account for the presence of the
11 aforementioned complex flow features. The behaviour of this criterion and comparisons of the dual-mesh
12 predictions against pure RANS, pure coarse LES and Direct Numerical Simulation (DNS) results are also
13 presented in the current paper.

14 **1. Introduction**

15 The buoyancy driven flow in a heated cavity is a key benchmark for many civil or power-generation engineering
16 applications such as solar collectors or passive safety nuclear plant designs. One important difference between the
17 square and the tall buoyant cavities is that the former features a stronger stable stratification that results in
18 significant damping of turbulence. As a result, the Rayleigh number required for the transition to turbulence is
19 higher in the square cavity than in a tall cavity. According to Henkes & Le Quéré (1996) and Xin & Le Quéré
20 (2001), the critical Rayleigh number at which transition to turbulence occurs in a square cavity configuration with
21 perfectly conducting horizontal walls is of the order of 10^6 . On the other hand, the Rayleigh numbers of the flow
22 in the cavity with a 28:1 aspect ratio (with height = 28*width) studied experimentally by Betts & Bokhari (2000)
23 were $0.86 * 10^6$ and $1.43 * 10^6$ and the flow was fully turbulent. Wall-resolved Large Eddy Simulation (LES) or
24 Direct Numerical Simulation (DNS) such as Sebilliau (2016), Wu et al. (2017a), Wu et al. (2017b), Wu et al.
25 (2019), Benhamadouche et al. (2020) and Ahmed et al. (2020) are very expensive for high Reynolds and/or
26 Rayleigh number flows as it requires a very fine mesh in the near-wall regions in all three directions to resolve the
27 turbulence structures.

28 Hybrid RANS-LES methods can provide a cheaper way of computing the square cavity flow compared to LES,
29 Revell et al. (2020). In these hybrid methods, the near-wall region is handled by the RANS model which allows
30 wall normal refinement with high-aspect ratio cells that are at odds with LES theory. The dual-mesh hybrid RANS-

31 LES technique used in this work was developed by Xiao & Jenny (2012) for isothermal flows and a number of
32 improvements were suggested by Tunstall et al. (2017) and Tunstall (2016) who also extended the idea of the
33 approach to heat transfer problems.

34 In previous studies of the square cavity in the literature, separate LES and RANS works can be found. Peng &
35 Davidson (2001) performed an LES study for a Rayleigh number of $1.58 * 10^9$. For this Rayleigh number the
36 levels of the turbulence in the cavity are relatively low. The dynamic Smagorinsky model yielded good predictions
37 of the mean quantities of the flow and thermal fields despite the fact that some discrepancies were observed in the
38 prediction of the second moments.

39 One example of a RANS study of the square cavity can be found in Omranian et al. (2014) where both eddy
40 viscosity and Reynolds stress models were used with different turbulent heat flux models. In addition, different
41 near-wall treatments were tested, namely the low Reynolds-number treatment, the standard wall function (which
42 is based on the logarithmic velocity distribution) and the analytical wall function (see Craft et al. (2002)).

43 As regards hybrid RANS-LES simulations of the square cavity flow, Abramov & Smirnov (2006) studied the
44 case at a Rayleigh number of $1.58 * 10^9$ using a Detached Eddy Simulation (DES) based on the one equation
45 model that solves for the turbulent kinetic energy. The predictions of the mean flow and thermal fields were
46 reasonable. However, close to the downstream ends of the vertical walls, the authors observed an under-prediction
47 of the vertical walls' boundary layer thickness and an overprediction of the vertical velocity peaks in these
48 boundary layers. Another hybrid RANS-LES study can be found in Kocutar et al. (2015), where the boundary
49 elements method was used to study both laminar and turbulent natural convection.

50 Most of the studies found in the literature are limited to low Rayleigh numbers, as there was a lack of
51 experimental and DNS data for high Rayleigh numbers. In fact, until recently the maximum Rayleigh number
52 reported in experiments and in DNS studies was of the order of 10^9 which can be found in Ampofo & Karayiannis
53 (2003) and Puragliesi & Leriche (2012), respectively. However, Sebilleau (2016) conducted DNS studies in which
54 the Rayleigh numbers were 10^8 , $1.58 * 10^9$, 10^{10} and 10^{11} . The author generated fine DNS data (was later
55 published in Sebilleau et al. (2018)) which he used to perform an extensive analysis of different RANS closure
56 techniques. The present work utilizes this DNS data to shed some light on whether hybrid RANS-LES can provide
57 an alternative to both LES and RANS for simulating high Rayleigh number square cavity flows.

58 The organisation of this paper is as follows. The second section provides an explanation of the square cavity
59 configuration studied here. The third section gives insight into the dual-mesh approach by explaining both the flow
60 and the heat transfer related parts of the method. This section also briefly mentions the RANS and the LES models
61 that were chosen to conduct this work. The fourth section highlights the code and the discretization techniques that

62 were used here. The results obtained here are included in the fifth section which is followed by the concluding
63 section.

64 2. The differentially heated square cavity

65 The square cavity test-case shown in Fig. 1 (with periodic boundary conditions in the z -direction to represent a
66 cavity that is infinitely long in this direction) is computed for a Rayleigh number (Ra) of 10^{11} , a fluid Prandtl
67 number (Pr) equal to 0.71 and a linear temperature boundary condition at the horizontal walls (i.e. the temperature
68 varies linearly between the hot wall temperature (T_h) and the cold wall temperature (T_c)). This linear temperature
69 variation represents the case of ‘‘highly conductive’’ horizontal walls more relevant to industrial components with
70 thick steel walls. Note that Ra of 10^{11} is also industrially relevant (similar to a Reynolds number of 10^5).

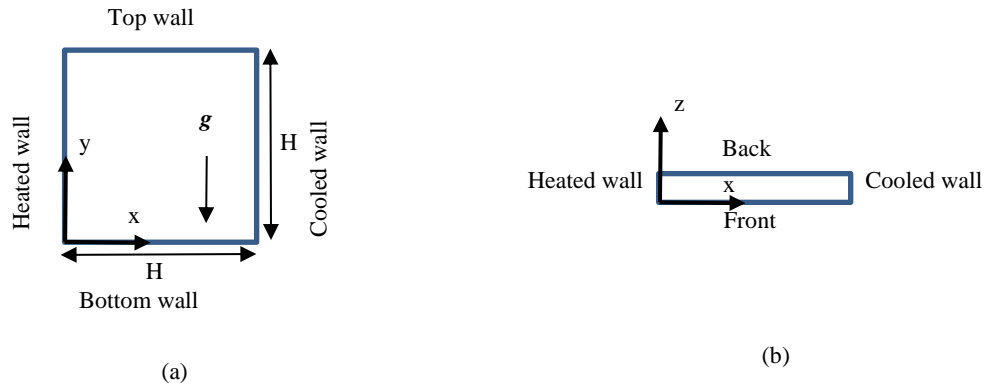


Fig. 1. Schematic representation of different cross sections of the buoyant square cavity. g is the gravity vector.

71 In this study, pure unsteady RANS, pure coarse LES and dual-mesh hybrid RANS-LES simulations were run
72 and the results were compared to the DNS data of Sebilliau et al. (2018). The LES and RANS meshes were both
73 generated using STARCCM+ v11.02 in which the available hyperbolic tangent grid stretching function was used
74 when creating the two grids. The length of the domains in the spanwise direction was chosen to be $0.15 H$, where
75 H is the cavity height as in the DNS study of Sebilliau et al. (2018) who checked the decay of two-point
76 correlations.

77 The RANS mesh consists of $250 \times 250 \times 1$ cells with near-wall grid spacing of $0.0002 H$. The same near-wall grid
78 spacing was used in the RANS simulations of Sebilliau (2016) and it allows the near-wall nodes to be located
79 within the viscous sublayer. Using a finer RANS grid was found to have little impact on the results.

80 On the other hand, the LES mesh has $150 \times 150 \times 23$ cells with near-wall grid spacing of $0.003137 H$. The LES
81 mesh had to be refined in the wall normal direction because of the small thickness of the boundary layers. However,
82 the grid is still too coarse for the LES to fully resolve the near-wall region. Indeed, using the local DNS wall shear

83 stress values, the average value of x^+ ($x^+ = \frac{x \sqrt{\tau_w}}{\nu}$, where x is the wall-distance of the near-wall node and τ_w , ρ
84 and ν are the wall shear stress, fluid density and kinematic viscosity, respectively) over the hot wall is
85 approximately 14. Note that x^+ better represents this quantity compared to y^+ , since the direction normal to the
86 hot wall here is the x direction. The local values of this parameter as well as Δy^+ and Δz^+ ($\Delta y^+ = \frac{\Delta y \sqrt{\tau_w}}{\nu}$ and
87 $\Delta z^+ = \frac{\Delta z \sqrt{\tau_w}}{\nu}$, where Δy and Δz are the near-wall grid spacings in the y and z directions, respectively) over the
88 hot wall are shown in Fig. 2.

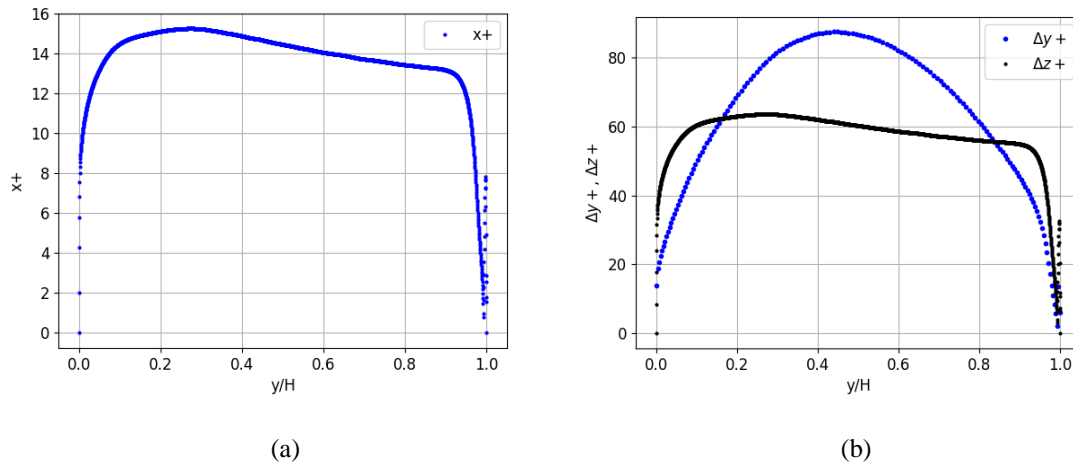


Fig. 2. Local values of x^+ (shown in (a)), Δy^+ and Δz^+ (both are shown in (b)) along the hot wall. These values were estimated using the local wall shear stress from the DNS data of Sebilliau (2016). H is the cavity height. y was used here to represent the vertical distance from the bottom wall.

The LES mesh of 0.5 million cells plus the negligible cost of the RANS simulation provide enormous economy compared to the 726 million nodes DNS simulation.

3. Methodology

3.1. The dual-mesh approach

In the dual-mesh approach, two computational domains are overlapped, one of these domains is used to solve the RANS equations and in the other domain, LES equations are solved. The two solutions are “nudged” together on the fly similarly to two-phase flow modelling where drift terms couple the fields of both phases, here the RANS and the time averaged LES fields, which could be imagined as high and low inertia phases respectively, e.g. solid particles in gas flow in the two fluid model of Zhang & Reese (2003).

103 The advantage of this overlapping flow-models approach is that it avoids the interface problem that occurs with
 104 single-mesh hybrid methods that try to match the highly fluctuating LES quantities with the smooth RANS
 105 ensemble-averaged quantities. On the other hand, in the dual-mesh approach the RANS quantities are compared
 106 to corresponding LES quantities that are averaged in time. Following Xiao & Jenny (2012), the averaging operator
 107 here is an Exponentially Weighted Averaging operation $\langle \cdot \rangle^{EWA}$:

$$\langle \phi \rangle^{EWA}(t) = \int_{-\infty}^t \phi(t') \frac{1}{T_{avg}} \exp\left(-\frac{(t-t')}{T_{avg}}\right) dt' \quad (1)$$

108 where ϕ can be any variable, t denotes the current point in time, t' represents times that precede the current time,
 109 T_{avg} is the averaging time scale.

110 A first order approximation of this operation allows the exponentially weighted averaged (EWA) quantities to
 111 be estimated as:

$$\langle \phi \rangle^{EWA,n} = (1 - \alpha) \phi^n + \alpha \langle \phi \rangle^{EWA,n-1} \quad (2)$$

112 where n represents the current time step, $n - 1$ refers to the previous time step and $\alpha = \frac{1}{1 + \frac{\Delta t}{T_{avg}}}$ in which Δt is the
 113 time step size.

