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Andreas Papoutsakis (✉ andreas.papoutsakis@city.ac.uk)

City University of London

Manolis Gavaises

City University of London

Research Article

Keywords: impulses, exhaled, Fully Lagrangian Approach, Fast Fourier Transform

Posted Date: August 17th, 2021

DOI: <https://doi.org/10.21203/rs.3.rs-784401/v1>

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Version of Record: A version of this preprint was published at Scientific Reports on March 10th, 2022. See the published version at <https://doi.org/10.1038/s41598-022-07717-z>.

Droplet nuclei caustic formations in exhaled vortex rings

Andreas Papoutsakis^{1,*} and Manolis Gavaises¹

¹City University of London. School of Mathematics, Computer Science and Engineering, Department of Mechanical Engineering and Aeronautics, London, EC1V 0HB, UK.

*andreas.papoutsakis@city.ac.uk

+these authors contributed equally to this work

ABSTRACT

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 large distances. The present study is the first implementation of the second order Fully Lagrangian Approach (FLA) for three-dimensional realistic flow-fields obtained by means of Computational Fluid Dynamics (CFD) and provides a method to calculate the occurrence and the intensity of caustic formations.

The carrier phase flow field is resolved by means of second order accurate Direct Numerical Simulation (DNS) based on a Finite Difference approach for the momentum equations, while a spectral approach is followed for the Poisson equation using Fast Fourier Transform (FFT). The effect of the undulations of the carrier phase velocity due to large scale vortical structures and turbulence is investigated. The evaluation of the higher order derivatives needed by the second order FLA is achieved by pre-fabricated least squares second order interpolations in the three dimensions.

The method allows for the simulation of the clustering of droplets and droplet nuclei exhaled in ambient air in conditions akin to light cough. Given the ambiguous conditions of vortex-ring formation during cough instances, three different formation numbers $n = UT/D$ are assumed, i.e. under-developed ($n = 2$), ideal ($n = 3.7$) and over-developed VRs ($n = 6$). The formation of clusters results in the spatial variance of the airborne viral load. This un-mixing of exhaled aerosols is related to the formation of localised high viral load distributions that can be linked to super-spreading events.

Introduction

Respiratory infections can be transmitted through droplets ($> 5\mu\text{m}$) and droplet nuclei ($< 5\mu\text{m}$)¹⁻³. According to the World Health Organization (WHO) report² COVID-19 in particular, is primarily transmitted through droplets and contact⁴⁻⁶. The airborne route is a potentially important transmission pathway for viral infection in indoor environments since contact transmission can be limited by fast inactivation of the virus on hands. Furthermore, contact transmission often incorporates an initial airborne path where large inocula droplets deposit on surfaces through sneezing⁷. The interaction of the carrier phase flow field with the exhaled droplets dictates the intensity of the viral load and the infection distance. Recent research⁸⁻¹⁰ has shown that vortex rings can be produced in coughs and can enhance the transport of fine cough droplets. Vortex ring structures occur in light or hoarse cough configurations⁸. These instances consist of short impulses of exhaled air result to a self-contained structure that can travel large distances. Increased concentrations of airborne viral loads have been related to super-spreading events¹¹, and have been attributed to individual behaviours of coughing and sneezing¹² and specific activities¹³.

