8.0 Large Eddy Simulation

Theoretically, the Navier-Stokes equations can be used to simulate turbulent flows. The computational grid used in such a simulation would have to be fine enough to allow the smallest turbulent length scales to be realized and the computational time step would have to be small enough to simulate the highest frequencies of the turbulent spectrum. In practice, such computations are prohibitively expensive for high Reynolds numbers. The Reynolds averaged Navier-Stokes (RANS) equations were derived assuming that all of the unsteadiness due to the turbulent nature of the flow could be modeled with empirically derived correlations. This reduces the time and length scales that must be simulated, but also limits the applicability of the simulation for unsteady flows. Large eddy simulations (LES) were developed to extend the simulation of unsteady flows beyond DNS. The desired result of an LES computation is to obtain a DNS equivalent solution for the large-scale turbulence on a much coarser grid than is required for DNS. An LES simulation requires:

1. A grid fine enough to discretize the small nearly isotropic scales of the turbulence
2. A low dissipation numerical scheme
3. A filter function to determine the division of the turbulent spectrum into grid realized and subgrid regions
4. A subgrid turbulence model

A true LES simulation is more than a high Reynolds number computation run without a turbulence model. Although the resulting solution from such a simulation may resemble turbulent flow, the resulting solution will most likely not represent an equivalent DNS solution.

8.1 The Filtering Operation

The filtering operation is critical to LES. Consider a filtering operation with a uniform characteristic filter width $\Delta$ (which implies isotropic grid elements). Leonard defined the following filter in physical space

$$\bar{\phi}(x) = \int_{-\infty}^{\infty} G(x - \xi)\phi(\xi)d\xi$$

(8.1)

Note that in this chapter the over bar represents a filtered quantity, not a time averaged quantity as in the previous chapters. The filtering operation is a spatial operation as opposed to the Reynolds averaging operation discussed in Chapter 2 that is a temporal operation. The original function $\phi$ is then decomposed into a filtered field (or grid resolved) and a “subgrid” term

$$\phi = \bar{\phi} + \phi'$$

(8.2)
The function $G$ defined in Eq. 8.1 is the “filter function”. The filter function may be any function defined on an infinite domain that satisfies the following requirements (Ref. 1):

1. $G(-\xi) = G(\xi)$

2. $\int_{-\infty}^{\infty} G(\xi) d\xi = 1$

3. $G(\xi) \to 0$ as $|\xi| \to 0$ such that all moments $\int_{-\infty}^{\infty} G(\xi)\xi^n d\xi$ ($n \geq 0$) exist

4. $G(\xi)$ is “small” outside $\left(-\frac{\Delta}{2}, \frac{\Delta}{2}\right)$

One important and useful feature of this choice of filter is

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial x}$$

(8.3)

Three common filters are

Spectral cutoff filter: $G(\xi) = \frac{\sin\left(\frac{\pi\xi}{\Delta}\right)}{\frac{\pi\xi}{\Delta}}$ (8.4)

Gaussian filter: $G(\xi) = \frac{1}{\Delta\sqrt{\pi}} \exp\left(\frac{C\xi^2}{\Delta^2}\right)$ (8.5)

Box filter: $G(\xi) = \begin{cases} \frac{1}{\Delta} & \text{if } |\xi| < \frac{\Delta}{2} \\ 0 & \text{otherwise} \end{cases}$ (8.6)

The spectral cutoff filter is normally applied in spectral space as

$$\hat{\phi}(k) = \hat{G}(k)\hat{\phi}(k)$$

(8.8)
The constant $C$ in the Gaussian filter (Eq. 8.5) is somewhat arbitrary, and values from 2 to 6 have been used in practice. Note that the box filter (Eq. 8.6) is valid on both finite and infinite domains. For this reason box filters are often used to relate DNS to LES for physical space numerical schemes.

There are advantages to using spectral and pseudo-spectral solution methodologies for LES. The first advantage is that the approximate field, which is discrete in spectral space, is a finite sum of continuous functions in physical space. Thus the approximate field, the spectral filter, and their derivatives are continuous functions in physical space. The spectral filters defined in Eqs. 8.8 and 8.9 have the following additional useful properties

\[
\phi = \phi \\
\phi' = 0
\]  

(8.10)

(8.11)

This says that filtering a grid resolved quantity yields the original grid resolved quantity and that the spectral filter of a subgrid quantity is equal to zero.