114 3.1.1. Consistency of the flow fields

115 In the dual-mesh approach, the classic RANS and LES momentum equations, with Boussinesq approximation
 116 for density variation and eddy viscosity models for turbulent stresses, are supplemented with the “drift force”
 117 source terms Q^R and Q^L :

$$\begin{aligned} \frac{\partial \langle U_i \rangle}{\partial t} + \langle U_j \rangle \frac{\partial \langle U_i \rangle}{\partial x_j} &= -\frac{1}{\rho_{ref}} \frac{\partial \langle p \rangle}{\partial x_i} \\ &+ \frac{\partial}{\partial x_j} \left((\nu + \nu_t) \left(\frac{\partial \langle U_i \rangle}{\partial x_j} \right) \right) \\ &+ (1 - \beta) (\langle T \rangle - T_{ref}) g_i \\ &+ Q_i^R \end{aligned} \quad (3)$$

118

$$\begin{aligned}
& \frac{\partial \bar{U}_i}{\partial t} + \bar{U}_j \frac{\partial \bar{U}_i}{\partial x_j} = - \frac{1}{\rho_{ref}} \frac{\partial \bar{p}}{\partial x_i} \\
& + \frac{\partial}{\partial x_j} \left((v + v_{sgs}) \left(\frac{\partial \bar{U}_i}{\partial x_j} \right) \right) \\
& + (1 - \beta (\bar{T} - T_{ref})) g_i \\
& + Q_i^{L,u} + Q_i^{L,g} \tag{4}
\end{aligned}$$

119 where the angle brackets $\langle \rangle$ and the overbar $\bar{\quad}$ denote Reynolds averaged and spatially filtered quantities,
120 respectively, v_t is the RANS eddy viscosity and v_{sgs} is the sgs viscosity. β is the thermal expansion coefficient
121 and T_{ref} and ρ_{ref} represent the reference temperature and reference density, respectively. The drift terms are
122 defined as:

$$Q_i^R = \sigma^L \frac{\langle \bar{U}_i \rangle^{EWA} - \langle U_i \rangle}{\gamma_{r1}} \tag{5}$$

$$Q_i^{L,u} = (1 - \sigma^L) \left(\frac{\langle U_i \rangle - \langle \bar{U}_i \rangle^{EWA}}{\gamma_{l1}} \right) \tag{6}$$

$$Q_i^{L,g} = (1 - \sigma^L) \left(\frac{G_i}{\gamma_{l2}} \right) \tag{7}$$

123 where γ_{r1} , γ_{l1} and γ_{l2} are timescales that control how fast the solutions relax towards each other and G_i is a
124 function of the resolved LES velocity fluctuation.

125 The drift term added to the RANS momentum equation (Q_i^R in Equation (3)) drives the RANS velocity field
126 towards the EWA LES velocity field where the LES is superior to the RANS (far from the walls). On the other
127 hand, the source term in the LES momentum equation ($Q_i^{L,u}$ in Equation (4)) acts to modify the LES velocity field
128 in a way that makes the LES EWA velocity field consistent with the RANS velocity field at locations where one
129 knows that the RANS performs better than the LES (near the walls).

130 The switch function σ^L takes values 0 or 1 (depending on whether the RANS drives the LES or vice versa) in
131 most of the domain except in a narrow model-transition layer, the position and width of which is defined by the
132 specific choice of the σ^L function. Its choice depends on the user-chosen or affordable LES grid. This re-opens
133 the large research topic of quality criteria for LES (Salvetti et al. (2010)) and will be revisited in section 5.2.

134 To disconnect LES mesh requirements from viscous scaling and avoid the difficult buffer layer resolution, i.e.
135 to start trusting the LES only in the fully turbulent Log-layer, Tunstall et al. (2017) specified the interface below
136 which the RANS drives the LES and above which the LES drives the RANS as the location where the quantity

137 $Re_y = \frac{\sqrt{k^R} y}{\nu}$ equals 200:

$$\sigma^L = 0.5 \left(1 + \tanh\left(\frac{Re_y - 200}{10}\right) \right) \quad (8)$$

138 k^R is the RANS turbulent kinetic energy, y is the wall distance and ν is the kinematic viscosity.

139 Similar to the velocity fields, the total turbulent kinetic energies of the RANS and the LES are made consistent
 140 by the addition of source terms to the momentum and turbulence equations. In regions where the LES is under
 141 resolved, the source term $Q_i^{L,g}$ (in Equation (4)) adjusts the LES resolved fluctuations to make the LES total
 142 (EWA) turbulent kinetic energy (k^{EWA}) equal to the RANS turbulent kinetic energy (k^R). In order to enhance
 143 this consistency in regions where the contribution of the modelled turbulent kinetic energy to the total turbulent
 144 kinetic energy is significant, Tunstall et al. (2017) decided to adjust the subgrid-scale (sgs) turbulent kinetic energy
 145 k_{sgs} through the addition of a source term ($Q^{k_{sgs}}$) to the k_{sgs} transport equation (Equation (11)), which is solved
 146 when using the one equation k LES model. The function G_i in Equation (7) reads:

$$G_i = \left(1 - \frac{k_{sgs}^{EWA}}{k^{EWA}} \right) \frac{k^R - k^{EWA}}{k^R + k^{EWA}} (\bar{U}_i - \langle \bar{U}_i \rangle^{EWA}) \quad (9)$$

$$k^{EWA} = \langle 0.5 u_i'' u_i'' \rangle^{EWA} + k_{sgs}^{EWA} \quad (10)$$

147 where k_{sgs} is the sgs turbulent kinetic energy, $u_i'' = \bar{U}_i - \langle \bar{U}_i \rangle^{EWA}$ is the resolved LES velocity fluctuation and
 148 k^{EWA} is the EWA total LES turbulent kinetic energy. The LES sgs k equation reads:

$$\begin{aligned} \frac{\partial k_{sgs}}{\partial t} + \frac{\partial}{\partial x_j} (k_{sgs} \bar{U}_j) &= 2\nu_{sgs} \overline{S_{ij}^2} \\ &+ \frac{\partial}{\partial x_j} \left(\nu_{sgs} \frac{\partial k_{sgs}}{\partial x_j} \right) - \varepsilon_{sgs} + G_{k_{sgs}} \\ &+ Q^{k_{sgs}} \end{aligned} \quad (11)$$

149

$$Q^{k_{sgs}} = (1 - \sigma^L) \frac{k_{sgs}^{EWA}}{k^{EWA}} \frac{k^R - k^{EWA}}{\gamma_{r2}} \quad (12)$$

150 where ε_{sgs} and $\overline{S_{ij}}$ are the sgs dissipation rate and the filtered strain rate tensor, respectively. $G_{k_{sgs}}$ is a buoyancy
 151 production term (see Appendix B).

152 On the other hand, in regions where the LES is well resolved, the RANS turbulent kinetic energy is forced
 153 towards the LES “total EWA turbulent kinetic energy” by modifying the turbulent kinetic energy production term
 154 in the RANS turbulence equations as shown in Equation (13).

$$P_k = P_k^{model} + \sigma^L \frac{k^{EWA} - k^R}{\gamma_{r2}} \quad (13)$$

155 where P_k is the modified RANS turbulent kinetic energy production term and P_k^{model} represents the original

156 RANS turbulence production term. The quantities γ_{l1} , γ_{l2} , γ_{r1} and γ_{r2} are called the relaxation time scales and
157 are defined as:

$$\gamma_{l1} = \gamma_{r1} = \max\left(C_{\gamma1} \frac{k^R}{\varepsilon^R}, \Delta t\right) \quad (14)$$

$$\gamma_{l2} = \gamma_{r2} = \max\left(C_{\gamma2} \frac{k^R}{\varepsilon^R}, \Delta t\right) \quad (15)$$

158 where ε^R is the RANS turbulence dissipation rate, $C_{\gamma1} = 0.1$ and $C_{\gamma2} = 0.01$.

159 Even though the forcing of the turbulence levels of the LES towards the RANS turbulence levels described above
160 only enforces consistency between the total turbulent kinetic energies, one can choose to make all the components
161 of the LES total turbulent stress tensor consistent with their RANS counterparts instead. A drift term formulation
162 that can accomplish this consistency can be found in Xiao & Jenny (2012) who pointed out that the stress
163 consistency would be better justified when the estimated RANS turbulent stress tensor can be trusted (e.g. when
164 using a Reynolds stress model) compared to when using an eddy viscosity model.

165 Another drift term that enforces the stress consistency was suggested by de Laage de Meux et al. (2015) in the
166 framework of anisotropic linear forcing for the generation of turbulence near the inlet of an LES domain. The
167 authors added a drift term to the LES momentum equation to drive the LES mean velocity and resolved stresses
168 towards target RANS velocity and stresses provided by a RANS simulation that used the elliptic blending Reynolds
169 stress model (see Manceau & Hanjalić (2002)). However, the same forcing strategy used by the authors can be
170 used in the dual-mesh framework.

171 It is also worth noting that some dual-mesh methods proposed in the literature enforce the consistency between
172 the LES and the RANS not via a relaxation forcing but in implicit ways that effectively correct the LES total
173 turbulent stresses. More details about these methods can be found in Xiao et al. (2016) and Nguyen et al. (2020).
174 Furthermore, another dual-mesh method was suggested by Davidson (2019) in which the author coupled a DES
175 solution with a steady RANS solution and the coupling strategy involved using relaxation forcing.

176 **3.1.2. Consistency of the thermal fields**

177 Regarding the thermal fields, Tunstall (2016) decided to achieve the consistency between the RANS and the
178 LES fields by ensuring consistency between the RANS temperature and the LES EWA temperature as well as
179 making the LES total EWA temperature variance consistent with the RANS temperature variance. Consequently,
180 when using the dual-mesh approach to solve heat transfer problems one needs to solve transport equations for the
181 RANS temperature variance and the LES sgs temperature variance where the later gives the modelled part of the

182 LES total temperature variance.

183 By using an eddy-diffusivity hypothesis to model the heat flux, the RANS and LES temperature equations read,
 184 respectively:

$$\frac{\partial \langle T \rangle}{\partial t} + \langle U_j \rangle \frac{\partial \langle T \rangle}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\left(\frac{\nu}{Pr} + \frac{\nu_t}{Pr_t} \right) \frac{\partial \langle T \rangle}{\partial x_j} \right) + Q^{(T)} \quad (16)$$

$$\frac{\partial \bar{T}}{\partial t} + \bar{U}_j \frac{\partial \bar{T}}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\left(\frac{\nu}{Pr} + \frac{\nu_{sgs}}{Pr_{sgs}} \right) \frac{\partial \bar{T}}{\partial x_j} \right) + Q^{\bar{T}} \quad (17)$$

185 For both the turbulent Prandtl number Pr_t and the sgs Prandtl number Pr_{sgs} a value of 0.9 was used in this study.

186 The drift terms in the above temperature equations are defined as:

$$\begin{aligned} Q^{\bar{T}} &= (1 - \sigma^L) \frac{\langle T \rangle - \langle \bar{T} \rangle^{EWA}}{\gamma_{t3}} \\ &+ (1 - \sigma^L) \left(1 - \frac{\theta^{EWA}_{sgs}}{\theta^{EWA}} \right) \frac{\theta^R - \theta^{EWA} \bar{T} - \langle \bar{T} \rangle^{EWA}}{\theta^R + \theta^{EWA}} \frac{\langle \bar{T} \rangle^{EWA}}{2\gamma_{t4}} \end{aligned} \quad (18)$$

$$Q^{(T)} = \sigma^L \frac{\langle \bar{T} \rangle^{EWA} - \langle T \rangle}{\gamma_{r3}} \quad (19)$$

187 where $\theta^{EWA}_{sgs} = \overline{\langle T'^2_{sgs} \rangle}^{EWA}$ is EWA of the LES sgs temperature variance and θ^{EWA} is the EWA total LES
 188 temperature variance defined as $\theta^{EWA} = \langle (\bar{T} - \langle \bar{T} \rangle^{EWA})^2 + \overline{T'^2_{sgs}} \rangle^{EWA}$. $\theta^R = \langle T'^2 \rangle$ is the RANS temperature
 189 variance.

190 In regions where the LES is expected to be under-resolved, the mean temperature of the LES is modified by a
 191 source term that is added to its transport equation (Equation (17)). This source term is the first part of $Q^{\bar{T}}$ (defined
 192 in Equation (18)) and it increases or decreases the LES temperature to match the LES EWA temperature with the
 193 RANS temperature. At the other locations, the RANS temperature is driven towards the LES EWA temperature
 194 through the drift term $Q^{(T)}$ in the RANS temperature equation (Equation (16)).

