Droplet nuclei distribution in exhaled vortex rings. Study of caustic formations with the second order Fully Lagrangian Approach.

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Vortex ring structures occur in light or hoarse cough configurations. These instances consist of short impulses of exhaled air resulting to a self-contained structure that can travel great distances. In this study we investigate the clustering of droplets and droplet nuclei exhaled in ambient air in conditions akin to light cough. The carrier phase flow field is resolved by means of second order accurate Direct Numerical Simulation (DNS) based on finite difference approach for the momentum equations. The Poisson equation is resolved using Fast Fourier Transform (FFT). The second order Fully Lagrangian Approach (FLA2) is utilised for the solution of the particle dispersion. The evaluation of the higher order derivatives needed by the FLA2 is achieved by pre-fabricated least squares second order interpolations in the three dimensions. The higher moments provided by FLA2 represent the dispersed continuum by deformed spheroids. Given the ambiguous conditions conditions of vortex-ring formation during cough instances three different formation numbers are assummed, i.e. $U*T/D=2$ for under-developed VRs , ideal VRs (3.7) and overdeveloped VRs (6).

I. INTRODUCTION

According to Simha et al.[5] vortex rings produced by coughs can enhance the transport offine cough droplets. Vortex ring structures occur in light or hoarse cough configurations. These instances consist of short impulses of exhaled air resulting to a self-contained structure that can travel great distances. The importance of vortex rings in viral transmitions has been exhibited by Dhanak et. al[4].

In order to simulate the generation of VRs in coughs, we use a nominal cough velocity of $U_0 = 5m/\mathrm{sec}$ which is within the bounds for cough measurements[1,5]. Assumming an orifice opening of $D = 410^{-}4m^2$ (see Bourouiba et al.[2]) and a kinematic viscosity $\nu = 1810^6 m^2/2$, the Reynolds number of the flow,

$$Re = \frac{U_0 D}{\nu}\,, \tag{1}$$

is equal to $Re = 5555.5$. The characteristic time of the flow $t_0 = D/U_0$ is equal to $4m\mathrm{sec}$. While the injection time T is related to the formation number n as:

$$n = \frac{1}{D}\int_{t=0}^{t=T} U(t)dt \sim U_0 T/D\,, \tag{2}$$

where $U(t)$ is the injection profile

$$U(t)/U_0 = \begin{cases} 3\left(\frac{t}{0.2T}\right)^2 - 2\left(\frac{t}{0.2T}\right)^3, \text{if } x < 0.2T \\ 1, \text{if } 0.2T < x < 1.4T \\ 3\left(\frac{1.6T-t}{0.2T}\right)^2 - 2\left(\frac{1.6T-t}{0.2T}\right)^3, \text{if } 0.14T < x < 1.6T \\ 0, 0.16T < x \end{cases} \tag{3}$$

The exhaled droplet and droplet nucleii relaxation time τ_0 is defined as:

$$\tau_0 = \frac{\rho_{air} d^2}{18\nu}\,, \tag{4}$$

and for the conditions of the present study the relaxation time is $\tau_0 = 3m\mathrm{sec}$ assumming a droplet diameter equal to 10μm. Droplet size distributions are provided[6] in Table II. The cough volume has been measured by Bourouiba, Dehandschoewercker, and Bush [2], in the range $0.25-1.25$lt. In our implementation care is taken to represent all droplet sizes by defining droplet nuclei parcels that correspond to $1/c$ droplets.

From the second order FLA the number density for each droplet size is obtained by the model equation

$$\hat{c} = \begin{cases} \frac{2c_0}{\sqrt{J^2+2HR_\varepsilon}+\sqrt{J^2-2HR_\varepsilon}} & \text{if } J^2-2HR_\varepsilon > 0 \\ \\ \frac{c_0\sqrt{J^2+2HR_\varepsilon}}{2R_\varepsilon H} & \text{if } J^2-2HR_\varepsilon < 0\,. \end{cases} \tag{5}$$

As a function of the initial number density assigned to the parcel c_0.

TABLE I. Flow conditions for cough in literature

Author	u	D	T	d
Simha et al.[4]	$2m/\mathrm{sec}$-$6m/\mathrm{sec}$	-	-	10μ
Burbuida et al.[2]	-	2cm	-	-
Duguid[6]	-	-	-	-
Tang et al.[1]	2-25m/sec	-	-	2μ m

TABLE II. Droplet size distribution N as number of nucleii per cough.

Bin	1	2	3	4	5	6	7	8	9	10
d	2	4	8	16	24	32	40	50	75	100
St	$7.5^{-}4$	0.05								7.7
n	50	290	970	1600	870	420	240	110	140	85
c	50	290	970	1600	870	420	240	110	140	85
α	50	290	970	1600	870	420	240	110	140	85

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TABLE III. Cases simulated

Name	Domain size	$n\theta \times nr \times nz$	T ($m$sec)	n	Re	T_{CPU} on 32 Cores
C2DN2	$2D \times 16D$	$1 \times 512 \times 4096$	8sec	2	5555,5	$< 12h$
C2DNI	$2D \times 16D$	$1 \times 512 \times 4096$	14.8	3.7	5555,5	$< 12h$
C2DN8	$2D \times 16D$	$1 \times 512 \times 4096$	32	4	5555,5	$< 12h$
C3DNT	$1D \times 2D$	$513 \times 256 \times 512$	8	2	5555,5	$12h$
C3DN2	$2D \times 4D$	$513 \times 512 \times 1096$	8	2	5555,5	$48h$
C3DNI	$2D \times 4D$	$513 \times 512 \times 1096$	14.8	3.7	5555,	$4days$
C3DN8	$2D \times 8D$	$513 \times 512 \times 2096$	32	4	5555,5	$16days$

II. METHOD

The carrier phase flow field is resolved by means of second order accurate Direct Numerical Simulation (DNS) based on finite difference approach for the momentum equations. The Poisson equation is resolved using Fast Fourier Transform (FFT).

