NUMERICAL SIMULATION OF SPATIALLY DEVELOPING FORCED AND NATURAL MIXING LAYERS WITH L.E.S.

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Abstract

The purpose of the present work is to simulate numerically the spatially developing plane mixing layer solving the three dimensional incompressible Navier-Stokes equations in the primitive variables $u - p$ formulation with the Large Eddy Simulation model of turbulence. Discretization in space is achieved using a finite volume technique on a staggered grid. Different discretization schemes for the convective term have been compared; laminar and subgrid stresses are discretized with centered second order accurate formulae. A second order predictor-corrector Adam-Bashforth method is employed to advance the solution in time.

Calculations have been performed for both natural and forced mixing layer and reasonable agreement found with both experimental data and numerical simulation. The influence of the data sampling technique upon the quality of the results has also been brought in evidence.
List of Symbols

$C_s$  "Linking" coefficient for S.G.S. model
$C_i$  Advection velocity of the perturbation wave on the boundary
$f_{jk}$  Convective flux along the $j^{th}$ direction for the
         momentum balance along the $k^{th}$ direction
$f_p$  Inviscid shear layer frequency for the $p^{th}$ harmonic
$H$  Space operator
$l$  Length scale of the subgrid eddies
$l, m, n$  Mesh indices in the streamwise, spanwise and
           transversal directions
$L_x, L_y, L_z$  Dimensions of the computational domain
               in the $x$, $y$ and $z$ directions, respectively
$N_x, N_y, N_z$  Grid points of the computational domain
               in the $x$, $y$ and $z$ directions, respectively
$p$  Pressure
$r$  Freestream velocity ratio
$Re_{\delta\omega_0}$  Reynolds number based on $\Delta u$, $\delta\omega_0$ and $\nu$
$S_{ij}$  Strain rate tensor of the resolved scale
$T$  Time
$u_i$  $i^{th}$ component of velocity vector
$\bar{u}_i$  Filtered $i^{th}$ component of velocity vector
$u'_i$  Subgrid $i^{th}$ component of velocity vector
$u, v, w$  Streamwise, spanwise and transversal velocity components
$u_1, u_2$  Upper and lower freestream velocities, respectively
$\bar{u}_i^p$  $i^{th}$ component of velocity perturbation vector
$u_m$  Mean velocity of the layer
$x, y, z$  Streamwise, spanwise and transversal coordinate
$z_{aver}$  Transversal coordinate of the mean velocity of the layer
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<tr>
<td>$\delta_\omega$</td>
<td>Local vorticity thickness</td>
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<td>$\delta_{\omega 0}$</td>
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<td>$\Delta$</td>
<td>Filter width (linear dimension of the grid cell)</td>
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<td>Turbulent eddy viscosity</td>
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<td>$\Phi_i$</td>
<td>$i^{th}$ component of the perturbation function</td>
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<td>$\omega_p$</td>
<td>Inviscid shear layer oscillatory frequency for the $p^{th}$ harmonic</td>
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1. INTRODUCTION

A plane mixing layer is a free shear flow generated by the interaction of two coflowing parallel streams with different mean velocities joining together downstream of the trailing edge of a splitter plate (Fig. 1.1).

Phenomena which can be likened to plane mixing layers exist in a variety of practical cases, like flow around the trailing edge of a turbine blade, flow around the lip of the intake valve of an internal combustion engine, heterogeneous combustion and meteorological flows, etc.; moreover, the interaction between vortical structures which occurs during mixing layer development is responsible for the generation of acoustic noise. These few examples show the wide range of applications for which the understanding of the main physical features of mixing layers and their correct prediction is of fundamental importance.

Layer growth in the transversal direction and turbulent mixing between the two flows are the most important features of mixing layer phenomenology. These phenomena are strictly connected to the evolution of the vortical structures generated in the layer, which increase their own size by entrainment of surrounding fluid; therefore, the transversal size of the layer increases with distance from the splitter plate. Many authors studied the physics of the mixing layer and found coherent vortical structures to be present. The vortices start to appear some distance downstream of the separation plate and, by their interaction, generate more complex structures further downstream. Winant & Browand [1] found that the growth dynamics for a natural mixing layer is governed by the vortex pairing process. Basically three distinct regions can be identified downstream of the splitter plate. Close to the plate linear unstable waves of small amplitude are generated by the interaction of the two flows (i.e., a wake is originated from the boundary layers of the two incoming flows). This is the linear instability region. Downstream of this region the presence of single periodic vortices generated by the growth of the unstable linear waves is observed. These vortices increase their size entraining fluid from the irrotational flow outside of the vortical layer. Further downstream the vortices join each other in pairs and begin to roll up, generating structures of a typical elongated form (Fig. 1.1), which exhibit a high level of coherence. These structures further interact pairing off in the same way as before (Fig. 1.1). Vortex pairing is responsible for the generation of acoustic waves [1].

Up to now research has focused upon two different types of mixing layer: natural and forced. The term natural indicates a mixing layer where the vortical structures are allowed to develop naturally from the random initial perturbations present in the flow while in the forced one a periodic perturbation is superimposed to the inlet flow to promote their development. In the former case the flow is self-similar and the layer grows linearly in the streamwise direction.
Fig. 1.1 - Sketch of spatially developing mixing layer

Fig. 1.2 - Sketch of streamwise vortices in a mixing layer
Vortex pairing takes place randomly in time and space [1],[2]. On the other hand the forced layer is not self-similar and is characterized by regions of enhanced and retarded growth (i.e., the growth rate is not linear). Vortex pairing is a well organized phenomenon with regular spacing between structures. In order to obtain meaningful information on the physics of flow mixing the forcing has to act only as catalyst for the instabilities present in the flow without modifying it in a fundamental way; therefore the forcing amplitude must be small (i.e., the r.m.s. level of the perturbation must be kept low) [2].

The investigation of Ho & Huang [3] on the effect of subharmonic forcing on the merging 1 of vortical structures and its influence on the growth of the layer has shown to be possible to influence the merging process varying the forcing frequency. It was also found out that the effect of low frequency forcing with high amplitude increases the spreading rate of the layer through the formation of large vortical structures generated by the coalescence of small vortices. This process is known as collective interaction.

The previously mentioned works [1], [2] and [3] consider a 2D layer, and focus on the study of the physics of the spanwise vortices. Other experimental activities have been carried out to investigate the development of the streamwise vortices which exhibit a mushroom-like shape (Fig. 1.2).

All together, these investigations have brought an enhanced understanding of the physical behaviour of mixing layers; at the same time analytical work has also been carried out, and worth mentioning is the contribution by Monkewitz & Huerre [4] who performed a study on the linear instability associated with the typical mean velocity profile. At the same time the availability of increasingly powerful computers has made possible the development of new turbulent models and the solution of Navier-Stokes equations without any model for turbulent flows at low Reynolds number.

At the present time two approaches are available for very accurate simulations of turbulent flows: Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES). With the DNS technique all the turbulent length scales of the flow are solved directly, using a number of computational points large enough to account for the smallest scales of the motion. Therefore the computational time and the machine storage space needed are very high, and as the spatial resolution needed increases with $Re^{9/4}$, the simulation is restricted to low Reynolds number flows. On the other hand in the LES approach the large scales of the flow are solved directly while the smallest scales are modeled through a subgrid scale model. In this case the choice of the grid size must be such that the modeled scales lie within the inertial subrange. The large eddy technique permits the simulation of turbulent flows at higher Reynolds numbers than possible with DNS. Nevertheless the simulation is still limited by the computing capabilities of the available machines (e.g. up

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1 So called because more than two vortex can join together to generate a single coherent vortical structure.
to \( Re = 10^5 \). The first simulations with DNS and LES were limited to the time development of a flow, or in other words, to a Lagrangian study of the layer (see [5] and [6]). For this type of simulation the basic assumption is that the computational domain can be regarded as a moving control volume advected at the mean velocity of the layer; consequently only the time development of the flow structures can be studied and the computational time needed is not prohibitive. From a numerical point of view the boundaries treatment is very simple because periodic boundary conditions can be applied at the inlet and outlet planes of the domain. It is also evident that no data can be gathered concerning flow development in space. Moreover time development simulations cannot represent some features of the mixing layers, like the deflection of the center of the mixing region toward the low speed side which results in an asymmetric development of the layer. They can nevertheless provide useful information on the physics of turbulent structures in this class of flows.

In the last few years spatially developing mixing layers have also been simulated. Lowery & Reynolds [7] and Sandham & Reynolds [8] have studied, respectively, 3D and 2D forced mixing layers with DNS. In both studies the evolution of the mixing layer is investigated superimposing to the mean inlet velocity profile time dependent oscillatory perturbations proportional to the eigenvalues and eigenfunctions of the Rayleigh equation for the inviscid shear layer problem. Sandham and Reynolds also tested the case where a random phase is added to the perturbation in order to simulate a natural mixing layer. Comte et al. [6] have performed a 2D LES simulation of a natural mixing layer obtained superimposing to the inlet mean velocity profile white-noise random perturbations of small amplitude. In this case the additional energy supplied at each timestep destabilizes the most unstable mode which starts to grow at the rate predicted by the linear instability theory.