195 As regards the temperature fluctuations, at locations where the LES is under-resolved, both the resolved and
 196 modelled temperature fluctuations of the LES are adjusted to drive the EWA total LES temperature variance
 197 towards the RANS temperature variance. The resolved temperature fluctuations are modified by the second part
 198 of the source term $Q^{\bar{T}}$ (see Equation (18)) in the LES temperature equation (Equation (17)) and the modelled

199 temperature fluctuations are altered by adding a source term ($\overline{Q^{T'^2}_{sgs}}$) to the sgs temperature variance transport
 200 equation:

$$\begin{aligned} & \frac{\partial \overline{T'^2_{sgs}}}{\partial t} + \bar{U}_j \frac{\partial \overline{T'^2_{sgs}}}{\partial x_j} = \\ & 2 \left(\frac{\nu}{Pr} + \frac{\nu_{sgs}}{Pr_{sgs}} \right) \frac{\partial \bar{T}}{\partial x_i} \frac{\partial \bar{T}}{\partial x_i} - \frac{1}{Pr} \frac{\varepsilon^L}{k_{sgs}} \overline{T'^2_{sgs}} \\ & + \frac{\partial}{\partial x_j} \left(\left(\frac{\nu}{Pr} + \frac{\nu_{sgs}}{Pr_{sgs}} \right) \frac{\partial \overline{T'^2_{sgs}}}{\partial x_j} \right) + \overline{Q^{T'^2}_{sgs}} \end{aligned} \quad (20)$$

201 where:

$$\overline{Q^{T'^2}_{sgs}} = (1 - \sigma^L) \frac{\theta^{EWA}_{sgs} \theta^R - \theta^{EWA}}{\theta^{EWA} \gamma_{l4}} \quad (21)$$

202 and

$$\varepsilon^L = 2\nu \overline{S_{ij} S_{ij}} + \nu_{sgs} \overline{S_{ij} S_{ij}} \quad (22)$$

203 On the other hand, at locations where the LES is well-resolved, the RANS temperature variance is relaxed
 204 towards the EWA total LES temperature variance by the term $Q^{(T'^2)}$ in the RANS temperature variance equation:

$$\begin{aligned} & \frac{\partial \langle T'^2 \rangle}{\partial t} + \langle U_j \rangle \frac{\partial \langle T'^2 \rangle}{\partial x_j} = 2 \frac{\nu_t}{Pr_t} \frac{\partial \langle T \rangle}{\partial x_i} \frac{\partial \langle T \rangle}{\partial x_i} \\ & - \frac{1}{R_t} \frac{\varepsilon^R}{k^R} \langle T'^2 \rangle + \frac{\partial}{\partial x_j} \left(\left(\frac{\nu}{Pr} + \frac{\nu_t}{Pr_t} \right) \frac{\partial \langle T'^2 \rangle}{\partial x_j} \right) \\ & + Q^{(T'^2)} \end{aligned} \quad (23)$$

205 where R_t (the thermal to dynamic time scales ratio) was set equal to 0.5 and the drift tem $Q^{(T'^2)}$ reads:

$$Q^{(T'^2)} = \sigma^L \frac{\theta^{EWA} - \theta^R}{\gamma_{r4}} \quad (24)$$

206 The relaxation time scales of the thermal field read:

$$\gamma_{l3} = \gamma_{r3} = \max \left(R_t C_{\gamma 1} \frac{k^R}{\varepsilon^R}, \Delta t \right) \quad (25)$$

$$\gamma_{l4} = \gamma_{r4} = \max \left(R_t C_{\gamma 2} \frac{k^R}{\varepsilon^R}, \Delta t \right) \quad (26)$$

207 3.2. Turbulence models

208 The LES and RANS models used here are the one equation k model and the $BL v2/k$ model of Billard &
 209 Laurence (2012), respectively. The equations of the versions of these models that were used in this study are

210 provided in the Appendix. Details of the RANS model can be found in Billard and Laurence (2012), Uribe (2006),
211 Hanjalić et al. (2004), Manceau et al. (2002) and Durbin (1991). The reader is also referred to Yoshizawa and
212 Horiuti (1985) and Fureby et al. (1997) for details about the LES model.

213 **4. Computational implementation and discretization techniques**

214 All the simulations of this study were run in OpenFOAM 2.3.x using the dual-mesh code of Tunstall (2016).
215 However, the heat transfer part of the dual-mesh formulation of Tunstall (2016) has been implemented as part of
216 this work. Additionally, the dual-mesh code was combined with “buoyantBoussinesqPimpleFoam”, which is an
217 OpenFOAM solver for buoyant flows. The buoyancy related terms were also added to the equations of the RANS
218 model.

219 A second-order accurate backwards scheme is used for the temporal discretization of both the RANS and the
220 LES simulations. Regarding the spatial discretization, central differencing was used for the LES. On the other
221 hand, the van Leer scheme (van Leer (1974)) was used for all the RANS equations with the exception of the
222 momentum equation in which the second-order accurate upwind scheme was employed. The adjustable time step
223 option in OpenFOAM was used to ensure that the Courant number remains less than 1. The pressure velocity
224 coupling was handled using the PISO algorithm (Issa (1986)). The solver and the discretization procedures have
225 been extensively tested and benchmarked over a variety of heat transfer and thermal hydraulics applications in the
226 past, see Guleren et al. (2010), Han et al. (2012), Afgan et al. (2008), Kahil et al. (2019), Abed & Afgan (2017),
227 Abed & Afgan (2020), Abed et al. (2020a), Abed et al. (2020b) and Benhamadouche et al. (2020).

228 **5. Results**

229 In the results presented here, the same nondimensionalization as the one chosen by Sebilliau et al. (2018) was
230 used:

$$231 \mathbf{U} = \frac{\mathbf{U} H Pr}{\nu Ra^{0.5}}, T = \frac{T - \left(\frac{T_h + T_c}{2}\right)}{\Delta T}, \mathbf{x} = \frac{\mathbf{x}}{H} \quad (27)$$

232 where \mathbf{U} is the velocity vector, T is the temperature, \mathbf{x} is the position vector, H is the cavity height and ΔT is the
233 temperature difference: $T_h - T_c$. It should be noted that the terms “hybrid RANS” and “hybrid LES” are used
234 for the RANS and the LES simulations that are run simultaneously when using the dual-mesh approach. On the
235 other hand, what is meant by “pure RANS” and “pure coarse LES” are the RANS and coarse LES simulations
236 that are run without being corrected and forced towards each other. The second moments of all the simulations
237 reported in this section were calculated as the sum of their resolved and modelled components. For details about
how this calculation can be done, the reader can refer to Sebilliau (2016).

238 Regarding the parameters of the dual-mesh method, the only parameter that needs to be chosen before the
239 simulation which is the averaging period (T_{avg}) has been specified here as $32 \frac{H}{\sqrt{g\beta H\Delta T}}$, where $\sqrt{g\beta H\Delta T}$ is a buoyant
240 velocity scale (see for example Kumar & Dewan (2016) and Ammour et al. (2013)).

241 In section 5.1, the results obtained from the pure RANS and pure coarse LES simulations are reported. This
242 allows the reader to get an idea of some of the shortcomings of these standalone simulations. In section 5.2, a new
243 “resolution based” criterion for determining σ^L is suggested. Section 5.3 discusses the dual-mesh results obtained
244 when σ^L was evaluated using the new criterion.

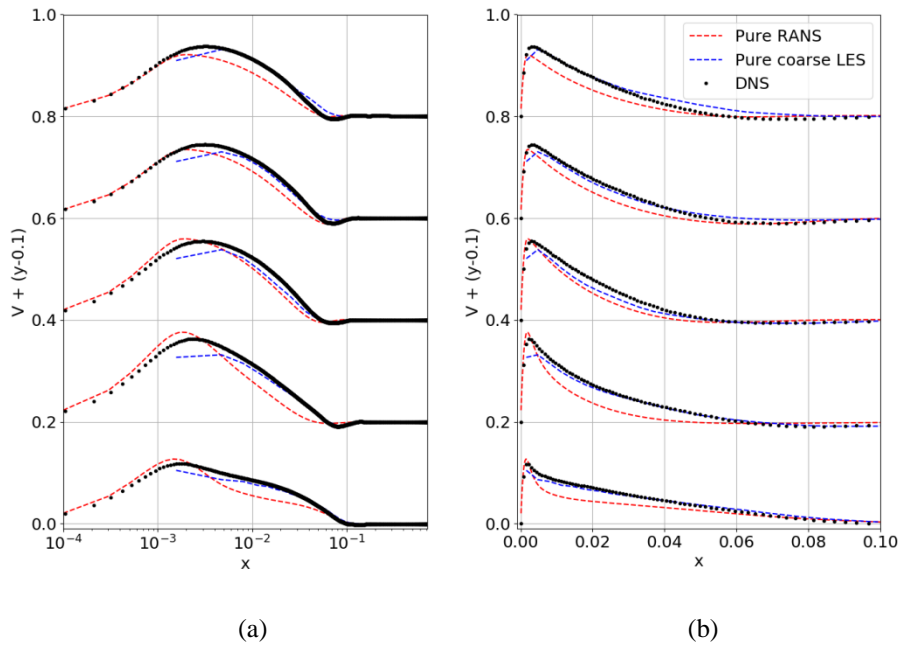
245 **5.1. Pure RANS and pure coarse LES results:**

246 Profiles of the mean velocity, total turbulent kinetic energy, total turbulent shear stress¹ and mean temperature
247 from the pure RANS and pure coarse LES simulations are shown in Fig. 3-Fig. 5. All these statistics have been
248 computed using the classic arithmetic mean operation (not to be confused with the EWA operation). It can be seen
249 that the coarse LES predictions of the velocity and temperature are reasonable away from the wall. The LES
250 predictions of the turbulent shear stress can be observed to improve towards the outer edge of the boundary layer.
251 However, the coarse LES cannot be relied upon to provide wall parameters such as the Nusselt number and the
252 wall shear stress.

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¹ It should be noted that the quantities called the total turbulent kinetic energy and the total turbulent shear stress do not only represent the fluctuations due to turbulence but also the fluctuations that are caused by mean flow instabilities.



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257 Fig. 3. Plots showing the pure coarse LES and pure RANS predictions of the mean vertical velocity profiles near
 258 the hot wall at horizontal lines that correspond to cavity heights equal to $0.1H$, $0.3H$, $0.5H$, $0.7H$ and $0.9H$. (a)

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is a semi logarithmic plot (b) is a linear plot.

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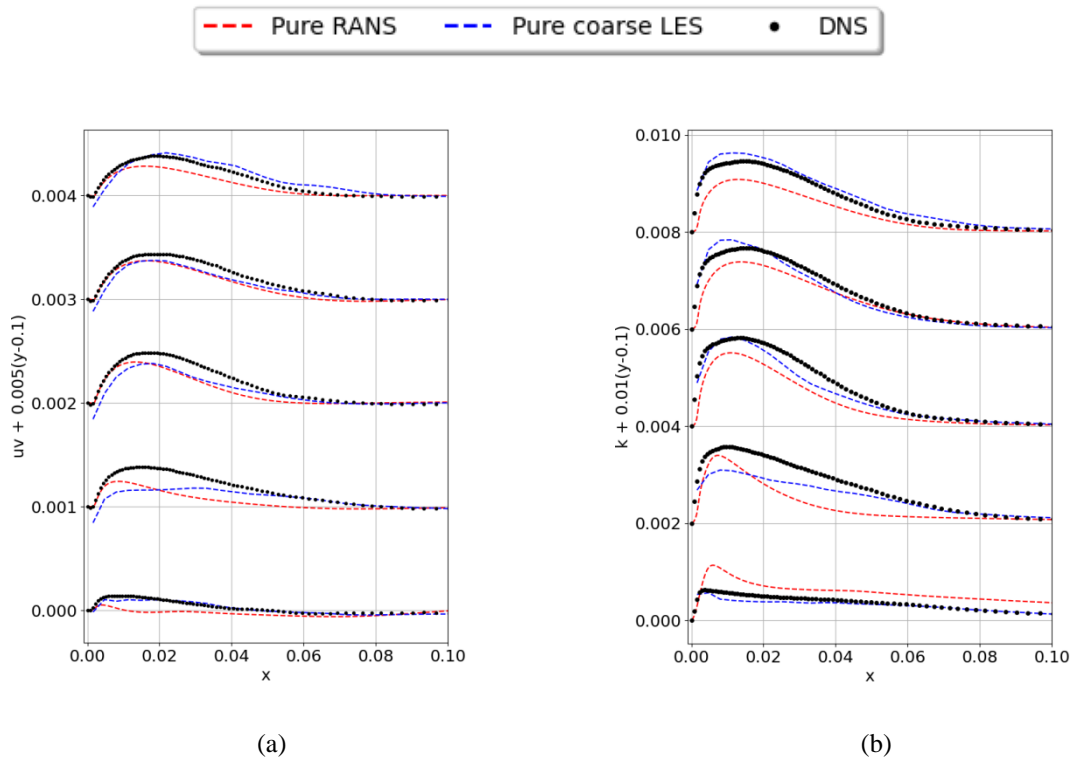


Fig. 4. Plots showing the pure coarse LES and pure RANS predictions of the profiles near the hot wall at horizontal lines that correspond to cavity heights equal to $0.1H, 0.3H, 0.5H, 0.7H$ and $0.9H$. (a) turbulent shear stress (b) total turbulent kinetic energy.

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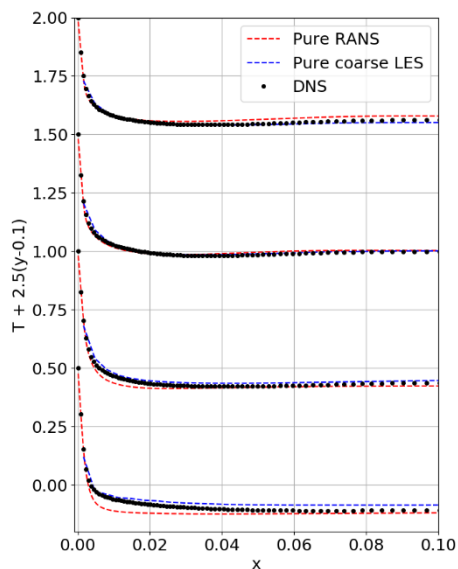
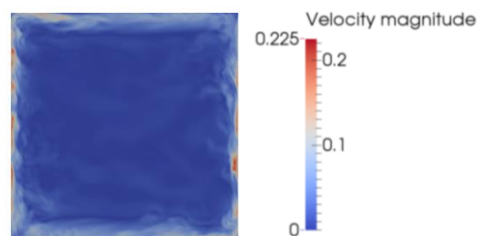


Fig. 5. A plot showing the pure coarse LES and pure RANS predictions of the mean temperature profiles near the hot wall at horizontal lines that correspond to cavity heights equal to $0.1H, 0.3H, 0.5H$ and $0.7H$.

285 The pure RANS predictions of the velocity profiles are unsatisfactory. At the heights of $0.1H$ and $0.3H$, the
286 velocity in the immediate vicinity of the wall is overpredicted. This is because at these locations there is an
287 underprediction of the wall normal mixing of wall parallel momentum clearly seen in the turbulent shear stress
288 profiles at these locations (Fig. 4 (a)). The inadequate wall normal mixing of the RANS at $y=0.1H$ and $0.3H$ is
289 consistent with the fact that the RANS underpredicts the thickness of the momentum boundary layer at the height
290 of $0.3H$ as well as the width of the thermal boundary layer at both $y=0.1H$ and $0.3H$. At the vertical locations of
291 $y = 0.7H$ and $0.9H$, the pure RANS seems to underpredict the velocity in the entire boundary layer. The total
292 turbulent kinetic energy (TTKE) is underpredicted at all the locations apart from the height of $0.1H$ at which the
293 RANS overpredicts the TTKE. The pure coarse LES predictions of the TTKE are in better agreement with the
294 reference DNS data than the pure RANS.

