Large-Eddy Simulation of Subsonic Jets

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Abstract. The present study deals with development and validation of a fully explicit, compressible Runge-Kutta-4 (RK4) Navier-Stokes solver in the opensource CFD programming environment OpenFOAM. The background motivation is to shift towards explicit density based solution strategy and thereby avoid using the pressure based algorithms which are currently proposed in the standard OpenFOAM release for Large-Eddy Simulation (LES). This shift is considered necessary in strongly compressible flows when \(Ma > 0.5\). Our application of interest is related to the pre-mixing stage in direct injection gas engines where high injection pressures are typically utilized. First, the developed flow solver is discussed and validated. Then, the implementation of subsonic inflow conditions using a forcing region in combination with a simplified nozzle geometry is discussed and validated. After this, LES of mixing in compressible, round jets at \(Ma = 0.3, 0.5, 0.65\) are carried out. Respectively, the Reynolds numbers of the jets correspond to \(Re = 6000, 10000, 13000\). Results for two meshes are presented. The results imply that the present solver produces turbulent structures, resolves a range of turbulent eddy frequencies and gives also mesh independent results within satisfactory limits for mean flow and turbulence statistics.

1. Introduction

During the past decade the role of opensource programs has become more and more significant in carrying out large scale parallel computational fluid dynamics (CFD) simulations. The attractive features of such programs include the lack of license fees together with the complete freedom of implementation of new flow solvers within a reasonable time. In the present study the high-level programming environment OpenFOAM is utilized in order to implement a new flow solver for compressible Large-Eddy Simulations with specific interest in fuel jet mixing.

The background objective of our study lies in internal combustion engine applications where natural gas (NG), i.e. methane, is considered as an interesting alternative fuel. NG could for example replace diesel fuels in several combustion applications with only minor modifications to the existing engines. The advantage of NG combustion lies in the significant reduction of NOx and soot emissions which are typically considered to be the most unwanted diesel emissions. However, the typical port injection NG engine concept has also certain caveats. For example, the incomplete combustion of NG in cavities may result in the release of the fuel into the atmosphere. Such a 'methane slip' would be highly unwanted since methane is a harmful greenhouse gas. This effect could be reduced by direct injection strategy and charge preparation in the cylinder. Thereby, the premixing process of gaseous methane with air needs to be well understood.
The physical features of properties of gaseous sprays and jets have been studied extensively in the past using computational methods (Boersma & Lele, 1999; Bogey, 2003; Freund, 1997; Moore, 2009; Wang, 2010; Vuorinen, 2010). The aeroacoustics in jet applications plays an especially important role in jet engine and combustor applications where combustion control and noise reduction are often the target objectives (Colonius & Lele, 2004). However, in many practical cases, such as fuel injection systems in combustion engines, the jet acoustics is believed to be of less importance. In such applications one is more interested on the transient behavior of the jet and the connection between injection parameters (such as injection pressure and ambient conditions) to turbulent mixing (Vuorinen, 2010).

The present study deals with Large-Eddy Simulation of subsonic gaseous jets at idealized conditions. In specific, we study the role of injection pressure on the jet mixing. As a prototype problem a simplified model problem in which a round jet is injected through a long injector into a chamber enclosed by walls. In such conditions the jet mixing can be effectively studied.

The organization of the paper is as follows. First, the theoretical background is introduced including the governing equations and the solution approaches. After this the simulation setup is introduced together with the description of the boundary conditions. Also validation examples are considered. Subsequently, the results are presented and finally, conclusions are drawn.

