The SGS kinetic energy and the viscous dissipation equations as closure relations in LES

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Abstract

In this paper the main drawbacks of the large eddy simulation models, present in literature, are analysed and a new LES model is proposed. The closure relation for the generalised SGS turbulent stress tensor: a) complies with the principle of turbulent frame indifference; b) takes into account both the anisotropy of the turbulence velocity scales and turbulence length scales; c) removes any balance assumption between the production and dissipation of SGS turbulent kinetic energy. In the proposed model: a) the closure coefficient which appears in the closure relation for the generalised SGS turbulent stress tensor is theoretically and uniquely determined without adopting Germano's dynamic procedure; b) the generalised SGS turbulent stress tensor is related exclusively to the generalised SGS turbulent kinetic energy (which is calculated by means of its balance equation) and the modified Leonard tensor. In this paper the main drawbacks associated with the calculation of the viscous dissipation by means of an algebraic model are shown. The calculation of the viscous dissipation is carried out by integrating its exact balance equation. The velocity field obtained from the numerical simulation is analysed by using vortex identification methods *D*, *Q* and λ_2. The comparative analysis of each identification method is also carried out, highlighting how methods *D* and *Q* improperly associate the presence of a vortex to zones of high vorticity while the λ_2 method identifies a vortex only when it coincides with a minimum of pressure.
Keywords: LES, sub grid kinetic energy viscous dissipation, balance equation anisotropy, scale similarity, vortex identification.

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1 Introduction

Among the most common LES models present in literature are the Dynamic Smagorinsky-type SGS Models (*e.g.* Dynamic Smagorinsky Model DSM [2], Dynamic Mixed Model DMM, Lagrangian Dynamic Model LDM [3]), in which the generalised SGS turbulent stress tensor is related to the resolved strain-rate tensor by means of a scalar eddy viscosity. It is assumed in these models that the eddy viscosity is a scalar proportional to the cubic root of the generalised SGS turbulent kinetic energy dissipation and that such dissipation is locally and instantaneously balanced by the production of the generalised SGS turbulent kinetic energy. Consequently, it is evident that the dynamic Smagorinsky-type SGS models are subject to three relevant drawbacks. The first drawback is represented by the scalar definition of the eddy viscosity; the second one is related to the assumption of a local and instantaneous balance between the production and dissipation of the generalised SGS turbulent kinetic energy, whilst the third drawback is related to the dynamic calculation of the coefficient used to model the eddy viscosity (Smagorinsky coefficient).

The scalar definition (first inconsistency) of the eddy viscosity is equivalent to assuming that the principal axes of the generalised SGS turbulent stress tensor, or the unresolved part of it (represented by the cross and Reynolds terms), are aligned with the principal axes of the resolved strain-rate tensor. This assumption has been disproved by many experimental tests and by DNS, which demonstrate that there is no alignment between the generalised SGS turbulent stress tensor, or the unresolved part of it, and the resolved strain-rate tensor. Moreover, as is well known, the eddy viscosity is, in the most general case a symmetric fourth order tensor given by the product of two-second order tensors which represent respectively the turbulence length scale and the turbulence velocity scale. The scalar definition of the eddy viscosity, used in the above-mentioned dynamic Smagorinsky-type SGS models, presupposes the existence of a single turbulence velocity scale and a single turbulence length scale. This is equivalent to assuming that the turbulence is isotropic but, as shown by several authors, even in the dissipation range of the smallest turbulence scales there are high anisotropy levels, even at high Reynolds numbers.

The second inconsistency of the Smagorinsky dynamic models is related to the assumption of a local and instantaneous balance between production and dissipation of the generalised SGS turbulent kinetic energy, formulated in the above-mentioned models to obtain the turbulent viscosity expression. The balance between production and dissipation of the generalised SGS turbulent kinetic energy is confirmed statistically and never instantaneously, and only locally at the scales associated with wave-numbers within the inertial subrange and the latter exists only for isotropic turbulence and at high Reynolds numbers. Moreover, since the dissipation of the generalised SGS turbulent kinetic energy is, by definition, positive, the assumption of local balance implies that the production of generalised SGS turbulent kinetic energy is also positive. This assumption is equivalent to neglect back-scatter i.e. the energy transfer from the smallest unresolved scales to the largest ones.