295 One important thing to note is that this flow features the presence of unstably stratified flow regions particularly
296 near the top right and bottom left corners. This unstable stratification is caused by the linear temperature profile at
297 the horizontal walls. As explained by Sebilliau et al. (2018), this unstable stratification causes the appearance of
298 buoyant plumes which rise along the hot wall and fall along the cold wall. This instability is the main reason why
299 turbulence levels in this cavity are greater than what the turbulence levels would be in a cavity with horizontal
300 walls that are adiabatic at the same Rayleigh number. These large turbulence levels can be observed in Fig. 6 in
301 which a snapshot of the velocity field of the pure coarse LES simulation is shown.

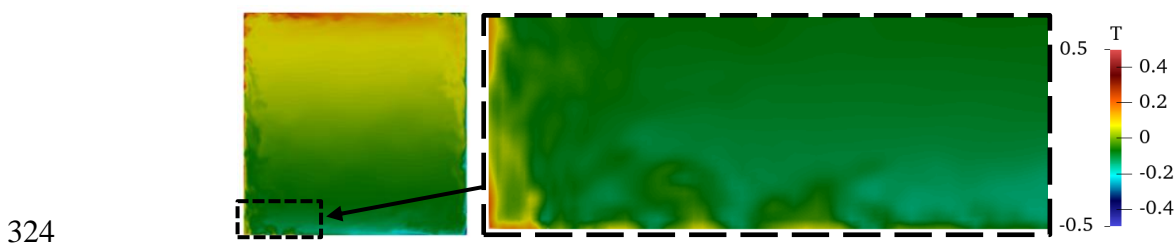


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303 Fig. 6. An instantaneous snapshot of the LES velocity magnitude from the pure coarse LES simulation.

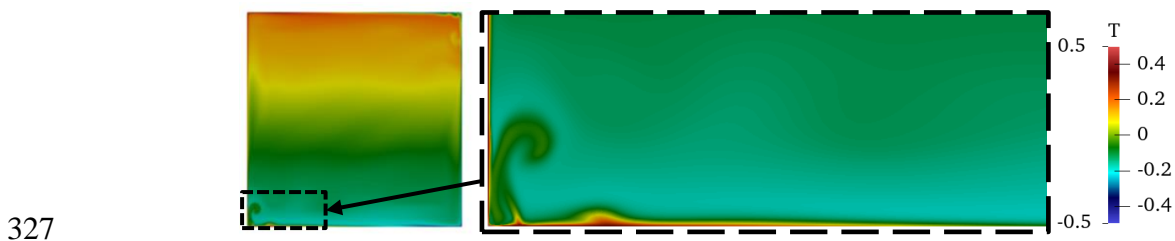
304 The high turbulence levels and the instabilities present in this flow are the reasons why no problem regarding
305 the transition of the flow to a turbulent state was faced when the one-equation k model was used even though this
306 model is dissipative and the LES grid is coarse. The same LES model was one of the models used by Kumar &
307 Dewan (2016) in their wall-resolved LES study of the square cavity. The temperature variation imposed by the
308 authors at the horizontal walls is likely to be the reason why no transition problem was reported. On the other
309 hand, Barhaghi & Davidson (2007) experienced a transition delay problem when using the Smagorinsky model
310 (which is also dissipative) to simulate a tall buoyant cavity which can be attributed to the adiabatic condition at

311 the horizontal walls of the cavity. Contrarily, the authors attained a good transition prediction with the dynamic
312 Smagorinsky model.

313 Snapshots of the instantaneous temperature fields from the pure RANS and pure coarse LES simulations are
314 shown in Fig. 7 and Fig. 8. In order to well visualize the aforementioned instability, a closer view of the flow near
315 the bottom left corner is provided for both the pure RANS and the pure coarse LES temperature snapshots. In the
316 RANS zoomed-in view, the unstable stratification that triggers the instability can be clearly seen near the bottom
317 wall. This stratification increases from right to left (following the flow direction) until it is strong enough to allow
318 the instability to form. It can be observed that the onset location of the pure coarse LES instability is upstream of
319 the location where the RANS instability starts. However, the RANS instability appears to have a larger lengthscale
320 than the LES instability. This might be the reason why the RANS predicts a high TTKE at the height of $0.1H$ since
321 at this location the RANS resolved variances are significantly greater than the modelled variances. The dominance
322 of the RANS resolved component of the TTKE over the modelled one in the boundary layer was observed to
323 almost vanish near the midheight of the cavity.



325 Fig. 7. An instantaneous snapshot of the temperature from the pure coarse LES simulation. A zoomed-in view of
326 the contours near the bottom left corner is provided as well.



328 Fig. 8. An instantaneous snapshot of the temperature from the pure RANS simulation. A zoomed-in view of the
329 contours near the bottom left corner is provided as well.

330 **5.2. Estimating the LES zone weight (σ^L) by comparing the turbulence lengthscales and**
331 **the grid size**

332 One of the main purposes of this study is to design a new criterion that determines σ^L by assessing the resolution
333 of the LES grid and successfully use this criterion in a dual-mesh simulation of the square cavity flow. The basic
334 idea behind a criterion of this type is that it gives $\sigma^L = 1$ at the locations where the LES is well-resolved and gives
335 $\sigma^L = 0$ at the remaining locations. The development of this criterion was motivated by the complexity that is
336 present in this flow as it features coexistence of laminar and turbulent zones. The Re_y criterion (see Equation (8))
337 gives $\sigma^L = 0$ in the laminar regions and thus cannot distinguish between the laminarization in these regions and
338 the laminarization that occurs in the viscosity affected region. Details of this behaviour as well as the results
339 obtained using the Re_y criterion are included in Appendix C.

340 Three important studies in which the LES resolution was assessed by comparing the grid size to the turbulence
341 lengthscales are the studies of Xiao et al. (2014), Addad et al. (2008) and Uribe et al. (2010). Xiao et al. (2014)
342 designed a criterion that assesses the grid resolution in the three different directions by defining a turbulence
343 lengthscale associated with each direction and comparing it to the filter width in that direction. In this study,
344 however, for simplicity we base our criterion on turbulence lengthscales that are scalar quantities rather than
345 vectors or tensors. Addad et al. (2008) argued that the LES can be considered to be well-resolved at locations
346 where the grid size (Δ) satisfies the following condition:

$$\Delta < \max\left(\lambda, \frac{L_{RM}}{10}\right) \quad (28)$$

347 where L_{RM} and λ are the RANS predictions of the integral and Taylor lengthscales, respectively:

$$L_{RM} = \frac{k^{3/2}}{\varepsilon} \quad (29)$$

$$\lambda = \sqrt{\frac{10\nu k}{\varepsilon}} \quad (30)$$

350 The lengthscale $\frac{L_{RM}}{10}$ was introduced as a lower limit in Equation (28) because for high Reynolds numbers, the
351 grid size does not need to be as small as the Taylor lengthscale (λ) and the resolution can be considered adequate
352 if the grid allows resolving eddies with lengthscales greater than one tenth of the integral lengthscale (Addad et al.
353 (2008)).

354 In the study of Uribe et al. (2010), the authors formulated their RANS-LES blending functions as:

$$f_b = \tanh\left(C_1 \frac{\varphi k^{3/2}}{\varepsilon \Delta}\right)^n \quad (31)$$

355 where C_1 and n are constants. This function assesses the resolution of the LES grid by comparing the grid spacing
 356 Δ to the lengthscale $\frac{\varphi k^{3/2}}{\varepsilon}$ which represents the integral lengthscale $\frac{k^{3/2}}{\varepsilon}$ multiplied by the wall-normal anisotropy
 357 $\varphi = \frac{\langle v^2 \rangle}{k}$ (the ratio of the wall-normal Reynolds stress to the turbulent kinetic energy). Multiplying the integral
 358 lengthscale by φ provides a damping of the former in the near-wall region as $\frac{k^{3/2}}{\varepsilon}$ can become large in this region.
 359 A comparison of $\frac{k^{3/2}}{\varepsilon}$ and $\frac{\varphi k^{3/2}}{\varepsilon}$ in the near-wall region of a channel flow can be found in Uribe (2006).

360 In this study we first choose to combine the resolution criteria of Addad et al. (2008) and Uribe et al. (2010).
 361 This was done by starting from Equation (28) and multiplying both the integral and Taylor lengthscales by a
 362 damping function as:

$$\Delta < \max(\psi \lambda, \psi \frac{L_{RM}}{10}) \quad (32)$$

363 where the damping function ψ was defined using the elliptic blending parameter α (see Appendix A) as follows:

$$\psi = \frac{3}{2} \left((1 - \alpha^3) \varphi + \alpha^3 \frac{2}{3} \right) \quad (33)$$

364 Using this function in Equation (32) damps the integral and Taylor lengthscales close to the wall since as the
 365 wall is approached the values of α and φ go to 0 and as a result the damping function ψ becomes approximately
 366 equal to $\frac{3}{2} \varphi$ which approaches 0. On the other hand, at locations far enough from the wall for α to become close
 367 to 1, ψ approaches 1 and thus the lengthscales λ and $\frac{L_{RM}}{10}$ in Equation (32) are not damped. ψ was not formulated
 368 using $\psi = \frac{3}{2} \varphi$ since far from the wall φ is not guaranteed to become equal to $\frac{2}{3}$ (meaning ψ can be smaller than 1
 369 at large wall distances). For instance even in the centreline of a channel, turbulence is not isotropic (the three
 370 normal Reynolds stresses are not equal at this location) and thus φ does not equal $\frac{2}{3}$ (see for example the DNS data
 371 of Kawamura et al. (1998)).

372 In contrast to the flow studied here, the test cases in Xiao et al. (2014), Addad et al. (2008) and Uribe et al. (2010)
 373 do not feature unsteadiness, buoyancy forces or flow laminarization. Therefore, the new criterion has to be
 374 designed to account for these flow features. This gives the new criterion the advantage that it can be used for
 375 buoyancy driven flows, where the aforementioned features are quite often found.

376 One point worth noting is that the lengthscales λ and L_{RM} were calculated here using the total RANS turbulent
 377 kinetic energy (k^R_{Total}) and the total RANS dissipation rate (ε^R_{Total}) which were calculated from the pure RANS
 378 results as:

$$L_{RM} = \frac{k_{Total}^R{}^{3/2}}{\varepsilon_{Total}^R} \quad (34)$$

379

$$\lambda = \sqrt{\frac{10\nu k_{Total}^R}{\varepsilon_{Total}^R}} \quad (35)$$

380 where k_{Total}^R and ε_{Total}^R were calculated as:

$$k_{Total}^R = \{k^R\} + k_{Res}^R \quad (36)$$

381

$$\varepsilon_{Total}^R = \{\varepsilon^R\} + \varepsilon_{Res}^R \quad (37)$$

382 where $\{\}$ is used here to represent quantities averaged in time using a simple arithmetic mean operation. k^R and
 383 k_{Res}^R are the pure RANS modelled and resolved turbulent kinetic energies², respectively. k_{Res}^R was calculated
 384 as:

$$k_{Res}^R = 0.5 * \{u_i''^R u_i''^R\} \quad (38)$$

385 where $u_i''^R = \langle U_i \rangle - \{\langle U_i \rangle\}$ represents the resolved RANS velocity fluctuation. In addition, ε^R and ε_{Res}^R are the
 386 pure RANS modelled and resolved turbulent dissipation rates³, respectively. ε_{Res}^R was estimated using:

$$\varepsilon_{Res}^R = 2\nu\{\langle S_{ij} \rangle \langle S_{ij} \rangle\} \quad (39)$$

$$\langle S_{ij} \rangle = 0.5 \left(\frac{\partial \langle U_i \rangle}{\partial x_j} + \frac{\partial \langle U_j \rangle}{\partial x_i} \right) \quad (40)$$

387 The problem with Equation (32) is that in laminar zones it is difficult to predict the behaviour of the lengthscales
 388 L_{RM} and λ . The definitions in Equations (34) and (35) are not guaranteed to give lengthscales that are greater than
 389 0 in all the laminar zones. If L_{RM} and λ both become equal to 0 at a particular location, Equation (32) will see that
 390 the grid size is greater than the turbulence lengthscales, which is a false indication of an under-resolved LES at
 391 this location. As a result, in the dual-mesh context the LES will be forced towards the RANS at this location. This
 392 can be problematic at the laminar locations where instabilities that enhance the turbulence levels form (in this
 393 cavity flow these instabilities exist near the top right and bottom left corners). Forcing the LES fluctuations at
 394 these locations can destroy the LES instabilities and affect the predicted turbulence levels. In addition, one would

² What is meant here by the RANS resolved turbulent kinetic energy is the kinetic energy of the unsteady motions resolved in the RANS simulation which represent mean flow instabilities rather than turbulence.

³ The RANS resolved turbulent dissipation rate term was used to represent the rate at which the energy of the unstable motions resolved in the RANS simulation is dissipated into heat.

395 want the LES to drive the RANS at all the laminar locations as the LES does a better job than the RANS in
 396 predicting the interaction of the laminar zones with the turbulent ones.