2. Theoretical Background

2.1. Governing Equations

Compressible flows can be described using the full Navier-Stokes (NS) equations describing the conservation of mass, momentum and total energy. In the present simulations the NS-equations are introduced for the conservative variables \((\rho, \rho u_i, \rho e)\) which represent the density, momentum density and total energy density of the flow at a given point and time. The NS-equations read:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_j)}{\partial x_j} &= -\chi \sigma(x,y,z)(\rho - \rho^*) \\
\frac{\partial \rho u_i}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} &= \frac{\partial}{\partial x_j} (-p \delta_{ij} + \sigma_{ij}) - \chi \sigma(x,y,z)(\rho u_i - \rho^* u_i^*) \\
\frac{\partial \rho e}{\partial t} + \frac{\partial (\rho e + p) u_j}{\partial x_j} &= \frac{\partial}{\partial x_j} (\sigma_{ij} u_i) + \frac{\partial}{\partial x_j} \left( \lambda \frac{\partial T}{\partial x_j} \right) - \chi \sigma(x,y,z)(\rho e - \rho^* e^*).
\end{align*}
\]

Here, the equations (1)-(3) have been introduced together with source terms that may be used to drive the solution towards target states \((\rho^*, u_i^* \text{ and } e^*)\) within a relaxation time scale \(\tau = 1/\chi < \Delta t\). The source terms can be activated within desired regions of the flow using a mask function \(\sigma = \sigma(x, y, z)\), where \(0 \leq \sigma \leq 1\). In fact, this approach is quite common in the literature for introducing damping regions within different flow configurations (e.g. non-reflecting walls or outlets) or, alternatively, forcing the solution towards desired target values or profiles (Bogey, 2003; Freund, 1997). In the present study the forcing regions are applied for imposing subsonic inflow conditions for determining the jet injection pressure (see next section).

The pressure is assumed to be coupled to density and temperature via the equation of state and the internal energy of the flow is given as a sum of thermodynamic and kinetic energies

\[
p = \rho RT \text{ and } e = c_v T + 1/2 u^2.
\]

Once \(\rho, \rho u_i\) and \(\rho e\) are known the pressure and temperature can be constructed from equation (4). The temperature dependence of the specific heat \(c_v(T)\) is modeled using a polynomial form where the properties of nitrogen are used. Furthermore, the temperature dependence of the gas viscosity is modeled using the Sutherland’s law.
2.2. The Numerical Methods
In the present work LES is applied to solve the equations (1)-(3) within the finite-volume framework. For time integration method we implemented the RK4-method to the OpenFOAM code as a top-level solver. The RK4 method is frequently used in the field of compressible flow simulations and it represents a standard state-of-the-art method (Bogey, 2003; Colonius & Lele, 2004; Moore, 2009). The compact, low storage and fully explicit formulation of RK4 is chosen here (Ferziger & Perić, 1999). In the RK4 method the change in variables (i.e. $\delta \rho$, $\delta \rho u_i$ and $\delta \rho e$) is evaluated four times per timestep at cell centroids using equations (1)-(3). In fact, the repetitive evaluation of the terms in (1)-(3) within each substep is the time consuming part of the algorithm in the finite volume framework as the fluxes need to be evaluated. The boundary conditions and thermodynamics need to be adjusted accordingly in-between the RK4-substeps.

The convection terms in the equations (1)-(3) are discretized using a flux formulation which leads to skew symmetric discretization of the equations (Ferziger & Perić, 1999). This is the kinetic energy conserving form in the inviscid limit which is preferred for more robust computations and minimization of the aliasing errors. For the purposes of this work the relatively high Reynolds numbers of the studied cases forced us to choose a limited scheme for the convection terms which is however second order accurate in space. The accuracy of the solver is checked using the well-known lid-driven cavity flow data at a low Mach and Reynolds number ($Ma = 0.3$, and $Re = 400$) and a comparison of the present solvers to the DNS-data of Ghia et al. (1982) is shown in Figure 1. The L2-error of the velocity components is shown in Figure 2 which implies that the discretization is formally of second order accuracy. The presented test case implies that the discretization of the governing equations has been implemented correctly and forms the basis for the actual simulations to be described in the next section.