The third inconsistency concerns the ineffectiveness, in the wall region, of Germano's dynamic procedure for the calculation of the coefficient which appears in the closure relation for the generalised SGS stress tensor. In fact, in the wall region the dimensions of the filters used in the dynamic procedure are larger than those of the largest eddies governing the energy and momentum transfer. Under these conditions the dynamic procedure is not able to fully account for the local subgrid dissipative processes that affect the entire domain.

In this paper a new LES model is proposed which overcomes the above drawbacks. The closure relation for the generalised SGS turbulent stress tensor: a) complies with the principle of turbulent frame indifference [1]; b) takes into account both the anisotropy of the turbulence velocity scales and turbulence length scales; c) removes any balance assumption between the production and dissipation of SGS turbulent kinetic energy. In the proposed model: a) the closure coefficient which appears in the closure relation for the generalised SGS turbulent stress tensor is theoretically and uniquely determined without adopting Germano's dynamic procedure; b) the generalised SGS turbulent stress tensor is related exclusively to the generalised SGS turbulent kinetic energy (which is calculated by means of its balance equation) and the modified Leonard tensor.

The velocity fields obtained by the numerical simulation are analysed by using the so-called *D* [6], *Q* [7] e λ_2 [8] methods for the identification of vortices. From the comparative analysis of vortex structures identified by the three different methods mentioned above, the inconsistencies and drawbacks of these methods are shown.

2 A new LES model

In order to remove the assumption of alignment between the unresolved part of the generalised SGS turbulent stress tensor and the resolved strain rate tensor and to take into account the anisotropy of the unresolved scales of turbulence, the generalised SGS turbulent stress tensor is expressed in the following form:

$$\tau_{ij} = L_{ij}^{\ m} - 2\nu_{ijmn}\overline{S}_{mn} \tag{1}$$

in which $\overline{S}_{mn}$ is the resolved strain rate tensor and L_{ij}^{m} is the modified Leonard tensor. The eddy viscosity is expressed in the above-mentioned equation by a fourth-order tensor proportional to the product of a second-order tensor, b_{ij}, which represents the turbulence velocity scales, and a second-order tensor, d_{mn}, which represents the turbulence length scales, according to the following equation:

$$\nu_{ijmn} = Cb_{ij}d_{mn}\ , \text{ where } \quad b_{ij} = b_{ji}\ , \quad d_{mn} = d_{nm}\,. \tag{2}$$

The expression of the eddy viscosity in terms of a fourth-order tensor enables the anisotropic character of the turbulence to be fully represented, since it does not either assume the existence of a single turbulence velocity scale and or a single turbulence length scale, as is found in models in which the viscosity is expressed as a scalar. The second-order tensor which represents the turbulence velocity scales is defined as follows:

$$b_{ij} = \sqrt{E}\,\frac{L_{ij}^{m}}{L_{ij}^{m}} \tag{3}$$

where E is the SGS turbulent kinetic energy. In this manner it is assumed that the anisotropy of the unresolved turbulence velocity scales, expressed by tensor b_{ij}, is equal to the anisotropy of the smallest resolved scales, associated with the modified Leonard tensor. This assumption is based on scale similarity, according to which the scales that are contiguous in the wavenumber space have strict dynamic analogies related to the energy exchange processes which occur between them.

Introducing equation (2) and (3) into (1) gives:

$$\tau_{ij} = (1+r)L_{ij}^{m} \quad \text{where} \qquad r = -2Cd_{mn}S_{mn}\frac{\sqrt{E}}{L_{kk}^{m}} \tag{4}$$

In order to close the equations governing the turbulent flows, it is necessary to determine the coefficient C which appears in equation in (4.a) or anywhere else, the coefficient r which appears in equation (4.b).

In this paper the coefficient r is determined without Germano's dynamic procedure, the inconsistencies of which are fundamentally linked to the fact that in the wall region the dimensions of the filters used in the dynamic procedure are larger than those of the largest eddies governing the energy and momentum transfer.