For both DNS and LES a difficult numerical problem lies in the mathematical treatment of outflow boundaries. In fact the flow must leave the domain without any reflection and the solution at interior points must not be influenced by the presence of the boundaries. The problem is further complicated by the presence of coherent vortical structures which must not be distorted when crossing the boundary plane.
2. LARGE EDDY SIMULATION PRINCIPLE

For each class of turbulent flow it is possible to consider two broadly different classes of flow structures ("eddies") : the large eddies and the small eddies.

The large eddies interact directly with the mean flowfield, from which they extract energy. This energy is dissipated by the smallest scales of motion at the end of a process of continuous energy transfer to smaller and smaller flow structures (i.e., energy cascade). Basically the large eddies are responsible for the transfer of mass, momentum and energy within the flow and their size is related to the dimension and the geometry of the mean flow scales. Their time scale is of the same order of magnitude as for the mean flow.

The small eddies on the other hand are generated by the interaction between large eddies and have a dissipative behaviour. They are characterized by a tendency towards isotropy and a time scale smaller than large eddies. Due to the decreasing size of the scales involved, small eddies are generated and destroyed more rapidly than the large ones.

The basic idea of LES is to solve directly the anisotropic part of the flow (large eddies) which is flow dependent and model the isotropic flow structures (small eddies) whose behaviour is universal. The possibility of computing explicitly the non isotropic flow structures is one of the main advantages with respect to other turbulent models where all the structures are modeled. Nevertheless, one practical limitation exists, namely the need for a large amount of cpu time because the 3D unsteady Navier-Stokes equations for the large scales must be solved numerically.

For the present work a finite difference discretization of the Navier-Stokes equations is adopted. For this type of discretization the model for the isotropic small scales is related to the grid size which acts like a filter. The filtered part of the flow is modeled with a Subgrid model (S.G.S.) which must reproduce the removal of energy from large to small eddies. The right choice of grid size depends on the type of flow to be simulated. For wall bounded flows a problem arises close to the walls where it is practically impossible to solve all the flow scales on a finite mesh because the dimensions of the length scales decrease approaching the wall. To overcome the problem approximate wall boundary conditions are usually applied [9], [10], [11].

For free turbulent shear flows a problem of resolution exists in the region of mean shear and can be solved only increasing the number of grid points across that region. In other words, the regions of high vorticity must be discretized as finely as possible. The domain has to be long enough to allow the transversal growth of the flow and to make possible the development of long wavelength instabilities in the streamwise direction.
3. FILTERING

The principle of large eddy simulation leads to the need to define a separation between large and small scales which can be achieved with the application of a filter. For a continuum mathematical treatment it is possible to define a sharp separation between the two ranges of scales (i.e., in Fourier space a "cutoff" wavenumber is considered). On the other hand, this cannot be easily done in a discrete numerical simulation of the problem. The filter must be applied to the governing equations which, in the present case, are the 3D unsteady Navier-Stokes equations for incompressible flow:

\[
\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re} \frac{\partial^2 u_i}{\partial x_j \partial x_i} \tag{1}
\]

coupled with the continuity equation:

\[
\frac{\partial u_i}{\partial x_i} = 0 \tag{2}
\]

Equations (1) and (2) are made non-dimensional with respect to the typical velocity and length scales of the flow (see section 7). The instantaneous flowfield is then split in large scale motion and subgrid component:

\[ u_i = \overline{u}_i + u'_i \tag{3} \]

where \(\overline{u}_i\) corresponds to the part of the flow computed directly and \(u'_i\) is the part cut by the filter (small scales). The filtered Navier-Stokes equations are rewritten as:

\[
\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial \overline{u}_i \overline{u}_j}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \frac{1}{Re} \frac{\partial^2 \overline{u}_i}{\partial x_j \partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} \tag{4}
\]

\[
\frac{\partial \overline{u}_i}{\partial x_i} = 0 \tag{5}
\]

The term \(\tau_{ij}\) is the subgrid scale Reynolds stress tensor (S.G.S.) which represents the interaction between the small and the large scales. It simulates the subtraction of energy from the large scale motion and is defined as:

\[
\tau_{ij} = u'_i u'_j + \overline{u'_i \overline{u}_j} + \overline{u'_i u'_j} \tag{6}
\]

The convective flux \(\overline{u}_i \overline{u}_j\) in equation (4) is awkward to treat numerically. Applying Leonard's modification [10] the averaged momentum equation can be rewritten as:

\[
\frac{\partial \overline{u}_i}{\partial t} + \frac{\partial \overline{u}_i \overline{u}_j}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \frac{1}{Re} \frac{\partial^2 \overline{u}_i}{\partial x_j \partial x_i} - \frac{\partial \tau'_{ij}}{\partial x_j} \tag{7}
\]
where the last two terms \((-\bar{U}_i\bar{U}_j + \bar{U}_i\bar{U}_j)\) are Leonard's terms. It can be shown ([10], [11]) that these terms are responsible for a redistribution of energy among the large scales and are of the same order of magnitude as the truncation error for a second order space discretization scheme on a staggered grid. The approach followed in the present work is the one originally proposed by Deardoff and Schumann where the Leonard's terms are set to zero, for any order of accuracy of the discretization scheme, following the argument by Mason [12]. The following relationships are therefore obtained:

\[ \bar{U}_i\bar{U}_j = \bar{U}_i\bar{U}_j \]

\[ \tau'_{ij} = \bar{u}'_i\bar{u}'_j \]

Use of the Deardoff-Schumann approach requires the Navier-Stokes equations to be discretized on a staggered grid and integrated in space with the finite volume technique. The time derivative of the velocity averaged over the cell volume is given by the balance of momentum fluxes and viscous stress averaged over the cell surfaces. This formulation turns out to be similar to the solution of the integral form of the Navier-Stokes equations [11],[13] and the resulting equations are similar to those obtained applying the continuous averaging procedure:

\[ \frac{u(x + h) - u(x - h)}{2h} = \frac{d}{dx} \left\{ \frac{1}{2h} \int_{x-h}^{x+h} u(\xi) d\xi \right\} \]

Relation (11) shows how a discrete mesh filters out the scales smaller than the mesh size \(h\) [11]. In the following section the modelization of the filtered term will be presented.
4. SUBGRID MODEL

To have an effective L.E.S., the modeled scales must lie in the inertial subrange to respect the assumption of isotropy for the modeled part of the flow. This condition must be satisfied by means of a correct choice of the filter width \( \Delta \).

The subgrid effect to be modeled is the removal of energy from large to small eddies: the assumed isotropy of the small scales allows the application of eddy viscosity theory to the modelization of \( \tau_{ij}' \) to obtain the relationship:

\[
\tau_{ij}' = -\nu_t \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)
\]

relating the subgrid stresses to the local strain rate of the resolved scales.

The eddy viscosity is modeled using Smagorinski's subgrid scale model which is derived from the assumption that in the inertial subrange the production of energy is equal to the dissipation:

\[
\nu_t = \ell^2 \sqrt{2S_{ij}S_{ij}}
\]

where

\[
S_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)
\]

is the strain rate tensor of the resolved scales.

In equation (13) \( \ell \) is the length scale of the subgrid eddies which must be related to the filter width \( \Delta \). Since in the simulation the filtering is done directly by the grid, \( \Delta \) must depend on its size. For a non equally spaced mesh the relations are:

\[
\Delta = (\Delta x \Delta y \Delta z)^{\frac{1}{3}}
\]

and

\[
\ell = C_s \Delta
\]

The "linking" coefficient \( C_s \) relates the S.G.S. model to the physics of the inertial subrange and depends on the form of filter used. Theoretically \( C_s = 0.17 \) for a sharp cut-off filter in wavenumber space and \( C_s = 0.23 \) for a top hat filter in the physical space [12]. For a finite difference method a sharp cut-off is not achieved and the effect due to the highest non resolved scale is not taken into account by the model, because \( C_s \) is not uniquely defined in a numerical simulation. Mason [12] has shown that \( C_s \) must decrease with grid size. Therefore a small value of \( C_s \) generates an accumulation of energy at the smallest resolved scales [9]. Typical values for \( C_s \) in the present simulation are in the range 0.06-0.2.
5. NUMERICAL METHOD

The present section is devoted to the description of the numerical solution of the governing equations.

In the past most simulations with LES and DNS have been done using spectral methods because of their high spatial accuracy; the last years, however, have seen an increasing use of finite differences. Finite differences present some advantages with respect to spectral methods such as the possibility to use stretched grids, easier handling of complex flow geometries (e.g. curved walls, steps, etc.) and user friendliness. Their major drawback is that they are less accurate than spectral methods.

In order to understand the accuracy requirements the numerical discretization has to satisfy, it is worth reminding that the spatially developing mixing layer is characterized mainly by streamwise advection of coherent vortical structures generated by the growth of unstable waves and can therefore be regarded as an advection dominated flow where high gradient regions are present. This feature leads to a need to pay particular attention to the treatment of the non linear convective terms in order to avoid aliasing errors. Moreover, problems of energy conservation related to the local and global accuracy of the scheme can also arise. It is therefore necessary to use a finite difference scheme with high local spatial accuracy and with the characteristic of controlling aliasing errors [14].

In the following subsections the representation of equations (7), (12), (13) in space and time will be discussed.