![Figure 1](image1.png)  
**Figure 1.** Vertical and horizontal velocity profiles for the lid-driven cavity case. Zero-gradient and no-slip boundary conditions are applied.

![Figure 2](image2.png)  
**Figure 2.** L2-error in the velocity components implying the second order accuracy of the present discretization.

3. Simulation Setup
3.1. Geometry of the Injection Chamber
The simulation geometry is shown in Figure 3. The setup consists of an injector with exit diameter $D = 0.001m$ and the actual injection chamber that is enclosed by walls. The diameter and height of the chamber are $40D$ and $50D$ respectively. The flow is not allowed to leave the domain which is the situation in real engines where the valves are closed during the
injection. Initially, the chamber is filled with nitrogen at temperature $T = 393\, K$ and pressure $p = 100000\, Pa$. A nitrogen jet is then injected into the chamber through the nozzle at a given injection pressure. Hence, at this stage of the study, we do not study actually methane injection which is a reasonable approximation since the properties of methane and air are rather similar.

The total simulation time is $1\, ms$ during which the total injected mass is of order $\sim 10^{-3}$ of the total gas mass in the chamber. Thus, one can assume that the average pressure and density in the chamber are constant during the injection. The injector region is needed in order to accelerate the flow with a pressure gradient. A special advantage of making the injector region very long is that the flow variables may be forced to target values very far away from the actual region of interest which minimizes the possible influence of the forcing approach to the results (see next section). Special attention is put on refining the grid adequately in the jet region. Mesh effects are studied with a coarse and fine grid consisting of 3.5M and 9.5M cells respectively. The finest grid is shown in Figure 3 in which the smallest cells are of size $\Delta x_{\text{min}} = D/36$ in all directions whereas for the coarsest grid $\Delta x_{\text{min}} = D/24$.

**Figure 3.** a) Short-time averaged temperature field in the chamber showing the clear cooling of the gas due to expansion in the injector region. b) Short-time averaged velocity field showing the acceleration of the jet. c) Instantaneous passive scalar field showing mixing in the jet. Note that the passive scalar is forced to unity in the nozzle region. d) Zoom to the nozzle inlet region.

### 3.2. Boundary Conditions and Simulation Cases

Imposing correct boundary conditions for compressible turbulent flows is a rather complex and widespread research field of its own (Colonius & Lele, 2004). The problematic boundary condition types are subsonic inlets and outlets. Also wall boundary conditions need special attention. In specific, if reflection of strong acoustical waves or shocks from walls is considered important, simple boundary conditions like the zero gradient condition might be inadequate (Colonius & Lele, 2004; Moore, 2009).

In the present study, the standard no-slip BC for velocity is applied on the walls and the slip BC is applied inside the injector since no boundary layers are resolved with the present grid. For
the thermodynamic quantities the zero gradient condition is applied at the walls which enforces also the equation of state to be fulfilled automatically at the boundary cell faces.

In a practical gas jet injection system the injection pressure needs to be very high (tens of bars). In a converging nozzle this leads to very high velocities which, however, can not exceed the choked state ($Ma = 1$). In the present case the injection system is modeled using a simple gas injector through which the jet is accelerated using a pressure gradient. The injector starts at point $z/D = -77$ and the fluid exits to the chamber through the nozzle exit hole at point $z/D = 0$. As the flow is subsonic, special emphasis needs to be put on the implementation of the inflow boundary conditions. The inflow region is defined as the region $-77 \leq z/D \leq -73$ where the flow is forced to desired target values $\rho^*, \rho^* u_i^*$ and $\rho^* e^*$. This can be done conveniently by activating the source terms in the equations (1)-(3) and by letting them smoothly vanish to zero within the region $-73 \leq z/D \leq -71$ using a hyperbolic tangent function. Different variants of the forcing approach have been tested in various applications (Colonius & Lele, 2004; Freund, 1997). The back pressure ($p^*$) is modified by varying $\rho^*$ since $T^* = 393$K. The simulated cases corresponding to three injection pressures and two meshes are shown in Table 1.

