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Particle dispersion produced by a turbulent free convection flow in a room-sized cubical cavity

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Abstract. This paper introduces the framework for the ongoing "2024 International CFD Challenge on the Long-Range Indoor Dispersion of Pathogen-Laden Aerosols." The Challenge is designed as a blind test to assess the accuracy of computationally efficient turbulence modeling techniques, including URANS and LES, in replicating both the hydrodynamics and aerosol dispersion in an idealized indoor environment. To evaluate the simulations, DNS data of turbulent natural flow at a high Rayleigh number within a room-sized enclosure will serve as a reference benchmark. Participants have the flexibility to conduct simulations of the same flow configuration using their preferred CFD software, employing URANS, LES, and/or hybrid methods. The Challenge was officially launched on October 16, 2023, and has garnered participation from 31 teams representing 18 different countries, with the expected submission of results in May 2024. The outcomes of the comparison between the different modelling approaches and the reference DNS will be presented and discussed during the conference.

1. Introduction

Computational Fluid Dynamics (CFD) is a useful tool for predicting and investigating physical aspects associated with the transmission of infectious diseases via aerosols such as SARS, human influenza H1N1, avian influenza (H5N1) and tuberculosis [1]. These pathogen-laden aerosols may be expelled by an infected person when sneezing, coughing, talking or singing. The short-term, short-range dispersion of the flow and aerosol clouds has been considered in the past successful "2022 International Computational Fluid Dynamics Challenge on violent expiratory events" [2]. The objective of this Challenge was to determine the ability of Unsteady Reynolds Averaged Navier-Stokes (URANS) and Large-Eddy Simulation (LES) techniques to simulate the flow and the evaporative aerosol cloud dispersion generated just after the end of an isolated cough ejecting warm fluid into a quiescent colder ambient. Seven research groups from 6 different countries presented 12 different simulations of the same flow configuration using URANS, LES and/or hybrid techniques. The comparison of some dispersion metrics of the particle cloud with the reference Direct Numerical Simulation (DNS) showed that, in general, URANS and LES underpredict the vertical mixing of the thermal puff and the particle cloud.

The aerosol indoor dispersion process just after the violent expiratory events, which have a typical duration of 0.5 s [3], has short length-scales, of the order of 1 m, and short time-scales, typically, of about 2s. After this time, the decaying jet velocities are reduced to the values of the background air currents and the dispersion process within the indoor space is governed by the forced or natural ventilation system. The relevant length-scale of the subsequent dispersion of the aerosol cloud is the dimension of the room and the time-scales depend strongly on the type and intensity of the ventilation. As the natural continuation of the past CFD Challenge, focused on the short-term dispersion, this new edition is directed towards the determination of the accuracy of the RANS and LES techniques to predict the long-term dispersion of aerosol clouds in an indoor environment produced by a pure natural convection turbulent flow enclosed in a prototypical cubical room. Existing DNS results are used as reference data. The focus of the comparison is focused on the performance of RANS and LES for predicting correctly (1) the time-averaged flow field and the spatial distribution of the turbulent kinetic energy and (2) the dispersion velocity of different aerosol clouds released in different locations of the cubical room.