5.1 Spatial discretization

The simple flow geometry of the mixing layer allows the use of an orthogonal computational domain discretized with a cartesian grid in three dimensions. Stretching is used only in the direction which corresponds to transversal flow development (z-dir see Fig. 1.1). Equations (4) and (5) are discretized applying a finite volume technique over a staggered grid, which is the variable layout offering the best conservation properties for incompressible flow calculations (for more details see Harlow & Welch [15]). In figure 5.1 the staggered configuration is shown for a 2D case; generalization to three dimensions is obvious.

Over a staggered grid the control volumes for \( x \), \( y \) and \( z \)-momentum balances do not coincide. With respect to the physical grid cell the control volume for momentum is displaced half way between two grid cells in the direction where the momentum balance is made, as sketched in figure 5.1.

The large scale momentum equation (7) can be rewritten as follows:

\[
\frac{\partial \bar{u}_i}{\partial t} = H(\bar{u}_i, \bar{u}_j) - \frac{\partial \bar{p}}{\partial x_i}
\]  \hspace{1cm} (17)
The computational variables \( p, u, w \) are situated as follows:

\( p \) in the center of the cell, \( u \) at \((l + \frac{1}{2}, n)\) and \( w \) at \((l, n + \frac{1}{2})\) locations.

where \( H \) is the space operator containing resolved terms, subgrid Reynolds stresses and molecular viscous stresses. As anticipated, the main difficulty lies with the proper discretization of the non-linear advective term \( \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} \).

Due to the different locations of the velocity components, interpolations are needed to calculate the fluxes on the center of the six control surfaces as shown in figure 5.2 for the 2D \( x \)-momentum balance.

The convective fluxes along the \( j^{th} \) direction for the momentum balance in the \( k^{th} \) direction are given by the following cross-interpolation formulae:

\[
\begin{align*}
    f_{jk}^+ &= (\bar{u}_j)_i^+ (\bar{u}_i)_j^+ \\
    f_{jk}^- &= (\bar{u}_j)_i^- (\bar{u}_i)_j^-
\end{align*}
\]

\((i, j, k = 1, 2, 3)\) (18)

where \((\bar{u}_j)_i^+\) is the \( j^{th} \) velocity component interpolated along the \( i^{th} \) direction and vice-versa \((\bar{u}_i)_j^+\) is the \( i^{th} \) velocity component interpolated along the \( j^{th} \) direction.\(^1\) The velocities \((\bar{u}_j)_i\) may be interpolated using different formulae depending on the direction along which the interpolation is made.

When the fluxes are interpolated along orthogonal directions the resulting balances are non-conservative and aliasing errors can affect the solution. The aliasing error phenomenon

\(^1\) The velocity components \( \bar{u}_1, \bar{u}_2, \bar{u}_3 \) refer respectively to the \( x_1, x_2, x_3 \) coordinates; in the present work the velocity components are defined also with \( \bar{u}, \bar{v}, \bar{w} \) and the coordinates with \( x, y, z \).
is due to the appearance of high frequency modes that cannot be handled directly in the calculation (i.e., frequencies with wavelength smaller than the grid size). These frequencies appear in the resolved flow as a low frequency contribution and can destabilize the numerical solution (for more details see Hirsch [16]). The requirement for the discretization scheme to be conservative and to limit aliasing errors can be solved in two different ways: 1) applying a conservative centered relationship or 2) using upwind interpolation formulae. In the former case the lowest order scheme is the 2nd order one obtained using linear interpolations. The requirement that mean momentum and energy be conserved by the numerical scheme has often been satisfied in Large Eddy Simulation of channel flows applying the conservative Arakawa’s form [9],[17]:

\[
\frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = \frac{1}{2} \left\{ \frac{\delta (\bar{u}_i \bar{u}_j)}{\delta x_j} + \bar{u}_j \frac{\delta (\bar{u}_i)}{\delta x_j} + \bar{u}_i \frac{\delta (\bar{u}_j)}{\delta x_i} \right\}
\]

(22)

where \( \frac{\delta }{\delta x_j} \) is the central difference operator in the \( j \) direction. With such a formulation the aliasing error phenomenon cannot be completely avoided and the typical instability generated by the centered scheme can still affect the computation as will be shown later.

With the upwind approach the artificial dissipation introduced controls the aliasing errors leading to a stable solution even if the scheme is not conservative. However, the grid size must be small enough to avoid that the information corresponding to the highest resolvable frequencies be “smeared out” of the simulation by numerical dissipation.

In the Large Eddy Simulation of a spatially developing mixing layer done by Comte et al.[6] the 2D Navier-Stokes equations in the vorticity stream-function formulation have
been solved using a second order centered discretization with the conservative Arakawa’s formulation of the advection term. On the other hand, Lowery & Reynolds [7] and Sandham & Reynolds [8] in their Direct Simulation of the same flow use the primitive variables formulation and solve the governing equations with a second order upwind formulation along the streamwise coordinate and a centered second order scheme in the two other directions.

In the present work some tests have been performed in order to understand the effect of different schemes used in the literature and their results will be discussed later (see appendix). Only the conclusions are reported here in order to justify the final choice for the discretization of the advection term. The first scheme tested was the centered 2nd order scheme in the Arakawa formulation obtained by linear interpolation of the nodal values of the variables. As said above this scheme has been quite successful for channel flow calculations with L.E.S. but when applied to the mixing layer problem a “wiggly” solution was found even if the scheme is energy conserving.

In a second test QUICKEST scheme [19] was used for the z-direction together with 2nd order formulae for y and z directions. QUICKEST is an upwind scheme, 3rd order accurate over a uniform mesh. The results show the presence of a damping effect, which leads to a stable solution. However, the damping is very high and the contribution of the subgrid scale term is completely obscured (i.e., results insensitivity is found with respect the variation of coefficient $C_s$ in the modeled term).

The two tests made clear that an accurate simulation required use of an upwind formulation to avoid instability, but with accuracy higher than QUICKEST to prevent unacceptable levels of numerical damping.

To fulfil the requirements of high local precision the terms $(\bar{u}_i)_j$ are interpolated over four points with a 3rd order polynomial formula. For the interpolation along x-direction an upwind-biased relationship proposed by Kawamura et al. [18] is used while centered formulae are applied for $(\bar{u}_i)_2$ and $(\bar{u}_i)_3$. The centered interpolation formula for $(\bar{u}_i)_3$ takes into account the variable grid size along the transversal coordinate. The interpolations along the three directions for the $\bar{u}_1$ velocity component in the case of the x-momentum balance are given below as example (see also Fig. 5.2):

$$
(\bar{u}_1)_1^+ = \frac{1}{6} \left[ \bar{u}_1(l+2,m,n) - \bar{u}_1(l+1,m,n) + \bar{u}_1(l,m,n) - 2 \bar{u}_1(l-1,m,n) \right] 
$$
(19)

$$
(\bar{u}_1)_2^+ = \frac{1}{12} \left[ -\bar{u}_1(l,m+2,n) + 7 \bar{u}_1(l,m+1,n) + 7 \bar{u}_1(l,m,n) - \bar{u}_1(l,m-1,n) \right] 
$$
(20)

2 Quadratic Upstream Interpolation for Convective Kinematics with Estimated Streaming Terms.
Using relations (19), (20), (21) and the corresponding ones for the other components, the flux balances along $x$ and $z$-directions become third order accurate while the flux balance along $y$ is fourth order accurate. On the boundaries, for lack of points outside the computational domain, the interpolations are made with standard central second order formulae. By doing so the overall precision of the scheme is reduced but the local higher accuracy for the interior points is preserved [14].

The dissipation introduced by (19) takes the shape of a fourth order derivative and can be written as follows:

$$
\frac{\Delta x_1^3}{4} \frac{\partial^4 \bar{u}_i}{\partial x_1^4}
$$

To confine the effect of this term to controlling the aliasing error the grid size $\Delta x_1$ must be kept as small as possible.

At this point it is worthwhile to make some comments on the use of upwind schemes for L.E.S. Boris [20] proposes the use of monotone non linear algorithms (e.g. Flux-Corrected Transport (FCT), Total Variation Diminishing (TVD), etc.) which have been developed for the calculation of flows with sharp gradients and work on the principle of reducing the local accuracy of the scheme in the regions of steepest gradients to avoid the onset of oscillations. Obviously this feature is in direct contrast with the need to achieve high local accuracy, but Boris arguments that these schemes already contain both a built-in filter and a built-in subgrid model. It is not clear yet [20] whether the built-in model provides enough diffusion to entirely replace the modelled subgrid term.

However, practical experience shows that, when these algorithms are applied care must be taken in the treatment of the subgrid modeled terms to avoid an over-estimation of the overall (numerical and modeled) dissipation as shown by QUICKEST's results.

From the discussion carried out it is clear that the "correct" treatment of convective terms is related to the availability of algorithms which can handle gradients in a correct way (e.g. without introducing high damping) while retaining the high accuracy which is of fundamental importance in the calculation of turbulent flows. Further work remains to be done before a solution fully satisfactory from both points of view will become available.
The laminar stress term \( \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_i} \) is discretized with a centered formula:

\[
\frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_i} = \frac{\partial}{\partial x_i} \left( \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}_i}{\partial x_i} \right)
\]

(24)

the derivatives in parentheses are evaluated with a centered formula at the center of the control volume surfaces (see Fig. 5.2). Formula (24) is 2nd order accurate on uniform or moderately stretched meshes, while with high stretching the accuracy drops to first order [14], [21].