The coefficient r is uniquely and theoretically determined by using the relation between the generalised SGS turbulent kinetic energy and the generalised SGS turbulent stress tensor. In fact, by definition, the generalised SGS turbulent kinetic energy is equal to half the trace of the generalised SGS turbulent stress tensor.

$$\tau_{kk} = 2E = (1+r)L_{kk}^{m}, \quad \text{i.e.} \qquad r = \frac{2E - L_{kk}^{m}}{L_{kk}^{m}} \tag{5}$$

introducing (5) into (4) gives:

$$\tau_{ij} = \left(1 + \frac{2E - L_{kk}^{m}}{L_{kk}^{m}}\right)L_{ij}^{m} = \left(\frac{2E}{L_{kk}^{m}}\right)L_{ij}^{m} \tag{6}$$

The closure relation (6) is obtained without any assumption of local balance between the production and dissipation of generalised SGS turbulent kinetic energy and may thus be considered applicable to LES with the filter width falling into the range of wave numbers greater than the wave number corresponding to the maximum turbulent kinetic energy.

The closure relation for the generalised SGS turbulent stress tensor (6): a) complies with the principle of turbulent frame indifference given that it relates only objective tensors [1]; b) takes into account both the anisotropy of the turbulence velocity scales and turbulence length scales; c) assumes scale similarity in the definition of the second-order tensor representing the turbulent velocity scales; d) guarantees an adequate energy drain from the grid scales to the subgrid scales and guarantees backscatter; e) overcomes the inconsistencies linked to the dynamic calculation of the closure coefficient used in the modelling of the generalised SGS turbulent stress tensor.

The generalised SGS turbulent kinetic energy, E, is calculated by solving its balance equation, defined by the following equation:

$$\frac{DE}{Dt} = -\frac{1}{2}\frac{\partial \tau(u_k,u_k,u_m)}{\partial x_m} - \tau_{mk}\frac{\partial \bar{u}_k}{\partial x_m} - \frac{\partial \tau\left(p,u_m\right)}{\partial x_m} + \nu\frac{\partial^2 E}{\partial x_m \partial x_m} + \tau\left(F_{Ok},u_k\right) - \nu\tau\left(\frac{\partial u_k}{\partial x_m},\frac{\partial u_k}{\partial x_m}\right) \quad (7)$$

Equation (7) is form-invariant under Euclidean transformations of the frame and frame-indifferent [1]. The last term on the right of (7) is defined viscous dissipation :

$$\varepsilon = \nu\tau\left(\frac{\partial u_i}{\partial x_j},\frac{\partial u_i}{\partial x_j}\right) \quad (8)$$

From a thermodynamic point of view this quantity describes an internal process, *i.e.* the viscous dissipation in the turbulent flow, and therefore can be considered as an internal variable, and its evolution can be described by a transport equation. Some authors [4] model ε with the following expression:

$$\varepsilon = \frac{C^* E^{3/2}}{\bar{\Delta}} \quad (9)$$

and calculate the scalar coefficient C^* which appears in (9) by means of a dynamic procedure based on the following scalar Germano identity:

$$C_* \frac{E^{T3/2}}{\bar{\Delta}^T} - \left\langle C_* \frac{E^{3/2}}{\bar{\Delta}} \right\rangle = \nu\left\langle \frac{\partial \bar{u}_k}{\partial x_m}\frac{\partial \bar{u}_k}{\partial x_m} \right\rangle - \nu\frac{\partial\left\langle \bar{u}_k \right\rangle}{\partial x_m}\frac{\partial\left\langle \bar{u}_k \right\rangle}{\partial x_m} \quad (10)$$

The term on the right of eqn. (10) expresses the viscous dissipation of turbulent kinetic energy which occurs locally in the range of the wavenumbers falling between the two filter dimensions. At high Reynolds numbers the dynamic procedure, expressed in (10) and carried out with grid and test filters of which the dimensions are associated with the wavenumbers lower than those belonging to the inertial subrange, is not applicable because it is subject to three relevant inconsistencies. Equation (10) (first inconsistency) allows the calculation of the closure coefficient C^* only if the dimensions of the test and grid filters are associated with wave numbers belonging to the inertial subrange.

The second inconsistency concerns the calculation of the term on the right of (10), which at high Reynolds numbers is negligible if the dimensions of the filters used in the dynamic procedure are associated with wavenumbers lower than those belonging to the inertial subrange.