2. Physical and mathematical model

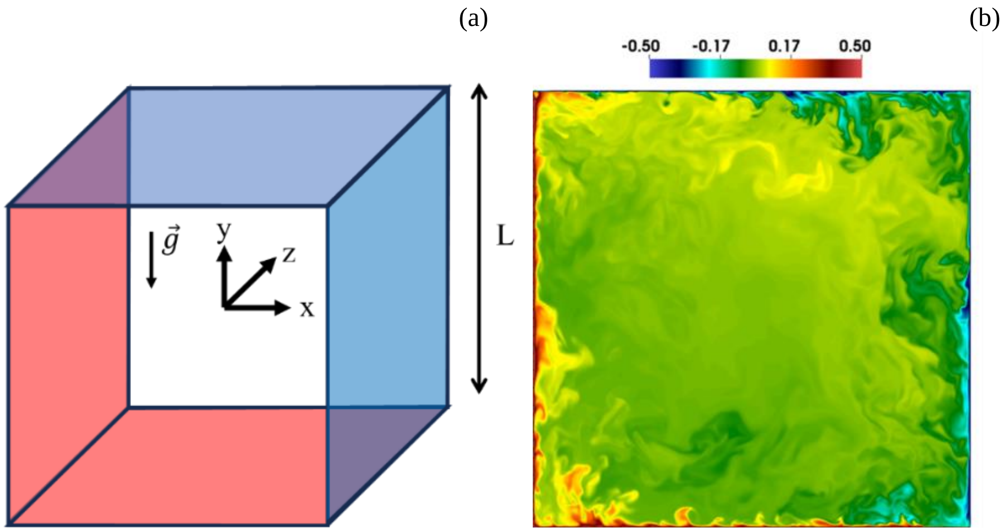

Figure 1. (a) Physical model. (b) Instantaneous contours of non-dimensional temperature ($\theta = \frac{T-T_0}{T_H-T_C}$) on the vertical symmetry plane of the cavity ($z = 0$).

We examine the dispersion of solid micron-sized spherical particles within a turbulent natural convection flow occurring in a three-dimensional room-sized cubic cavity. This physical model of the cubic cavity, measuring $L = 2.5\,m$, is depicted in Figure 1a along with the Cartesian coordinate system used. In this setup, the lower and the vertical rear walls are kept at constant and uniform temperature (T_H), which is higher than the constant and uniform temperature (T_C) of the upper and the front vertical opposite walls. The other two vertical sidewalls are assumed to be perfectly adiabatic. The fluid being used is air at ambient pressure and temperature (T_0=$(T_H + T_C)/2$). The physical properties of the fluid are considered constant with respect to temperature, except for density, according to the Boussinesq approximation. The Rayleigh number (Ra), calculated as $Ra = g\beta(T_H - T_C)\,L^3/\nu\alpha$, and the Prandtl number (Pr), defined as $Pr = \nu/\alpha$, have values of $3.6 \cdot 10^9$ and 0.7, respectively.

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To generate the DNS database, the governing equations are numerically solved using NEK5000 [Deville, 2003], an open-source, high order spectral element method-based solver. The computational grid, with a total of approximately 300 million nodes, ensuring explicit resolution of all spatial scales according to the resolution criteria proposed by Scheel et al. [2013] for turbulent Rayleigh-Bénard flows. The minimum and maximum grid cells are $\Delta x_{min} = \Delta y_{min} = \Delta z_{min} = 1.4 \cdot 10^{-4} L$ and $\Delta x_{max} = \Delta y_{max} = \Delta z_{max} = 3.3 \cdot 10^{-3} L$, respectively. Lagrangian Tracking of individual particles under the one-way coupling hypothesis is used to analyze the particle dispersion.

As an illustration of the turbulent natural convection flow, Figure 1b displays non-dimensional temperature contours on the $z = 0$ plane (see Fig. 1a). This flow exhibits a main upward motion near the left warm vertical sidewall and a downward motion near the right cold wall, resulting in a large-scale circulation pattern within the cavity. One can observe ascending and descending plumes near the lower hot wall and the upper cold wall, respectively. Thin thermal boundary layers are attached to the thermally active walls. This particular flow configuration was chosen because the orientation and direction of fluid rotation within the large-scale circulation are fixed and determined by the thermally active vertical walls. This is in contrast to the classical Rayleigh-Bénard problem in a cubic cavity, heated from below and cooled from above, with the remaining vertical walls being adiabatic. In that scenario, the large-scale circulation changes orientation at a very low frequency (Valencia et al. 2007). Additionally, at this high Rayleigh number, the thermal boundary layers on the horizontal walls are fully turbulent, while those attached to the thermally active vertical walls, although unsteady, are primarily laminar [Lavrinenko et al. 2023].