The S.G.S. term \( \frac{\partial \tau_{ij}}{\partial x_j} \) are discretized with a centered 2nd order accurate formula. In the treatment of the turbulent subgrid stresses care must be taken in the calculation of the strain rate tensor \( S_{ij} \) as well as the turbulent viscosity \( \nu_t \), particularly with regard to their positioning over the grid. Two different procedures have been tested, namely the classical one suggested by Mason [12] and an “ad hoc” one developed in order to reduce the number of interpolations necessary for the calculation of \( \tau_{ij} \). In the former case \( S_{ij} \) and \( \nu_t \) are calculated on the middle of the upper surface of the cell \( (l, m, n + \frac{1}{2}) \) and interpolations are needed for the calculation of \( \frac{\partial \tau_{ij}}{\partial x_j} \) at the locations required by the numerical control volume of the different momentum equations. In the other case four different location points are used to compute \( S_{ij} \) and \( \nu_t \) (see table 5.1 and Fig. 5.3) at the same locations as the different velocity components.

The last term in equation (17) is the pressure gradient computed over the control volume relative to the \( x \), \( y \) and \( z \)-momentum balance. In a staggered grid the pressure nodes are located on the surfaces of the control volume for the velocity and its gradient computed using consecutive nodal values is the natural driving force for the velocity component under calculation. The discretization is by a centered 2nd order accurate formula. The pressure term for the \( x \)-momentum balance is given below as an example:

\[
\frac{\partial \bar{p}}{\partial x_1} \bigg|_{l+\frac{1}{2},m,n} = \frac{\bar{p}(l+1,m,n) - \bar{p}(l,m,n)}{x(l+1,m,n) - x(l,m,n)}
\]

(25)

5.2 Time advancement

The governing equations are advanced in time using the 2nd order accurate explicit predictor-corrector Adams-Bashforth scheme [9].

Starting from equation (17) the velocity field at time level \( (n+1) \) is guessed from the velocity fields at time levels \( (n) \) and \( (n-1) \) and the pressure at \( (n-1) \):

\[
\frac{\bar{u}_i^{(n+1)} - \bar{u}_i^{(n)}}{\Delta t} = \frac{3}{2} H(\bar{u}_i, \bar{u}_j)^{(n)} - \frac{1}{2} H(\bar{u}_i, \bar{u}_j)^{(n-1)} + \frac{1}{2} \frac{\partial \bar{p}^{(n-1)}}{\partial x_i}
\]

(26)
Fig. 5.3 - Subgrid stresses locations for the cell l,m,n

<table>
<thead>
<tr>
<th>$S_{ij}$</th>
<th>locations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_{11}$</td>
<td>$l,m,n$</td>
</tr>
<tr>
<td>$S_{12}$</td>
<td>$l + \frac{1}{2}, m + \frac{1}{2}, n$</td>
</tr>
<tr>
<td>$S_{13}$</td>
<td>$l + \frac{1}{2}, m, n + \frac{1}{2}$</td>
</tr>
<tr>
<td>$S_{22}$</td>
<td>$l,m,n$</td>
</tr>
<tr>
<td>$S_{23}$</td>
<td>$l,m + \frac{1}{2}, n + \frac{1}{2}$</td>
</tr>
<tr>
<td>$S_{33}$</td>
<td>$l,m,n$</td>
</tr>
</tbody>
</table>

Table 5.1 - Locations of $S_{ij}$

the predicted velocity field $\bar{u}_i^{(n)}$ is corrected applying equation:

$$\frac{\bar{u}_i^{(n+1)} - \bar{u}_i^{(*)}}{\Delta t} = -\frac{3}{2} \frac{\partial p^{(n)}}{\partial x_i}$$  (27)

Continuity of $\bar{u}_i^{(n+1)}$ is enforced through the Poisson’s equation:

$$\frac{\partial^2 p^{(n)}}{\partial x_i^2} = \frac{2}{3 \Delta t} \frac{\partial \bar{u}_i^{(*)}}{\partial x_i}$$  (28)

from which the pressure can be calculated once the predicted velocity field is known. Equation (28) is obtained taking the divergence of equation (27) and applying the continuity equation [22]. The successive steps of the solution are to guess the velocity field from equation (26), derive the pressure field at time level ($n$) by mean of the Poisson’s equation (28) and finally use equation (27) to provide the corrected velocity field at time level ($n+1$).
Equation (28) is solved using a Fast Poisson solver [23] based upon a Fourier transform method which solves simultaneously the whole pressure field without any iterative procedure. The main drawback lies in the fact that stretching is allowed only along one coordinate direction.

The timestep $\Delta t$ is taken constant and chosen to satisfy everywhere on the mesh the stability requirements given by the C.F.L. condition for the advective terms and for the diffusive terms [9]:

\[
(CFL)_a = \Delta t \left[ \frac{|U|}{\Delta x} + \frac{|V|}{\Delta y} + \frac{|W|}{\Delta z} \right]_{max} \leq 0.5
\]  

\[
(CFL)_d = \frac{1}{\nu_{tot}} \left[ \frac{\Delta t}{\Delta x^2}, \frac{\Delta t}{\Delta y^2}, \frac{\Delta t}{\Delta z^2} \right]_{max} \leq 0.1
\]  

where $\nu_{tot}$ is the sum of molecular ($\nu$) and turbulent ($\nu_t$) viscosities.
6. BOUNDARY CONDITIONS

One of the major theoretical problems related to the accurate numerical simulation of spatially developing flows is the correct handling of the boundary conditions. A non appropriate definition of the boundary conditions can affect the interior flow solution in two different ways: numerically, introducing a weakness in the system of equations which generates instabilities in space as well as in time, or physically if the boundary equations do not provide the correct physical information to the computational domain. The difficulty becomes more noticeable when turbulent inflow and outflow conditions must be specified along the direction of flow development.

For the inlet boundary condition the problem lies in the need to introduce into the flow “pseudoturbulent” perturbations strong enough to destabilize it and make possible a proper development of turbulence. A widely used procedure is to start from the mean velocity profile and superimpose time dependent perturbations simulating the instantaneous turbulent velocity fluctuations.

For the other boundaries, the problem lies with the need to define a finite domain of numerical integration while dealing with a physically unbounded flow. Some techniques allow the use of an infinitely large domain, like the mapped spectral method developed by Cain et al. [24] and applied by Lowery & Reynolds [7] and Sandham & Reynolds [8] for the treatment of free stream boundaries in their mixing layer simulations. A mapping scheme with stretched grid can be also applied along the streamwise direction although the problem of setting the boundary conditions at infinite is not well defined; this technique has been applied by Davis & Moore [25]. In the present simulation a finite domain is used, leading to the implementation of ad hoc open boundary conditions for outflow boundaries. The free stream boundaries must also be treated as inflow-outflow boundaries, to take into account entrainment in the transversal direction [26] and transversal oscillations of the main stream which must not be constrained by the mathematical boundary conditions. On the other hand, when an infinite domain is considered there is neither inflow nor outflow at the free stream location and the slip wall condition can be applied [7,8].

In the following subsections streamwise inlet and outflow conditions are discussed first, then spanwise and transversal boundary conditions and finally initial condition.

6.1 Inlet boundary condition

The objective of the present work is to study the main development of a plane mixing layer. The area interested by the main growth is located far away from the separation plate. Therefore, in order to capture the formation of vortical structures without having recourse to a very long computational domain the plate itself is not modeled and the mean velocity profile at the inlet boundary is assumed to satisfy a \( \tanh \) distribution, which represents quite well the mean velocity profile of the mixing layer in its initial development stage (see
Fig. 1.1). The mean streamwise velocity profile on the inlet plane is then defined by the relation:

\[
< \bar{u}_i(z) > = \frac{1}{2} \left\{ \frac{1}{\lambda} + \tanh(2z) \right\} \quad (i=1) \tag{31}
\]

where \( \lambda = \frac{u_1 - u_2}{u_1 + u_2} \); \( u_1 \) and \( u_2 \) are the free stream velocities for the two flows [6],[7],[8]. The profile does not take into account the wake generated downstream the splitter plate. The adimensional parameter characterizing the flow is \( r = \frac{u_2}{u_1} \), which defines the shearing intensity of the layer; when \( r = 0 \) (lower limit) only one stream is present and no shear takes place, while the maximum shear corresponds to the case of \( r = 1 \) (upper limit) (e.g. the wake behind an obstacle). In the present simulation \( \lambda = \frac{1}{3} \) and \( r = 0.5 \). When the streamwise velocity profile (31) is imposed at the inlet of the computational domain without superimposing any perturbation the flow remains laminar along the whole development and the typical features of the turbulent mixing layer (i.e., rolling up into vortices, vortex pairing, etc.) do not develop.

Three dimensional perturbations must be superposed to reproduce the turbulent field generated in the early stages of the flow development, namely within the linear instability region. The time dependent inlet velocity profile is defined by the following relation:

\[
\bar{u}_i(0, y, z, t) = < \bar{u}_i(z) > + \bar{u}_i^P(y, z, t) \quad (i=1,2,3) \tag{32}
\]

where \( \bar{u}_i^P(y, z, t) \) are the time dependent perturbations imposed on the inlet section \( (x = 0) \). The form of perturbations to be used is different for the forced and the natural mixing layer.

