1. Introduction

Optimization of the nozzle contour to obtain maximum thrust under the limitations of an engine envelope is one of the most important design factors for an effective rocket engine. The classical design approach is based on ideal contours (designed by the method of characteristics, delivering a uniform flow at the nozzle exit), but being significantly truncated to limit the overall thrust chamber length [1]. The demand of higher performance of rocket launchers is inherently associated with the requirement of increasing expansion ratios. However, the presence of flow separation and coupled complex shock structures inside the nozzle cause significant mechanical and thermal loads at higher expansion ratio.

Flow separation is typically undesirable since it incurs high energy losses and lateral forces on the structure of the nozzle. The knowledge of the transient process in a supersonic nozzle is important to predict the unsteady behavior of these loads during the startup and shutdown phases. Additionally, the shape of the nozzle (planar, conical or contoured) has an important influence on the type of flow separation (free- or restricted-shock separation). It is considered that for the parabolic and compressed-truncated perfect (CTP) nozzles, the transition of the flow structure, from free-shock separation (FSS) to restricted-shock separation (RSS) and vice-versa, create the sudden change of the pressure distribution along the nozzle wall, resulting in the generation of strong side-loads [2–9]. Especially for RSS, the excessive heat load associated with the re-attached supersonic flow at the nozzle wall and the side-load characters have to be mastered by the thermo-mechanical design. Fundamentally, the complex flow features consist of phenomena like shock propagation, shock reflection, shock
boundary layer interaction, shock mixing/shear layer interactions. Experimental and numerical studies of shock structures in the plume pattern are presented by many researchers [1–11]. However, and despite its importance, only a few researchers [12–19] have investigated transient nozzle flows during engine start-up.

Experimental investigations have been performed by Smith [12], Amann [13], Saito et al. [14] in a laboratory shock tube setup. Amann, for instance, studied the influence of several parameters such as nozzle half-angle, throat width and nozzle inlet radius, on the starting process of supersonic nozzles driven by a shock. Besides, special interest has been paid to the duration of the starting process, since it decreases the useful testing time of short-duration facilities. However, the evolution of the complex wave structures has also been shown. A comprehensive review of the nozzle flow separation is presented by Hadjadj and Onofri [10].

From a numerical point of view, a few studies were undertaken to simulate nozzle flow transients (startup and shutdown) [15–19]. Nevertheless, most of those simulations were two-dimensional planar or axisymmetric, owing to the large amount of CPU time required for three-dimensional computations. It is noted that, all these numerical predictions were typically able to reproduce the principle phenomena of shock propagation, speeds of secondary shock wave/contact discontinuity. However, their main inadequacy lies in the fact to resolve the 3D turbulence and its strong interactions with the complex shock wave structures and the location of the flow separation. The resolution of all these issues and the associated computational costs are still highly challenging areas of scientific research to be explored.

Concerning rocket nozzles, Chen et al. [20] examined the flow structures of the start-up and shutdown processes using a Navier–Stokes solver. The configuration they studied was a sub-scale nozzle of a J-2S rocket engine (i.e. a precursor of the American Space Shuttle main engine). Also, Mourouval et al. [18,19] studied numerically the early transient flow induced in an expanding nozzle by an incident planar shock wave and the appearance of a strong secondary shock wave. A detailed analysis of the wave structure was given and the mechanism of formation of vortices on the contact surface has been shown.

As can be seen, most of the previous works are either experimental studies and have limited higher order turbulent statistical data or two-dimensional numerical simulations that deal with the prediction of the main flow features (namely the primary and secondary shock waves, multiple shock wave reflections and slip surfaces). However, a detailed three-dimensional numerical investigation of transient shock/boundary layer interactions in such configurations has not been done so far. Therefore, the present work is an initial attempt dedicated to partially fill this gap in the literature.

Here, we use the large-eddy simulations (LES) to study the shock induced transient flow in a three-dimensional planar nozzle (associated to a shock tube). Several test cases are carried out to investigate the propagation of shock waves, flow separation and complex shock wave/boundary layer interaction associated with shock induced transient flows through planar nozzles. The computational domain has been chosen similar to the experimental setup of a shock-tube facility of the Ben-Gurion University, Beer-Sheva, Israel. Fundamentally, this study can be useful to strengthen the understanding of the shock-driven turbulence amplification associated with fast transient fluid flow. The quantification of interaction of turbulent fluctuations and its effect and mutual dependencies on overall dynamics of the complex flow evolution are important issues to deal with.