Another advantage of the spectral approach is that derivatives yield an exact value for the approximate field. In other words, if one is approximating a function using $N$ Fourier modes, then as long as one has at least $2(N+1)$ points in physical space, it does not matter if one has 20 or 20 million points: the value of the derivative at any given point is the same. Therefore one can take a flow field generated with a spectral DNS code, filter and coarsen the solution, and produce a flow field which satisfies the governing equations for LES.

There are drawbacks to spectral filters. First, they have limited applicability in realistic flow situations because of boundary constraints. Also, spectral filters are non-positive (i.e. the filter function is negative at some points in space). The latter condition results in a subgrid stress tensor that does not satisfy the Reynolds stress realizability conditions outlined in Chapter 2.

Both Gaussian filters (Eq. 8.5) and box filters (Eq. 8.6) are positive functions, and thus the Reynolds stress realizability conditions outlined in Chapter 2 will be satisfied on the resulting subgrid stress tensor. Unfortunately Eq. 8.10 and Eq. 8.11 are not valid for these filters. Furthermore, if a spatial numerical solver is to be used the filter must also be discretized. Therefore it is necessary to examine the discretized system that is solved in the actual code because discrete systems
sometimes have different properties than the original continuous systems from which they were derived.

### 8.2 Derivation of the LES Equations

The Favre averaged or filtered Navier-Stokes equations were derived in Chapter 2. The Favre filter can be defined for any variable as

\[
\tilde{\phi} = \frac{\rho \phi}{\bar{\rho}}
\]  

(8.12)

Note that the over bar signifies a spatially filtered quantity, and the tilde represents a Favre filtered, or grid resolved, quantity. Thus the Favre filter may be thought of as a density weighted filter in space. Applying this filtering operation to the Navier-Stokes equations, and assuming that the filtering commutes with the derivative operation, the LES equations are

\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_i}{\partial x_i} = 0
\]  

(8.13)

\[
\frac{\partial \bar{\rho} \bar{u}_i}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_j \bar{u}_j}{\partial x_j} = -\frac{\partial \bar{\rho}}{\partial x_i} + \frac{\partial \bar{\tau}_{ij}}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \bar{\tau}_{ij} - \bar{\tau}_{ij} \right) - \frac{\partial}{\partial x_j} \bar{\rho} \left( \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j \right)
\]  

(8.14)

\[
\frac{\partial \bar{\rho} \bar{E}}{\partial t} + \frac{\partial}{\partial x_i} \left( \bar{\rho} \bar{E} + \bar{p} \right) \bar{u}_i = -\frac{\partial \bar{\rho}}{\partial x_i} \left( \bar{E} \bar{u}_i - \bar{E} \bar{u}_i \right) - \frac{\partial}{\partial x_i} \left( \bar{p} \bar{u}_i - \bar{p} \bar{u}_i \right) + \frac{\partial \bar{u}_j \bar{T}_{ij}}{\partial x_i} + \frac{\partial}{\partial x_i} \left( \bar{k} \frac{\partial \bar{T}}{\partial x_i} - \bar{k} \frac{\partial \bar{T}}{\partial x_i} \right)
\]  

(8.15)

The resolved viscous stress tensor in Eqn. 8.14 takes the form

\[
\bar{\tau}_{ij} = 2 \bar{\mu} \left[ \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial \bar{u}_k}{\partial x_k} \delta_{ij} \right]
\]  

(8.16)

The viscosity and thermal conductivity is assumed to be calculated from the Favre averaged temperature (\(\bar{T}\)). The total energy (\(\bar{E}\)) is defined as

\[
\bar{E} = \bar{e} + \frac{1}{2} \bar{u}_i \bar{u}_j + k_{sgs}
\]  

(8.17)

The subgrid kinetic energy, \(k_{sgs}\), is defined as the effect of the subgrid scales on the kinetic energy of the resolved field.
Finally, the LES equation of state is

$$\overline{\rho} = \overline{\rho} R T$$  \hspace{1cm} (8.19)