The shape of the perturbation for the forced case is chosen taking into account the fact that the mixing layer is characterized by an unstable behaviour which can be viewed as the superposition of interacting instability waves propagating and amplifying in the downstream direction [27]. To calculate the most unstable wave (corresponding to the natural frequency of the layer \( f_n \)) the linear instability theory can be applied. The procedure followed by many authors (Monkewitz & Huerre [4] and Lowery & Reynolds [7], among the others) is resumed below for a 2D problem. The small perturbation:

\[
\frac{1}{2} \left\{ \hat{u}_j(z) \exp[i(\alpha x - \omega_p t)] + c.c. \right\} \quad (j=1,3) \tag{33}
\]

is superimposed on the mean streamwise velocity profile (31) (c.c. is the complex conjugate) and inserted in the linearized inviscid Navier-Stokes equation (Rayleigh problem):

\[
\dddot{\bar{u}}_3 = \left[ \frac{\dddot{\bar{u}}_1}{\bar{u}_1 - c + \alpha^2} \right] \dddot{\bar{u}}_3 \tag{34}
\]

\[
\bar{u}_1 = \frac{1}{\alpha} \dddot{\bar{u}}_3
\]
where the symbol "'" stands for the operator $\frac{d}{dz}$. The solution of the eigenvalue problem (34) gives the streamwise mode $\alpha$ and the eigenfunctions $\tilde{u}_1$ and $\tilde{u}_3$, whose oscillation frequency is $\omega_p$. The ratio $\frac{\omega_p}{\alpha} = c$ is the propagation speed of the wave in the $x$-direction.

In the present study no attempt is made to solve (34) and the forcing perturbation function is chosen to obey the relation:

$$\Phi_i(y, z, t) = u'_i [\sin(\omega_p t) + \cos(\omega_p t)] \quad (i=1,3)$$  \hspace{1cm} (35)

where $u'_i$ is the amplitude of the perturbation, and $\omega_p$ is taken equal to fundamental frequency $\omega_0$, which for the $\text{tanh}$ profile (31) depends from the parameters $\lambda$ and $r$. Solving (34) Lowery & Reynolds [7] found that for $\lambda = \frac{1}{3}$ and $r = 0.5$ the Strouhal number corresponding to the most unstable mode is $St = 0.018$ (Oster & Wygnanski [2] found a value of $St = 0.02$ from experimental measurements), where the Strouhal number is defined as:

$$St_0 = \frac{f_0 \theta_0}{2u_m}$$  \hspace{1cm} (36)

with $f_0 = \frac{\omega_0}{2\pi}$, $\theta_0$ is the momentum thickness which takes the value $\frac{1}{4}$ for profile (31), $u_m$ is the mean velocity of the layer ($\frac{u_1 + u_2}{2}$). This formulation gives a value $\omega_0 = -\frac{4}{3}$ for the frequency of the fundamental mode. In the simulation the first and the second subharmonics are added to the fundamental mode to promote vortex pairing.

The energy provided to the flow triggers the unstable behaviour of the layer causing the appearance of structures well organized in time as well as in space. Obviously this is not appropriate for the natural mixing layer where the perturbations should be random, or, from the theoretical point of view, should not be periodic and satisfy the criterion to supply an equal amount of energy at each timestep. In this way the unstable modes of the profile (31) grow naturally whereas the stable ones are damped, and the growing of the unstable waves is not "artificially" promoted. For this purpose a 3D white noise random field is generated and superimposed to the mean velocity profile at the inlet section. The perturbation function for the natural case is rewritten as follows:

$$\Phi_i(y, z, t) = u'_i \Psi(y, z, t) \quad (i=1,2,3)$$  \hspace{1cm} (37)

where $\Psi(y, z, t) \in [-1:1]$ is a random field with uniform distribution and $u'_i$ is the amplitude of the perturbation.

In order to introduce the strongest perturbation in the region of maximum shear $\Phi_i(y, z, t)$ is modulated with the exponential function $e^{-\sigma |z-z_c|}$ where $z_c$ is the mixing layer centerline transversal coordinate and $\sigma$=2.63. Finally the perturbations are calculated with the following relation:

$$\bar{u}'_i(y, z, t) = \Phi_i(y, z, t)e^{-\sigma |z-z_c|} \quad (i=1,2,3)$$  \hspace{1cm} (38)
the perturbation amplitude $u'$ is 0.03 for the forced mixing layer and 0.12 for the natural one.

### 6.2 Outflow boundary condition

In the previous sections it has already been stressed that the boundary condition applied on the outflow section must not be "reflective". In this context non "reflective" means that the flow solution within the computational domain must not be influenced by the presence of the boundary acting as a discontinuity. In order to minimize, if not entirely eliminate, the region of backward influence many authors have developed several conditions for different flows (hyperbolic, elliptic, parabolic). The mixing layer simulated in the present work is an advection dominated flow and can be assumed to be hyperbolic along the streamwise coordinate. Therefore information from external points ($x > L_x$) are not needed to calculate the flow field on the plane at $x = L_x$. This assumption makes possible to use a wave equation to find the boundary values of velocity [28]. The wave equation cannot be applied explicitly to the pressure equation because of its elliptic behaviour. Therefore a Neumann condition is used. The wave equation used is:

$$\frac{\partial \bar{u}_i}{\partial t} + C_i \frac{\partial \bar{u}_i}{\partial x_1} = 0 \quad (i=1,2,3) \tag{39}$$

where $C_i$ is the advection velocity of the wave. Equation (39) is valid for linear waves like the Sommerfeld radiation condition for which the technique was developed by Orlanski. In the case of turbulent flows boundary equation (39) has been applied successfully by different authors [6],[7],[8] even if the perturbations generated inside the domain are not linear. The procedure followed for the discretization of eq. (39) on the boundary location at time level ($n + 1$) is given in the following for the $\bar{u}_1$ velocity component (see Figs. 5.1 and 5.2):

$$\frac{\bar{u}_1^{(n+1)}(l,m,n) - \bar{u}_1^{(n-1)}(l,m,n)}{2\Delta t} = \frac{C_1}{\Delta x} \left\{ \frac{\bar{u}_1^{(n+1)}(l,m,n) + \bar{u}_1^{(n-1)}(l,m,n)}{2} - \bar{u}_1^{(n)}(l-1,m,n) \right\} \tag{40}$$

where $C_1$ is calculated from the above equation as function of the interior flow solution at locations ($l - 1, m, n$) and ($l - 2, m, n$) at time levels ($n$), ($n - 1$) and ($n - 2$):

$$C_1 = -\frac{\bar{u}_1^{(n)}(l-1,m,n) - \bar{u}_1^{(n-2)}(l-1,m,n)}{\bar{u}_1^{(n)}(l-1,m,n) + \bar{u}_1^{(n-2)}(l-1,m,n) - 2\bar{u}_1^{(n-1)}(l-2,m,n)} \Delta t \tag{41}$$

finally the new boundary value at time level ($n + 1$) is given by:

$$\bar{u}_1^{(n+1)}(l,m,n) = \frac{(1 - \gamma)}{(1 + \gamma)} \bar{u}_1^{(n-1)}(l,m,n) - \frac{2\gamma}{(1 + \gamma)} \bar{u}_1^{(n)}(l-1,m,n) \tag{42}$$

with $\gamma = \frac{\Delta t}{\Delta x} C_1$. 

20
In order to check the effect of the boundary condition on the interior flow solution a comparison has been made of the results for two different domains; the first with \( L_z = 130 \) and the second with \( L_z = 65 \), using the inlet condition is given by relation (35). At the same time level \( T = 87.5 \), \( \overline{u}_3 \) presents the same flow structures in the two cases (fig. 6.1) although the results slightly disagree in the region just before the outlet plane (3 units length from the outlet as shown in Fig. 6.1b). The structures are neither stretched nor compressed close to the boundary and their coherence is preserved. The result is in agreement with those of Comte et al. [6] and Lowery & Reynolds [7] who apply the same boundary condition to spatially developing mixing layers. The test shows that the treatment of the boundary with the wave equation does not affect the internal flow solution even if applied to the propagation of non linear wave with a high degree of coherence.

![Transversal velocity component for the forced mixing layer at time level T=87.5, L_z=130](image)

**Fig. 6.1a - Transversal velocity component for the forced mixing layer at time level T=87.5, L_z=130**

![Transversal velocity component for the forced mixing layer at time level T=87.5, L_z=65](image)

**Fig. 6.1b - Transversal velocity component for the forced mixing layer at time level T=87.5, L_z=65**

6.3 Transversal boundary condition

The flow is not hyperbolic along the transversal coordinate and a condition allowing both inflow and outflow must be adopted. On the free stream boundaries \( z = 0 \) and \( z = L_z \) the wave eq (39) is no longer valid. To satisfy the inflow-outflow requirement, continuity
is invoked for the velocity component normal to the boundary plane [26]:

$$\frac{\partial \bar{u}_3}{\partial x_3} = - \frac{\partial \bar{u}_1}{\partial x_1} - \frac{\partial \bar{u}_2}{\partial x_2}$$  \hspace{1cm} (43)

while, to calculate the velocity component $\bar{u}_1$ and $\bar{u}_2$ the stress-free condition is adopted:

$$\frac{\partial^2 \bar{u}_1}{\partial x_3^2} = \frac{\partial^2 \bar{u}_2}{\partial x_3^2} = 0$$  \hspace{1cm} (44)

The above boundary condition is valid for free stream boundaries where small gradients are present.