The manuscript is organized as follows: A brief description of the numerical tools be presented in section 2. Section 3 illustrates the formulation of the numerical setup followed by the results and discussion in section 4. Finally, conclusions and future work are presented in section 5.

2. Numerical method

2.1. Filtered Navier–Stokes equations

An implication of Kolmogorov’s (1941) theory of self-similarity is that the large eddies of the flow are dependent on the geometry while smaller scales are more universal in nature. This feature allows one to explicitly solve for the large eddies in a numerical simulation and implicitly account for the smaller eddies by using a subgrid scale (SGS) model. The triumphant journey of LES started with the pioneering work of Smagorinsky [21], Lilly [22], Deardorff [23], Germano [24] and others. Comprehensive accounts on LES are provided by Sagaut [25] and Pope [26] and reviews at different stages of the development are provided in [27–30].

The definition of any filtered quantity with a filter function \( G_\Delta \) and associated filter width \( \Delta = (\Delta_x \times \Delta_y \times \Delta_z)^{1/3} \) can be given by,

\[
\bar{f}(\bar{x}, t) = \frac{1}{\int \int \int} \int f(\tilde{x}, t) G_\Delta(\tilde{x} - \bar{x}) d\tilde{y} \tag{1}
\]

To reduce the SGS terms, the Favre averaged definition is generally used in compressible flow simulations, defined as, \( \bar{f} = \rho \tilde{f} / \bar{\rho} \). Applying the above definitions and neglecting the SGS terms having negligible contributions [31], the filtered compressible Navier–Stokes system of equations can be written as,

\[
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial (\bar{\rho} \bar{u}_i)}{\partial x_j} = 0 \tag{2}
\]

\[
\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial \bar{p} \bar{u}_i}{\partial x_j} + \frac{\partial \bar{p} \bar{u}_j}{\partial x_i} = \frac{\partial \bar{\sigma}_{ij}}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} \tag{3}
\]

\[
\frac{\partial \bar{E}}{\partial t} + \frac{\partial \bar{p} \bar{E}}{\partial x_j} \bar{u}_j = \frac{\partial (\bar{\theta} \bar{u}_i)}{\partial x_j} \bar{u}_j - \frac{\partial \bar{q}_{ij}^{SGS}}{\partial x_j} - \frac{\partial \bar{\tau}_{ij}}{\partial x_j} \tag{4}
\]

where \( \bar{\sigma}_{ij} \) is the resolved stress tensor, \( \bar{E} \) is the resolved energy, \( \tau_{ij} = \rho (\bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j) \) and \( \bar{q}_{ij}^{SGS} \) are the SGS stress and the SGS heat flux respectively, both of which have to be modeled in order to close the system of equations. In the present work, the Wall-Adapting Local Eddy-viscosity (WALE) model is used to close these SGS terms.

2.2. WALE model

The WALE model proposed by Nicoud and Ducros [32] is basically designed to reproduce more accurate scaling for simulations containing wall boundary conditions. It includes the effect of both the strain and the rotation and thereby gives a better prediction in the region where vorticity dominates rotational strain. The WALE model reproduces a proper near wall scaling so that the eddy viscosity is \( v_t = C_W(y^+)^3 \). It is estimated from the velocity gradient tensor’s invariant as follows,

\[
v_t = C_w \Delta^2 \frac{(\tilde{u}^2_{ij} + \tilde{v}^2_{ij})^{3/2}}{(\tilde{u}^2_{ij} + \tilde{v}^2_{ij})^{5/4}} \tag{5}
\]

where \( C_w \) is a model constant, \( \tilde{s}_ij = \frac{1}{2} \left( \frac{\tilde{u}_i}{\mbox{\wedge} \nu} + \frac{\tilde{u}_j}{\mbox{\wedge} \nu} \right) \) and \( \tilde{g}^2_{ij} \) is the traceless symmetric part of the square of the resolved velocity gradient tensor (\( \tilde{g}_{ij} = \bar{u}_i \bar{u}_j / \bar{\rho} \)), namely, \( \tilde{g}^2_{ij} = \frac{1}{2} \left( \frac{\tilde{g}^2_{ij}}{\mbox{\wedge} \nu} + \frac{\tilde{g}^2_{ij}}{\mbox{\wedge} \nu} \right) - \frac{1}{2} \tilde{\delta}_{ij} \tilde{g}^2_{kk} \) with \( \tilde{g}^2_{kk} = \bar{g}_{ii} \bar{g}_{jj} \). The model constant \( C_w = 0.5 \) is recommended to be optimal from priori tests of freely decaying isotropic homogeneous turbulence. It can be emphasized that, the LES model based on \( \tilde{g}^2_{ij} \tilde{g}^2_{ij} \) detects turbulence structures with either (large)
strain rate, rotation rate or both. Moreover, it avoids any dynamic procedure while maintaining the desired near wall scaling. No eddy-viscosity is being produced in case of wall bounded laminar flow (Poisueille flow). This is distinctively advantageous over the Smagorinsky model (based on $S_{ij} S_{ij}$, but not on rotation rate) which is capable of reproducing the laminar to turbulent flow transition. The WALE model based on the $S_{ij} S_{ij}$ invariant is known to be capable of handling the transitional pipe flow [32].