397 To prevent the condition in Equation (32) from being violated in the laminar zones, the lengthscales were limited
 398 by making use of the pure RANS prediction of the Kolmogorov lengthscale (η) as:

$$\Delta < \max(\psi\lambda, \psi \frac{L_{RM}}{10}, 8C_{kolm}\eta) \quad (41)$$

399 where:

$$\eta = \left(\frac{\nu^3}{\{\varepsilon^R\}} \right)^{\frac{1}{4}}, \quad (42)$$

400

$$C_{kolm} = \begin{cases} 1 & \text{for } d \geq \Delta_{max}, \\ 0.3125 & \text{for } d < \Delta_{max} \end{cases} \quad (43)$$

401 where d is the wall distance and $\Delta_{max} = \max(\Delta_x, \Delta_y, \Delta_z)$ is the largest cell size in the three directions.

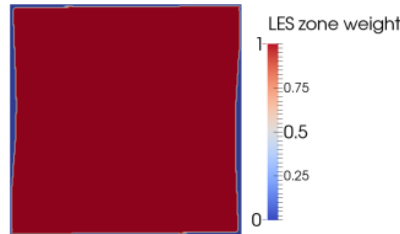
402 It can be observed that the time average of the RANS modelled dissipation rate ($\{\varepsilon^R\}$) is used in the definition
 403 of the Kolmogorov lengthscale and not the total dissipation rate ε^R_{Total} (ε^R_{Total} was used in the definitions of the
 404 integral and Taylor scales). This is to make the product 8η much larger than the grid size Δ in the laminar zones
 405 where $\varepsilon^R \rightarrow 0$. This in turn allows the criterion in Equation (41) to correctly predict that the LES is well-resolved
 406 at the laminar zones. 8η is multiplied by C_{kolm} in order to provide a damping in the viscous sublayer as 8η becomes
 407 much larger than $\psi\lambda$ and $\psi \frac{L_{RM}}{10}$ and might become larger than the grid size in this region. This damping thus
 408 prevents the quantity $8C_{kolm}\eta$ from becoming larger than the grid size in the viscosity affected region (otherwise
 409 the criterion might falsely indicate that the LES is well-resolved at some locations in the sublayer).

410 In Equation (43), it is assumed that wall distances lower than the value of Δ_{max} correspond to the viscous
 411 sublayer. The justification for this assumption is that the purpose of damping the Kolmogorov lengthscale using
 412 C_{kolm} is to prevent the maximum lengthscale in Equation (41) from becoming larger than the grid size near the
 413 wall for coarse LES grids. For these grids, a wall distance equal to the maximum grid spacing Δ_{max} corresponds
 414 to a y^+ that is definitely greater than 11. Thus, the Kolmogorov damping we introduced remains active over the
 415 entire viscous sublayer (the viscosity affected region extends up to a y^+ of about 11). The criterion in Equation
 416 (41) can be used to estimate the LES zone weight (σ^L) in the hybrid simulation using:

$$\sigma^L = \begin{cases} 1 & \text{for } \Delta < \max(\psi\lambda, \psi \frac{L_{RM}}{10}, 8C_{kolm}\eta) \\ 0 & \text{for } \Delta > \max(\psi\lambda, \psi \frac{L_{RM}}{10}, 8C_{kolm}\eta) \end{cases} \quad (44)$$

417 One observation that can be made about this equation is that σ^L does not need to be calculated repeatedly during
 418 the entire dual-mesh hybrid simulation. This is because all the turbulence lengthscales in Equation (44) are
 419 calculated from the pure RANS results. The use of hybrid RANS to estimate these lengthscales was avoided as the
 420 relaxation forcing in the LES regions can pollute predictions of the turbulence quantities in these regions.
 421 Therefore, one can run the pure RANS simulation, calculate the required lengthscales and then run the dual-mesh
 422 simulation (it is a good practice to run the pure RANS before the dual-mesh simulation since the pure RANS
 423 results give good initial conditions for the hybrid RANS simulation). σ^L can then be calculated at one of the initial
 424 time steps of the dual-mesh simulation since nothing in Equation (44) changes during this simulation. In order to
 425 calculate σ^L in the hybrid simulation, the turbulence lengthscales in Equation (44) need to be interpolated into the
 426 LES grid so that they can be compared to Δ , which we chose to calculate as the cubic root of the volume of the
 427 cell⁴ $(\Delta_x \Delta_y \Delta_z)^{1/3}$. After this σ^L can be interpolated into the RANS grid so that it can be used in the RANS
 428 equations.

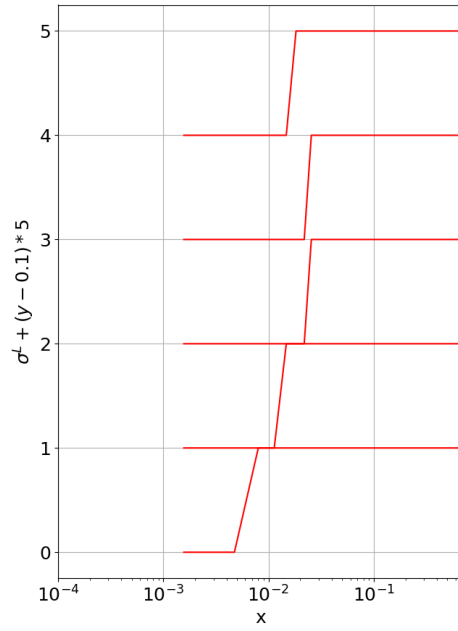
429 In Fig. 9, a contour plot of σ^L from a hybrid simulation in which it was estimated using the new lengthscale
 430 criterion is presented. It can be seen that Equation (44) gives the required behaviour of σ^L . σ^L is equal to 1 in the
 431 laminar core and the regions where σ^L is equal to 0 (RANS regions) near the top right and bottom left corners are
 432 very thin. Profiles of σ^L near the hot wall are also shown in Fig. 10.



433
 434 Fig. 9. Contours of the LES zone weight (σ^L) from a hybrid simulation in which it was estimated using Equation
 435 (44).

436
 437

⁴ Δ was not calculated as $\max(\Delta_x, \Delta_y, \Delta_z)$ in order to avoid ending up with thick RANS regions (with $\sigma^L = 0$) close to the horizontal walls.



438

439 Fig. 10. Mean values of the LES zone weight (σ^L) from a hybrid simulation in which it was calculated using
 440 Equation (44). This figure shows σ^L profiles at horizontal lines that correspond to cavity heights equal to $0.1H$,
 441 $0.3H$, $0.5H$, $0.7H$ and $0.9H$. The horizontal axis is in log scale.

442 Plots of the lengthscales $\psi\lambda$, $\psi \frac{L_{RM}}{10}$, $8C_{kolm}\eta$, 8η and Δ at four cavity heights are shown in Fig. 11 (a)-(d). The
 443 damping of the integral and the Taylor lengthscales that is introduced by the function ψ results in a relatively
 444 smooth change of these lengthscales with the wall distance in the wall vicinity compared to the behaviour of the
 445 undamped lengthscales λ , $\frac{L_{RM}}{10}$ which can be seen in Fig. 12. The undamped lengthscales can also be observed to
 446 become quite large close to the wall.

447 It can be seen from Fig. 11 that close to the wall, the quantity 8η becomes much larger than the lengthscales $\psi\lambda$
 448 and $\psi \frac{L_{RM}}{10}$. On the other hand, the quantity $8C_{kolm}\eta$ which equals 2.5η at wall distances less than Δ_{max} (see
 449 Equation (43)) appears to provide a much more reasonable estimation of the near-wall turbulence lengthscale than
 450 8η . $8C_{kolm}\eta$ can be observed to become quite large at $x = 0.1$ (which corresponds to an average x^+ of around
 451 885). This is because of the almost vanishing turbulence at this location (see the pure RANS turbulent kinetic
 452 energy profiles in Fig. 4 (b)) which causes a small value of ε^R which leads to a large estimation of $8C_{kolm}\eta$ (see
 453 the definition of η in Equation (42)).

454 Fig. 11 shows that $\psi \frac{L_{RM}}{10}$ and $\psi\lambda$ are not close to 0 at $x = 0.1$. This is because these two lengthscales have been
 455 based on the RANS total turbulent kinetic energy (k^R_{Total}) and the RANS total dissipation rate (ε^R_{Total}). These

456 two quantities do not approach 0 at $x = 0.1$. Even though at this location the turbulent fluctuations are very weak
457 (meaning both k^R and ε^R approach 0), the unsteady motion of the core makes k^R_{Res} and ε^R_{Res} non-zero resulting
458 in nonzero values of k^R_{Total} and ε^R_{Total} . The large values of $\psi \frac{L_{RM}}{10}$ and $\psi\lambda$ serve to prevent σ^L from falling to
459 zero, and hence prevent the RANS from driving the LES outside the boundary layer.

460 As mentioned previously, the lengthscale $8C_{kolm}\eta$ is used in Equation (44) to provide an additional safeguard
461 that prevents the condition in the equation from being violated in laminar zones, where the lengthscales $\psi \frac{L_{RM}}{10}$ and
462 $\psi\lambda$ are not guaranteed to become large. In Fig. 11 (e), a plot of the turbulence lengthscales at a vertical line located
463 at a horizontal distance of $0.1H$ from the hot wall is shown. This location features low turbulence levels but is
464 dominated by the unsteady motions which have been discussed previously. The low turbulence levels at this
465 location result in a low ε^R and make $8C_{kolm}\eta$ larger than the other lengthscales ($\psi \frac{L_{RM}}{10}$ and $\psi\lambda$) up to a wall
466 distance of about $0.01H$. This relatively high near-wall value of $8C_{kolm}\eta$ makes σ^L rise to 1 at a distance of about
467 0.008 from the wall as a consequence of Δ becoming less than $8C_{kolm}\eta$ at this wall distance (Fig. 13).

468 If one was relying only on the lengthscales $\psi \frac{L_{RM}}{10}$ and $\psi\lambda$, the distance at which σ^L becomes 1 would have been
469 larger than 0.008 . This can be observed from Fig. 11 (e) which shows that the wall distance after which Δ becomes
470 smaller than the lengthscales $\psi \frac{L_{RM}}{10}$ and $\psi\lambda$ is larger than the distance where Δ starts becoming smaller than the
471 lengthscale $8C_{kolm}\eta$. It is better to minimize the wall distance at which σ^L becomes 1 near the top right and bottom
472 left corners in order to avoid the risk of damping the instabilities present in the hybrid LES simulation at these
473 locations. Introducing the lengthscale $8C_{kolm}\eta$ as an argument in Equation (44) thus serves as a shield against a
474 late RANS-LES switch near the top right and bottom left corners. However, one still needs to avoid having a large
475 grid size Δ near these corners as this can result in a delay of the RANS-LES switch.

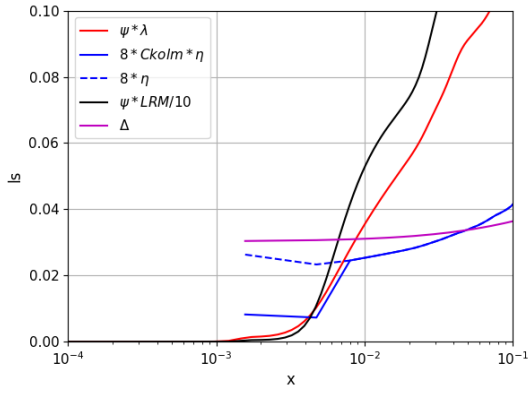
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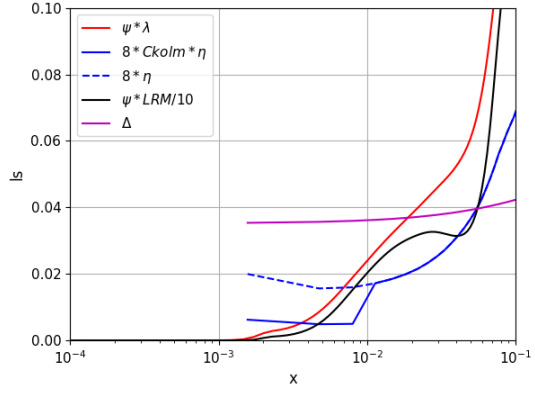
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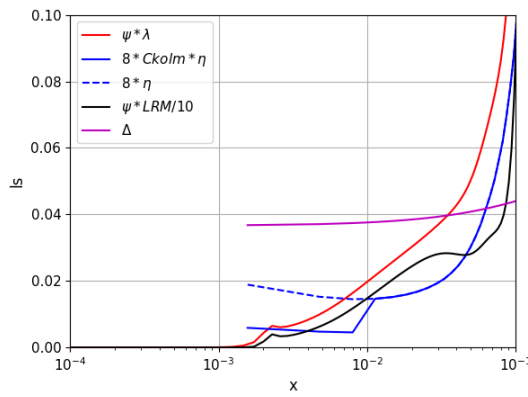
(a)



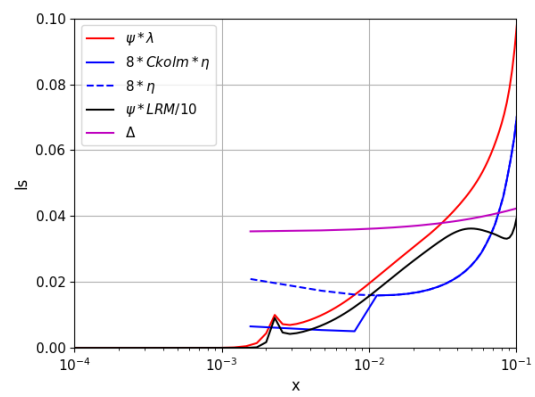
(b)