As with Reynolds averaging, the filtering operation produces terms that must be modeled in order to close the equation set. The LES momentum equation, Eqn. 8.14, contains two such terms. The first, $$\frac{\partial}{\partial x_j} (\overline{r}_{ij} - \overline{\tau}_{ij})$$, represents the difference in the viscous terms between Favre and “straight” filtering. The second term, $$\frac{\partial}{\partial x_j} (u_{ij} \overline{u}_j - \overline{u}_i \overline{u}_j)$$, arises from the convection terms and has been observed to behave much like a viscous stress. Thus it is frequently redefined in terms of the “subgrid stress tensor” $$\tau_{ij}^{sgs}$$ defined as

$$\tau_{ij}^{sgs} = \overline{\rho} \left( \overline{u}_i \overline{u}_j - \overline{u}_i \overline{u}_j \right)$$  \hspace{1cm} (8.20)

The LES energy equation, Eq. 8.15, contains four subgrid terms. The first term, $$\frac{\partial}{\partial x_i} (\overline{Eu}_i - \overline{E\overline{u}}_i)$$, arises from the convection term. The second term is a pressure-velocity correlation term, $$\frac{\partial}{\partial x_i} (pu_i - \overline{p\overline{u}}_i)$$, which is also related to the convection term. The third term, $$\frac{\partial}{\partial x_i} (u_j \overline{r}_{ij} - \overline{u}_j \overline{r}_{ij})$$, is a viscous subgrid term similar to the term in the LES momentum equation. This term represents the transfer of energy due to subgrid viscous forces. The fourth term, $$\frac{\partial}{\partial x_i} \left( \kappa \frac{\partial T}{\partial x_i} - \frac{\partial \overline{T}}{\partial x_i} \right)$$, is a heat flux subgrid term. The subgrid kinetic energy, $$k^{sgs}$$, used in the definition of the Favre filtered total energy in Eq. 8.7 must also be defined for closure.

The subgrid stress tensor, $$\tau_{ij}^{sgs}$$, is usually treated in a similar manner as the Boussinesq approximation for the RANS equations (Chapter 2)
\[ \tau_{ij}^{sgs} = -2\bar{p}v_i \left( \tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{kk} \delta_{ij} \right) + \frac{2}{3} \bar{p} k^{sgs} \delta_{ij} \] (8.21)

In the above equation, \( \tilde{S}_{ij} \) represents the resolved rate of strain tensor

\[ \tilde{S}_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \] (8.22)

Note that a subgrid eddy viscosity, \( \nu_t \), has been introduced in Eq. 8.21. The subgrid eddy viscosity accounts for the turbulence that cannot be resolved on the computational grid.

Introducing the subgrid stress tensor into Eq. 8.14 and assuming that the straight filtered stress tensor is equal to the Favre filtered stress tensor \( (\tilde{T}_{ij} = \tilde{T}_{ij}) \) the LES momentum equation becomes

\[
\frac{\partial \bar{p} \tilde{u}_i}{\partial t} + \frac{\partial \bar{p} \tilde{u}_i \tilde{u}_j}{\partial x_j} = \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \tilde{T}_{ij}}{\partial x_j} = \frac{\partial \tau_{ij}^{sgs}}{\partial x_j}
\] (8.23)

The LES energy equation (Eq. 8.15) can be further simplified as follows. Using the definition of total enthalpy

\[ H = E + \frac{p}{\rho} \] (8.24)

two of the subgrid terms can be combined to form

\[ -\frac{\partial}{\partial x_i} \left( \bar{p} E_{u_i} - \bar{p} \tilde{E}_{u_i} \right) = \frac{\partial}{\partial x_i} \left( \bar{p} u_i \right) = \frac{\partial}{\partial x_i} \left( \bar{p} \tilde{H}_{u_i} - \bar{p} \tilde{H}_{u_i} \right) \] (8.25)