At time $t = 0$ the pressure inside the injector is given by the hyperbolic tangent function to change smoothly from the back pressure value $p = p^*$ to the ambient conditions $p = 100000Pa$. The initial hyperbolic tangent profile vanishes smoothly to zero in the region $-7 \leq z/D \leq -5$. Figure 4 shows the mass flow profiles that are measured from data close to the nozzle exit (i.e. very far from the forcing region). It can be seen that the implemented boundary condition behaves as desired: low injection pressure gives a lower flow velocity and mass flow than a high pressure. As seen, the profiles are also mesh independent and provide a very steady mass flow after the initial transient phase has passed by.

Figure 4. The mass flow for different pressure ratios $p_{rel}$ for two different meshes. A constant mass flow level is achieved after an initial transient suggesting that the boundary condition is working as expected.
Figure 5. Jet visualization for three different pressure ratios $p_{\text{rel}}$ for the coarsest grid. Snapshots from three different times. **Left:** $p_{\text{rel}} = 1.1$. **Middle:** $p_{\text{rel}} = 1.2$. **Right:** $p_{\text{rel}} = 1.4$. 
| Case | $p_{rel}$ | $p^*$ (Pa) | $\rho^*$ (kg/m$^3$) | $U_o$ (m/s) | Mass flow (kg/s) | Mesh size |
|------|----------|------------|---------------------|------------|-----------------|-----------|
| Case 1 | 1.4      | 140000     | 1.199               | 260.0      | 1.95e-4         | 3.5M      |
| Case 2 | 1.2      | 120000     | 1.028               | 188.0      | 1.35e-4         | 3.5M      |
| Case 3 | 1.1      | 110000     | 0.942               | 132.0      | 0.92e-4         | 3.5M      |
| Case 4 | 1.4      | 140000     | 1.199               | 260.0      | 1.95e-4         | 9.5M      |
| Case 5 | 1.2      | 120000     | 1.028               | 188.0      | 1.35e-4         | 9.5M      |
| Case 6 | 1.1      | 110000     | 0.942               | 132.0      | 0.92e-4         | 9.5M      |

4. Results

4.1. Flow Visualization

For flow visualization and mixing studies we solve an additional equation for a passive scalar. Such visualizations are shown in Figure 5 in which snapshots from several instants of time are seen for the coarse mesh. It can be observed that in the beginning of the simulation all the three injection pressures (Case 1-Case 3) tend to produce a rolling tip vortex. Also the growing Kelvin-Helmholz instability can be clearly observed. At later time the initially laminar jet becomes turbulent and enhanced mixing can be observed. Figure 5 implies that the jets with lower Reynolds and Mach number have more visible generation of inlet vortices during the whole simulation although the issue is definitely dependent on the inflow boundary conditions.

Figure 5. Simulation Cases

![Figure 5. Simulation Cases](image)

Figure 6. Inverse of the mean $z$-component of velocity along the $z$-axis.

Figure 7. Mean temperature along the $z$-axis.

4.2. Mean Flow

The inverse of the mean axial velocity of the jets along the $z$-axis are shown in Figure 6. It is observed that the potential cores of the jets extend until a distance of 5 – 6D from the nozzle exit after which the velocity begins to decay with a slope comparable to 1/6.5 (see e.g. Moore (2009)). The lower Mach number jets seem to have somewhat longer potential cores than the higher Mach number cases. A slight effect of the inflow boundary conditions is also observed: at the nozzle exit the grid refinement leads to sharper gradients leading thereby to a slightly more rapid decay of the core.

![Figure 6. Inverse of the mean $z$-component of velocity along the $z$-axis.](image)

![Figure 7. Mean temperature along the $z$-axis.](image)
Figure 7 shows a plot of the mean temperature along the $z$-axis. Clearly, the fine and the coarse grids give very similar characteristic behavior. At the jet exit the incoming gas is cooler than the surrounding gas due to the adiabatic expansion during the acceleration stage. The inlet temperature values are in close agreement with the adiabatic expansion theory.