The SGS heat flux, $q_{\text{gs}}^{\text{dev}}$ is modeled using the eddy-diffusivity hypothesis assuming constant $P_{\text{rt}} = 0.9$ and is given by,

$$q_{\text{gs}}^{\text{dev}} = -\frac{\mu_{\text{t}} c_p}{P_{\text{rt}}} \frac{\partial \Theta}{\partial x_j}$$

An in-house three-dimensional compressible Navier–Stokes solver equipped with a fifth-order WENO scheme [33], LES models and an immersed boundary method [34,35] is used for the present simulations. The use of low-dissipation, high-order shock-capturing schemes is an essential ingredient for computing complex compressible flows with shock waves. The objective is to avoid excessive numerical damping of the flow features over a wide range of length scales as well as to prevent spurious numerical oscillations near shock waves and discontinuities. For instance, the family of WENO schemes is a good choice to achieve this goal. The diffusion terms are determined by means of fourth-order compact central difference formulas. The discretized equations are integrated in time by means of the explicit third-order total variation diminishing Runge–Kutta algorithm (RK3-TVD). The CFL number is set to 0.7 for all simulations. Detailed description of the applied methodology is reported in our previous work [36–39]. Three-dimensional LESs are carried out for all the cases presented in this paper. The simulations are performed on a SGI Altix ICE 8200EX and an IBM Power6 parallel computer of France.

### 3. Problem formulation

Fig. 1 shows the computational setup of the current study. A shock wave with a prescribed shock Mach number ($M_s$) is allowed to pass through the nozzle situated at the end test section of the shock-tube arrangement. The Rankine–Hugoniot relations for a moving shock ($M_i = 1.86$) for air are used to set the left state (shocked gas, subscripted as ‘2’) and right state ( stagnant gas, subscripted as ‘1’) of the shock wave. Geometric and flow parameters of the nozzle are: the radius of curvature of the nozzle converging section $R_n = 10$ mm, length of the nozzle $L_n = 142.871$ mm, nozzle angle = 15°, throat length, $L_t = 9.5$ mm, $p_i = 98800$ Pa, $T_1 = 291.5$ K, $Re = 4.1 \times 10^5$ (based on $L_t$ and properties at the left state) and $L_d$ is the nozzle location.

![Fig. 1](image1.jpg)

**Table 1** Parameters for different LES test cases performed in the present work.

<table>
<thead>
<tr>
<th>Case</th>
<th>$C_1$</th>
<th>$C_2$</th>
<th>$C_3$</th>
<th>$C_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial turbulent velocity</td>
<td>Zero</td>
<td>White random noise</td>
<td>Homogeneous isotropic</td>
<td>Homogeneous isotropic</td>
</tr>
<tr>
<td>Domain (mm$^3$)</td>
<td>$450 \times 80 \times 4.75$</td>
<td>$450 \times 80 \times 4.75$</td>
<td>$350 \times 80 \times 2\pi$</td>
<td>$160 \times 40 \times 9.5$</td>
</tr>
<tr>
<td>Grid (million points)</td>
<td>172</td>
<td>169</td>
<td>188</td>
<td>343</td>
</tr>
<tr>
<td>$\Delta_x, \Delta_y, \Delta_z$ (mm)</td>
<td>140, 140, 140</td>
<td>120, 50, 170</td>
<td>98.49, 196</td>
<td>49.49, 49</td>
</tr>
<tr>
<td>Nozzle location, $L_d$ (mm)</td>
<td>152</td>
<td>152</td>
<td>94.248</td>
<td>56.5</td>
</tr>
</tbody>
</table>

The flow-field has been averaged in the homogeneous direction to compare the experimental and numerical schlieren pictures. Comparisons of the early stage shock wave structures are shown in Fig. 2. A part of the incident shock (IS) reflects and returns back upstream of the nozzle section as reflected shock (RS), while the part which entered in the opening variable flow section of the nozzle evolves as primary shock (PS) front, followed by a typical mushroom shaped contact surface (CS) and the boundary layer interaction with transverse reflections gives rise to a secondary shock (SS). It can be seen from these figures that the numerical simulation is able to capture the dominant wave structures of the flow-field.

