In-silico analysis of airflow dynamics and particle transport within a human nasal cavity
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Abstract

We present a numerical investigation of the airflow dynamics and droplet transport through an averaged human nasal cavity. The effect of droplet size and breathing rate on the deposition patterns are explored. The simulations reveal that smaller droplets penetrate deeper into the airway, whereas larger droplets agglomerate near the anterior portion of the nasal cavity. Increasing the flow rate augmented the penetration of the droplets. The complex interplay of the finite droplet size and the flow inertia decided the spatial deposition of the
droplets. The findings from this study demonstrate the efficacy of state-of-art simulation frameworks for targeting respiratory disorders.

**Keywords:** Computational fluid dynamics, lattice Boltzmann, nasal flow, droplet deposition

1. **Introduction**

The dynamics of airflow and droplet transport through a human nasal cavity has been extensively studied in recent years owing to its fundamental importance in understanding a plethora of respiratory diseases [1][2]. In the context of the present Covid-19 pandemic, investigations of respiratory flows have received a great deal of attention. Similar to other airborne viral diseases, penetration of the Severe Acute Respiratory Syndrome-CoronaVirus-2 (SARS-CoV-2) into the upper airways is the first step of the infection. It is widely believed that the CoV-2 virus is primarily transmitted through droplets released during respiratory secretions, such as coughing or sneezing [3]. These released droplets maybe inhaled during direct contact or proximity, which are subsequently transported along the nasal airway. It has been proposed in recent studies that the nasal epithelial cells are favorable sites for initiating response/interaction with the Covid virus [4]. The virus loaded droplets inside the nasal airway may get trapped in the nasal mucosa. Subsequently, the virus may cross the mucosal interface and locate the appropriate molecular receptors, thereby initiating infection. Additionally, the SARS-CoV-2 is believed to be able to cross over the neural-mucosal interface in the olfactory region, thereby gaining access to the central nervous system [5]. Thus, it is of paramount importance to understand the dynamics of transport of these droplets during respiration, in an effort to predict the disease transmission and devise suitable methods for treatment. This knowledge can thus indicate how to protect us against air-borne infections and, at the same time, how to design specific aerosols to deliver drugs with the highest efficacy [6][7]. For the latter, ongoing efforts are focusing on devising specific technologies for protecting the nasal mucosae against infections [8] and
on delivering vaccines via nasal sprays for pediatric purposes [9].

Owing to the inherent structural and physiological complexity of the nasal airway, obtaining spatially resolved in vivo flow measurements is a challenging task. With the rapid increase in computational prowess, numerical simulations have emerged as a powerful tool to analyse the flow behaviour inside the nasal cavity. A plethora of numerical investigations have been carried out in recent years to understand the rich and complex dynamics of nasal airflow and aerosol transport. The effect of breathing rate on the airflow characteristics was explored by Li et al. [10]. Barbarite et al. [11] studied the fluid dynamic causes of nasal obstruction and associations with patient-reported outcome in a large cohort of patients. Covello et al. studied the transport of water droplets in the human nasal cavity under steady inspiration conditions and analyzed the deposition patterns corresponding to different breathing rates. The performance of nasal sprays for topical drug delivery was explored in the extensive works of Basu et al. [12, 7]. The consequence of surgery induced physiological changes in the nasal cavity on the airflow pattern and particle deposition has been examined by Bahmanzadeh et al. [13]. The various modelling aspects and challenges pertinent to airflow in the human nose has been provided in the comprehensive review of Doorly et al. [14].

In spite of a host of previous studies on nasal airflow and particle/droplet transport, many open questions still remain to be answered. It is worth recalling that, the transport of passive point particles in the airflow are dictated by the fluid streamline they belong to at the time of injection. Thus, given the no-slip conditions at the cavity walls, particles cannot be deposited at the nasal mucosa. On the other hand, finite-size droplets can depart from the initial streamlines which provides a mechanism for impinging the walls, particularly in the narrow passages of the nasal cavity. This paper thus addresses the question on how the finite size of the droplet influence the deposition patterns inside the nasal cavity. It further elaborates on the role of breathing rate and flow condition (laminar or turbulent) on the droplet dynamics. It is worth recalling that the transient nature of flow has been often neglected in previous studies on nasal
airflow, which may be an unreasonable assumption under realistic breathing conditions. In our present study, we attempt to address some of these pertinent issues related to droplet transport and deposition.

