Large-eddy simulations of variable-density turbulent jets

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Abstract. We perform Large-eddy simulations (LES) of turbulent variable-density jets. A fully developed turbulent pipe flow of air at the Reynolds number of Re = 5300 enters a large reservoir of air, helium or carbon dioxide. The impulsely starting jets as well as the fully developed stationary flows are considered. In the first case we show that the air stream propagates faster in the light medium of helium as compared to other gas pairs, while in the fully developed case the same helium-air pair exhibits the lowest level of turbulent fluctuations.

Keywords: turbulence, jet flow, variable density, mixing

1. Introduction

Turbulent jets represent a wide class of flows in hydrodynamics being of high relevance in technological applications. The variable density of the medium is encountered in combustion and mixing processes motivating research in this area. One of the first experiments with variable-density jets were performed by Ahmed et al.\cite{Ahmed2001}, where they considered the impact of swirl on the intensity of mixing. The stability of air/helium jets were considered by Sreenivasan et al.\cite{Sreenivasan1990}. Monkewitz et al.\cite{Monkewitz1994, Monkewitz1995} investigated the rate of entrainment and mixing in transitional heated jets. Panchapakesan and Lumley\cite{Panchapakesan1982} performed extensive measurements of air/helium jets. The main emphasize was on the far field and self-similar characteristics. Djeridane and Amielh\cite{Djeridane2004} presented experimental measurements of helium, air and carbon dioxide jets, which are frequently employed for the verification of numerical simulations\cite{Djeridane2005}. General feature of most simulations and experiments is that the air serves as the environment, while the jet is generated using different gases\cite{Djeridane2006, Djeridane2007}. While this approach is used in practice, it is challenging to compare different cases due to changing Reynolds number because of the variable-density properties. In this work we investigate a fully developed turbulent pipe flow of air entering a large reservoir of air, helium or carbon dioxide, thus, fixing the inflow conditions for all the cases.