Turbulence results in the mixing of droplets and droplet nuclei¹⁴ and in the increase of settling velocity^{15,16}. As the droplet size and Stokes number increases, the particle trajectory memory becomes pronounced; thus, un-mixing^{17,18} and Random Uncorrelated Motion (RUM)¹⁹ are also observed. Un-mixing results in the segregation of droplets by a preferential concentration, clustering mechanism²⁰. Clustering is exhibited as the formation of narrow local droplet accumulation regions in the zones of low vorticity and high strain rate²¹ and have been associated with zero-acceleration points²². For high Stokes number regimes, inertia droplets sample the carrier phase velocity field as a white noise²³, in an ergodic fashion, forming clusters due to a multiplicative amplification mechanism²³⁻²⁵. This multiplicative process of amplification and dilatation was identified by¹⁹ as the deformation of the Lagrangian volume of the dispersed phase²⁶ transported along a particle trajectory. The Lagrangian volume may vanish, giving rise to instantaneous singularities in the particle concentration field identified as caustics or caustic formations. In the same work¹⁹, in addition to mixing and un-mixing (clustering), RUM was identified as a third type of characteristic response of the dispersed phase in turbulent flows, applicable to all Stokes numbers. The occurrence of RUM was linked with the occurrence of singularities due to trajectory intersections related to the trajectory history. Particle motion, as the overlapping of a mesoscopic smoothly varying component and RUM, was identified in²⁷⁻²⁹. RUM results in a multi-valued velocity field of the dispersed phase due to the folding of the dispersed continuum, playing a significant role in

collision processes.

The intensity of caustics is important to a great variety of environmental, biological, engineering and cosmological^{30–34} flows, (e.g. environmental pollution³⁵, the impact of radioactive particles³⁶ and the potency of spray delivered medication³⁷, are strongly dependent on the formation of such accumulation regions³⁸, and recently has become the focus of experimental³⁹ and theoretical work⁴⁰. The Fully Lagrangian Approach, (FLA or Osipov method)⁴¹, treats the particulate phase as a pressureless continuum⁴⁰, by introducing the Jacobian matrix determinant $|\mathbf{J}|$ (i.e. $\rho_0 = |\mathbf{J}|$)⁴². Thus, continuous fields for the particle number density and the particle velocity can be defined on the Lagrangian dispersed continuum. Due to the absence of pressure, the continuum can intersect itself creating overlapping folds. Particle collisions may occur among particles that are attached to overlapping folds⁴³, thus a low particle loading constrained needs to be incorporated in order to support the pressureless continuum assumption. The use of the FLA in turbulent flows^{19,44} resulted in the identification of the concentration distribution and the identification of the mechanisms involved in the segregation process^{18,19}. A turbulent diffusion model was introduced for the First order FLA, implemented for numerical experiments in homogeneous isotropic turbulence where the modelling of turbulent diffusion was exhibited and assessed in comparison with DNS simulations using a standard Lagrangian approach for the dispersed phases⁴⁵. In the same paper it was also exhibited that the singularities of the point wise number density inferred from the standard FLA infects the spatially averaged results. A second order closure was presented for the spatially filtered number density was presented, where the FLA number density was interpreted alongside with the spatial structure of the dispersed continuum, and was connected to a length scale⁴⁰.

The introduction of the FLA into the study of turbulent flows⁴⁴ resulted in the identification and analysis of spatial structures of the dispersed phase distribution using the moments of concentration. The analysis by¹⁹ showed that the distribution of the particle concentration in the long term is log normal. This is consistent with the analysis by⁴⁶ where, using Voronoï tessellation, the authors observed the same log normal distribution. Also, FLA studies on DNS of homogeneous and isotropic turbulence led to identification of the mechanisms involved in the segregation process^{18,19}. The introduction of the FLA in the study of turbulent flows resulted in the quantification of the singularities related to trajectory intersections and the establishment of a relation between the frequency of their occurrence and the Stokes number.

In this paper we present the first implementation of the second order Fully Lagrangian Approach (FLA) for three-dimensional realistic flow-fields obtained by means of Computational Fluid Dynamics (CFD) and provides a method to calculate the occurrence and the intensity of caustic formations. This is achieved by calculating a principal direction of the caustic front based on the tensor of the Hessian of the deformed continuum. The structure of the paper is as follows. The range of the conditions and the configuration of the cases studied are presented in the Results section. In the same section the FLA and the FLA2 results are presented and discussed. Specifically, the solution of the number density for the exhaled Lagrangian clouds is presented for low-Re two dimensional and also high-Re fully turbulent configurations, for three distinct formation numbers. In the Method section the implementation of the FLA2 for CFD configurations is presented and the results are further discussed in the Discussion section. The DNS methodology and the implementation of the second order FLA for three-dimensional turbulent flow fields is presented in the Supplementary Material.