6.4 Spanwise boundary condition

The spanwise direction for a spatially developing plane mixing layer is the only one along which the flow is homogeneous allowing the application of cyclic boundary conditions for all the flow field quantities.

6.5 Pressure and predictor step boundary conditions

The pressure on the boundaries is calculated applying the Neumann boundary condition:

$$\frac{\partial p}{\partial n} = 0$$  \hspace{1cm} (45)

where $n$ denotes the direction normal to the boundary plane.

The boundary conditions discussed above are applied to the corrector step, while for the predictor step the Neumann boundary condition is applied on the boundary planes except in the spanwise direction where the cyclic condition is still valid [26],[29].

6.6 Initial condition $t=0$

At time $t=0$ the velocity and the pressure fields are set to zero, only the streamwise component is initialized everywhere using velocity profile (31) without any perturbation.
7. RESULTS

The results presented in this section aim to show the capability of the L.E.S. technique to predict turbulent spatially developing forced and natural mixing layers. The Reynolds number has therefore been chosen to compare the present results with D.N.S. calculations of Lowery & Reynolds [7] and experimental measurements of Oster & Wygnanski [2].

Before going into the details of the results, the conditions of the calculation and main parameters characterizing the problem will be resumed. The computational variables have been cast in non dimensional form with respect to the characteristic dimensional quantities of the flow, namely the free stream velocity difference $\Delta u = u_1 - u_2$, and the inlet vorticity thickness $\delta_{w_0}$ which can be obtained from the general definition of vorticity thickness

$$\delta_w = \frac{1}{\frac{\partial \Omega}{\partial z}}_{\text{max}}$$

using the velocity profile (31) which gives $\delta_{w_0} = 1$. The Reynolds number of the problem is defined as:

$$Re = \frac{\Delta u \delta_{w_0}}{\nu}$$

where $\nu$ is the molecular viscosity. The local momentum thickness is calculated using the formula:

$$\theta = \int_{-\infty}^{+\infty} (u_1 - \bar{u})(\bar{u} - u_2)dz$$

For the present calculations, the values of the different parameters are:

$$\delta_{w_0} = 1; \quad \Delta u = 1; \quad Re = 100; \quad \theta_0 = \frac{1}{4}$$

for $\lambda = \frac{1}{3}$ and $r = 0.5$ (see section 6.1).

In order to capture the spatial development of the mixing layer it is necessary to have a "long" computational domain with a sufficient resolution. To achieve this result with limited computer resources the spanwise perturbation $u'_2$ has been set to zero, and the calculation performed using a very coarse mesh in $x_2$. The dimensions of the computational domain were $L_x = 130$, $L_y = 1.8$ and $L_z = 35$ with $N_x = 340$, $N_y = 6$ and $N_z = 40$ grid points. The grid was stretched in the transversal direction ($z$-dir).

Two sets of calculations are presented in the following subsections, respectively for the forced and the natural mixing layer. The results are arranged in the following way: the instantaneous spanwise vorticity fields are shown first, followed by integral quantities such as momentum and vorticity thickness and by mean and turbulent field statistics,
plotted versus the non dimensional coordinate $\eta = \frac{z - z_{aver}}{\theta}$, where $z_{aver}$ is the value of the transversal coordinate for which the mean streamwise velocity component is equal to the mean velocity of the layer $u_m = 1.5$.

Two sampling procedures have been applied to the calculation of mean streamwise velocity and rms turbulence fluctuations. With the first procedure (procedure A) the data are sampled each timestep over the time interval $87.5 < T < 262.5$ (the period $0 < T < 87.5$ is a transient and no meaningful information can be gathered). The results obtained making use of procedure A represent a complete average over the whole set of samples and tend to smooth out the effect of discrete large scale structures. With the other procedure (procedure B) which was suggested by Lowery & Reynolds [7] the data are sampled each time unit over the time interval $175 < T < 262.5$ to put in evidence the periodic nature of the simulated flow. For the natural mixing layer calculation only the procedure A is employed. The timestep used in the calculations was kept constant at $\Delta t = 0.025$.

Additionally a full 3D computation was performed for the natural mixing layer. The domain used for this case has the dimensions: $L_x = 40$, $L_y = 10$ and $L_z = 35$ with $N_x = 105$, $N_y = 20$ and $N_z = 40$ grid points. The instantaneous streamwise vorticity ($\omega_x$) field in the plane $y-Z$ at $x = 25$ is presented at end of this section.

All the calculations were performed on the Alliant $f_{x} 80$, the CPU time required was $3.2 \times 10^{-4}$ seconds.

### 7.1 Forced mixing layer
#### 7.1.1 Vorticity field

In figures 7.1 and 7.2 the instantaneous spanwise vorticity ($\omega_y$) contours are presented at two time levels, $T = 262.5$ and $T = 269.5$ respectively.

At time level $T = 262.5$ four well defined coherent structures are present, with vortex pairing occurring at the streamwise locations $x \approx 37$ and $x \approx 112$. The first vortex pairing is difficult to detect in figure 7.1, but becomes clearly visible comparing in figure 7.2 where the structure is located at $x \approx 47$ and its transversal dimension is increased by the entrainment of irrotational fluid during the rolling up process. In the region $50 < x < 100$ vortex pairing is inhibited and single vortices are present. Further downstream at $x \approx 112$ the pairing of two vortices is quite visible and their rolling up can be followed in figure 7.2 ($x \approx 124$). The presence of two vortex pairing is strictly related to the use of the first and second subharmonics of the fundamental frequency in the forcing function. As shown by Oster & Wygnanski [2] these subharmonics must be present in order to promote vortex pairing.
In figure 7.1 it can be seen that the structures in the region of the first vortex pairing have a wavelength in the range $6.5 < \Lambda < 8.5$ comparable with the wavelength of the fundamental frequency is $\Lambda_0 = 6.9$. In the region of inhibited pairing $\Lambda$ is close to the wavelength of the first subharmonic $\Lambda_1 = 13.8$. In the last part of the domain the value of $\Lambda$ approaches the second subharmonics wavelength $\Lambda_2 = 27.7$. During the calculations the vortical structures appear periodically at the same streamwise coordinate like in the experimental investigations of Oster & Wygnanski [2] and Ho & Huang [3].

From both figures it is also possible to verify that the advection velocity of the vortices is close to the mean velocity of the layer $u_m$. Moreover figures 7.1 and 7.2 put in evidence the suitability of boundary condition (39) : the structures leave the domain without any remarkable deformation.

### 7.1.2 Integral variables

In figure 7.3 momentum thickness ($\frac{\theta}{\delta u}$ curve 1) and vorticity thickness ($\delta_\omega$ curve 2) are plotted. Momentum thickness is an integral quantity which gives an indication of the layer thickness (i.e., the transversal growth). As found by Oster & Wygnanski [2] the forced mixing layer exhibits regions of enhanced and retarded growth. As a consequence of this behaviour $\theta$ and $\delta_\omega$ are not linear with respect to the streamwise coordinate. The three regions defined in the previous subsection can be easily recognized from curves 1 and 2 of figure 7.3.

The growth rate of $\theta$ ($\frac{d\theta}{dx}$) is about 1%, in agreement with the calculation of Lowery & Reynolds [7].

More information concerning the locations of vortex pairing can be extracted from the vorticity thickness curve which shows the variations of the maximum mean streamwise velocity gradient. An increase of the slope reveals the presence of a vortex pairing process while a constant value of $\delta_\omega$ is associated with absence of any pairing. The three regions found in the calculation correspond to the ones identified by Oster & Wygnanski [2]: region I where the growth rate exceeds the one of the *natural* layer; region II characterized by a reduction of the growth rate, which can even becomes negative in case of high amplitude forcing ; region III where the same growth rate as region I is experienced.

Oster & Wygnanski [2] provide an analytical relation to determine the boundaries of the three regions. In particular the region of inhibited pairing (i.e., region II) begins at $x = \frac{u_m}{\Lambda f_r}$ and ends at $x = \frac{2u_m}{\Lambda f_r}$ where $f_r$ is the frequency response of the layer in this region. The same relations can be applied to calculate the location of region III using the appropriate value of $f_r$ as defined in the previous subsection (for region II the frequency $\Lambda = \frac{u_m}{f}$)
response corresponds to the first subharmonic, whereas for region III it coincides with the second subharmonic). Applying the previous relations it is found that region II lies in the area $42 < x < 85$ and region III in $85 < x < 170$; obviously region I ends at the streamwise location $x \approx 42$. In the present simulation region $I$ ends at $x \approx 45$, while region II ends at about $x \approx 100$, value which is about 15 units length higher than expected. The computed slopes in regions $I$ and $III$ are the same (i.e., $\frac{d\delta_{\omega}}{dx} \approx 0.08$), while $\frac{d\delta_{\omega}}{dx} \approx 0.02$ in region $II$. Comparing this result with D.N.S. calculations of Lowery & Reynolds [7], good agreement is found except for the length of the inhibited pairing area $II$. The predicted growth rate is lower in the first and last region and higher in region $II$ than the ones given by D.N.S. The disagreement is directly related to the different forcing function used in the present work (see section 6).