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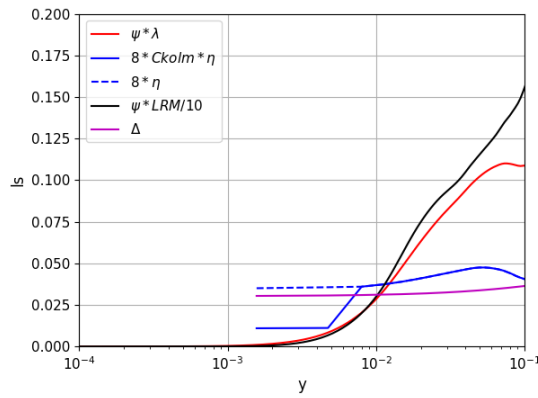
(c)



(d)

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(e)

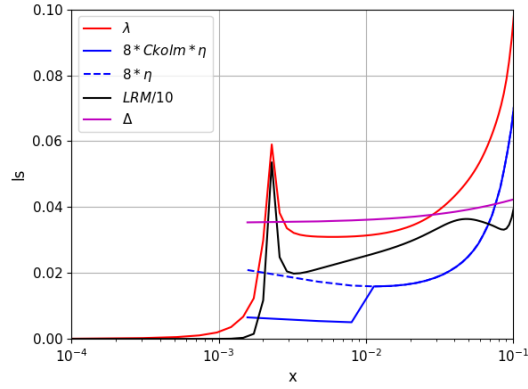
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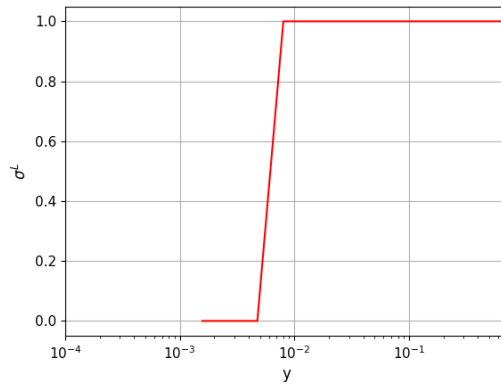
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Fig. 11. Plots of the lengthscales $\psi\lambda$, $\psi\frac{LRM}{10}$, 8η and $8C_{kolm}\eta$ as well as the filter width Δ (calculated as the cubic root of the volume of the cell) at horizontal lines that correspond to cavity heights equal to (a) $0.1H$ (b) $0.3H$ (c) $0.5H$ (d) $0.7H$. The profiles of the lengthscales and the filter width shown in (e) are at a vertical line that is located at a distance of $0.1H$ from the hot wall. The horizontal axis is in log scale.



489

490 Fig. 12. A plot of the lengthscales λ , $\frac{LRM}{10}$, 8η and $8C_{kolm}\eta$ as well as the filter width Δ (calculated as the cubic
 491 root of the volume of the cell) at a horizontal line that corresponds to the cavity height equal to $0.7H$. The
 492 horizontal axis is in log scale.



493

494 Fig. 13. A plot of the LES zone weight (σ^L) at a vertical line that is located at a distance of $0.1H$ from the hot
 495 wall. This plot is from a hybrid simulation in which σ^L was estimated using Equation (44). The horizontal axis
 496 is in log scale.

497 5.3. Dual-mesh results obtained using the new resolution criterion

498 The fact that the regions in which σ^L is 0 near the top right and bottom left corners are thin causes the hybrid
 499 RANS instability to be almost eliminated (see Fig. 15). The reason why the hybrid RANS becomes steady is the
 500 vigorous forcing of the RANS towards the LES in these regions. The averaged LES field is steady (the chosen
 501 EWA averaging period is large enough to smooth the LES field) and forcing the RANS towards it in a significant
 502 part of the region where the RANS instability forms eliminates the unsteadiness.

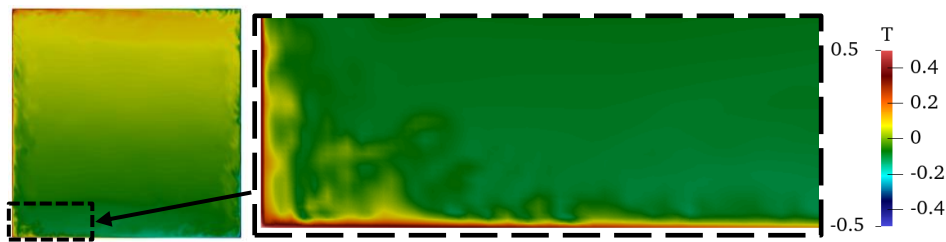
503 The fact that the hybrid RANS becomes steady simplifies the application of the dual-mesh approach as one does
 504 not need to take into account the time dependency of the RANS simulation when coupling the RANS and the LES.

505 In this case, the only requirement that has to be satisfied by T_{avg} is that it has to be large enough to smooth the
506 LES quantities and remove all the fluctuations. Although not shown here, the fact that the results of this section
507 hardly changed when the averaging time scale was doubled suggests that $T_{avg} = 32 \frac{H}{\sqrt{g\beta H\Delta T}}$ is large enough to
508 smooth out the turbulence structures.

509 The hybrid simulations perform well in predicting the vertical velocities near the hot wall as shown Fig. 16 (a).
510 This is because the hybrid RANS-LES coupling does not damp the instability in the hybrid LES simulation as can
511 be seen from the snapshot of the hybrid LES temperature field shown in Fig. 14. The reason why the LES instability
512 is not damped is that at the locations where the LES instability is dominant (near the top right and bottom left
513 corners), the LES is forced towards the RANS in only a thin layer close to the wall. Capturing this instability
514 allows the LES to predict the high turbulence levels along the vertical walls as these high levels are triggered by
515 the flow unsteadiness.

516

517



518 Fig. 14. An instantaneous snapshot of the LES temperature from a hybrid simulation in which the LES zone
519 weight was calculated using Equation (44). A zoomed-in view of the contours near the bottom left corner is
520 provided as well.

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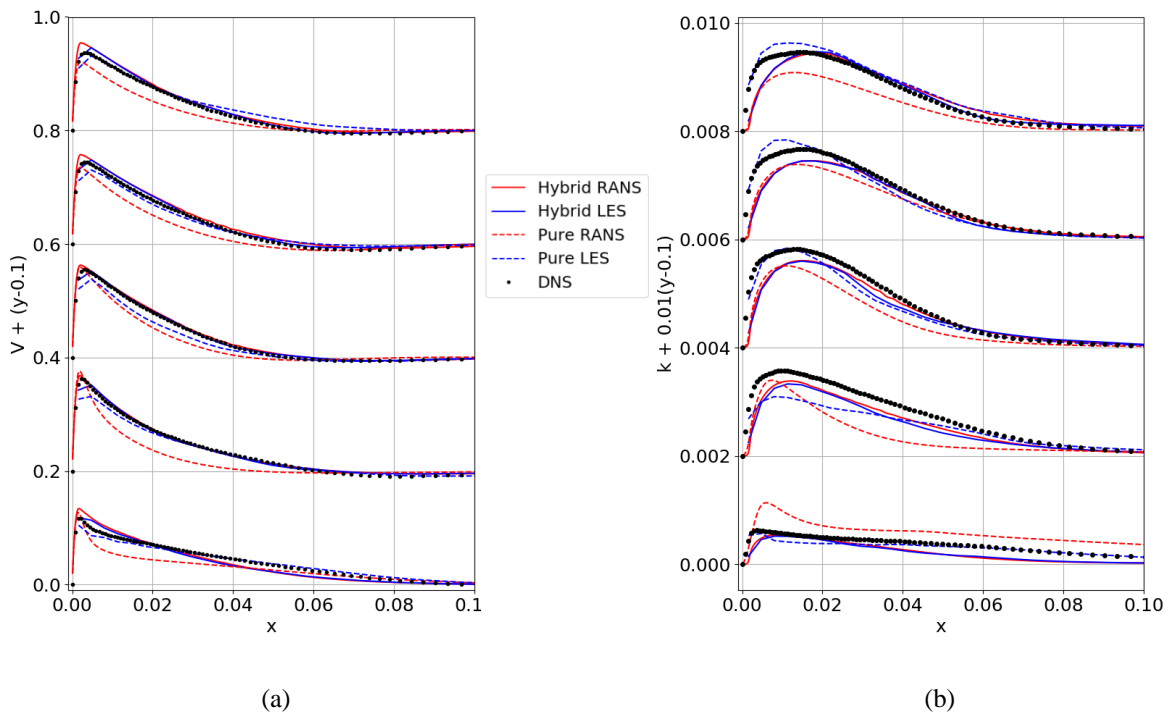


522 Fig. 15. An instantaneous snapshot of the RANS temperature from a hybrid simulation in which the LES zone
523 weight was calculated using Equation (44). A zoomed-in view of the contours near the bottom left corner is
524 provided as well.

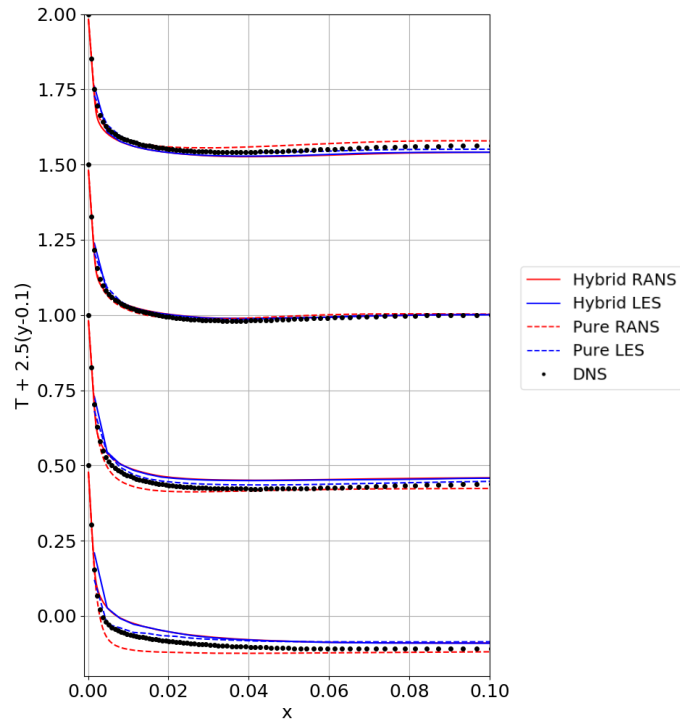
525 The predictions of the total turbulent kinetic energy profiles of the flow near the hot wall are shown in Fig. 16
526 (b). The reasonable hybrid predictions of these profiles at the downstream locations of the boundary layer are a

527 consequence of not damping the plume instability in the hybrid LES simulation. However, admittedly the hybrid
 528 method's predictions of the TTKE profiles worsen as the bottom wall is approached due to the low turbulence
 529 levels in the upstream region of the hot wall's boundary layer. The significant underprediction of the TTKE at the
 530 height of $0.1H$ is consistent with the poor hybrid velocity predictions at the same location. Fig. 17 also shows that
 531 the temperature profiles are of reasonable accuracy at all the locations apart from the height of $0.1H$.

532 It can be observed from Fig. 16 (a) that the hybrid LES simulation does a good job in capturing the interaction
 533 of the turbulent boundary layer with the laminar core. Note that the coarseness of the LES grid only allows
 534 capturing the outer edge of the boundary layer, since only the first and second cells contain the peak of the velocity
 535 profile, and the wall-jet side is fairly well modelled with the hybrid RANS. Conversely, the pure RANS simulation
 536 performed rather poorly on the cavity side but the RANS is aptly corrected by the LES when run in a hybrid
 537 simulation (the continuous red line is almost overlapped by the DNS symbols at most of the locations).



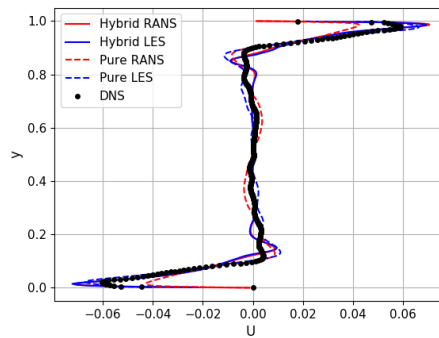
538
 539
 540 Fig. 16. Plots showing the pure RANS, pure LES, hybrid RANS and hybrid LES predictions of the profiles of
 541 the mean vertical velocity (shown in (a)) and the total turbulent kinetic energy (shown in (b)) near the hot wall at
 542 horizontal lines that correspond to cavity heights equal to $0.1H$, $0.3H$, $0.5H$, $0.7H$ and $0.9H$. In the hybrid
 543 simulations σ^L was calculated using Equation (44).



544

545 Fig. 17. A plot showing the pure RANS, pure LES, hybrid RANS and hybrid LES predictions of the mean
 546 temperature profiles near the hot wall at horizontal lines that correspond to cavity heights equal to $0.1H$, $0.3H$,
 547 $0.5H$ and $0.7H$. In the hybrid simulations σ^L was calculated using Equation (44).

548 The horizontal velocity profiles at the midwidth obtained using the different simulations are shown in Fig. 18. It
 549 can be seen from this figure that the hybrid simulations and the pure coarse LES do a much better job in predicting
 550 the velocity profile than the pure RANS. This is because the pure RANS performs worse than the other simulations
 551 in predicting the velocities at the hot wall boundary layer (Fig. 16 (a)).



552

553 Fig. 18. A plot showing the pure RANS, pure LES, hybrid RANS and hybrid LES predictions of the mean
 554 horizontal velocity at the cavity midwidth. In the hybrid simulations σ^L was calculated using Equation (44).