Results

In order to investigate the occurrence of caustics of droplet nuclei in coughs due to large scale vortical structures and due to turbulence we performed a series of DNS of cough configurations. Scope of this analysis is the calculation of the droplet distribution, the investigation of the occurrence of caustics and finally the calculation of the intensity of the droplet nuclei clustering. The exhaled droplet nuclei distribution is modelled by solving for representative droplet clouds using a standard Lagrangian approach based on the fully resolved carrier phase flow field. The number density of the droplet nuclei for each representative cloud is calculated using the Fully Lagrangian Approach^{26,47} also highlights the occurrence of caustics. The second order FLA is used to calculate the intensity of the caustics by providing a measure of the number density at a given length-scale. The numerical implementation of the method is described in detail in the supplementary material of this paper.

Cases setup

Given the ambiguous conditions of the human coughs as described in literature^{8,10,48,49} we focus in simulations within the limited vortex ring formation period, assuming Reynolds and Stokes numbers related to human cough conditions. Vortex rings form during injection impulses with a finite duration T in an ambient medium. The resulting vortex ring for an average injection speed U issuing from an orifice with diameter D is characterised by the formation number $n = TU/D$. Long duration of exhalation impulses as the ones observed in a typical cough result to large formation numbers (i.e. $n > 100$), which lead to the formation of jets. The formation number n is related to the temporal injection profile and the average injection velocity U_0

Table 1. Flow conditions for cough in literature

Author	u	D	T	d
Simha et al. ¹⁰	2m/sec-6m/sec	-	-	10 μ
Burbuida et al. ⁵⁰	-	2cm	-	-
Tang et al. ⁵¹	2-25m/sec	-	-	2 μ m

Table 2. Cases simulated

Name	Domain size	$n\theta \times nr \times nz$	T (msec)	n	Re
C2DN2	$2D \times 4D$	$1 \times 512 \times 4096$	4	2	1000
C2DN4	$2D \times 8D$	$1 \times 512 \times 4096$	8	3.7	1000
C2DN6	$2D \times 12D$	$1 \times 512 \times 4096$	12	6	1000
C3DN2	$1.5D \times 3D$	$513 \times 256 \times 512$	4	2	10000
C3DN4	$1.5D \times 6D$	$513 \times 256 \times 1024$	8	3.7	10000
C3DN6	$1.5D \times 9D$	$513 \times 256 \times 1536$	12	6	10000

as:

$$n = \frac{1}{D} \int_{t=0}^{t=T} U(t) dt \sim U_0 T / D, \text{ where } U(t) \text{ is the injection profile } U(t)/U_0 = \begin{cases} 3 \left(\frac{t}{0.2T} \right)^2 - 2 \left(\frac{t}{0.2T} \right)^3, & t < 0.2T \\ 1, & 0.2T < t < 1.4T \\ 3 \left(\frac{1.6T-t}{0.2T} \right)^2 - 2 \left(\frac{1.6T-t}{0.2T} \right)^3, & 0.14T < t < 1.6T \\ 0, & 0.16T < t \end{cases} \quad (1)$$

A coarse estimate for the formation number of a cough can be derived from the volume V of the air exhaled $V = \pi/4 T U D^2$, as $n = TU/D = 4V/\pi D^3$. The typical exhaled volume from a cough has been calculated in the range of 0.25 to 1.25 litres^{9,50}. Thus, the formation number for coughs at this exhaled volume range spans from $n = V/D^3 = 40$ to 199, assuming a mouth opening of 0.02m. Such high formation numbers correspond to jets rather than vortex rings with short trails. Given the evidence of vortex rings in coughs, however, in cases of intermittent inlet conditions⁸⁻¹⁰, it is legitimate to focus in the narrow region of exhalation regimes characterised by low formation numbers which indeed correspond to the formation of vortex rings rather than fully developed jets. Specifically, three different formation numbers $n = UT/D$ are assumed, i.e. $n = 2$ for under-developed vortex rings, $n = 3.7$ for ideal vortex rings and $n = 6$ for overdeveloped vortex rings.