2. Governing equations

We use the low-Mach number approximation of the Navier-Stokes equations to describe the flow of two different gases, which is valid when the characteristic flow velocity $U$ is much smaller than the velocity of the sound $c_0$. This approximation allows us to eliminate acoustic waves, which impose additional restrictions on the resolution of the computational grid and time step. Further all the variables are nondimensionalized using $L, U, \rho_0$, which are the characteristic length, velocity and dynamic viscosity, respectively. The resulting equations are summarized as follows\cite{Ismail2016}:
\[
\frac{\partial u_j}{\partial x_j} = -\frac{1}{\rho} \frac{D\rho}{Dt},
\]
(1)
\[
\rho \left( \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \right) = \frac{\partial p^{(0)}}{\partial x_i} + \frac{1}{Re} \frac{\partial \tau_{ij}}{\partial x_j},
\]
(2)
where \( u_i \) is the \( i \)-th component of the velocity field, \( \rho \) is the density field, \( Re = UL/\mu_0 \) is the Reynolds number,
\[
\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right)
\]
denotes the viscous stress tensor. The decomposition \( p = p^{(0)} + p^{(1)} \), of the pressure field is used, where \( p^{(0)} \) is the so-called hydrodynamic pressure, which behaves similarly to the pressure field in the incompressible case, and \( p^{(0)} \) is the thermodynamic pressure, which does not depend on space and is connected to temperature and density by the equation of state (given below). We consider a constant-temperature mixing process of air coming from the pipe with different ambient gases (air, helium, carbon dioxide), thus, \( p^{(0)} \) depends only on the density field. To describe the mixing process, we consider the equation for concentration \( c \) field:
\[
\rho \left( \frac{\partial c}{\partial t} + u_j \frac{\partial c}{\partial x_j} \right) = \frac{1}{Re \, Sc} \frac{\partial}{\partial x_i} \left( \rho \frac{\partial c}{\partial x_i} \right),
\]
(4)
where \( Sc = \mu / (\rho D_{\text{diff}}) \) is the Schmidt number, \( D_{\text{diff}} \) is the tabulated value of the mutual diffusion. The value \( c = m_{\text{air}} / (m_{\text{gas}} + m_{\text{air}}) \) is the mass fraction of air, therefore at the inlet \( c = 1 \). In case of helium or carbon dioxide co-flow \( c = 0 \). The Mendeleev-Clapeyron equation of state with a constant mixture temperature gives:
\[
\rho = \rho^{(0)} \frac{M_{\text{air}} M_{\text{gas}}}{R_a T M_{\text{air}} + c (M_{\text{gas}} - M_{\text{air}})},
\]
(5)
where \( R_a, M_{\text{air}}, M_{\text{gas}} \) denote the universal gas constant, the molecular mass of air and the molecular mass of the co-flowing gas, respectively. The dynamic viscosity of the mixture of \( n \) non-reactive gases is as follows [11]:
\[
\mu = \sum_{j=1}^{n} \frac{X_j \mu_j}{X_j \sum_{k=1}^{n} \Phi_{jk}},
\]
(6)
where \( X_j \) is the mole fraction of the \( j \)-th component of the mixture, \( \mu_j \) is the dynamic viscosity of the \( j \)-th component, and \( \Phi_{jk} \) is the coefficient of viscous interaction of the \( j \)-th and \( k \)-th components.
\[
\Phi_{jk} = \frac{1}{4} \left( 1 + \left( \frac{\mu_j}{\mu_k} \right)^{1/2} \left( \frac{M_j}{M_k} \right)^{1/4} \right)^2 \left( \frac{2M_j}{M_j + M_k} \right)^{1/2}
\]
(7)
where \( M_j \) and \( M_k \) are the molar masses of the \( j \)-th and \( k \)-th components, respectively. The mole fraction \( X_j \) is connected with the mass fraction \( c_j \) by the relation:
\[
X_j = \frac{c_j}{\sum_{i=1}^{n} (c_i / M_i)}
\]
(8)
For example, in case of “air – He” pair, where we denote the quantities related to air by subscript 1 and to helium by subscript 2, the expression for the dynamic viscosity is:
\[
\mu = \frac{X_1 \mu_1}{X_1 + X_2 \Phi_{12}} + \frac{X_2 \mu_2}{X_1 + X_2 \Phi_{12}}.
\]
(9)
Table 1 summarizes all parameters for air, helium and carbon dioxide used in the study.
Table 1. The parameters of gases.

|       | $\rho$, kg/m$^3$ | $\mu \cdot 10^3$, Pa·sec | $D_{air}$, cm$^2$/sec | $M$, g/mole |
|-------|------------------|-------------------------|----------------------|-------------|
| Air   | 1.293            | 1812                    | -                    | 28.98       |
| He    | 0.179            | 1946                    | 0.62                 | 4.002       |
| $CO_2$| 1.977            | 1463                    | 0.21                 | 44.01       |

3. Results
The main computational domain represents a cylinder of radius $6D$ and length $17D$, where $D$ is the diameter of a pipe supplying the fluid (see Fig. 1a). Further we use the cylindrical coordinate system $(z, r, \phi)$ located in the center of the end of the pipe. The axis $z$ is a streamwise coordinate, $r$ and $\phi$ denote the radial and azimuthal directions, respectively. The inflow is generated in a precursor simulation of the pipe with periodic boundary conditions. The velocity field in some fixed plane $r-\phi$ is then copied each time step into the main area.

Figure 1. Geometry of the main computational domain (a) and the example of an instantaneous and time averaged velocity fields (b). White horizontal lines on the right side of (b) indicate the cross-sections where the radial profiles are analyzed below.