This term can then be modeled with an eddy diffusion model as

\[ \frac{\partial}{\partial x_i} \left( \bar{p} \tilde{H}_{u_i} - \bar{p} \tilde{H}_{u_i} \right) \approx \frac{\partial}{\partial x_i} \left( -c_e \bar{p} \sqrt{k^{sgs}} \Delta \frac{\partial \tilde{H}}{\partial x_i} \right) \] (8.26)

where \( \Delta \) is the local grid spacing and \( c_e \) is an empirical coefficient. The thermal conductivity term, \( \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} - \tilde{k} \frac{\partial \tilde{T}}{\partial x_i} \right) \), is neglected based on the assumption that the thermal conductivity is locally constant and that the Favre filtering is equivalent to the straight filtering. The viscous transport term is modeled as
\[
\frac{\partial}{\partial x_i} \left( u_i \tau_{ij} - \tilde{u}_i \tilde{\tau}_{ij} \right) \approx \frac{\partial}{\partial x_i} \left( \bar{\mu} \frac{\partial k_{sgs}}{\partial x_i} \right)
\]  

(8.27)

This term is generally small and is often neglected in practice.

Thus the modeled LES energy equation may now be written as

\[
\frac{\partial \bar{p} E}{\partial t} + \frac{\partial}{\partial x_i} \left( \bar{\rho} \bar{E} + \bar{p} \right) u_i = \frac{\partial}{\partial x_i} \left( c_e \bar{\rho} \sqrt{k_{sgs}} \Delta \frac{\partial \bar{H}}{\partial x_i} \right) + \frac{\partial \tilde{u}_i \tilde{\tau}_{ij}}{\partial x_i} + \frac{\partial}{\partial x_i} \left( \tilde{k} \frac{\partial \bar{T}}{\partial x_i} \right)
\]  

(8.28)

Inspection of the modeled LES equations (Eqs. 8.13, 8.23, and 8.28) shows that these equations are quite similar to the RANS equations incorporating the Boussinesq approximation derived in Chapter 2. It should be noted that the time averaging process used to derive the RANS equations and the spatial filtering operations used to derive the LES equations are quite different, and hence the terms in the two equation sets are not the same.

Three things are required to close the modeled LES equations:

1. The subgrid turbulent kinetic energy \( k_{sgs} \)
2. The subgrid eddy viscosity \( \nu_t \)
3. The empirical coefficient in the energy equation, \( c_e \)

### 8.3 Smagorinsky Model

As with the RANS equations, there are numerous models for the LES eddy viscosity. One of the earliest models for the LES eddy viscosity was proposed by Smagorinski\(^2\) and is given by

\[
\nu_t = \left( C_s \Delta_g \right)^2 \left( 2 \tilde{S}_{ij} \tilde{S}_{ij} \right)^{1/2}
\]  

(8.29)

where \( C_s \) is the Smagorinsky coefficient and \( \Delta_g \) is the local grid spacing. This model ignores the subgrid kinetic energy \( k_{sgs} \). The Smagorinsky model provides a simple closure for the LES equations and has been used effectively for a number of applications. But, like its algebraic counterpart in the RANS regime, it has been shown to be lacking in simulating complex turbulent flows. The Smagorinsky model is not valid near walls, and a wall damping term (Ref. 3) is often added to the model. The wall-damped form is given by
\[ \nu_t = (C_s \Delta \left( 1 - e^{-x^2/25} \right)^2 \left( 2 \overline{S}_y \overline{S}_y \right)^{1/2} \]  \tag{8.30}

The coefficient \( C_s \) must be defined for this model. In practice no universal value of \( C_s \) exist.

### 8.4 Dynamic Smagorinsky Model

Several investigators have attempted to dynamically calculate \( C_s \) based on equating the highest wave number resolved turbulent stresses with the subgrid stress. One dynamic LES closure model outlined in Ref. 4 can be described as follows. The subgrid stress tensor is written as

\[ \tau_{ij}^{gs} = -C(x,t)\Delta^2 |S(\tilde{u})| S_{ij}(\tilde{u}) \]  \tag{8.31}