Participants of the Challenge are encouraged to conduct flow simulations using their preferred computational fluid dynamics (CFD) software, utilizing any of the available turbulence modeling techniques (such as RANS, LES, or RANS-LES hybrid methods). A mesh independence test is required to select an adequate grid resolution for the simulation.

We are investigating the unsteady dispersion of two clouds of solid particles, when the flow is statistically fully developed. Initially, both clouds have a spherical shape with a dimension of $D_c = 0.5\, m$. Cloud #1 is located near one of the lower corners of the cavity, where the hot horizontal and vertical walls intersect, while Cloud #2 is situated at the geometric center of the cavity. The coordinates of the cloud centers, relative to the coordinate system depicted in Figure 1, are as follows: for Cloud #1, $x_{c1} = y_{c1} = z_{c1} = -1\, m$, and for Cloud #2, $x_{c2} = y_{c2} = z_{c2} = 0$. The particles are assumed to be perfectly spherical with a constant diameter ($d_p = 0.5\, \mu m$) and a density of $\rho_p = 1350\, kg/m^3$. The number of particles in each cloud should be larger than 1000.

The turbulent dispersion of these clouds is determined by tracking the time evolution of the mean squared distance between particles belonging to a specific cloud, defined as follows:

$$D_{xyz}^2 = \frac{1}{N} \sum_{i,j} \left(\left[x_i - x_j\right]^2 + \left[y_i - y_j\right]^2 + \left[z_i - z_j\right]^2 \right) \quad (1)$$

where x, y, and z represent the coordinates of the position of the particles, and N is the number of all possible particle pairs. The value of D_{xyz}^2 for a large number of particles uniformly distributed in a cube of dimension is $D_{xyz}^2 = L^2/2$. The mean squared distance within the plane of rotation of the large-scale circulation (D_{xy}^2) and the mean squared distance along the perpendicular direction of the plane of rotation (D_z^2) are defined as

$$D_{xy}^2 = \frac{1}{N} \sum_{i,j} \left(\left[x_i - x_j\right]^2 + \left[y_i - y_j\right]^2 \right) \quad (2)$$

and

$$D_z^2 = \frac{1}{N} \sum_{i,j} \left(\left[z_i - z_j \right]^2 \right) \tag{3}$$

Participants are required to submit the distribution of the time-averaged velocity, time-averaged temperature and turbulent kinetic energy on the planes $x = 0$, $y = 0$ and $z = 0$. To evaluate the performance of the turbulence model on the prediction of the particle dispersion the time evolutions of D_{xyz}^2, D_{xy}^2 and D_z^2 for the two clouds considered are also required. These data submitted by the different teams will be compared among the participants and with the reference DNS. As an example, Figure 2 shows the time evolution of D_{xyz}^2, predicted by the DNS, for the two clouds considered.

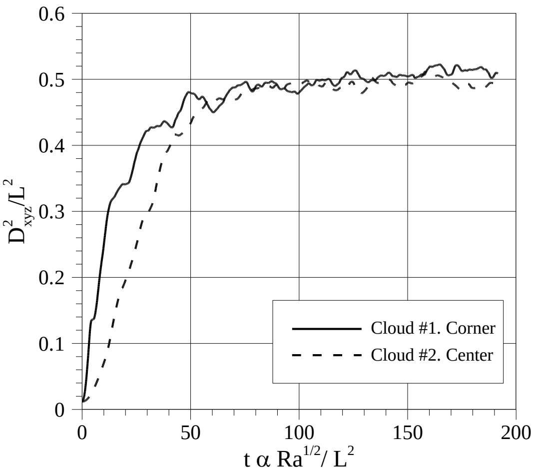

Figure 2. Time-evolution of the mean squared distance.

It can be seen that the cloud initially located near the corner of the cavity (Cloud#1) mixes faster than the cloud released at the center (Cloud#2). When the non-dimensional time reaches a value of 100, corresponding to a dimensional time of about 450 s, the particles of both clouds are essentially uniformly distributed within the cavity.

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