![Figure 7](image1.png)  
**Figure 7.** Plot of the mean temperature along the $z$-axis.

The radial distribution of the mean velocities (normalized by inlet velocity) in similarity coordinates are considered in Figure 8. The result is shown only for the highest injection pressure case for clarity since this case is considered the most challenging due to the highest Reynolds number. Figure 8 implies that the simulation result is nearly grid independent for the shown profiles although small differences are noted at the location $z/D = 10$. Similar observations are made for the passive scalar concentration which is shown in Figure 9.

![Figure 8](image2.png)  
**Figure 8.** Radial distribution of the $z$-component of velocity from several downstream locations.

**Figure 9.** Radial distribution of concentration from several downstream locations.

4.3. Turbulence Statistics

For turbulence statistics two tests are made. Figures 10 and 11 show the distribution of RMS of velocity along the $z$-axis and in the radial directions respectively. Clearly, some differences between the two meshes are seen but the statistics are rather close to one another.

![Figure 10](image3.png)  
**Figure 10.** Axial RMS of velocity.

![Figure 11](image4.png)  
**Figure 11.** Radial distribution of RMS of velocity.
4.4. Spectral Content and Small Scale Turbulence

The energy spectra of velocity time series are considered in Figures 12 and 13. It is seen that the algorithm captures a range of scales. Furthermore, the differences between the two grids becomes clear since the fine grid supports somewhat broader range of temporal frequencies. However, for a given injection pressure, at the lower frequencies the spectra are nearly mesh independent. This implies that the resolution of the grids is within reasonable limits.

Figure 12. Kinetic energy spectrum from $z/D = 10$ on the jet axis.

Figure 13. Kinetic energy spectrum from $z/D = 10$ and $r/D = 2$.

Figure 14. Visualization of the developing tip vortex and the Kelvin-Helmholtz instability from an early stage of injection using the $Q$-isosurface. The red (blue) color corresponds to positive (negative) $\omega_z$ revealing the direction of vortex rotation.

Figure 15. Visualization of the small scale vorticity from a late time when the turbulence has fully developed using the $Q$-isosurface. The red (blue) color corresponds to positive (negative) $\omega_z$ revealing the direction of vortex rotation.

The iso-surfaces of the flow field vortex structures may be visualized using the $Q$-criterion. Figure 14 shows the roll-up of vortex rings due to the growth of the Kelvin-Helmholtz instability and interaction with the quiescent gas at early times for the finest grid ($Ma = 0.65$, $Re = 13000$).
Also rather thin, axially oriented vortices are observed. The direction of vortex rotation is visualized by coloring the isosurfaces with the $z$-component of vorticity ($\omega_z$). Thus, a positive (negative) value implies that the vortex is rotating clockwise (counter-clockwise). At a later time the shear layer is still producing Kelvin-Helmholtz-like instabilities although they are somewhat hidden by the excessive amounts of small scale turbulence as seen in Figure 15.

5. Conclusions

A description of a newly implemented Runge-Kutta-4 algorithm has been given. The code has been validated using the lid-driven cavity case and tested on more challenging flow case i.e. LES of gas jets at various Mach and Reynolds numbers. In our opinion there should be no actual need to use the pressure based algorithms when $Ma > 0.5$.

There are also certain issues that need further investigation. First, we noted that the used discretization scheme might be somewhat too dissipative since the low-amplitude jet acoustics was not fully captured and thus other non-dissipative alternatives must be considered in the upcoming studies. Also the applied grids should be considered carefully since the 2:1 refinement ratio might be too steep. The future studies will focus on further development and testing of the present flow solver for combusting fuel jets, supersonic jets and sprays.

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