where \( C(x,t) \) is the Smagorinsky coefficient to be determined dynamically and \( \Delta \) is the grid spacing. For this purpose a second spatial filter, called the test-filter, of width larger than the grid filter is introduced. We choose the test-filter scale \( \overline{\Delta} = 2\Delta \). This filter generates a second set of resolvable-scale fields (denoted by \( \overline{\cdot} \)). Then, the dynamic SGS model of the \( \tau_{ij} \) at the grid filter and of the \( T_{ij} \) at the test-filter are written as:

\[
\begin{align*}
\tau_{ij} - \frac{\delta_{ij}}{3} \tau_{kk} &= -2C\overline{\Delta}^2 \overline{|S_{ij}|} \\
&= -2C\beta_{ij} \\
T_{ij} - \frac{\delta_{ij}}{3} T_{kk} &= -2C\overline{\Delta}^2 \overline{|S_{ij}|} \\
&= -2C\alpha_{ij}
\end{align*}
\]  \tag{8.32}

A least squares method is developed to predict \( C(x,t) \) as:

\[ C(x,t) = -\frac{1}{2} \frac{\ell_{ij} \left( \alpha_{ij} - \beta_{ij} \right)}{\alpha_{mn} - \beta_{mn} (\alpha_{mn} - \beta_{mn})} \]  \tag{8.33}

with \( \ell_{ij} = \ell_{ij} - (\delta_{ij} / 3) \ell_{kk} = -2C\alpha_{ij} + 2C\beta_{ij} \).

### 8.5 k-Equation Model

Another approach to closing the LES equations is to introduce a transport equation for the subgrid kinetic energy, \( k^{gs} \). The exact subgrid kinetic energy equation may be written
\[
\frac{\partial \rho k^{\text{sgs}}}{\partial t} + \frac{\partial}{\partial x_i} \left( \rho \frac{\partial k^{\text{sgs}}}{\partial x_i} \tilde{u}_i \right) = -\left( u_i \frac{\partial p}{\partial x_i} - \tilde{u}_i \frac{\partial p}{\partial x_i} \right) + \left( u_i \frac{\partial \tau_{ij}}{\partial x_i} - \tilde{u}_i \frac{\partial \tau_{ij}}{\partial x_i} \right) - 
\]

\[
\frac{\partial}{\partial x_i} \left( \rho k^{\text{sgs}} \tilde{u}_i \right) - \frac{\partial \tilde{u}_j \tau_{ij}^{\text{sgs}}}{\partial x_i} + \tau_{ij}^{\text{sgs}} \frac{\partial \tilde{u}_j}{\partial x_i} 
\]

(8.34)

This equation contains several subgrid terms. The equation is modeled in a similar manner as the RANS turbulent kinetic energy equation. The modeled equation is

\[
\frac{\partial \rho k^{\text{sgs}}}{\partial t} + \frac{\partial}{\partial x_i} \left( \rho k^{\text{sgs}} \tilde{u}_i \right) = \frac{\partial}{\partial x_i} \left( \rho \nu_t \frac{\partial k^{\text{sgs}}}{\partial x_i} \right) - \tau_{ij}^{\text{sgs}} \frac{\partial \tilde{u}_j}{\partial x_i} - \rho c_e \frac{k^{\text{sgs}}}{\Delta} \]

(8.35)

where the terms on the right-hand-side are the diffusion, production, and dissipation of the subgrid kinetic energy respectively. An algebraic expression for the dissipation is generally used instead of a transport equation as in two-equation RANS turbulence models. The turbulent viscosity is given by

\[
\nu_t = c_e \sqrt{k^{\text{sgs}}} \Delta 
\]

(8.36)

The LES energy equation dissipation coefficient \(c_e\) and the eddy viscosity coefficient \(\nu_t\) are determined dynamically by equating the highest wave number resolved turbulent properties with the subgrid properties. The dynamic process for determining these coefficients is described in detail in Ref. 5.

### 8.6 Inflow Turbulence Boundary Condition

Flows that include a developing boundary layer at the inflow plane of a simulation require a boundary condition that includes the specification of the inflow velocity fluctuations. Soteriou and Ghoniem\(^6\) show the development of an incompressible mixing layer with and without perturbation at the inflow plane. Compared to the perturbed case, the development of the mixing layer without perturbation is delayed significantly. This is because disturbances within the boundary layer are amplified and lead to the Kelvin-Helmholtz instability that eventually causes the shear layer to roll up. If these disturbances are not present in the boundary layer, then the shear layer will develop more slowly until disturbances are generated through minute numerical errors.