The nominal exhale velocities range between $U_0 = 1\text{m/sec}$ to $U_0 = 10\text{m/sec}$ which include experimentally measured coughs^{8,51} and breathing scenarios³. The Reynolds numbers reported vary between $Re = 1000$ and $Re = 16000$ ^{3,50}. A synopsis of the aerodynamic conditions of coughs as presented in the literature is shown in the table 1. A typical value of the orifice diameter is 2cm ($D^2 = 4 \cdot 10^{-4} \text{m}^2$ ⁵⁰) while a reasonable choice of the air kinematic viscosity is $\nu = 18 \cdot 10^{-6} \text{m}^2/\text{sec}$. In our simulations we selected two representative set of cases characterised by a low Reynolds number $Re = \frac{U_0 D}{\nu} = 1000$ (two dimensional laminar simulations) and a high Reynolds number set of cases with $Re = 10000$ (three dimensional laminar simulations).

For the droplet size distribution used in our simulations we used eight bins of representative particles with diameters from 0.5 μm to 100 μm in accordance to droplet nuclei sizes reported in literature^{3,49,50}. The laminar two dimensional simulations $Re = 1000$ correspond to $U_0 \sim 1\text{m/sec}$ and a characteristic time of the flow $t_0 = D/U_0 \sim 20\text{msec}$, the fully turbulent three-dimensional simulations $Re = 10000$ to $U_0 \sim 10\text{m/sec}$ and $t_0 \sim 2\text{msec}$. For the three-dimensional turbulent simulations the sinusoidal fluctuations described in the supplementary material were superimposed on the inlet velocity profile shown in 1, assuming $k_T = 0.1$ and $\varepsilon_T = 1$. The details of the transitional and fully turbulent simulations carrier out in our analysis are presented in the Table 2.

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

$$\tau_0 = \frac{\rho_d d^2}{18\mu_{air}}, \quad (2)$$

where, ρ_d is the droplet density and μ_{air} is the carrier phase dynamic viscosity and d is the droplet size. The range of droplet sizes simulated in our analysis are provided⁴⁹ in Table 3.

In our implementation care is taken to represent all droplet sizes by defining droplet nuclei parcels that correspond to $1/c$

Table 3. Droplet sizes and Stokes numbers used in the simulations.

Bin d (μ m)	1 0.5	2 1	3 2	4 5	5 10	6 20	7 50	8 100	$\delta_{0,\tau}$
St (Re=1.0 · 10 ³)	2.89e-05	1.16e-04	4.62e-04	2.89e-03	1.16e-02	4.62e-02	0.289	1.16	93.0 μ m
St_t (Re=1.0 · 10 ³)	9.13e-04	3.65e-03	1.46e-02	9.13e-02	0.37	1.46	9.13	36.5	16.5 μ m
St (Re=10.0 · 10 ³)	2.89e-04	1.16e-03	4.62e-03	2.89e-02	0.116	0.462	2.89	11.6	29.4 μ m
St_t (Re=10.0 · 10 ³)	2.89e-02	0.116	0.462	2.89	11.6	46.2	289.0	1155.0	2.94 μ m

droplets. The Stokes number of the particles $St = \tau_0 U / D$, is:

$$St = \frac{\rho_d}{18\rho_{air}} D_d^2 Re, \quad (3)$$

where $D_d = d/D$ is the non-dimensional droplet diameter. Droplet clustering occurs for local Stokes numbers greater than unity $St_t > 1$. Based on the macroscopic timescale D/U a critical diameter d_0 is defined as:

$$\delta_0^2 = \frac{18\rho_{air}}{\rho_d} Re^{-1}, \quad (4)$$

while for the turbulent time scales $D/URe^{-1/2}$ the Stokes number is defined as $St_t = \tau_0 U / (DRe^{-1/2})$ resulting to a critical diameter d_t defined as:

$$\delta_t^2 = \frac{18\rho_{air}}{\rho_d} Re^{-3/2}. \quad (5)$$

Droplets with diameter $d > \delta$ are expected to exhibit trajectory crossing³⁹. In our simulations we assume a range of droplet nuclei dimensions from 0.5 μ m up to 100 μ m. The critical droplet diameters δ_0 and δ_t for the macroscopic and the turbulent time scales are shown in last column of Table 3. In the same table we present the droplet nuclei characteristics for the eight (8) distinct representative sets of parcels (bins) issued during the cough simulation. As it can be deduced from Table 3 the selected diameters for the representative droplet nuclei parcels result in a wide range of Stokes numbers from nearly non-inertia droplets (i.e. $St < 10^{-3}$) to droplets well within the ballistic regime (i.e. $St > 10$)⁵² for the specific conditions of the flows simulated.

Droplet nuclei distribution

For the cases provided in the Table 2, C2DN2, C2DN4 and C2DN6 consist of two-dimensional axis-symmetric simulations of exhaled vortex rings that allow for the resolution of long injection times and longer transport distances. Each one of those cases corresponds to different formation numbers resulting to different ratios of droplet nuclei encapsulated within the vortex rings in relation to the particles left behind in the jet core. Cases C3DN2, C3DN4 and C3DN6 are three dimensional turbulent simulations of exhaled VRs that allow for the resolution of the finest turbulent scales ($\Delta x = 0.0039D \sim 2\eta = Re^{-3/4}D$). The three-dimensional cases are of increasing computational cost due to the larger computational domain and the increased simulation time as the formation number increases.

The vorticity magnitude iso-surfaces for the three-dimensional cases C3DN2, C3DN4 and C3DN6 are shown in the Figure 1 at times nT after the end of the injection (i.e. $t = 2nT$, where for the cases with $n \leq 3.7$ the flow field vorticity has been almost completely absorbed by the VR. The corresponding distribution of droplets with $d = 2\mu$ m at the same instances is shown in Figure 2. As it can be inferred from Figure 2 the vortex rings with $n = 2$ and $n = 3.7$ present a thin trail of droplets along the trail of the vortex rings. For $n = 6$ the trailing droplet nuclei are significant and lag the evolution of the VR. This results to the dilation of the trailing droplets as they lag behind expressed by the low number densities shown in blue.

In Figures 3 to 4 we present the FLA results for the number density and the FLA2 result for various filtering widths R_ϵ ; for droplets with diameters 2 μ m and 5 μ m respectively. The filtering widths correspond to different orders of magnitude from $R_\epsilon = 10^{-4}D$ to $R_\epsilon = 10^{-2}D$ which correspond to filter sizes from 2 μ m to 0.2mm. It can be observed that qualitatively, the solution converges to the FLA solution as R_ϵ tends to zero. For the larger filtering lengths the areas in the proximity of caustic regions are affected resulting to variations between FLA and FLA2 at larger areas as the filtering width increases.

Caustics occurrence

The quantitative comparison of the FLA2 results with the point wise number density provided by FLA is shown in the figures 5 to 7 for the three-dimensional DNS simulations at times $T = 2nT_0$, where n is the formation number. The droplet nuclei with low inertia $St_t < 1.0$ (see Table 3) show number densities below $10n_d^0$ and no caustic formations are observed since the volume filtered number density $\hat{n}_d$ does not deviate from the point wise number density $n_d = 1/J$ (see Figures 5 to 7 (a)-(c)).

Figure 1. Vorticity contour for the test cases C3DN2 (top) C3DN4 (middle) and C3DN6 (bottom) at time $t = 2nT$ equal to twice the formation period nT for each one of the cases simulated.

Figure 2. FLA number density for $d = 2.0 \mu\text{m}$ droplet nuclei. C3DN2 (top) C3DN4 (middle) and C3DN6 (bottom) at time $t = 2nT$ equal to twice the formation period nT for each one of the simulations shown.