A small co-flow of $U_{sw} = 0.04U$ is set at the bottom boundary as it is shown in Fig. 1, where $U$ is the bulk velocity of the pipe flow. The Reynolds number based on $U$ and $D$ is equal to 5300. On lateral and outflow boundaries, the Neumann conditions are imposed for the velocity field. The computational mesh for the precursor (pipe) simulation consisted of $6.55 \times 10^6$ nodes and more than $15.8 \times 10^6$ for the main domain. No subgrid-scale model is used in the Large-eddy simulation (LES) framework, while two high-frequency modes are filtered using a parabolic transfer function with amplitude of 5% for the latter mode [12]. To solve the equations, we use the spectral-element Nek5000 code [13] with a spatial discretization based on the Lagrange polynomials of degree $N = 7$. For the time discretization the semi-implicit time-stepping scheme of third-order accuracy is used. Our group has previously validated the simulations on a number of [14–16].
To validate the precursor simulation, we first compare the radial profiles of the time-averaged axial velocity component and their fluctuations with the data from the literature showing excellent agreement [17,18]. Further, the data [18] representing the results of a similar LES calculation will be used to compare the statistical characteristics of the pipe jet. Spectral-element simulations give results for a fully developed stationary jet flow, which are consistent with our previous finite-volume simulations [18]. A slightly different level of fluctuations of a periodic pipe leads to some discrepancies near the end of the nozzle (z/D = 1). However, the results are in excellent agreement in all the cross sections further downstream, Fig. 2.

Figure 2. The radial profiles of the time-averaged axial velocity component and their fluctuations for a fully developed air-air simulation. Three axial stations are shown: z/D = 1, 4, 7. The data from the literature [18] is shown by blue symbols.

First, we consider impulsively starting jets of air entering He or CO₂ environment. At time t = 0, a fully developed turbulent pipe flow is supplied to the inflow of the main domain. We track the propagation of the concentration front. Figure 3 shows the instantaneous concentration fields for different instants t. It is intuitively clear that a heavy gas will spread faster in a light medium (air – He) as compared to the light gas in a heavy environment (air – CO₂). The mixing process of helium and air is accompanied by relatively large vortex structures, as compared to air – CO₂ pair. This is probably due to the decrease in the local Reynolds number \( \text{Re}_{loc} = D \cdot \text{U}_{loc} \cdot \rho_{gas} / \mu_{loc} \) in the mixing layer.
according to Eqs. (5)-(9). Figure 4 shows the jet front coordinate against \( t^{1/2} \), together with the data from the literature [19], where the propagation air-air jet with an almost uniform laminar velocity profile at the nozzle at higher Reynolds numbers \( Re = 1.9 \times 10^5 \) was considered.

Figure 3. The concentration field for two calculations (He, CO\(_2\)) at different instants of time. The red color corresponds to the value \( c = 1 \) (air), blue - \( c = 0 \) (He or CO\(_2\)).

Figure 5 shows a comparison of the time-averaged axial velocity component and their fluctuations for fully developed simulations for all the cases. In case of “air – He” pair, the axial velocity decays more slowly than in other cases. Also the level of fluctuations is lower, which was previously associated with a decrease in the local Reynolds number in the mixing layers due to the lower density. Further work includes a more detailed analysis of the statistical characteristics as well as the study of the main vortical structures shaping the dynamics of the flow [20].

4. Conclusion
We studied variable-density jets using Large-eddy simulations. A fully developed turbulent pipe flow of air at the Reynolds number of Re = 5300 entered a large reservoir of air, helium or carbon dioxide. We considered the impulsively starting jets as well as the fully developed stationary flows. In the first case we showed that the air propagates faster in the light medium of helium as compared to other gas pairs, while in the fully developed case the same helium-air pair exhibits the lowest level of turbulent fluctuations.

Figure 4. Comparison of the speed of air jet propagation in the surrounding gas for “air-CO\(_2\)” system.
Figure 5. Comparison of time-averaged radial velocity profiles and RMS pulsations for all three calculations in cross sections $z/D = 1, 4, 7$.

5. Acknowledgements
This work is funded by the Russian Foundation for Basic Research No. 18-38-00717 and by the Federal Agency for Scientific Organizations (FASO of Russia) Project III.22.7. The computational resources are provided by Siberian Supercomputer Center SB RAS, Supercomputer Center of Novosibirsk State University and Joint SuperComputer Center of the Russian Academy of Sciences, Moscow.

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