Several approaches have been taken to add the perturbations to the inflow. The simplest approach is to add “white noise” to the velocity at the inflow plane as was done by Comte et al\(^7\). This approach is somewhat unphysical in that the perturbations have no correlation in space or time. A second approach is to add perturbations at discreet frequencies as was done by Soteriou and Ghoniem\(^6\). This can be effective for studying forced flows, but it must be remembered that turbulence is broadband and does not confine itself to discrete frequencies. A
third approach to this problem is to attempt to reconstruct the unsteady flow at the inflow using correlations for the perturbations. One example of this can be found in Ref. 5, in which a box of frozen turbulence is generated and saved. This box is scaled and applied as perturbations at the inflow of the simulation.

8.6 Other LES References

LES methods are still evolving as researches investigate methods for simulating the near-wall flow physics and methods to improve the performance of the subgrid models used in LES simulations. Fureby, et al\(^8\), provide a good summary of the LES methods currently being employed and investigated. Ref. 9 includes a wide range of experimental test cases for validation of LES simulations.

8.7 Spatial Mixing-Layer Example

The mixing layer experiment of Samimy and Elliot\(^6\) can be used to demonstrate the behavior of LES models. The data is also included in Ref. 10. The experimental setup had an upper supersonic stream and a lower subsonic stream mixing at a matched static pressure. Laser Doppler Velocimeter (LDV) measurements were made at several downstream locations between the trailing edge of the splitter plate and a station 210 mm downstream of the splitter plate. The flow parameters are given in Table 8.1.

<table>
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<th>(T_0, K)</th>
<th>(P_{01}, \text{kPa})</th>
<th>(M_1)</th>
<th>(M_2)</th>
<th>(M_c)</th>
<th>(U_1, \text{m/sec})</th>
<th>(U_2/U_1)</th>
<th>(\rho_2/\rho_1)</th>
<th>(\delta_1, \text{mm})</th>
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<td>479.5</td>
<td>0.355</td>
<td>0.638</td>
<td>8.0</td>
</tr>
</tbody>
</table>

Table 8.1 Flow parameters for the spatial mixing-layer case

The solutions were run for 30,000 time steps to wash out initial transients and then statistics were taken over the next 60,000 time steps. The time step used was \(5.0 \times 10^{-8}\) seconds. The flow solver used for these calculations was 4th order in space and 2nd order in time. The computational grid dimensions were 181 x 121 x 61. The inflow plane perturbations were specified using the “box of turbulence” approach from Ref. 5. Further details of the experiment and the computations can be found in Ref. 10.

All of the turbulence models investigated predict roughly the same mixing-layer thickness for this case as shown in Fig 8.1. The Hybrid \(k-\varepsilon\) model in Fig. 8.1 is the multi-scale hybrid RANS/LES turbulence model described in Chapter 9. The DES model is the Spalart-Allmaras DES hybrid model that is also described in Chapter 9. The traditional RANS models (\(k-\varepsilon\) and Spalart-Allmaras) have the worst agreement with the experimental data.
Figure 8.1  Mixing-layer thickness

The streamwise velocity 210 mm downstream of the splitter plate is shown in Fig. 8.2. Again all of the models are in reasonable agreement with the experimental data.

Figure 8.2  Nondimensional streamwise velocity at x=210 mm
The streamwise turbulence intensity, Reynolds stress, streamwise velocity fluctuation skewness, and streamwise velocity fluctuation flatness at $x=210$ mm are shown in Fig. 8.3-8.6. The performance of the traditional RANS models is seen to deteriorate as the order of the turbulent velocity fluctuation correlation increases. The LES and hybrid RANS/LES models are all in reasonable agreement with the experimental data.

Figure 8.3  Streamwise turbulence intensity at $x=210$ mm

Figure 8.4  Reynolds stress profiles at $x=210$ mm
Chapter 8 References:


