

Large Eddy Simulation (LES) for Steady-State Turbulent Flow Prediction

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Abstract The aim of this work is to simulate a steady turbulent flow using the Large Eddy Simulation (LES) technique in computational fluid dynamics (CFD). The simulation was done using an in-house code developed in the programming platform of Visual C++. The Finite Volume Method was used to compute numerically the solutions of the Navier-Stokes equation under turbulent conditions. The Quadratic Upstream Interpolation for Convective Kinetics (QUICK) numerical scheme was utilized with the Semi-Implicit Pressure Linked Equations (SIMPLE) as an algorithm. The code consists of a steady three-dimensional turbulent solver using the Large Eddy Simulation (LES) turbulent model. The simulated velocity flow profile was then compared against experimental data.

Keywords Computational fluid dynamics (CFD) • Large eddy simulation (LES) • Finite volume method • Turbulence • Navier-Stokes equations

1 Introduction

Large eddy simulation (LES) has been used in myriad studies to analyse turbulent flows in simple geometries and boundary conditions over the past 25 years [1, 2]. In the recent 5–10 years LES has been applied to predict increasingly complex flows [2]. These research efforts pioneered the idea of using the flow characteristics from the smallest resolved scales to predict the subgrid scale (SGS) stresses. This idea

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then gave rise to the scale similarity model and the mixed model. This way the required information from the smallest resolved scales were obtained mathematically by applying the filter operation twice. Bardina et al. [3] performed this method to rotating turbulent and to homogeneous isotropic flows. The follow-up work from Bardina et al. [3] was carried out by Germano et al. [4] who then proceeded to develop the dynamic subgrid scale model (DM).

Some simulations were done on the analysis of flows through cylindrical geometries using LES. For instance, Chang et al. [5] studied multiphase turbulent flows in pipes and Eggels and Nieuwstadt [6] used the Smagorinsky model to calculate flow properties in an axially rotating pipe. Besides that, the LES and DNS approaches were used to model a temporally evolving round jet at a low Reynolds number by Fatica et al. [7]. In this study, the Reynolds number was 800 (which was based on the radius and the centerline velocity of the jet) where the Smagorinsky model and the DM model were utilized.

In another study, the dynamic subgrid scale model (DM) model was used by Yang and Ferziger [8] to calculate the flow characteristics of a low Reynolds number turbulent flow in a channel with a two-dimensional obstacle mounted on one wall. The results were compared with another calculation performed using the Smagorinsky model with as well as the results from the DNS model. The overall results of the DM model were more consistent with the DNS solution as compared to the results from the Smagorinsky model. These comparisons conclude that the DM model is an improvement over the Smagorinsky model.

Hoffmann and Benocci [9] modelled a jet issuing from a two-dimensional slit onto a flat plate using LES. The DM model was modified to take into account the SGS stresses. The DM model was modified to utilizing test filtered variables (in contrast to the commonly used grid filtered variables) in the equation for the modelled parameter C . In these computations, no comparison against experimental data was carried out. However, the main physical features in the flow were captured.

Some work on the development of the LES method has been carried out in recent times [3, 6–8, 10]. These works were mainly on the modifications and development of the filtering component in the LES model used during the spatial averaging procedure.

The LES modelling method has gone through significant changes and improvements in the 1980s and in the 1990s. This is mainly due to the radical improvement in the advancement of computer systems. Besides that, these changes could also be attributed in the very rapid evolution of the SGS models where the DM model is proving to be quite promising. In a nutshell, there is a continuous and strong effort to advance the LES modelling approach to produce more realistic results for predicting characteristics of turbulent flows especially in engineering applications.

In this work, a solver was developed using the Finite Volume Method. The Quadratic Upstream Interpolation for Convective Kinetics (QUICK) numerical scheme [11] was used with the Semi-Implicit Pressure Linked Equations (SIMPLE) algorithm. The Large Eddy Simulation (LES) static turbulent model developed in

Smagorinsky [12] was used to compute the subgrid scale (SGS) stresses. Many simple experiments have been done in the past to observe turbulent flow phenomenon and to outline its characteristics. In this paper, two three-dimensional steady turbulent flow phenomenon was simulated and compared against the experimental results by Martinuzzi and Tropea [13] and Driver and Seegmiller [14].