Figure 3. Number density for $d = 2.0\mu\text{m}$ droplet nuclei. Case C2DN2. $T = 4\text{msec}$ (a) FLA (b) FLA2 $R_\epsilon = 0.01$ (c) FLA2 $R_\epsilon = 0.001$ (d) FLA2 $R_\epsilon = 0.0001$.

Figure 4. Number density for $d = 5.0\mu\text{m}$ droplet nuclei. Case C2DN2. $T = 4\text{msec}$ (a) FLA (b) FLA2 $R_\epsilon = 0.01$ (c) FLA2 $R_\epsilon = 0.001$ (d) FLA2 $R_\epsilon = 0.0001$.

This behaviour presents a global character for all formation numbers simulated as shown in all three Figures 5 to 7. For the droplets above the critical diameter $2.94\mu\text{m}$ the turbulent time scale Stokes number St_t becomes larger than unity as shown in the table 3 and this arises as a significant deviation of the FLA2 filtered number density from the FLA result (see Figures 5 to 7 (d)-(h)). The same behaviour is shown in the droplet nuclei conveyed by the laminar flow field in the low-Re case C2N2 shown in the figure 8. For the laminar flow field case the limiting values for the number densities appear in the plots 8 (f)-(h) which correspond to droplets with diameter larger than the critical diameter shown in Table 3.

Caustics intensity

From figures 5(f) to 7(f) it can be observed that at a length scale $R_\epsilon = 10^{-5}$ a limiting maximum for the number density appears at $20n_d^0$, at a larger length scale ($R_\epsilon = 0.0001$) this limit reduces to $10n_d^0$ and for $R_\epsilon = 0.001$, number densities higher than $3n_d^0$ are filtered out. For $R_\epsilon = 0.01$ this the highest limiting value reduces to $1n_d^0$. This limiting value at different length scales describes the intensity of the caustics providing a direct measure of the compression of the dispersed phase due to the large vortical structures of the flow but also on the effect of the turbulent scales on the compression and dilation of droplet nuclei. The VR seems to convey the droplet nuclei at large distances retaining the high initial number density of the exhaled plume n_d^0 at large distances from the orifice where it would have been expected to reduce due to the expansion of the cough jet.

Higher Stokes number nuclei present a ballistic behaviour⁵² which is characterised by high inertia particles moving on almost undisturbed trajectories. When crossing, these trajectories provide genuine Morse points with low J and low H thus the FLA2 and the standard FLA converge to very high number densities as shown in the figures 5(h), 6(h) and 7(h) where all points collapse on the $1/J$ curve.

In the Figures 8(a)-(h) we present the filtered number density scatter plot against the point-wise number density for the two dimensional simulations for the $n = 6$ formation number (i.e. case C2DN6 in Table 2). As shown in Table 3 the critical droplet nuclei diameter for the formation of caustics is $16.5\mu\text{m}$ which is in agreement with the appearance of a limiting maximum value for the filtered number densities shown in the figures 8(f)-(h). For the laminar cases, the predicted loading for the caustics reaches to $\hat{n}_d = 100$ for the smallest length scale shown (i.e. $R_\epsilon = 0.00001$). As expected the point-wise number density result (x-axis) is infected by singularities resulting to spurious point-wise number densities with $n_d > 10^4$. The much higher intensity of the caustics for the laminar case shown can be attributed to the lack of small scale fluctuations that are expected to disturb the caustic fronts and smooth their intensity.

Discussion and Conclusions

In this work we investigated the compression and dilation of droplet nuclei in vortex ring structures occurring in human cough configurations. These instances consist of short impulses of exhaled air, form at finite formation numbers dictated by the cough exhaled volume and the orifice diameter $n \sim V/d^3$, resulting to a self-contained structure that can travel large distances. Numerical simulations for turbulent and laminar configurations have been carried out. 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 and a spectral approach for the Poisson equation using FFT.