555 The wall shear stress (WSS) profiles along the hot wall are shown in Fig. 19 (a). It can be seen that the hybrid
556 LES does not accurately predict the WSS. This is because even though the EWA velocities at the near-wall nodes
557 of the LES are forced towards the corresponding RANS velocities, the wall distances of these nodes are large
558 enough to make the error associated with the finite difference approximation of the velocity gradient at the wall
559 non-negligible. This is the reason why the inaccuracy of the hybrid LES WSS is inevitable and one should consider
560 the hybrid RANS WSS predictions instead. In fact, the hybrid RANS gives reasonable predictions of the WSS
561 apart from a small overprediction between $y = 0.4$ and $y = 1$ which is caused by an overprediction of the velocity
562 peaks at these heights. This overprediction can be seen in the velocity profiles at the heights of $0.5H$, $0.7H$ and
563 $0.9H$ (Fig. 16 (a)). On the other hand, the pure RANS slightly overestimates the WSS at the bottom half of the hot
564 wall which is consistent with the overprediction of the velocity in the immediate wall vicinity which can be clearly
565 seen in Fig. 16 (a).

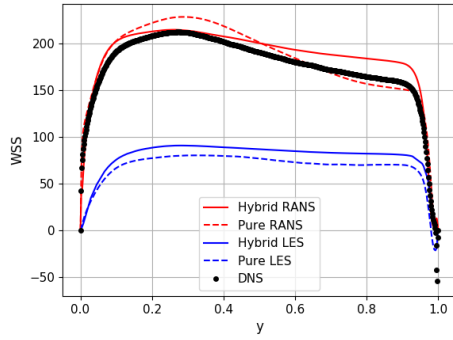
566 As regards the Nusselt number (Nu) predictions shown in Fig. 19 (b), the hybrid RANS does not seem to be
567 superior to the pure LES. However, one can observe that the hybrid RANS seems to give a more accurate prediction
568 of the locations of the local minima and local maxima of the Nu profile (between about $y = 0.2$ and 0.4) in
569 comparison to the pure coarse LES and pure RANS simulations. The local maxima and minima of the Nu are
570 related to a turbulence enhancement that occurs along the hot wall (Sebilleau (2016)). The fact that the locations
571 of these points are captured with the hybrid method suggests that the method is able to accurately predict the
572 location of the turbulence enhancement. The underprediction of the Nu by the hybrid RANS seems to be because
573 the RANS closure is incapable of accurately predicting the Nu in this flow. Future studies should focus on studying
574 the impact of using different RANS models and different turbulent heat flux treatments on the predicted Nusselt
575 number profile.

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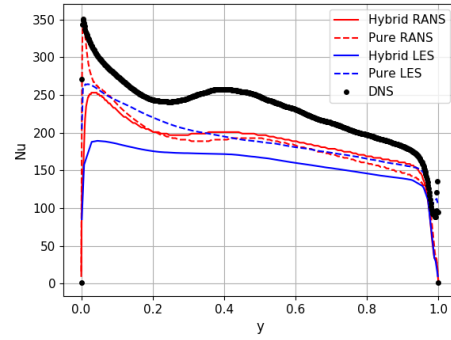
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(a)



(b)

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Fig. 19. Predictions of the wall shear stress (shown in (a)) and the Nusselt number (shown in (b)) along the hot wall of the pure RANS, pure LES, hybrid RANS and hybrid LES simulations. In the hybrid simulations σ^L was calculated using Equation (44).

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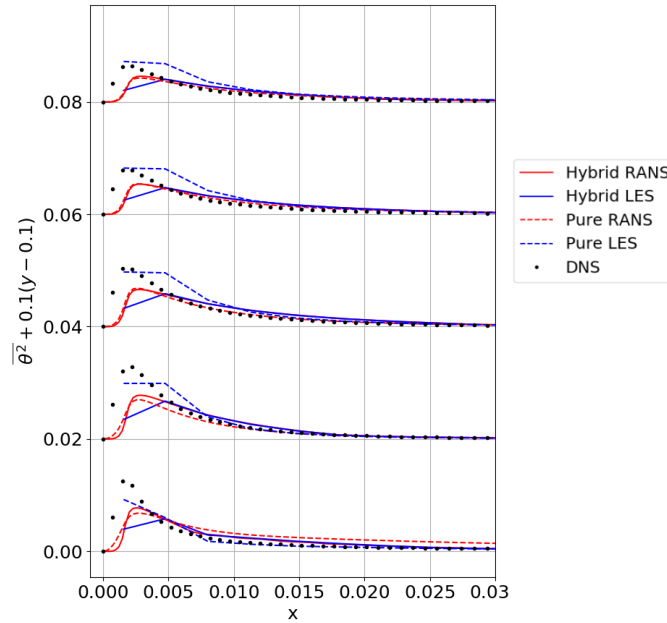
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The temperature variance predictions are presented in Fig. 20. It can be seen that at the heights of $0.3H$, $0.5H$, $0.7H$ and $0.9H$, the hybrid RANS and hybrid LES are superior to the pure coarse LES in predicting the temperature variance at locations to the right of the peaks of the variance. This is because forcing the LES towards the RANS close to the wall solves the problem of overpredicting the variance that is present in the pure coarse LES results. However, the peaks of the temperature variance are underestimated by the hybrid simulations at all the cavity heights. Again, the problem here lies in the RANS closure, which is unable to accurately predict the temperature fluctuations in the immediate near-wall region.



595

596 Fig. 20. A plot showing the pure RANS, pure LES, hybrid RANS and hybrid LES predictions of the temperature
 597 variance profiles near the hot wall at horizontal lines that correspond to cavity heights equal to $0.1H$, $0.3H$,
 598 $0.5H$, $0.7H$ and $0.9H$. In the hybrid simulations σ^L was calculated using Equation (44).

599 6. Conclusions

600 In this study, the performance of different turbulence modelling approaches in predicting a high Rayleigh number
 601 buoyant square cavity flow was assessed. This flow features boundary layers with a relatively small thickness (due
 602 to the high Ra), a laminar stably stratified core and unstably stratified regions near the downstream halves of the
 603 horizontal walls. The latter causes the presence of an instability in this flow that enhances the turbulence levels.
 604 The simulations that were run included a pure unsteady RANS, a pure coarse LES as well as dual-mesh hybrid
 605 RANS-LES simulations.

606 The RANS was found to perform poorly in capturing the flow in the later stages of the boundary layer. Contrarily,
 607 the coarse LES was found to be superior to the RANS in capturing the outer edge of the boundary layer. The main
 608 problem with the pure coarse LES is that it is unable to predict the near-wall part of the boundary layer. The
 609 reasons for this are mainly that the coarse LES does not capture the structures in the viscosity affected region and
 610 that the near-wall nodes are located at a distance large enough to prevent an accurate estimation of the near-wall
 611 gradients. In addition, an overestimation of the temperature fluctuations in the coarse LES results was observed.

612 It has been found that in order to successfully compute this flow with the dual-mesh approach, the σ^L determining
 613 criterion has to be able to distinguish the laminar zones in this flow from the viscosity affected near-wall regions
 614 of the turbulent zones. Consequently, a new criterion that can be considered to belong to the family of criterions

615 based on comparing the turbulence lengthscales and the grid size was developed and analysed here. This criterion
616 was designed in a way that makes it suitable for natural convection flows featuring laminar regions that coexist
617 with other regions that are turbulent. This criterion also has the advantages of the criteria of both Addad et al.
618 (2008) and Uribe et al. (2010) and can be used when computing non-buoyant flows. For these flows, however,
619 there is no need to include the lengthscale $8C_{k_{olm}}\eta$ in Equation (44).

620 The dual-mesh results yielded by the new lengthscale criterion for the square cavity flow were found to be of
621 reasonable accuracy. Future dual-mesh studies of the square cavity should focus on finding which RANS closures
622 can provide accurate estimations of the Nusselt number and the temperature variance in the immediate wall
623 vicinity. A subsequent paper will show that the new lengthscale criterion performs satisfactorily in determining
624 the RANS and the LES regions in a buoyant flow in a cylindrical annuli. These cylindrical annuli results can also
625 be found in the PhD thesis of the first author (Ali (2020)) and in Revell et al. (2020).

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764

765 **Appendix A. The ‘‘elliptic blending $k - \varepsilon - \nu^2/k$ ’’ or the $BL \nu^2/k$ model**

766

- 767 • The elliptic blending parameter (α) equation:

$$\alpha - L^2 \nabla^2 \alpha = 1 \quad (\text{A.1})$$

$$L = \sqrt{C_L^2 \left(\frac{k^3}{\varepsilon_h^2} + C_\eta^2 \frac{\nu^{1.5}}{\varepsilon_h^{0.5}} \right)} \quad (\text{A.2})$$

- 768 • Turbulent kinetic energy (k) equation:

$$\frac{Dk}{Dt} = P_k - \varepsilon_h + S_\varepsilon + \frac{\partial}{\partial x_j} \left(\left(\frac{\nu}{2} + \frac{\nu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right) + G_k \quad (\text{A.3})$$

$$P_k = \nu_t \langle S \rangle^2 \quad (\text{A.4})$$

$$\langle S \rangle = \sqrt{2 \langle S_{ij} \rangle \langle S_{ij} \rangle} \quad (\text{A.5})$$

$$\langle S_{ij} \rangle = 0.5 \left(\frac{\partial \langle U_i \rangle}{\partial x_j} + \frac{\partial \langle U_j \rangle}{\partial x_i} \right) \quad (\text{A.6})$$

$$S_\varepsilon = -2C_{\varepsilon 3} \nu_t \nu (1 - \alpha)^3 \frac{k}{\varepsilon_h} \left(\frac{\partial^2 \langle U_i \rangle}{\partial x_j \partial x_k} \right)^2 \quad (\text{A.7})$$

$$G_k = \beta g_i \frac{\nu_t}{Pr_t} \frac{\partial \langle T \rangle}{\partial x_i} \quad (\text{A.8})$$

769 where β is the thermal expansion coefficient, g_i is the gravity vector and G_k represents the buoyancy production
 770 of k (the exact buoyancy production has a turbulent heat flux which was modelled here using the Standard gradient
 771 diffusion hypothesis).

- 772 • Homogeneous dissipation rate (ε_h) equation:

$$\begin{aligned} \frac{D\varepsilon_h}{Dt} = & \frac{C_{\varepsilon 1} P_k - C_{\varepsilon 2}^* \varepsilon_h}{\tau} \\ & + \frac{\partial}{\partial x_j} \left(\left(\frac{\nu}{2} + \frac{\nu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon_h}{\partial x_j} \right) \\ & + G_k^\varepsilon \end{aligned} \quad (\text{A.9})$$

$$C_{\varepsilon 2}^* = C_{\varepsilon 2} + \alpha^3 (C_{\varepsilon 4} - C_{\varepsilon 2}) \tanh \left(\left| \frac{\frac{\partial}{\partial x_j} \left(\frac{\nu_t}{\sigma_k} \frac{\partial k}{\partial x_j} \right)}{\varepsilon_h} \right|^{\frac{3}{2}} \right) \quad (\text{A.10})$$

773 where the buoyancy production of the turbulence dissipation rate (G_k^ε) and the time scale τ read, respectively:

$$G_k^\varepsilon = C_{\varepsilon 1} \frac{G_k}{\tau} \quad (\text{A.11})$$

$$\tau = \sqrt{\left(\frac{k}{\varepsilon_h}\right)^2 + C_T^2 \left(\frac{\nu}{\varepsilon_h}\right)} \quad (\text{A.12})$$

774

775 • Turbulent viscosity (ν_t):

$$\nu_t = c_\mu \varphi k \min(\tau, \tau_{\min}) \quad (\text{A.13})$$

$$\tau_{\min} = \frac{C_t}{\sqrt{3} c_\mu \varphi \langle S \rangle} \quad (\text{A.14})$$

776 • Equation for the quantity $\varphi = \frac{\langle v^2 \rangle}{k}$ (where $\langle v^2 \rangle$ is the wall-normal Reynolds stress):

$$\begin{aligned} \frac{D\varphi}{Dt} = (1 - \alpha^3) f_w + \alpha^3 f_h - P_k \frac{\varphi}{k} \\ + \frac{\partial}{\partial x_j} \left(\left(\frac{\nu}{2} + \frac{\nu_t}{\sigma_\varphi} \right) \frac{\partial \varphi}{\partial x_j} \right) \end{aligned} \quad (\text{A.15})$$

$$f_h = \frac{-1}{\tau} \left(C_1 - 1 + C_2 \frac{P_k}{\varepsilon_h} \right) \left(\varphi - \frac{2}{3} \right) \quad (\text{A.16})$$

$$f_w = \frac{-\varepsilon_h \varphi}{2k} \quad (\text{A.17})$$

777 • The classic dissipation rate ε can be obtained from ε_h using:

$$\varepsilon = \varepsilon_h + 0.5 \nu \frac{\partial^2 k}{\partial x_j^2} \quad (\text{A.18})$$

778 The formulation of the Reynolds stress tensor that was suggested by Sebilliau (2016) for use in the turbulent

779 heat flux formulation when using the *BL* ν^2/k model was utilised here to estimate $\langle u_i u_j \rangle$:

$$\begin{aligned} \langle u_i u_j \rangle = \left[\frac{2}{3} \alpha^3 k \delta_{ij} - 2 \nu_t \langle S_{ij} \rangle \right] \\ + (1 - \alpha^3) \left[\varphi k n_i n_j + \frac{2}{3} k (\delta_{ij} - n_i n_j) \right] \end{aligned} \quad (\text{A.19})$$

780 It can be observed that the buoyancy production of φ which equals $-G_k \frac{\varphi}{k}$ was not added to Equation (A.15).