To close the present subsection one more integral parameter is presented, namely the value of the transversal coordinate ($z_{aver}$) where the mean streamwise velocity component $\overline{u}$ is equal to $u_m$. Curve 1 of figure 7.4 uses the mean velocity data for the interval $87.5 < T < 262.5$ while curve 2 refers to $87.5 < T < 175$. The evolution of $z_{aver}$ should show the "mean" tendency of the layer to move toward the low speed side. Curve 2 puts in evidence this trend while curve 1 shows an upward trend. This behaviour is interpreted as due to the presence of oscillations of the entire layer in the transversal direction. A longer sampling period would be necessary in order to average out these low frequency fluctuations and have $z_{aver}$ always negative along $x$ direction.

### 7.1.3 Mean streamwise velocity, turbulence intensities and Reynolds stresses

In the present subsection mean streamwise velocity profiles, turbulence intensities and Reynolds stresses, calculated employing averaging procedures A and B, are presented. As will be shown some results are strongly affected by the technique used. Seven streamwise stations lying within regions $II$ and $III$ have been monitored. The coordinates are: $x = 67.6$, $x = 73.4$, $x = 80.6$, $x = 86.0$, $x = 98.6$, $x = 117.3$ and $x = 129.2$. Figure 7.5 shows the mean streamwise velocity rescaled with respect to the low speed free stream velocity $u_2$ (i.e., $\frac{\overline{u} - u_2}{\Delta u}$) and calculated following sampling procedure A plotted versus the non dimensional coordinate $\eta$. In figure 7.6 the same quantity, calculated with procedure B, is presented.

The mean velocity profiles shown in figure 7.5, exhibit high degree of self similarity and appear unaffected by the forcing imposed at the inlet. On the other hand, when sampling procedure B is adopted the results should not be self similar, because the passage of large structures results in a larger lateral spread and a smaller mean velocity gradient in region $III$. However, this trend is not reproduced by the numerical result, the main reason being that $z_{aver}$ has a positive value (see Fig. 7.4) instead of the expected negative one, thus
leading to a smaller height of the interaction region. The result also shows the existence of a small velocity undershot (\( \approx 1.5\% \)) on the low speed side of the layer, related to the fact the flow has the maximum deflection in the pairing-off region (\( 45 < x < 110 \)). The same trend was also found by Lowery & Reynolds [7] who report a value around 2%. The thickness of the layer has a value of \( \Delta \eta \approx 10 \) in term of the self similarity coordinate in good agreement with [2].

The streamwise turbulent intensity \( (\sqrt{\frac{\nu^2}{\Delta \eta^2}}) \) is presented in figures 7.7 and 7.8. The different shapes put in evidence the effect of the different sampling procedures. In both cases the profiles do not show self-similarity. As shown by Oster & Wygnanski [2] in region II the streamwise rms velocity fluctuation is characterized by the presence of two lateral peaks with a minimum in the middle of the layer. This feature is not reproduced in the present simulation. However, in figure 7.8, a tendency towards this behaviour can be seen. In region III a bell shaped curve is found in agreement with the measurements [2].

The transversal rms velocity fluctuation \( (\sqrt{\frac{\nu^2}{\Delta \eta^2}}) \) is not affected by the sampling procedure as shown in figures 7.9 and 7.10. The typical bell shaped profiles are obtained, in good quantitative agreement with Oster & Wygnanski [2] data. The different dynamics of the layer in regions II and III do not affect the transversal distribution of \( \sqrt{\frac{\nu^2}{\Delta \eta^2}} \), which reaches an almost constant value in region II and becomes smaller downstream in agreement with the measurements [2]. When the sampling procedures A and B are applied to the calculation of the Reynolds stresses \( (\frac{-\nu'\nu'}{\Delta \eta^2}) \) the results are completely different as shown in the figures 7.11 and 7.12. The experimental results of Oster & Wygnanski [2] show that \( (\frac{-\nu'\nu'}{\Delta \eta^2}) \) is positive in region I, becomes smaller approaching the region of inhibited pairing to finally reach a negative value. Further downstream \( (\frac{-\nu'\nu'}{\Delta \eta^2}) \) increases attaining its maximum in the region of the second vortex pairing. This trend is found in the present calculation only when procedure B is applied (Fig. 7.12).

7.2 Natural mixing layer

7.2.1 Vorticity field

As pointed out in the previous sections the natural mixing layer is characterized by the random birth of vortical structures in time and space. This behaviour is well evidenced by the plots of the instantaneous spanwise vorticity \( (\omega_z) \) at different time levels (see Figs. 7.13-7.18 for the time levels \( T = 162.5, T = 175, T = 183.75, T = 227.5, T = 245 \) and \( T = 262.5 \)). The first three figures show the formation and the early stage of a vortex pairing. The last three vorticity fields show a vortex pairing and the formation of a single structure (i.e., a single vortex). This structure is generated at \( x \approx 77 \) at time \( T = 227.5 \), advected to \( x \approx 101 \) at time \( T = 245 \) and finally at time \( T = 262.5 \) reaches the position \( x \approx 126 \); during the advection process entrainment of surrounding fluid takes place increasing the original dimension of the structure. In the forced mixing layer the same
process takes place 30 units nearer to the inlet (see Fig. 7.1). Further interaction (vortex pairing) between the structures so generated occurs further downstream and cannot be observed in the present calculation due to the small length of the computational domain. Only the linear instability region and the initial non linear region [1] features can be simulated in the present calculation.

Figures 7.16-7.18 show the vortices born in the region $60 < x < 80$, which have a wavelength $\lambda_{x=74} \approx 20$ three times higher than the wave length $\Lambda_0 = 6.9$ of the most unstable mode (see section 7.1.1). This is consistent with the results of Oster & Wygnanski [2] for the unforced mixing layer (cfr. Fig. 29a of [2]), where downstream displacement between structures was found to be: $2\Lambda$, $2\Lambda$, $3\Lambda$, $4\Lambda$. In the present simulation the tendency of the layer to follow this displacement series is also shown in figure 7.18 (the wavelength is doubled at $x \approx 130$).

### 7.2.2 Integral variables

The momentum and vorticity thickness for the unforced mixing layer are presented in figure 7.19 ($\frac{\partial}{\partial x}$ curve 1, $\delta_\omega$ curve 2). As expected from the experimental investigations [1] and [2] the trend of these quantities is linear with respect to the streamwise coordinate, due to the non periodicity of the vortices generation. The growth rate of $\theta$ ($\frac{d\theta}{dx}$) is 0.008, smaller than the one found for the forced case ($\frac{d\theta}{dx} \approx 0.01$).

For the vorticity thickness the growth rate is $\frac{d\delta_\omega}{dx} = 0.038$, two times smaller than the corresponding one in regions I and III of the forced mixing layer. Oster & Wygnanski [2] also found that the growth rate of $\delta_\omega$ for the forced flow is twice the one for the unforced case.

The transversal coordinate $z_{aver}$ for the natural mixing layer is plotted in figure 7.20 and has the same behaviour as for the forced case (see Fig. 7.4). For the period $87.5 < T < 175$ (curve 2), the unforced layer has a smaller slope than the forced one while in curve 1 (relative to the period $87.5 < T < 262.5$) the maximum value of $z_{aver}$ is three times higher than the maximum value calculated for the forced case. This last result confirms that the flow is characterized by an oscillating behaviour with a period which is higher than the time interval $87.5 < T < 262.5$.

### 7.2.3 Mean streamwise velocity, turbulence intensities and Reynolds stresses

The mean streamwise velocity profiles ($\bar{u} - u_2$) for the natural mixing layer presented in figure 7.21 show the self similarity of the flow. Comparing those profiles with the corresponding ones for the forced case (see Figs. 7.5 and 7.6) the mean streamwise velocity
does not present the undershot typical of the forced mixing layer. On the high speed side the profiles are smoother due to the randomness present in the vortex generation process. The streamwise turbulent intensity $\sqrt{\frac{w'^2}{\Delta u'^2}}$ is plotted in figure 7.22. In the region $67 < x < 98.6$ the profiles are self similar, and the values are in quantitative agreement with the measurements of Oster & Wygnanski (they found a maximum value of 0.18 against 0.19 for the present calculation). In the last two stations lack of self similarity is found and the turbulence level is higher than for the upstream stations. As expected from the data of Oster & Wygnanski [2] the value of streamwise turbulent intensity for the present case lies within the ones calculated for regions $II$ and $III$ of the forced case (see Figs. 7.7 and 7.8).

The $\sqrt{\frac{w'^2}{\Delta u'^2}}$ profiles are shifted of $\Delta \eta \approx +1$ with respect to $\eta = 0$, which could be explained by the fact that $S_{\eta \eta}$ is greater than zero (see the discussion in section 7.1.3); this lack of symmetry affects all the profiles. The higher values found for the last two stations could be due to the need of an averaging period longer than the one chosen.

This last consideration is also confirmed by the transversal turbulence intensity results shown in figure 7.23 where the lack of self similarity is more evident. Moreover, the transversal oscillations of the layer play an important role in the calculation of the transversal turbulent intensity. The value of $\sqrt{\frac{w'^2}{\Delta u'^2}}$ is lower than the one of streamwise turbulence intensity; the maximum value found in the region $67 < x < 98.6$ is 0.16 against the 0.153 given by Oster & Wygnanski [2]. This value is also lower than the value calculated for the forced mixing layer (see Figs. 7.9 and 7.10).