The second order Fully Lagrangian Approach (FLA2) is utilised for the solution of the particle dispersion.

The evaluation of the higher order derivatives needed by the FLA2 is achieved by pre-fabricated least squares second order interpolations in the three dimensions. The higher moments provided by FLA2 represent the dispersed continuum by deformed spheroids.

Given the ambiguous conditions conditions of vortex-ring formation during cough instances three different formation numbers are assummed, i.e. $U * T/D = 2$ for under-developed VRs , ideal VRs (3.7) and overdeveloped VRs (6).

The cases simulated are provided in the Table III. Cases C2DN2,C2DNI and C2DN8 are two-dimensional axisymmetric simulations of exhaled VRs that allow for the resolution of long injection times and longer transport distances. Each one of those cases corresponds to different formation numbers allowing to calculate the encapsulation of particles within the VR in relation to the particles left back in the jet core.

Cases C3DN2,C3DNI and C3DN8 are three dimensional turbulent simulations of exhaled VRs that allow for the resolution of the finest turbulent scales ($\Delta x = 0.0039D \sim 2\eta = Re^{-3/4}D$), for the three different formation numbers as in the two-dimensional cases. The three-dimensional cases are of increasing computational cost due to the increase of the computational domain but also the required simulation time, given that for greater formation numbers the injection period T is longer.

The vorticity contour for the test case C3DNT is shown in the Figure 1.

[3456].

III. RESULTS

IV. CONCLUSION

ACKNOWLEDGMENTS

Appendix A: Appendixes

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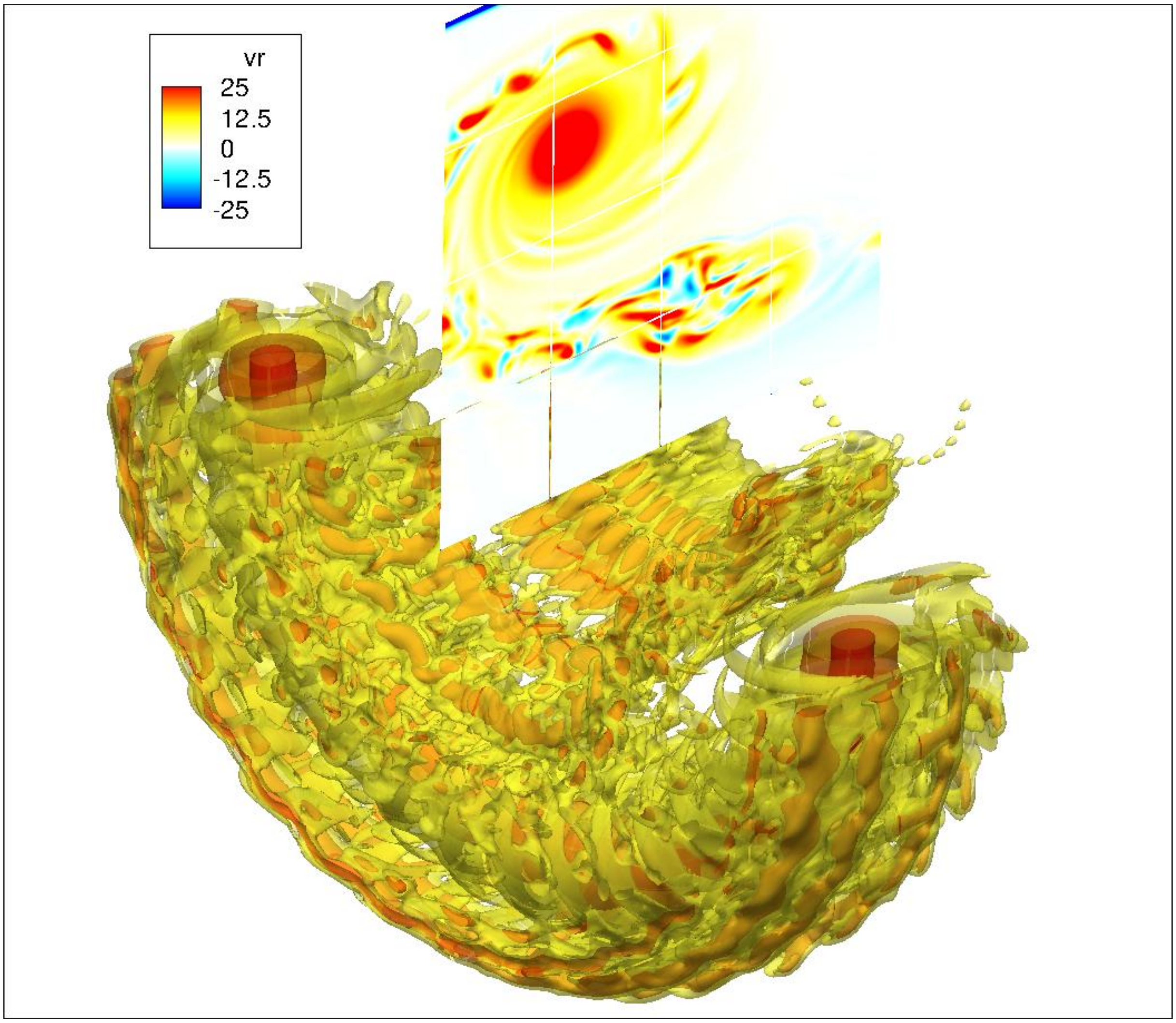

FIG. 1. Vorticity contour for the test case C3DNTU.