781 The reason for this is that in the core of the cavity, this source term becomes positive as the buoyancy production

782 G_k is negative in this region (because of the stable stratification). This can cause φ to increase until it becomes

783 unbounded eventually resulting in solution divergence (this was encountered particularly in the hybrid RANS

784 simulations). Another remedy of this problem would be to clip G_k to 0 which is the approach adopted in
 785 Code_Saturne.

786 Another point worth noting is that the divergence of the φ equation was also encountered because of the fact that
 787 in the hybrid RANS simulations, the production term P_k is modified (see Equation (13)), which can cause P_k to
 788 become negative at some locations. To fix this problem P_k in the φ equation was clipped to 0 using $\max(P_k, 0)$.

789 When attempting to replicate the RANS results produced here, attention should be paid to the version of the
 790 Elliptic blending $k - \varepsilon - v^2/k''$ model used. It has been observed that using a version similar to the one
 791 implemented in STARCCM+ v11.02 can yield different results. The difference mainly lies in that in STARCCM+
 792 v11.02 the term S_ε , which gives additional dissipation in the buffer layer, is removed from the k equation and an
 793 equivalent term is included in the dissipation equation.

$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	σ_k	σ_ε	σ_φ	c_μ
1.44	1.83	1	1.5	1	0.22
C_T	C_t	C_L	$C_{\varepsilon 3}$	$C_{\varepsilon 4}$	C_1
4	0.6	0.164	2.3	1	1.7
C_2	C_η				
0.9	75				

794 Table A.1. The BL v^2/k model constants.
 795

796 Appendix B. The one-equation eddy viscosity LES model

$$\begin{aligned} \frac{\partial k_{sgs}}{\partial t} + \frac{\partial}{\partial x_j} (k_{sgs} \bar{U}_j) \\ = 2\nu_{sgs} \bar{S}_{ij}^2 + \frac{\partial}{\partial x_j} \left(\nu_{sgs} \frac{\partial k_{sgs}}{\partial x_j} \right) \\ - \varepsilon_{sgs} + G_{ksgs} \end{aligned} \quad (\text{B.1})$$

$$\varepsilon_{sgs} = \frac{C_\varepsilon k_{sgs}^{3/2}}{\Delta} \quad (\text{B.2})$$

$$\nu_{sgs} = C_k k_{sgs}^{1/2} \Delta \frac{\kappa}{C_\Delta} \left(1 - y \exp\left(-\frac{y^+}{A^+}\right) \right) \quad (\text{B.3})$$

$$\bar{S}_{ij} = 0.5 \left(\frac{\partial \bar{U}_i}{\partial x_j} + \frac{\partial \bar{U}_j}{\partial x_i} \right) \quad (\text{B.4})$$

797 where the filter width Δ was evaluated as the cubic root of the cell volume. C_k , C_ε , κ , A^+ and C_Δ are constants. It
 798 can be noticed that the ‘‘van Driest damping function’’ is included in the definition of the lengthscale used to
 799 estimate the modelled sgs viscosity ν_{sgs} . The buoyancy production term G_{ksgs} was calculated as:

$$G_{ksgs} = \beta g_i \frac{\nu_{sgs}}{Pr_{sgs}} \frac{\partial \bar{T}}{\partial x_i} \quad (\text{B.5})$$

800 As regards the boundary condition of ν_{sgs} at the walls, a zero gradient condition was used. However, the subgrid-
 801 scale diffusivity $\frac{\nu_{sgs}}{Pr_{sgs}}$ (which appears in the equations of the thermal field) was strictly set to 0 at the walls. Using
 802 a zero gradient or a fixed value of 0 for both quantities was found to yield rather poor pure coarse LES results for
 803 the square cavity flow. However, the hybrid method’s results showed a weak sensitivity to the wall boundary
 804 condition of ν_{sgs} as the LES is forced towards the RANS in the near-wall cells in the dual-mesh simulation.

C_k	C_ε	κ	A^+	C_Δ
0.094	1.048	0.41	26	0.158

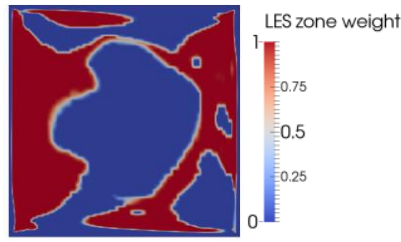
805 Table B.1. The ‘‘one-equation eddy viscosity model’’ constants.

806

807 **Appendix C. Results obtained with an LES zone weight (σ^L) based on Re_y**

808 Before discussing the dual-mesh results, it is useful to look at the behaviour of the LES zone weight in a hybrid
 809 simulation in which it was calculated using Equation (8). In Fig. C.1, a contour plot of the LES zone weight from
 810 the hybrid simulation is shown. As can be seen from this figure, σ^L is equal to 0 not only near the cavity walls but
 811 also at other locations far from the walls. This can be clearly seen near the core of the cavity and can be explained
 812 by the fact that the flow is laminar in this region since the stable stratification destroys turbulence and as a result,
 813 the quantity Re_y becomes small (even though at the outside of the boundary layer the wall distance is relatively
 814 high, the low turbulence levels make the product $k^R y$ small and thus result in a small Re_y)⁵. In other words, the
 815 criterion provided by Equation (8) gives a σ^L of 0 near the wall and in the cavity core as it fails to distinguish
 816 between the laminarization that occurs in the near-wall region due to the no-slip and no-penetration conditions and
 817 the far-from-the-wall laminarization caused by the stable stratification.

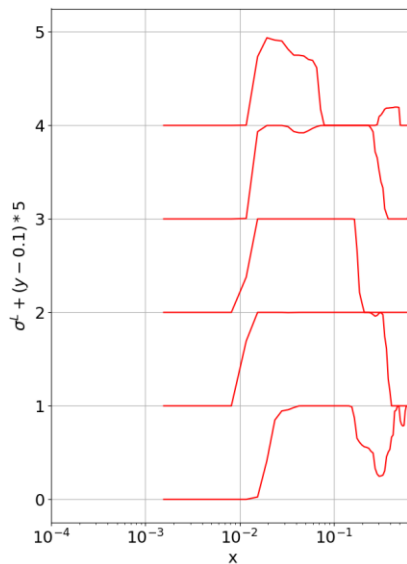
⁵ At the outside of the boundary layer, k^R (which is a hybrid RANS variable) is forced towards k^{EWA} (which is a hybrid LES variable). Although k^{EWA} approaches 0 in this region, it is greater than the pure RANS turbulent kinetic energy in the same region. If one replaces k^R in Equation (8) with the pure RANS turbulent kinetic energy, a different behaviour of σ^L would be obtained.



818

819 Fig. C.1. An instantaneous snapshot of the LES zone weight from a hybrid simulation in which it was calculated
 820 using Equation (8).

821 Small values of Re_y are also featured near the horizontal walls because these regions feature low turbulence
 822 levels. By looking at Fig. C.2 which shows time averaged values of σ^L , it can be seen that even with the time
 823 averaging, the behaviour of σ^L remains unsmooth.

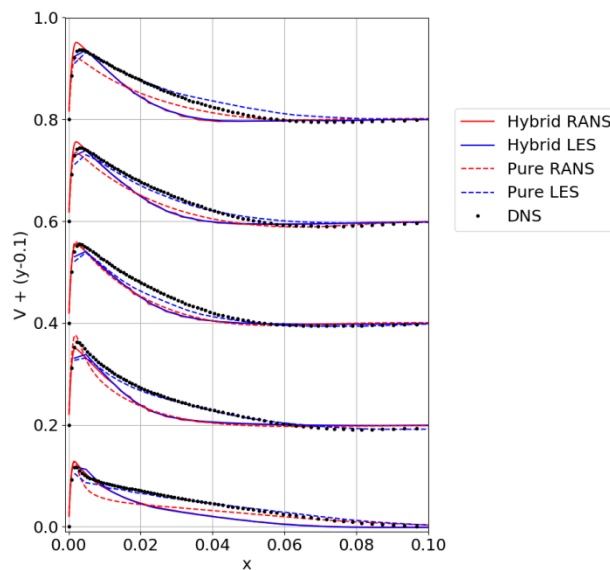


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825 Fig. C.2. Mean values of the LES zone weight (σ^L) from a hybrid simulation in which it was calculated using
 826 Equation (8). This figure shows σ^L profiles at horizontal lines that correspond to cavity heights equal to $0.1H$,
 827 $0.3H$, $0.5H$, $0.7H$ and $0.9H$. The horizontal axis is in log scale.

828 One important thing to note is that when using the dual-mesh approach, what happens when σ^L is 0 in regions
 829 where the unstable plumes are forming in the LES simulation is that the velocity and temperature fluctuations
 830 associated with these plumes are altered since the LES fluctuations are forced towards the RANS fluctuations.
 831 This weakens the plume fluctuations, which in turn causes the turbulence levels along the vertical walls to be low.
 832 This can be seen from Fig. C.3 in which the velocity profiles returned by the hybrid method show an
 833 underestimation of the hot wall boundary layer thickness (due to less mixing taking place). This means one should

834 try and reduce the forcing of the LES towards the RANS near the regions where the LES unstable plumes are
835 ejected by limiting the forcing as much as possible to the immediate near-wall region.



836

837 Fig. C.3. A plot showing the pure RANS, pure LES, hybrid RANS and hybrid LES predictions of the mean
838 vertical velocity profiles near the hot wall at horizontal lines that correspond to cavity heights equal to $0.1H$,
839 $0.3H$, $0.5H$, $0.7H$ and $0.9H$. In the hybrid simulations σ^L was calculated using Equation (8).

840 The weakening of the hybrid LES instability can be confirmed by looking at the temperature snapshot shown in
841 Fig. C.4 and comparing the instability near the bottom left or top right corners with that of the pure coarse LES
842 which can be visualized in Fig. 7. The drop in the turbulence levels along the hot wall in the hybrid LES simulation
843 can also be confirmed by comparing the snapshots of the velocity magnitude taken from the hybrid LES and the
844 pure coarse LES simulations (Fig. C.5 and Fig. 6, respectively). Indeed, the turbulent kinetic energy profiles plotted
845 in Fig. C.7 clearly show that the turbulent mixing along the hot wall in the hybrid LES simulation is less than the
846 one in the pure coarse LES. Fig. C.6 shows an instantaneous hybrid RANS temperature field in which the
847 instability can be seen although it appears to be weaker than the pure RANS instability shown previously in Fig.
848 8.

849

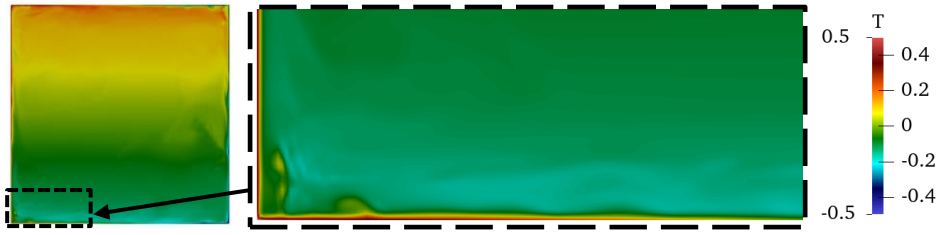
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Fig. C.4. An instantaneous snapshot of the LES temperature from a hybrid simulation in which the LES zone

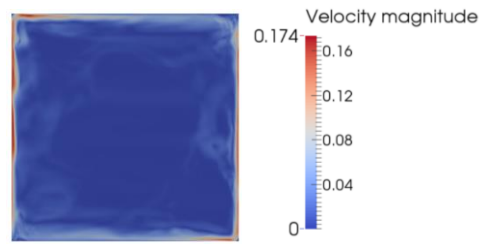
856

weight was calculated using Equation (8). A zoomed-in view of the contours near the bottom left corner is

857

provided as well.

858



859

Fig. C.5. An instantaneous snapshot of the LES velocity magnitude from a hybrid simulation in which the LES

860

zone weight was calculated using Equation (8).

861



862

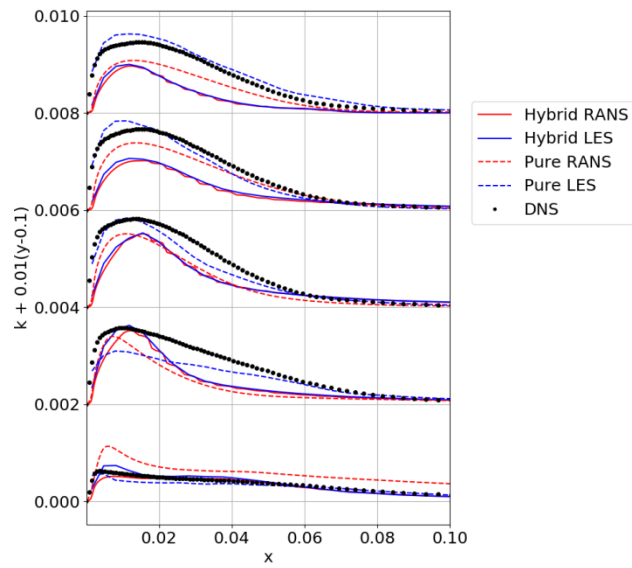
Fig. C.6. An instantaneous snapshot of the RANS temperature from a hybrid simulation in which the LES zone

863

weight was calculated using Equation (8). A zoomed-in view of the contours near the bottom left corner is

864

provided as well.



865

866

Fig. C.7. A plot showing the pure RANS, pure LES, hybrid RANS and hybrid LES predictions of the total
 867 turbulent kinetic energy profiles near the hot wall at horizontal lines that correspond to cavity heights equal to
 868 $0.1H$, $0.3H$, $0.5H$, $0.7H$ and $0.9H$. In the hybrid simulations σ^L was calculated using Equation (8).

868

869