### 4. Results and discussion

In order to visualize the propagation of different waves, the x–t diagram has been constructed from the transient density field.
Fig. 2. Comparison of experimental (top) and numerical (bottom) schlieren at (a) \( t \approx 15 \mu s \), (b) \( t \approx 65 \mu s \) and (c) \( t \approx 115 \mu s \); PS: primary shock, SS: secondary shock, RS: reflected shock, TW: transverse wave, SL: slip line and CS: contact surface.

Fig. 3. (a) \( x-t \) diagram based on density, (b) comparison with experimental data, non-dimensional distance \( \frac{x}{L_t} \) and non-dimensional time \( \frac{t_{a1}}{L_t} \).

Fig. 3a clearly shows the evolution of PS, CS and SS. From Fig. 3b, it can be seen that a very good agreement of the shock positions with the experimental results has been found. Deviation of the position of the secondary shock at the later stages, is inevitable due to the inaccuracy of the determination of the exact location of the secondary shock from the first derivative of the density field.

From the registered flow-field data we estimated the near wall properties at \( t \approx 613 \mu s \) (see Fig. 4). The position of the flow separation can be deduced from the wall shear stress \( \tau_{\text{wall}} = \mu \left( \frac{\partial u_t}{\partial \eta} \right)_{\text{wall}} \), where \( u_t \) is the tangential velocity and \( \eta \) the wall normal distance. However, it is also clear from this figure that \( \Delta_n^+ < 90 \) (\( \Delta_n^+ = \Delta_n u_t / \nu_w \), where \( u_t \) is the friction velocity, \( \nu_w \) is the kinematic viscosity at the wall and \( \Delta_n \) is the wall-normal distance of the near wall grid point). However, \( \Delta_n^+ \) decreases in downstream direction, beginning at the nozzle throat. This brings in the deviations of later stage flow structures when compared with the experimental results. It is evident that the immersed boundary method inherently produces non-smooth boundary (like steps) along the nozzle wall. However, it is also well known that without any artificial turbulence injection, the transition of laminar to turbulent flow will hardly take place numerically, given...
the present computational setting. The existence of high values of $\Delta_i^+$ clearly indicates the requirement of higher grid resolution for the improvement of the numerical prediction. In order to have an initial fluctuating flow-field, we have formulated case $C_2$ with an increased grid resolution. A random velocity field with zero mean and unity variance has been superimposed onto the mean flow-field assuming a turbulent intensity of 0.1 as an initial trial.

It is clear from Fig. 5 that the higher grid resolution for $C_2$ corroborates the fact that the calculated $\Delta_i^+$ is less than 60 which is lower than that of case $C_1$. It can also be noted that the flow separation point shifts upstream compared to case $C_1$ (shown with arrows, Fig. 5). As expected, the speeds of the principal shock waves show identical outcomes for $C_1$ and $C_2$. It is worth mentioning that the mean wall pressure and density profiles show symmetrical behavior on top and bottom walls. Nevertheless, inevitable differences in these profiles downstream of the flow separation point are also clearly visible in Fig. 6.

The three-dimensional numerical schlieren, $Q$ criterion (defined as $Q = 0.5(\Omega_i \Omega_j - S_i S_j)$, where, $S_i = 0.5(u_{i,j} + u_{j,i})$ and $\Omega_i = 0.5(u_{i,j} - u_{j,i})$, following the usual notation [40]) and vorticity field are shown in Fig. 7 to highlight the three-dimensional flow features and different scales of turbulence. On the other hand, Fig. 8 shows the anisotropic behavior of the Reynolds stresses, indicating that the shear layer region is dominantly turbulent. It can be seen from the velocity vector field (see Fig. 9) that, upstream of the separation zone, the flow is virtually laminar and the oblique shocks interact with these laminar boundary layers. This is distinctly different from the experimental observation. It is to be noted that the generation of a fluctuating flow-field with a white random noise generator produces a fluctuating flow-field without any correlation of fluctuating components of the velocities.