The Reynolds stresses profiles (Fig. 7.24) are self similar in the central part of the layer; as shown by the measurements [2] $-\frac{\tau_{xy}}{\Delta u'^2}$ is always positive. Oster & Wygnanski [2] found a maximum value of 0.013, against 0.015 for the present calculation.

7.2.4 Three dimensional natural mixing layer

The results presented in the present subsection aim to show the capability of the code to predict full 3D spatially developing mixing layers. In such a case the flow is characterized by the presence of streamwise vortical structures, having detected the presence of counter rotating vortices.

Due to the limited computer resources available, the 3D simulation carried out in the present work has been performed using a "short" domain of $L_x = 40$ along $x$ direction to have an acceptable spanwise resolution. This 3D calculation cannot be complete because of a longer domain would be needed to capture the development and the mutual interaction between spanwise and streamwise vortices. However, even if the structures cannot fully develop inside the computational domain some features of the vortical streamwise dynamics have been reproduced.
In figures 7.25 and 7.26 the spanwise negative and positive vorticity ($\omega_z$) fields for time level $T = 55$ are presented at the plane $x = 25$ which lies in the linear instability region of the natural mixing layer. Two main counter-rotating vortices can be seen centered in points $P(y,z) \equiv (4,17.5)$ and $P(y,z) \equiv (6,17.5)$. The symmetry of the structures is related to the imposition of cyclic boundary conditions. These vortices are generated by the growth of the most unstable waves in their complex 3D interaction. The presence of rotational fluid around the main couple of vortices is due to the interaction of the most stable waves, which are not yet damped in this region of the flow.
Fig. 7.1 - Instantaneous spanwise vorticity ($\omega_y$) at time level $T = 262.5$. Forced mixing layer

Fig. 7.2 - Instantaneous spanwise vorticity ($\omega_y$) at time level $T = 269.5$. Forced mixing layer
Fig. 7.3 - Momentum thickness (curve 1) and vorticity thickness (curve 2) for the forced mixing layer calculated from the mean streamwise velocity over the period $87.5 < T < 262.5$ with procedure A.

Fig. 7.4 - $z_{aver}$ for the forced mixing layer calculated from the mean streamwise velocity over the periods $87.5 < T < 262.5$ (curve 1) and $87.5 < T < 175$ (curve 2).
Fig. 7.5 - Mean streamwise velocity for the forced mixing layer calculated with procedure A over the period $87.5 < T < 262.5$

Fig. 7.6 - Mean streamwise velocity for the forced mixing layer calculated with procedure B over the period $175 < T < 262.5$
Fig. 7.7 - Streamwise turbulence intensity for the forced mixing layer calculated with procedure A over the period $87.5 < T < 262.5$.

Fig. 7.8 - Streamwise turbulence intensity for the forced mixing layer calculated with procedure B over the period $175 < T < 262.5$. 

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Fig. 7.9 - Transversal turbulence intensity for the forced mixing layer calculated with procedure A over the period $87.5 < T < 262.5$

Fig. 7.10 - Transversal turbulence intensity for the forced mixing layer calculated with procedure B over the period $175 < T < 262.5$
Fig. 7.11 - Reynolds stress for the forced mixing layer calculated with procedure A over the period $87.5 < T < 262.5$

Fig. 7.12 - Reynolds stress for the forced mixing layer calculated with procedure B over the period $175 < T < 262.5$
Fig. 7.13 - Instantaneous spanwise vorticity ($\omega_y$) at time level $T = 162.5$. Natural mixing layer

Fig. 7.14 - Instantaneous spanwise vorticity ($\omega_y$) at time level $T = 175$. Natural mixing layer
Fig. 7.15 - Instantaneous spanwise vorticity ($\omega_y$) at time level $T = 183.75$. Natural mixing layer

Fig. 7.16 - Instantaneous spanwise vorticity ($\omega_y$) at time level $T = 227.5$. Natural mixing layer
Fig. 7.17 - Instantaneous spanwise vorticity ($\omega_y$) at time level $T = 245$. Natural mixing layer

Fig. 7.18 - Instantaneous spanwise vorticity ($\omega_y$) at time level $T = 262.5$. Natural mixing layer
Fig. 7.19 - Momentum thickness (curve 1) and vorticity thickness (curve 2) for the natural mixing layer calculated from the mean streamwise velocity over the period $87.5 < T < 262.5$ with procedure A.

Fig. 7.20 - $z_{aver}$ for the natural mixing layer calculated from the mean streamwise velocity over the periods $87.5 < T < 262.5$ (curve 1) and $87.5 < T < 175$ (curve 2)
Fig. 7.21 - Mean streamwise velocity for the natural mixing layer calculated with procedure A over the period $87.5 < T < 262.5$

Fig. 7.22 - Streamwise turbulence intensity for the natural mixing layer calculated with procedure A over the period $87.5 < T < 262.5$
Fig. 7.23 - Transversal turbulence intensity for the natural mixing layer calculated with procedure A over the period $87.5 < T < 262.5$

Fig. 7.24 - Reynolds stress for the natural mixing layer calculated with procedure A over the period $87.5 < T < 262.5$
Fig. 7.25 - Negative streamwise vorticity ($\omega_x$) for the natural mixing layer at $x = 25$, time level $T = 55$

Fig. 7.26 - Positive streamwise vorticity ($\omega_x$) for the natural mixing layer at $x = 25$, time level $T = 55$
8. CONCLUSIONS

The present work has dealt with the simulation of spatially developing natural and forced mixing layers using the Large Eddy Simulation technique and a finite difference discretization implemented over a finite computational domain.

From the point of view of numerical techniques two main conclusions can be drawn:

- Both 2nd order centered and 3rd order upwind (QUICKEST) finite differences have been found inadequate to the task of reproducing correctly all the features of the flow. Satisfactory results have been obtained using a 4th order upwind biased formulation in the direction of spatial development and 4th order centered schemes in the other two.

- It is possible to reproduce correctly the physical behaviour of the mixing layer using a finite computational domain by a proper choice of boundary conditions. In particular, use of a "wave equation" at the outflow boundary, together with the continuity equation on the freestream boundaries makes it possible for the large scale structures generated into the flow to exit the computational field without being perturbed.

Due to limitations in available computer power, most of the effort has been confined to 2D simulations. Perturbations of the inlet velocity profile have been used to initiate the development of turbulence; time dependent periodic perturbations have been superimposed to the inlet mean velocity profile in order to simulate the forced mixing layer, while white-noise random perturbations have been used for the calculation of the natural mixing layer.

In the forced mixing layer simulation two vortex pairing processes take place inside the computational domain while for the natural one the length of the domain was not enough to capture the second vortex pairing. Analysis of the momentum and vorticity thickness shows that the natural layer exhibits a smaller growth rate than the forced flow one.

The mean field and turbulence statistics are in agreement with the results of both Direct Numerical Simulation [7] and measurements [2]. For the forced case the profiles are not self-similar due to the presence of the forcing imposed on the inlet profile. In the natural case the profiles are self-similar with the exception of the transversal rms velocity fluctuation which is affected by the presence of large scale low frequency oscillations of the layer. Two sampling procedures have been employed, and the results show that the statistics are strongly affected by the different techniques used.

Finally a full 3D simulation of the natural mixing layer has been carried out. The vorticity fields show the early stage development of the streamwise vortical structures.
References


APPENDIX

A discussion concerning the suitability of different discretization schemes for the advective terms of the governing equations (7), (12), (13) has been carried out in section 5. As an example results obtained making use of the centered conservative scheme and the upwind QUICKEST method are shown in this appendix. The main conclusion is that with the centered scheme the appearance of aliasing errors cannot be avoided while with the upwind one the damping introduced by the numerical formulation generates a highly smoothed solution and the physical features of the simulated flow are not reproduced correctly.

The results presented refer to a forced mixing layer with a computational domain characterized by the following dimensions: $L_x = 75$, $L_y = 1.8$ and $L_z = 40$ with $N_x = 100$, $N_y = 6$ and $N_z = 40$ grid points, the mesh was stretched along $z$-dir.

When the centered scheme is applied the presence of high frequency errors is clearly visible in figure A.1. The spanwise vorticity $(\omega_y)$ contours at time level $T = 50$ show that the large vortical structures develop correctly inside the domain and remain coherent during the advection process. Approaching the boundary the appearance of the spatial instability generates small narrower structures.

Figure A.2 shows the spanwise vorticity contours for the same flow when the QUICKEST scheme is used. For this case the solution is free of oscillations which puts in evidence the effect of the filtering action exercised by the scheme. The presence of numerical viscosity tends to smooth the solution, damping the growth of the most amplified wave. The result of figure A.2 corresponds to a computation carried out with a $C_s$ coefficient of 0.04. No changes were found in the vorticity field varying the value of $C_s$. This shows that the contribution of the modeled part of the flow (subgrid motion) is sensibly smaller than the filtering effect of the scheme.
Fig. A.1 - Instantaneous spanwise vorticity ($\omega_y$) at time level $T = 262.5$. Forced mixing layer Calculation with conservative centered scheme

Fig. A.2 - Instantaneous spanwise vorticity ($\omega_y$) at time level $T = 262.5$. Forced mixing layer Calculation with QUICKEST scheme