This paper is organized as follows: Sect. 2 presents the Mathematical Formulation and Computational Techniques while Sect. 3 provides the solver parameters used in the LES simulation. Section 4 describes the experimental details of the flow application at which the LES simulation was implemented and Sect. 5 consists of the analysis of the results and some comparative studies. Section 6 provides some discussions on the error distribution between the simulation and the experimental results. Finally, this paper ends with some conclusions and recommendations for future work.

2 Mathematical Formulation and Computational Techniques

The mass flow rate across the faces of the fluid element is the product of density, area and the velocity component normal to the face. The summation will be in the form of a differential which will result as the following:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0 \quad (1)$$

where u , v and w are the velocity components in the x , y and z —direction respectively.

The momentum conservation principles are required in order to form a partial differential equation (Navier-Stokes). The solution to this partial differential equation would describe the behavior of the momentum in the flow. The final form of the momentum equation will be as the following:

$$\frac{\partial(\rho u)}{\partial t} + \text{div}(\rho uv) = \text{div}(\Gamma \cdot \text{gradu}) + S_u \quad (2)$$

where the $\partial(\rho u)/\partial t$ is the unsteady term, $\text{div}(\rho uv)$ is the convective term, $\text{div}(\Gamma \cdot \text{gradu})$ is the diffusive term and S_u is the source term. The Γ in the diffusion term is the diffusion coefficient which is a function of the viscosity. The SIMPLE algorithm was employed in this simulation and it is shown in Fig. 1.

The LES model computes the subgrid scale stresses. Large eddies depend and extract energy from the bulk flow, their behavior is more anisotropic than small eddies (which are isotropic at high Reynolds number flows). A model such as the Reynolds Averaged Navier-Stokes (RANS) equations also describe the solution that comprises of the behavior of eddies in a time-averaged fashion. However, the

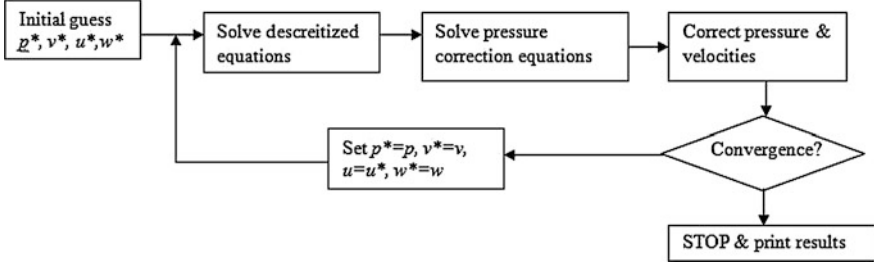


Fig. 1 The SIMPLE algorithm

LES model provides a means to compute a certain range of eddy scales (large eddies) through a statistical filtering procedure (spatial-averaging).

The filtering procedure is done by performing a convolution on the Navier-Stokes equation and the filter function (Gaussian filter, Fourier filter or the Tophat filter) producing the spatial-averaged Navier-Stokes equation.

The convolution averages-off the small eddies (which effects are estimated using semi-empirical models called sub- grid scale (SGS) models) where computation is only done on the large eddies. The LES model gives spatial-filtered Navier-Stokes equations:

$$\frac{\partial(\rho \bar{u}_i)}{\partial t} + \text{div}(\rho \bar{u}_i \bar{u}_j) = -\frac{\partial(\bar{p}_i)}{\partial x_i} + \text{div}(\Gamma \cdot \text{grad} \bar{u}_i) - \frac{\partial \tau_{ij}}{\partial x_j} \quad (3)$$

$$\tau_{ij} = \overline{\rho u_i u_j} + \rho \bar{u}_i \bar{u}_j \quad (4)$$

The terms $\bar{u}_i$ are the filtered velocities, $\bar{p}$ is the filtered pressure, the term τ_{ij} is the stress tensor that results from the statistical procedure (analogous to the Reynolds stresses in the RANS equations).