To improve the initial turbulent flow fluctuations, we formulated the case $C_3$ with homogeneous isotropic turbulent velocity
fluctuations in the shocked gas region. A prescribed energy spectrum of Passot-Pouquet, $E(k^*) = \mathcal{A} \left(\frac{k^*}{l^*}ight)^4 e^{-2(\frac{k^*}{l^*})^2}$ has been assumed to generate the initial velocity field. An open source (http://www.cerfacs.fr) turbulent flow-field generator code has been used first to get an initial box of turbulent flow-field and this periodic data has been repeatedly assigned to fit in the computational domain of $350 \times 80 \times 2\pi$ mm$^3$ (see Table 1). To generate a $(2\pi)^3$ box of turbulent flow-field, the following inputs are to be assumed, i) Acoustic Reynolds number $Re_{ac}$, ii) non-dimensional turbulent velocity $u'_p$, and iii) most energetic length scale $l^*_p$. The different parameters used to generate this flow-field are summarized in Table 2.

![Figure 8](image)

**Fig. 8.** Resolved Reynolds stress contour for $C_2$. (a) $\sqrt{\bar{R}_{11}/U_2}$, (b) $\sqrt{\bar{R}_{22}/U_2}$, (c) $\sqrt{\bar{R}_{33}/U_2}$, where $R_{ij} = \langle \tilde{\phi} \tilde{\phi}_j \rangle / \langle \tilde{\phi} \rangle$. Any average resolved quantity $\langle \hat{\phi} \rangle$ is defined as the spatial averaged quantity over homogeneous direction and the resolved fluctuating component $\hat{\phi} = \hat{\phi} - \langle \hat{\phi} \rangle$.

![Figure 9](image)

**Fig. 9.** Velocity vector plot $C_2$.

A comparison among the three test cases is illustrated in Fig. 10. It can be seen from the experimental Schlieren that the secondary shock is related to a Mach reflection and is attached with the turbulent separated zone. The experimental picture clearly indicates that the boundary layer upstream of the flow separation is turbulent in nature, resulting in a strong shock interaction with the boundary layer. It can also be seen that for $C_2$, the oblique shock reflections are close to a regular reflection rather than a Mach reflection. The flow features depict the inability to reproduce the turbulent flow-field and coupled interactions. Moreover, the strong expansion fan after the throat region is a clear indication of lacking grid resolution. On the other hand, the existence of a turbulent separation zone and improved shock boundary layer interactions are visible for $C_2$ and $C_3$. Again, it can be noted that the deviation from the experimental flow structures are essentially related to the onset of turbulence in the region between throat and flow separation point. The weak Mach reflections predicted by the simulations are related to the nature of the boundary layer upstream of the flow separation. Nevertheless, it is clearly visible that there exists a progressive improvement in the predictions from case $C_1$ to case $C_3$.

Knowing the flow symmetry in the computational domain, shown for the case of $C_2$, and having proper flow field initialization, obtained in the case of $C_3$, the test case $C_4$ is designed to deeper investigate the flow features and turbulent statistics. In this case the lower half of the nozzle is chosen for simulation with approximately four times higher mesh resolution. The initial turbulent flow fluctuations are assigned as homogeneous isotropic turbulent velocity fluctuations in the shocked gas region as in the case of $C_3$. However, this time turbulent flow-field generator code has been used to get a box of turbulent fluctuations to fit into the smaller computational domain of $160 \times 40 \times 9.5$ mm$^3$. For this case, an analysis of flow turbulence is presented on the basis of spatially averaged mean quantities over homogeneous spanwise z-direction. Any averaged resolved quantity $\langle \hat{\phi} \rangle$ is used to define a resolved fluctuating component $\hat{\phi}'' = \hat{\phi} - \langle \hat{\phi} \rangle$.

Same as before, a part of the incident shock (IS) reflects and returns back upstream of the nozzle section as reflected shock (RS), while the part which entered into the nozzle, evolves as primary shock (PS) front, followed by a typical mushroom shaped contact surface (CS), while the boundary layer interaction with reflected transverse waves gives rise to a secondary shock (SS). It can be seen from Fig. 11 that the numerical simulation of $C_4$ at time $\approx 165$ μs is able to capture the shape of the separation shock, secondary shock, separation region and the finer structures associated with the mushroom structure (MS) of contact discontinuity (compare also the experimental Schlieren picture Fig. 10).