The third inconsistency is related to the boundary conditions for ε. As is well known, in wall bounded turbulent flows the viscous dissipation of SGS turbulent kinetic energy, ε, balances the viscous diffusion of E at the wall

$$\varepsilon_W = \nu\frac{\partial^2 E}{\partial x_m \partial x_m} \quad (11)$$

The dissipative processes occurring in the wall region affect the energy cascade process of the entire domain, since in this region the kinetic energy both produced locally and transferred from the rest of the domain is dissipated. Since E is zero at the wall, eqn. (10) implies null values of ε at the wall. This contradicts eqn. (11). In order to remove these drawbacks, and therefore to operate simulations of high Reynolds number flows, in the proposed LES model a further transport equation is introduced for the subgrid viscous dissipation ε. This equation, expressed in terms of the generalised central moments, takes the form

$$\frac{\partial \varepsilon}{\partial t}+\frac{\partial \bar{u}_k \varepsilon}{\partial x_k}-\frac{\partial^2 \varepsilon}{\partial x_k \partial x_k}+\nu\frac{\partial}{\partial x_k}\tau\left(u_k,\frac{\partial u_i}{\partial x_j},\frac{\partial u_i}{\partial x_j}\right)+2\nu\frac{\partial}{\partial x_k}\left(\frac{\partial \bar{u}_i}{\partial x_j}\tau\left(u_k,\frac{\partial u_i}{\partial x_j}\right)\right)+2\nu\frac{\partial}{\partial x_k}\tau\left(\frac{\partial u_k}{\partial x_i},\frac{\partial p}{\partial x_i}\right)-$$

$$2\nu\frac{\partial}{\partial x_k}\left(\frac{\partial \bar{u}_i}{\partial x_j}\frac{\partial \tau_{ik}}{\partial x_j}\right)+2\nu\tau\left(\frac{\partial u_i}{\partial x_k},\frac{\partial u_k}{\partial x_j},\frac{\partial u_i}{\partial x_j}\right)+2\nu\frac{\partial \bar{u}_k}{\partial x_j}\tau\left(\frac{\partial u_i}{\partial x_k},\frac{\partial u_i}{\partial x_j}\right)+2\nu\frac{\partial \bar{u}_i}{\partial x_k}\tau\left(\frac{\partial u_k}{\partial x_j},\frac{\partial u_i}{\partial x_j}\right)+$$

$$2\nu\frac{\partial \bar{u}_i}{\partial x_j}\tau\left(\frac{\partial u_i}{\partial x_k},\frac{\partial u_k}{\partial x_j}\right)+2\nu\frac{\partial \tau_{ik}}{\partial x_j}\frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_k}+2\nu^2\tau\left(\frac{\partial^2 u_i}{\partial x_j \partial x_k},\frac{\partial^2 u_i}{\partial x_j \partial x_k}\right)=0 \qquad (12)$$

The first term on the left-hand side of eqn (12) is the local derivative, the second one expresses the convection term, the third is the viscous diffusion term, the 4th-7th are the turbulent transport terms, the 8th- 12th are the production terms of ε, and the last one expresses its destruction.

The sum of the fourth, fifth and sixth terms on the left of (12) is the divergence of the viscous dissipation turbulent transport vector, $\left(F_\varepsilon\right)_k$, which is modelled according to:

$$\left(F_\varepsilon\right)_k = C_{F\varepsilon}\frac{E}{\varepsilon}\tau_{kl}\frac{\partial \varepsilon}{\partial x_l} \text{ which, for (6), is equivalent to } C_{F\varepsilon}\frac{E^2}{\varepsilon}\frac{L^m_{kl}}{L^m_{jj}}\frac{\partial \varepsilon}{\partial x_l} \qquad (13)$$

The scalar coefficient $C_{F\varepsilon}$ in (13) is dynamically calculated by means of a Germano identity applied to the turbulent transport vector of ε.

The sum of the 8th, 9th, 10th and 11th unknown terms of (12) constitutes a production term of ε which is modelled in the following way:

$$P_\varepsilon = C_{P\varepsilon}\frac{\varepsilon\left(-\tau_{ij}\bar{S}_{ij}\right)}{E}, \text{ which, for (6), is equivalent to } -C_{P\varepsilon}\frac{\varepsilon L^m_{ij}\bar{S}_{ij}}{L^m_{kk}} \qquad (14)$$

The dynamic calculation of the coefficient $C_{P\varepsilon}$ is carried out by applying a Germano identity to the viscous dissipation production terms. The last term in (12) represents the destruction of ε. This is modelled, according to the closure relation presented in the following way:

$$D_\varepsilon = C_{D\varepsilon}\frac{\varepsilon^2}{E} \qquad (15)$$

The calculation of coefficient $C_{D\varepsilon}$ is carried out dynamically by applying a Germano identity to the viscous dissipation destruction term.

3 Vortex identification

The velocity fields obtained from the numerical simulation are analysed by using vortex identification methods *D* [6], *Q* [7] and λ_2 [8].

The first two methods are based on the relations existing between the invariants of the velocity gradient, A_{ij}. The third method identifies a vortical structure from the analysis of the symmetric matrix given by the sum of the square of the strain rate tensor S_{ij} with the square of the anti-symmetric part of the velocity gradient W_{ij}. Both the *D* method and the *Q* method formulate hypotheses on the trajectories of the particles in the neighbourhood of a point by analysing the eigenvalues and eigenvectors of the velocity gradient. If there exist two complex and conjugated eigenvalues of the velocity gradient, the path of the particles takes on a spiral shape. The *Q* method identifies the existence of a vortex if the second invariant, *Q*, of the velocity gradient is positive:

$$Q = \frac{1}{2} \cdot \left[P^2 - S_{ij} S_{ji} - W_{ij} W_{ji} \right] > 0 \tag{16}$$

where P is the trace of the velocity gradient. The above relation is verified when the enstrophy is greater than local strain intensity. This method fails in the vortex identification, since for negative values of *Q*, also two complex and conjugated eigenvalues, associated to a vortex, may exist. The *D* method identifies a vortex when the discriminant of the characteristic polynomial associated with the velocity gradient is positive:

$$D = \left(\frac{Q}{3} \right)^3 + \left(\frac{R}{2} \right)^2 > 0 \quad \text{where} \quad \mathrm{R} = \det(\mathrm{A}) \tag{17}$$

This method cannot identify the vortex core; furthermore, when the second invariant is greater than the third, the method shows the same drawbacks as the *Q* method. Moreover, when the third invariant is greater than the second one, such a method identifies a vortex where high vorticity exists: therefore the method fails since it identifies a vortex even where it does not exist, as high vorticity is neither a necessary nor a sufficient condition for the presence of a vortex. The λ_2 method [8] identifies a vortex when the symmetric matrix

$$\Lambda_{ij} = S_{ik} S_{kj} + W_{ik} W_{kj} \tag{18}$$

has two negative eigenvalues. By differentiating the Navier-Stokes equation, it holds:

$$\frac{DS_{ij}}{Dt} - \nu \frac{\partial^2 S_{ij}}{\partial x_k \partial x_k} + S_{ik} S_{kj} + W_{ik} W_{kj} = -\frac{1}{\rho} \cdot \frac{\partial^2 P}{\partial x_i \partial x_j} \tag{19}$$

If the first and second terms in equation (19) are negligible, the symmetric matrix Λ_{ij} is proportional to the opposite of the pressure Hessian matrix. When the symmetric matrix Λ_{ij} has two negative eigenvalues, the above mentioned Hessian matrix has two positive eigenvalues. In the plane identified by the eigenvectors associated with the two positive eigenvalues of the Hessian matrix, the quadratic form associated with the two eigenvalues is positive and, consequently, the pressure has a minimum. The criterion, therefore, is substantially based on the identification of zones corresponding to a minimum pressure. But the existence of a minimum pressure is neither a necessary nor a sufficient condition for a vortex.

4 Numerical set-up and results

The proposed LES model is used for the simulation of a turbulent channel flow (between two flat parallel plates) at Reynolds number $Re^*=u^*\delta/\nu$ =2340, where u^* is the friction velocity, δ is the channel half width and ν is the cinematic viscosity. The dimensions of the computational domain are $2\pi\delta$ in the streamwise direction and 2δ in spanwise direction. The computation is carried out with 128 x 96 x 96 grid points, respectively, in streamwise (x) spanwise (y) and wall-normal (z) directions.

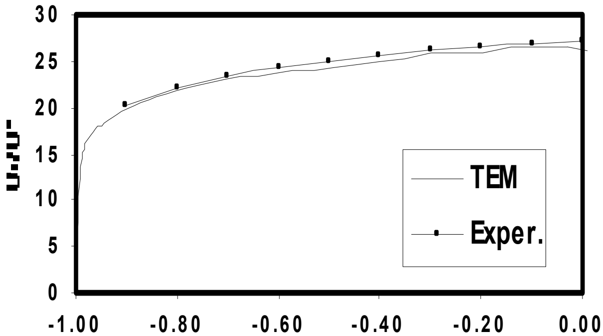

Figure 1: Time averaged streamwise velocity component at Re^*=2340. (Comparison with experimental data).