The LES Reynolds stresses arise due to the convective momentum transport which is a result of the interactions among SGS eddies per se and is modelled with a SGS turbulence model. The SGS turbulence model used in this computer code is the Smagorinsky-Lilly SGS model. In this computation, the Cross stress C_{ij} , Leonard stresses, L_{ij} and Reynold stresses, R_{ij} are implemented together in the finite volume method:

$$L_{ij} = (\rho \bar{u}_i \bar{u}_j - \rho \bar{u}_i \bar{u}_j) \quad (5)$$

$$C_{ij} = (\rho \bar{u}_i u'_j - \rho u'_i \bar{u}_j) \quad (6)$$

$$R_{ij} = \rho u'_i u'_j \quad (7)$$

Thus, resulting in one SGS turbulence model which can be formulated as the following:

$$\tau_{ij} = -2\mu_{SGS}\bar{S}_{ij} + \frac{1}{3}\tau_{ii}\delta_{ij} \quad (8)$$

Where μ_{SGS} is the artificial or the sub-grid scale viscosity which acts as the constant of proportionality and $\bar{S}_{ij}$ is the average strain rate. The size of the SGS eddies are determined by the filter choice as well as the filter cut-off width which is used during the averaging operation. The SGS viscosity can be obtained by the following semi-empirical formulation:

$$\mu_{SGS} = \rho(C_{SGS}\Delta)^2 \left| \sqrt{2\bar{S}_{ij}\bar{S}_{ij}} \right| \quad (9)$$

where Δ is the filter cut-off width and is an CSGS empirical constant which is usually specified in a range, $0.19 < C_{SGS} < 0.24$.

3 Solver Parameters

Prior to execution of the numerical solver, a number of parameters are required to be specified. These parameters are the numerical coefficients that are employed in the numerical scheme and the algorithm. These parameters influence the number of iterations, computational time, stability of computations and the convergence rate. The parameter types and the values that are used in this work can be summarized as in Table 1:

Table 1 Numerical setting for solver parameters

Properties	Experiment 1	Experiment 2
	Parameters	Parameters
Iterations for velocity and pressure	3,496	3,470
Relaxation factor for velocity	0.9	0.9
Relaxation factor for pressure	0.9	0.9
Convergence criterion for pressure correction matrix	1 %	1 %
Mesh size (x, y, z) in (meters)	(0.032, 0.05, 0.04)	(0.02, 0.0034, 0.0051)
C_{SGS} , SGS Constant	0.2	0.2

4 Experimental Descriptions

4.1 Experiment 1: Flow Over a Surface-Mounted Cubicle Obstacle

The experimental data from this experiment which was performed by Martinuzzi and Tropea [13] was compared against the simulation results. The fluid used in this experiment was water (incompressible flow) with the density of $1,000 \text{ kg/m}^3$ and viscosity of 0.001 kg/ms . The experiment was performed in a rectangular channel with a single cubicle obstacle mounted on the surface of the channel (internal flow). The Reynolds number (which is based on the channel height) was 12,000 with the inlet velocity of 0.467 m/s .

The experiment was conducted at atmospheric pressure. The length (x -direction), height (y -direction) and width (z -direction) are respectively $1.6 \times 0.16 \times 1.0 \text{ m}^3$. The obstacle was mounted at 0.8 m from the inlet (x -direction) and 0.46 m in the z -direction. This experiment was performed in a fully developed turbulent channel flow. The cubicle obstacle was placed at 5 times the channel height from the inlet (x -direction) and at the centerline of the width (z -direction). A detailed description of the experimental technique can be found in Dimaczek et al. [15]. A schematic illustration of the setup is shown in Fig. 2:

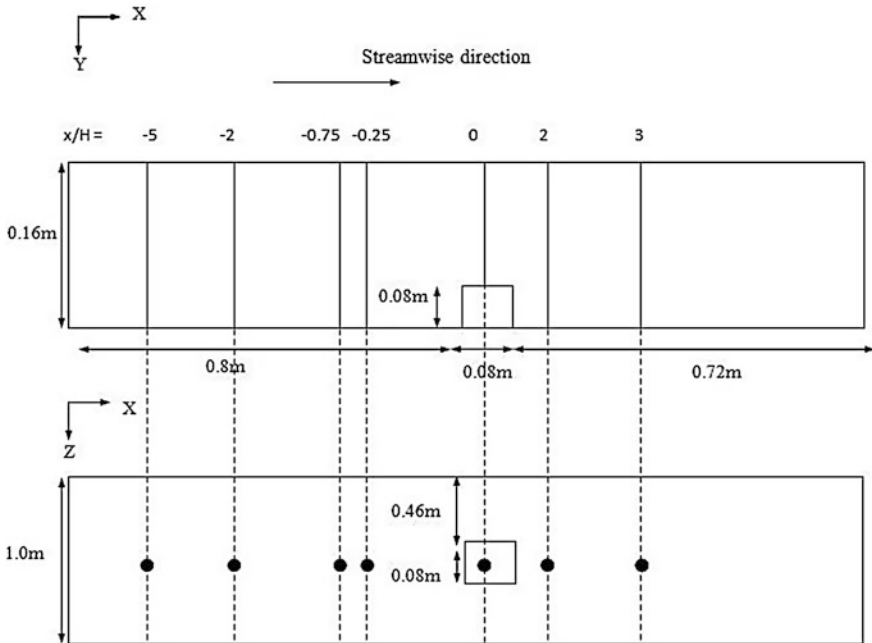


Fig. 2 Schematic representation of the setup in Experiment 1

4.2 Experiment 2: Flow Over a Backward-Facing Step with Opposite Wall

The experimental results from this experiment which was performed by Driver and Seegmiller [14] are used for the second validation of the LES solver. The fluid used in this experiment was air (incompressible at the Mach number of 0.128) with the density of 1.0 kg/m^3 and viscosity of $1.02 \times 10^{-5} \text{ kg/ms}$ at ambient temperature. This experiment was performed in a rectangular channel with a backward-facing step that diverges the channel. The Reynolds number based on momentum thickness with the boundary layer thickness of 0.019 m was 5,000 with the inlet velocity of 44.2 m/s . Hence, the fluid at the inlet is incompressible and undergoes fully turbulent flow. The experiment was conducted at atmospheric pressure. The length (x -direction), height (y -direction) and width (z -direction) are respectively $1.0 \times 0.101 \times 0.152 \text{ m}^3$. The backward step begins at 0.06 m from the inlet (in the x -direction). A schematic illustration of the setup is shown in Fig. 3:

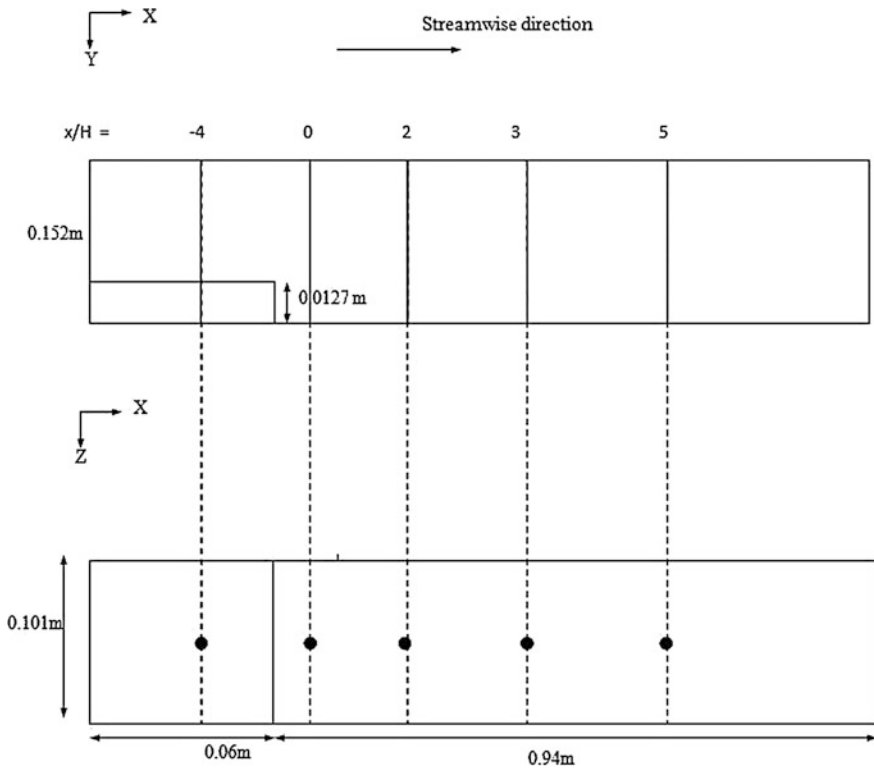


Fig. 3 Schematic representation of the setup in Experiment 2

5 Results Analysis

5.1 Experiment 1: Flow Over a Surface-Mounted Cubicle Obstacle

The velocity distributions obtained by the solver is compared with that obtained from the experiment. For the purpose of comparison, the most significant velocity gradients that influence the flow behaviour are taken. To identify the significant velocity gradients, a scaling argument was used. From the analysis, the velocity gradients, was identified as the most significant term for the given dimensions of the setup and the flow conditions. Thus, the u -velocities (streamwise velocities) are taken with respect to the y -axis at different points in the x -direction.

The velocity distributions in the experimental results are normalized to the inlet velocity that is U/U_0 . Similarly the distances in the experimental results are also normalized to the height of the obstacle which is respectively x/H , y/H , and z/H .

Seven sets of experimental results of the u -velocity distributions are obtained throughout the test section. Four sets of velocity distributions are used in the comparison at the region before the obstacle, one set right above the obstacle and two sets at the flow after the obstacle (the dissipation region). The normalized distances in the x , y and z -direction (x/H , y/H , and z/H) is at $(0, 0, 0)$ is right above the obstacle. The following are the first four sets of velocity distributions which are taken for comparison. These sets are taken at the upstream region before the obstacle at $x/H = -5$, $x/H = -2$, $x/H = -0.75$ and $x/H = -0.25$ which is shown in Figs. 4, 5, 6 and 7:

The computed streamwise velocities when compared with the experimental data at the near-wall region are seen to have deviations (Fig. 4 and 5). It can be seen that the usage of non-uniform grid produces more realistic results than a uniform grid for such cases. In Arnal and Friedrich [16] finer was used grid at the near-wall region. The simulations produced more accurate results as compared to the calculation done with a uniform grid which can be observed in Friedrich and Arnal [17]. Similar to Friedrich and Arnal [17], this work used a uniform grid which may be one of the reasons for inconsistencies mentioned above.

Fig. 4 Comparison of velocity distributions at $x/H = -5$

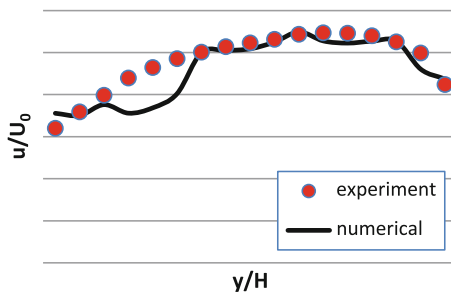


Fig. 5 Comparison of velocity distributions at $x/H = -2$

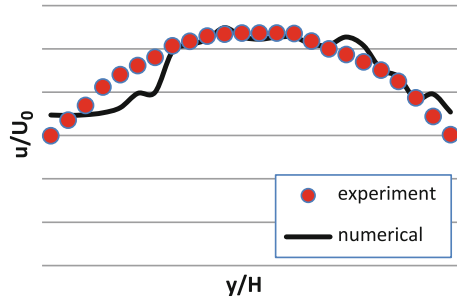


Fig. 6 Comparison of velocity distributions at $x/H = -0.75$

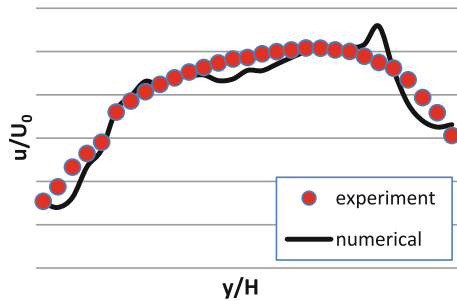
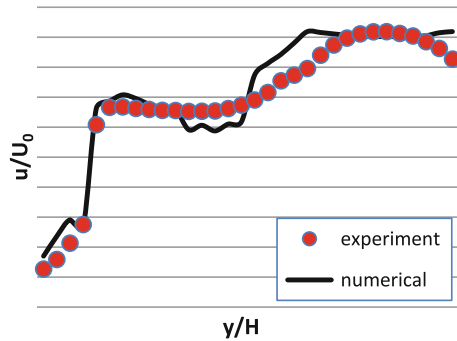


Fig. 7 Comparison of velocity distributions at $x/H = -0.25$



In Figs. 6 and 7, it can be observed that the simulation results produce a qualitatively similar trend as compared with that of the experiment. However, the velocity profile produced by the simulation appears to have slight irregularities ('wiggles'). Similar occurrences have been observed in Krajnovic and Davidson [18] while performing LES simulation on flow over a bluff body. In Krajnovic and Davidson [19], it was stated that these wiggles can be attributed to a combination of two factors, the coarseness of the mesh and the numerical scheme applied. Krajnovic and Davidson [18] also experienced these similar wiggles in the streamwise velocities in their simulation. Therefore, in Krajnovic and Davidson [19], it was suggested that a finer grid and a better numerical scheme may produce smoother trend in the streamwise velocities and hence eliminate these wiggles.

Figures 8, 9 and 10 are the velocity distributions which are taken right above the obstacle (at $x/H = 0$) and at the flow after the obstacle (the dissipation region at $x/H = 2$ and $x/H = 3$):

The solver had difficulty in accurately computing the flow behavior at the recirculation region (see Fig. 8). This may be attributed to the inability of the SGS model (Smagorinsky's model) to compute accurately the SGS stresses that heavily influences the flow during the recirculation phenomenon. One method to enhance the SGS model's accuracy is to modify it by including approximate boundary conditions. This was done in Morinishi and Kobayashi [20] where this method was stated to improve the accuracy of the computed SGS stresses. Another method was

Fig. 8 Comparison of velocity distributions at $x/H = 0$

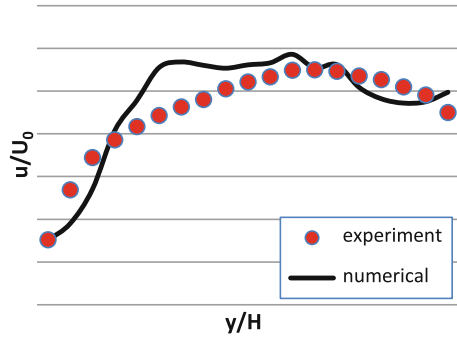


Fig. 9 Comparison of velocity distributions at $x/H = 2$

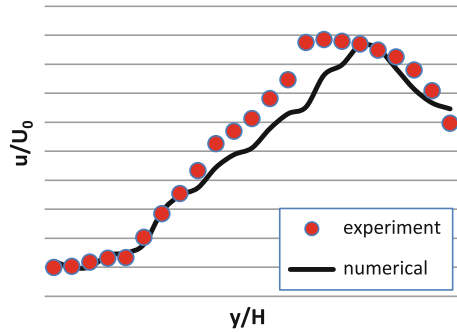
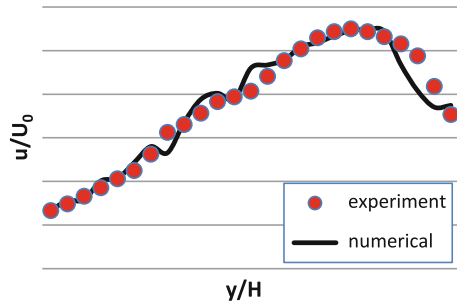


Fig. 10 Comparison of velocity distributions at $x/H = 3$



proposed in Yoshizawa [21] where a new parameter was introduced and was said to improve the accuracy of the Smagorinsky's model.

There are also slight inconsistencies for the velocities at the recirculation and the recovery region (refer to Figs. 9 and 10). To trace the vortex, the vortex center can be used where the velocity is zero. In this work, it can be observed that dissipation occurs gradually downstream after the obstacle or the step. Hence heading further downstream the vortex structure disappears which is consistent with the physical data. A similar work on identifying vortex dissipation downstream of flows was done in Roquemoire [22]. The dynamic Smagorinsky's model (DM model) was also stated to give more realistic results as compared with the static Smagorinsky's model.

5.2 Experiment 2: Flow Over a Backward-Facing Step with Opposite Wall

The velocity distributions obtained by the solver is compared with that obtained from the experiment. Similar to experiment 1, for the purpose of validation, the identification of the most significant velocity gradients is necessary and thus, the scaling argument was used. From the analysis, the velocity gradients, was identified as the most significant term for the given dimensions of the setup and the flow conditions. Therefore, the u-velocities (streamwise velocities) are taken with respect to the y-axis at different points in the x-direction.

The velocity distributions in the experimental results are normalized to the inlet velocity that is U/U_0 (dimensionless). Similarly, the distances in the experimental results are also normalized to the height of the backward-step which is respectively x/H , y/H , and z/H (dimensionless).

Seven sets of experimental results of the u-velocity distributions (velocities in the x-direction) are obtained throughout the test sections. Four sets of velocity distributions are used in the comparison at the region after the backward-step (the dissipation region) and before the backward-step. The following are the five sets of velocity distributions which are taken for comparison. These sets are taken at $x/H = -4$, $x/H = 0$, $x/H = 2$, $x/H = 3$ and $x/H = 5$ which are shown in Figs. 11, 12, 13, 14 and 15:

Fig. 11 Comparison of velocity distributions at $x/H = -4$

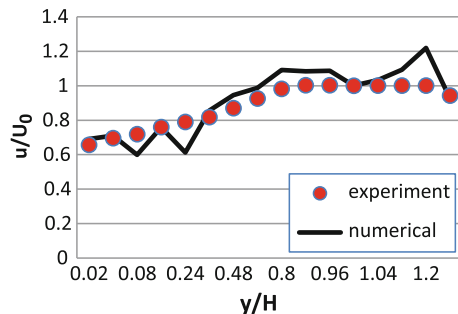


Fig. 12 Comparison of velocity distributions at $x/H = 0$

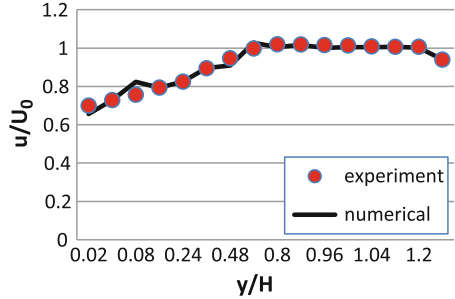


Fig. 13 Comparison of velocity distributions at $x/H = 2$

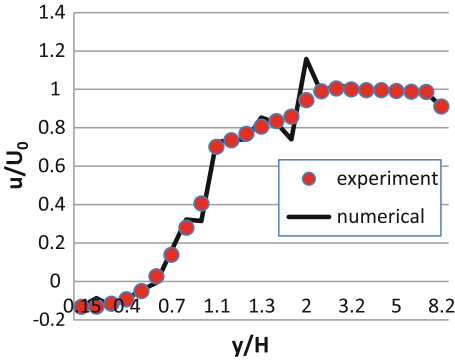
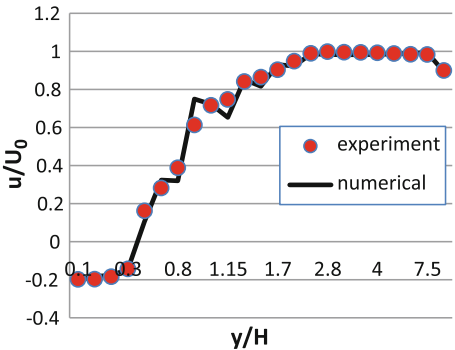


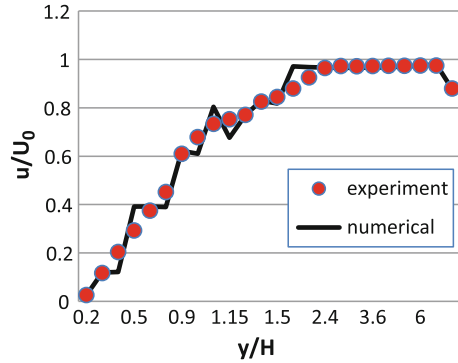
Fig. 14 Comparison of velocity distributions at $x/H = 3$



It can be seen in Fig. 11 that the wiggles have manifested themselves once more in the solver similar to experiment 1. However, these inconsistencies do not appear in Fig. 12. The factors of grid type and coarseness together with the numerical scheme play a critical role for the existence of these wiggles [18, 19].

The reattachment locations (the points where the wall-normal gradient of the stream wise velocity changes sign) obtained by the solver for experiment 2 is rather consistent with the physical results. This can be observed in Figs. 13, 14 and 15. Therefore, the incoherent vortex or the vortex stretching phenomenon is accurately

Fig. 15 Comparison of velocity distributions at $x/H = 5$



captured by the solver. The results of the solver capturing this phenomenon are not only consistent with the physical data but also similar to computational results of Balaras et al. [23]. To trace the vortex, the vortex center can be used where the velocity is zero. In this work for both experiments it can be observed that dissipation occurs gradually downstream after the obstacle or the step. Hence heading further downstream the vortex structure disappears which is consistent with the physical data. This can be observed in Figs. 13, 14 and 15. A similar work on identifying vortex dissipation downstream of flows was done by Roquemore et al. [22].

6 Deviation Analysis

The error in percentage (%) between the velocity distributions obtained by the numerical solver and the experimental results was computed using the following formulation:

$$error \text{ (\%)} = \left| \frac{u - u'}{u'} \right| \times 100 \% \quad (10)$$

where u' is the velocity obtained by the experimental results and u is the velocity obtained by the numerical solver. The average error obtained for the sets of velocity distributions in experiment 1 are as in Fig. 16:

In Fig. 16, as the flow approaches the obstacle, the average error is observed to increase. The average error at $x/H = -0.25$ which is right before the obstacle is at 15.545 %. This may be attributed to flow reversal, as could be observed in Fig. 5 (negative velocity values) when the fluid encounters the mounted-obstacle. This phenomenon is not accurately captured by the numerical solver and hence results in higher error values. The average error in the velocity distribution is observed to reduce as compared with that in the flow reversal region in front of the obstacle. This may be explained by the fact that the flow above the obstacle exhibits comparatively higher stability as the mean flow direction is preserved. The average error

Fig. 16 The average error distribution in the streamwise direction (For Experiment 1)

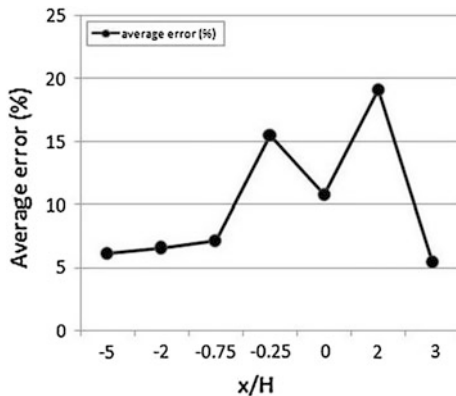
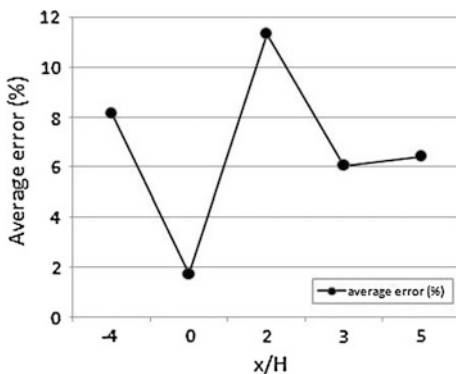


Fig. 17 The average error distribution in the stream wise direction (For Experiment 2)



at $x/H = 2$ has a higher value of 19.14 % due to inability of the numerical solver to capture the finer details of the flow recirculation phenomenon. Finally at $x/H = 3$, it can be observed that the average error reduces again during flow recovery. Thus the solver computes the velocity profile with fair amount accuracy.

The average error distribution in the streamwise direction for Experiment 2 can be seen in Fig. 17:

In Fig. 17, the average error is observed to reduce radically from $x/H = -4$ to $x/H = 0$. This is because at $x/H = 0$, the distribution at the velocity profile becomes more regular as compared to the profile near the inlet. However, at $x/H = 2$, it can be observed that the average error retains a high value of 11.34 %. This can be due to the numerical discrepancies in the solver which may give rise to difficulties in accurately capturing the flow recirculation phenomenon. Finally at $x/H = 3$ and at $x/H = 5$, it can be observed that the average error reduces and maintains a stable value. The intensity of backflow gradually reduces as the dissipation occurs. As the flow recovers and regains its stability, the solver computes the velocity profile more accurately.

The type of SGS stresses existing in turbulent flows are Reynolds stresses. Since stresses such as Leonard and Cross stresses are the result from the statistical

operation and thus, not measurable, the dominant SGS stresses which has any effect on the flow is assumed to be the Reynolds stresses. As can be observed in Fig. 17, the computational results in experiment 2 agree fairly well with the experimental data quantitatively and qualitatively with a less than 12 % average error at each measurement as compared to experiment 1 (Fig. 16). This is because; the complexity of the geometry of the experimental setup in experiment 2 is much lower than experiment 1. Hence, the Reynolds stresses from the flow is more intense in experiment 1 as compared to experiment 2 such that the simulation encountered more difficulties when predicting the flow in experiment 1 as compared to experiment 2.

7 Concluding Remarks

Based on the analysis performed it can be concluded that the results produced by the simulation are fairly consistent with the experimental results. Although the in-house source code equipped with the LES turbulence model is complete, further advancement and validation with empirical results with different flow conditions are necessary. For instance, the numerical scheme of the solver can be upgraded to third order QUICK or other UPWIND schemes to cut down the approximation errors during numerical operation. Besides that, based on recent work [18] the static Smagorinsky's model in this solver can be upgraded to the Dynamic Smagorinsky's model to accurately capture the flow fluctuations due to turbulence. The option for more meshing techniques could also be included as one of the features in the solver. These upgrades and testing will increase the capacity of the simulator to solve a greater variation of flow cases with optimum accuracy.

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