The quality of the mesh and the LES model effectiveness can be assessed from the dissipation length scale and the sub-grid-scale viscosity estimation by the LES model. Fig. 12 is presented to substantiate the reliability of the mesh resolution for the present LES at time $\approx 165$ μs. Kolmogorov scale is defined by $\eta = \left( \nu^3/\epsilon \right)^{1/4}$, where $\epsilon$ is the dissipation rate and $\nu$ is the kinematic viscosity. Following Pope [26] and assuming $\epsilon \approx \epsilon_{sgs} = C_\epsilon \kappa_{sgs}^3 / \Delta$, $k_{sgs} = (\nu_{sgs} \Delta / C_\epsilon)^{1/2}$, with $C_\epsilon = 0.7$, $C_\eta = 0.05$, the estimation of $\Delta / \eta$ can be obtained as a function of $\nu_{sgs}$ and model constants. It is argued in [26] that in an isotropic turbulence the maximum dis-

<table>
<thead>
<tr>
<th>$L_\infty$</th>
<th>$\bar{u}_{\infty}$/γ</th>
<th>$\bar{u}_{\infty}$/γ</th>
<th>$\bar{u}_{\infty}$/γ</th>
<th>$\kappa_*$</th>
<th>$\eta^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 mm</td>
<td>$c_{\infty}L_\infty$/γ</td>
<td>$u_{\infty}$/$c_\infty$</td>
<td>0.1$U_2$</td>
<td>6</td>
<td>$2\pi$/$\kappa_*$</td>
</tr>
</tbody>
</table>

---

Table 2

Reference state ($\infty$) is taken as the shocked gas state. $c_{\infty}$ and $\gamma_{\infty}$ are the speed of sound, viscosity at reference state. $u_p$ is the turbulent velocity, $l_p$ is the most energetic length scale and its associated wave number is $k_p$.
sipation takes place at length scales of about $24\eta$. As mentioned in [41,42] at least two points are necessary to resolve any flow feature, a grid spacing of $12\eta$ is needed to resolve the scale of $24\eta$. Inspecting the present outcome in Figs. 12a and 12b, it can be concluded that the resolution is not too far from the acceptable limit of the required grid resolution for LES. The presence of shocks gives rise to higher values of both $v_{\text{gs}}/v$ and $\Delta/\eta$ in the vicinity of the shocks. The contours of the ratio of $v_{\text{gs}}/v$ shows the effectiveness of the WALE model in the vicinity of flow separation and in the shear layer region. From the spatially averaged mean flow quantities and the near wall fluid point co-ordinates (x, y) we obtain the near wall mesh resolution.

Fig. 13a shows that on an average (red curve generated by a running average of the black curve) $\Delta_{w+}^+ < 10$ in the whole divergent section of the nozzle, and $\Delta_{w+}^+ < 5$ near the flow separation region ($\Delta_{w+}^+ = \Delta_{w+}u_{fr}/v_w$, where $u_{fr}$ is the friction velocity, $v_w$ is the kinematic viscosity at the wall and $\Delta_{w}$ is the wall-normal distance of the near wall grid point). Nevertheless, near the throat region it reaches a higher value. The range of the values of $\Delta_{w+}^+$ can be considered as acceptable and as better agreeing when compared with the previous test cases (i.e. $C_1$, $C_2$ and $C_3$) near wall resolution. The mean wall pressure (Fig. 13b) reveals the flow regions associated with favorable pressure gradient (FPG) and adverse pressure gradient (APG) in the nozzle.

Fig. 13b also shows the centerline pressure distribution depicting the location of PS and SS. The MS is clearly visible at the centerline density profile (see Fig. 14a). Its local Mach number ($M = \frac{\sqrt{\gamma}}{c}$, where $c$ is the local speed of sound) reaches a maximum value of $\approx 2.7$ in the divergent section and reduces to $\approx 1.2$ after the SS, relaxing to sonic and subsonic levels subsequently and being linked with the PS. The wall shear stress illustrates the flow separation region and flow reattachment. A smaller separation bubble is clearly visible along with the main separation bubble in Fig. 14b. An enlarged mean flow-field is depicted in Fig. 15. The streamlines and velocity vectors corroborate with the location of separation bubbles and the subsequent flow reattachment represented by zero wall shear stress.

The three-dimensional turbulent flow structures are visualized by plotting the positive iso-surfaces of second invariant of the velocity gradient tensor $Q$. Vortex convection and stretching are essentially nonlinear mechanisms through which fine-scale and intense vorticity fluctuations are generated and maintained. It can be emphasized that the baroclinic torque term due to non-collinear $\mathbf{V}T$ and $\mathbf{VS}$, in other words $\nabla \rho \times \nabla p \neq 0$ are expected to contribute to the production of vorticity in the vicinity of the SS interaction with the separated flow (see Fig. 15b). Vortical structures shown in Fig. 16, reveal the characteristics of compressible turbulent shear layers depicting deformed, stretched, coiled and elongated vortex tubes in the stream-wise, transverse and span-wise directions. The present LES for the case of $C_4$ has captured the larger and smaller turbulent structures associated with flow separation and the shear layer region interacting with the SS.

Instantaneous flow data and spatially averaged mean quantities are extracted from the region marked in red (data window shown in Fig. 15a). They are used to analyze the spatial structures at 165 $\mu$s. Fig. 16c illustrates the PDF of standardized in-
Fig. 12. Contours of (a) $\Delta_1/\eta$ and (b) $\nu_{sgs}/\nu$.

Fig. 13. (a) $\Delta_1^*$ along the nozzle wall, (b) wall pressure $\langle \bar{p}_{w} \rangle /p_1$ and centerline pressure $\langle \bar{p} \rangle /p_1$ (shifted by two units upwards). (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)

Fig. 14. (a) Centerline mean flow properties, (b) wall shear stress distribution.

Fig. 15. (a) Mean flow visualization, black solid curve represents the sonic line, (b) contours of the baroclinic torque term $|\nabla \rho \times \nabla p| L^2_{t}/(p_2 \rho_2)$. (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)
stantaneous quantities (vorticities and spatial derivatives of velocity components). The flatness values of these lie in the range of 6–12 indicating the similar properties of the double-exponential or exponential distribution of the probability density function (PDF) with non-zero low skewness values. On the other hand, the PDF of fluctuating velocity components assumes flatness values ≈ 5 with non-zero skewed distributions compared to a Gaussian distribution (see Fig. 17a). The two-point autocorrelation coefficients for fluctuating velocity components (at \( y = 0.026 \) mm) within this data window are computed to evaluate the effect of span-wise domain size on the turbulence. It is clear from this figure that the autocorrelation coefficients reduces to zero within half of the span-wise domain size, so that the domain is sufficiently large to enforce periodic boundary conditions without inhibiting the turbulence.

The resolved Reynolds stress terms reveal the prevailing anisotropy (see Fig. 18) in the interaction region. As expected, the dominant terms are \( R_{11} \), \( R_{22} \), \( R_{33} \) and \( R_{12} \). The estimated turbulent kinetic energy (Fig. 19a) attains a maximum value of ≈47% of the kinetic energy of the initial left state, indicating high turbulent intensity in the upper section of the compressible shear layer region. The scatter plots (Figs. 19b to 19d) of fluctuating components of the velocity field (within the data window) seem to show an anti correlation between stream-wise and transverse components. Other combinations appeared as without any preferential correlation.

We are aware of the fact that the extraction of fluctuating components based on only spatially averaged mean quantities suffers from insufficient stability of mean flow variables. We attempted to add temporal filtering to span-wise ensemble averaging, as an
Fig. 18.Resolved Reynolds stress $\sqrt{R_{ij}/U_2}$ where, $R_{ij}=\frac{\langle \tilde{\rho}'u''_i \tilde{u''_j} \rangle}{\langle \tilde{\rho} \rangle}$, (a) $R_{11}$, (b) $R_{22}$, (c) $R_{33}$, (d) $R_{12}$, (e) $R_{13}$ and (f) $R_{23}$.

Fig. 19.Turbulent kinetic energy $k/0.5U_2^2$ and scatter plots of the fluctuating velocity components.

Initial trial. A suitable filter length had to be estimated without affecting the unsteadiness of the flow for this purpose. The convective time scales associated with the speed of the dominant shocks (PS, SS) or the initial left state velocity together with the mesh size were used to define temporal filter lengths. The linear approximation of shock speeds from experimental findings yields Mach numbers of PS and SS as $M_{ps} \approx 1.8$ and $M_{ss} \approx 0.66$ respectively. Three test runs were carried out utilizing multiples of the filter length $\tau_f = \Delta/(\alpha_1M_{ss})$, where $\Delta$ is the minimum mesh size (49 μm).

It can be seen from Fig. 20 that the applied time filter produces deviations of the flow separation bubble, affecting the mean flow-
field. This problem could perhaps be cured by post-processing the flow data and including symmetric temporal filtering stencils at the corresponding instants of time. An alternative, to be tested in the future, would be ensemble-averaging of a number of flow realizations, obtained by slightly modifying the phases of the initial turbulent fields [43].