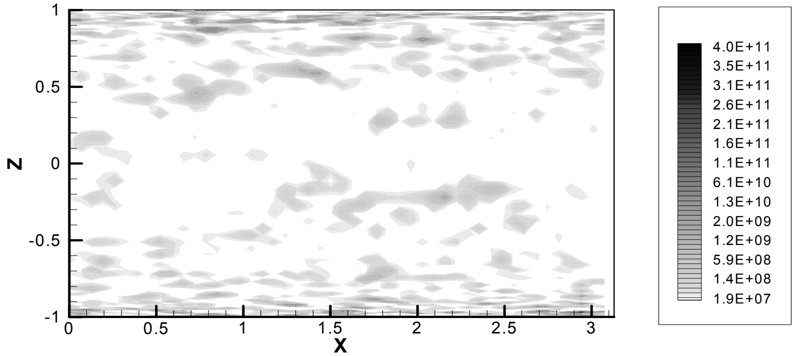

Figure 2: Vortex identification with D method, x-z plane.

In fig.1 the time-averaged streamwise velocity component is shown. The figure shows that LES and the experimental data agree quite considerably. Figs. 2–4 show the vortex structures, identified by means of the Q, D, λ_2 methods respectively, in the *x-z* plane (for a better visualisation only a limited part of the domain is shown). As shown by figs. 2 and 3, the D and Q methods improperly associate the presence of a vortex in high vorticity zones *i.e.* at the wall). Moreover, while the first method underestimates the vortex extension, the second one overestimates it. As shown in fig. 4, method λ_2 correctly identifies a vortex.

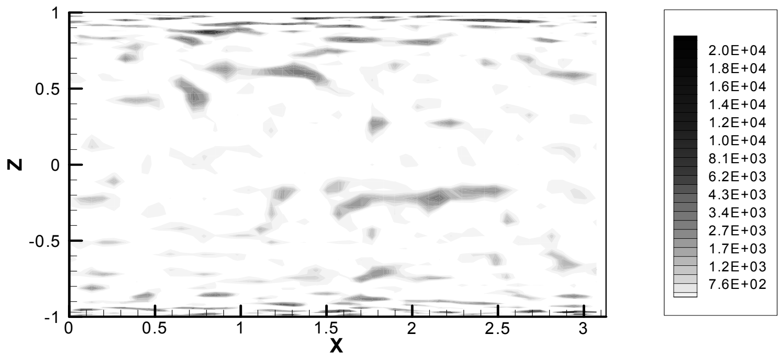

Figure 3: Vortex identification with Q method, *x-z* plane.

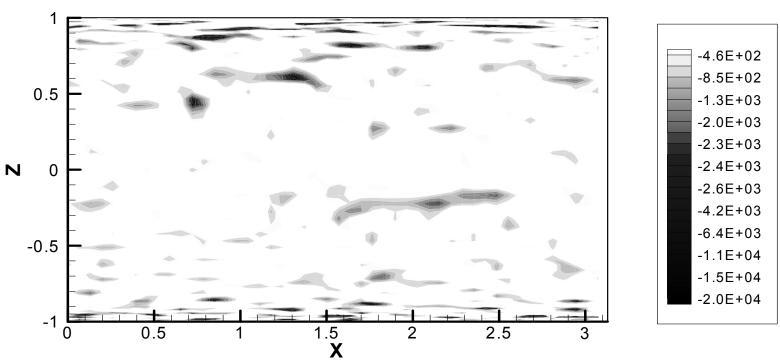

Figure 4: Vortex identification with λ_2 method, *x-z* plane.

In fig. 4 the near wall vortex structures (inside the turbulent boundary layer) are clearly identified: the dimensions of the spatial discretisation steps allow the optimal simulation of the above mentioned vortex structures that govern the transport, the production and the dissipation of the turbulent kinetic energy.

5 Conclusions

In this paper the main drawbacks of the LES models present in literature are analysed and a new closure relation is proposed for the generalised SGS turbulent stress tensor that: a) complies with the principle of turbulent frame indifference [1]; b) takes into account both the anisotropy of the turbulence velocity scales and turbulence length scales; c) removes any balance assumption between the production and dissipation of SGS turbulent kinetic energy. The figure shows that LES and the experimental data agree considerably well.

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