To obtain such predictions we developed and presented the implementation of the second order Fully Lagrangian Approach for Eulerian configurations of the method in the Computational Fluid Dynamics framework. The evaluation of the higher order derivatives needed by the second order FLA is achieved by pre-fabricated least squares second order interpolations in three dimensions and the primary direction of the caustics was calculated by means of Singular Value Decomposition.

The effect of the undulations of the carrier phase velocity due to large scale vortical and small scale turbulent structures on the concentration of exhaled nuclei and the corresponding viral load was investigated.

It was observed that the coherent vortical structures of the vortex ring as well as the turbulent fluctuations of the flow field induce significant caustic formations in agreement to the droplet nuclei Stokes number based on the smallest time scales of the flow. Furthermore, the intensity of the caustics was identified reaching up to 20 times the initial concentration for the turbulent cases and to 100 times the initial number density for the laminar configurations, at significant length scales ranging from $40\mu\text{m}$ to $400\mu\text{m}$, highlighting the smoothing effect of turbulent fluctuations to the intensity of the caustic fronts.

Eulerian CFD simulations⁵³ and Eulerian/Lagrangian approaches^{3,9} for coughing/breathing configurations in a variety of setups suggest the reduction of the number density of the exhaled droplets and droplet nuclei. In our work we observed instances of significant localised caustic formations³⁹ that result in high number densities sustaining or exceeding the initial number density of the droplet nuclei clouds when exhaled.

The following observations conclude our findings: i) The wake of the vortex ring conveys droplet nuclei resulting in the reduction of their number density.

ii) For the low formation number VR's studied, a significant amount of droplet nuclei is engulfed and conveyed within the VR.

Figure 5. Filtered FLA2 number density as a function of $1/J$. Case C3DN2. $T = 4msec$. (a)-(h) $D_d = 0.5\mu m - 100\mu m$

Figure 6. Filtered FLA2 number density as a function of $1/J$. Case C3DN4. $T = 8msec$. (a)-(h) $D_d = 0.5\mu m - 100\mu m$

Figure 7. Filtered FLA2 number density as a function of $1/J$. Case C3DN6. $T = 12\text{msec}$. (a)-(h) $D_d = 0.5\mu\text{m}-100\mu\text{m}$

Figure 8. Filtered FLA2 number density as a function of $1/J$. Case C2DN6. $T = 12\text{msec}$. (a)-(h) $D_d = 0.5\mu\text{m}-100\mu\text{m}$

- iii) The methodology proposed identifies the theoretical limit $St > 1$ for the formation of caustics for both laminar and turbulent simulations.
- iv) Even at significant length scales both the turbulent fluctuations and the macroscopic VR vortical structures result to high number densities sustaining or exceeding the initial number density of the droplet nuclei clouds when exhaled.
- v) The result for the laminar simulations showed increased intensity of the caustic fronts.

Methods

The carrier phase flow field is resolved by means of second order accurate Direct Numerical Simulation (DNS) which is also used for the integration of the laminar solution in a two-dimensional axis-symmetric domain. The droplet clouds are injected with the carrier phase velocity and the Jacobian and Hessian matrices are initialised according to the initial conditions of the initial value problem of the method⁴⁰ described in the supplementary materials. The droplet clouds are distributed uniformly along the radial and the azimuthal directions of the orifice. The instantaneous dispersed phase droplet number flow rate is integrated in time. The closest integer number of droplets is then emitted, while they are subtracted from the total influx integral.

The droplets are decomposed following the domain decomposition of the carrier phase computational domain. When crossing domains the droplet clouds are deleted and re-injected to the new partition. In order to avoid the re-allocation of memory addresses and retain the computational efficiency of memory arrays, erased particles result to empty memory entries which are re-used by newly injected droplet clouds.

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Acknowledgements

Author contributions statement

A.P. and M.G. contributed equivalently. All authors reviewed the manuscript.

Additional information

To include, in this order: **Accession codes** (N/A); **Competing interests** (The authors declare that they have no conflict of interest).

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