An estimation of four budget terms of the turbulent kinetic energy based on spatially averaged quantities are shown in Fig. 21. This rough estimation reveals that the turbulent kinetic energy production, turbulent transport and pressure dilatation terms are dominant for the non-equilibrium turbulent state. The plot of the pressure dilatation terms also shows fairly high positive and negative values (red and blue regions). However, they appear immediately downstream of the SS and not in the shear layer. It can be noted that the sporadic patches (dark blue region) of negative production of turbulent kinetic energy are predicted. This can be associated to density changes (shear layer subjected to compressions/expansions [44,45]) in this region and strongly out of equilibrium behavior of the turbulent flow can exist during the transient flow development. We are aware of the fact that the dissipation term cannot be reliably predicted in an LES. Nevertheless, it provides some interesting insight. A deeper and more reliable analysis of the turbulent budget terms will be made in our future study adopting phase averaging with more stable statistics.

5. Conclusions

In this work, we made an attempt to resolve numerically the complex flow features associated with shock induced supersonic flow inside a planar nozzle in a shock-tube arrangement. LESs are carried out with a flow solver equipped with a high-order WENO scheme and an immersed boundary technique. The global flow features of primary, secondary shock waves and contact discontinuity are well captured and in good agreement with the experimental data. Two simulations C1 and C2 with respectively, zero flow fluctuation and random noise, show quantitative agreement with experiments for the speed of the primary as well as the secondary shocks. Intersection points of the shock-wave on the central line matched qualitatively better with the simulation having initial fluctuations. It is observed that the initial flow-field greatly influences the separation point and the resulting oblique shock structure. The results of case C3 (computations with initial homogeneous isotropic turbulent fluctuating flow-field) show its superiority over the other cases. The lack of information of the initial level of turbulence in the experiments leads to the difficulties involved in the proper choice of the initial flow-field and the assumption of initial turbulent parameters.

Homogeneous isotropic turbulent flow fluctuations are then superimposed onto the shocked left state as initial fluctuating flow-field for the case of C4. Larger span-wise domain size (one throat length) and higher mesh resolution (isotropic mesh size of 49 μm) are used to simulate the transient nozzle flow in details. A symmetry condition on the mid-plane and a reduced stream-wise domain size are used compared to the previous test cases, in order to allow for an increased resolution, where it is needed. A preliminary analysis of the flow physics is made based on mean prop-

Fig. 20. Wall shear stress for various time filter width, C1: 10τr, C2: 20τr and C3: 50τr.

Fig. 21. Turbulent budget terms: (a) Production, (b) Transport, (c) Dissipation and (d) Pressure dilatation: black contour lines are values between −0.1 to 0.1, all terms are non-dimensionalized by \( U_1^2 \rho_2 / \tau_\alpha \). (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)
erties (ensemble averaged in span-wise direction) and a comparison with previous results and experimental data promises reliability. However, the computation of turbulence statistics (Reynolds stresses etc.), needs more stable (mean) flow variables. An attempt with extra temporal averaging during the simulation found to be inadequate, because the temporal filters are biased to the past information without any future information while calculating on the fly. To achieve stable statistics, further ensemble averaging has to be performed, based on 5–10 more simulations with little phase-incoherence in the free-stream isotropic turbulence. Physically meaningful fluctuations can thereby be received which are needed to compute correlations. Future work has to address this, before effects of flow acceleration on the mixing layer (which surrounds the separation bubble), of the dynamics of the separation bubble and of the shock unsteadiness can be investigated in a deeper analysis. Furthermore, the future work aims at further investigating the influence of the introduction of the fluctuating flow-field in the right state with zero mean velocity. A systematic comparison of the performance of different LES models should also be accomplished.

Conflict of interest statement

No conflict of interest

Acknowledgements

The authors gratefully acknowledge the financial support provided by the German Research Foundation (Deutsche Forschungsgemeinschaft – DFG) in the framework of the Sonderforschungsbereich Transregio 40 and the IGSSS (International Graduate School of Science and Engineering) at the TU München. We have utilized the computational facilities from GfCNI [CCRT/CINES/IDRIS] (grant t20162a7544) and Leibniz-Rechenzentrum München (LRZ). Authors are also grateful to Prof. G. Ben-Dor and Prof. O. Sadot (Ben-Gurion University) for providing some of their experimental results. Special thanks go to Prof. F. Hussain (Texas Tech. University), Prof. R. Friedrich (Technische Universität München) and Prof. T. Gatski (Center for Coastal Physical Oceanography, Old Dominion University, Norfolk, VA, USA) for their insightful comments and suggestions throughout this study.

References


A. Chaudhuri, A. Hadjadjy / Aerospace Science and Technology 53 (2016) 10–21