2. Methodology

2.1. Geometrical model of nasal cavity

The three dimensional model of the nasal cavity is adopted from the results of Brüning et al. [15], wherein a standardized geometry was generated by employing a statistical shape model on computed tomography (CT) scans of 25 healthy adults. The patient specific samples were obtained from the segmented medical images of the scans and an averaged geometry was derived from the 25 scanned geometries by employing a statistical model. The corresponding file of the averaged geometry has been freely distributed by the authors. We have obtained the aforementioned geometry file and adopted it for our computations. Given the level of sophistication of the surface mesh, identification of the nasal inlets and outlet (nares and trachea), inspection of the cavity geometrical details and post-processing of the airflow structure were done with the aid of the software Wicca developed by MedLea Srls and specialized to perform respiratory diagnostics, a tool previously validated in a number of nasal cavities reconstructed from tomographic images of phantoms and patients [16].

2.2. Computational model

The present numerical model is based on the software Moebius from Lexma Technology, as it allows multiphysics simulations of fluids and particles. Given the intricate structure of the nasal cavity with its plenty of narrow passages where air flows, special focus has been posed on the fluid dynamics method. In fact, the narrow gaps in the nasal turbinates can be millimeters across and flow velocities therein can locally reach 10 m/s. Therefore, the numerical method needs to comply with the transitional flow that takes place at physiological respiratory rates and rely on a computational mesh that is able to resolve the narrow passages with sufficient accuracy and stability.
To this end, we employed the Entropic Lattice Boltzmann Method (ELBM) for simulating 3D single phase fluid flow configuration \cite{17}. The ELBM is a powerful variant of the basic Lattice Boltzmann method \cite{18} based on a self-consistent tuning of the relaxation parameter so as to ensure compliance with local entropy growth (H theorem). ELBM is based on tracking the evolution of the discretized density distribution function, named populations $f_p(x, t)$, over a Cartesian grid. Here, $x$ and $t$ denote the spatial and temporal coordinates and subscript $p$ denotes a set of discrete speeds $c_p$ connecting the mesh points to its neighbors. The ELBM employed here is obtained by minimizing the lattice H-function $H[f] = \sum_p f_p \log(f_p/w_p)$, where $w_p$ is a set of normalized weight \cite{19}. In this study we employed the D3Q19 set of discrete speeds and associated weights \cite{20}.

The transitional nature of the air flow may develop strong gradients near the nasal walls posing a serious threat to the numerical stability. ELBM is a valid alternative to subgrid turbulence modeling \cite{21} since it is a parameter-free approach enabling to treat highly transitional and fully developed turbulent flows, while achieving large numerical stability. ELBM has been shown to provide highly accurate results from transitional \cite{22} to fully developed turbulence. At the same time a near-wall model has to be introduced to enforce the law of the wall. In the present study, we employed a wall function based approach by implementing a near-wall drag force \cite{23}.

Given the low volume occupied by each droplet as compared to the size of the nasal cavity, droplets are assumed to have a one-way coupling with the flow field, i.e. the droplets are affected by the flow field but not vice verse. Particles are described as extended, passive and massless rigid bodies. A droplet is assimilated to be a cluster made of $N_i$ beads and the position of its center of mass is given by, $R_i = \sum_k r_{ik}/N_i$, wherein, $r_{ik}$ is the individual bead position. Each cluster is propagated in time according to a first-order overdamped rigid body, such as

$$\dot{R}_i = a_i + u_i \delta(R_i - x)$$

(1)
where, $\tilde{\delta}$ is a smoothing function as used in the Immersed Boundary method and $\alpha_i$ is a fictitious acceleration obtained by virtual displacements, as used to compute the mechanical forces exerted by the surrounding fluid on each bead of the cluster. Similarly, the total torque acting on the cluster is computed and the orientational state is updated. Given the spherical shape of the cluster and the passive transport conditions, these elements can be safely neglected for the sake of simplicity. Finally the model does not take into account the effect of buoyancy.

2.3. Computational setup

A snapshot of the computational domain is presented in Fig. 1. The boundary of the domain is divided into three portions, wherein different boundary conditions are applied. The nostrils are considered as open boundaries maintained at constant ambient pressure. The air and droplets are driven through the nasal cavity by imposing a velocity condition at the boundary near the nasopharynx. To simulate a realistic respiratory cycle, a time varying velocity profile is imposed at the nasopharynx, considering a generic sinusoidal nature. For a healthy adult, the tidal volume ranges in 350-600 mL. Considering an

![Figure 1: Geometry of the averaged human nasal cavity - (a) isometric view and (b) top view, along with the inflow and outflow regions. The droplets are injected slightly upstream of the anterior nares, as shown in the highlighted region.](image-url)
inspiration time of 2 seconds, two breathing rates are considered with peak inspiration flow rates (PIFR) of 17 and 20 L/min, as shown in Fig. 2. It is to be noted that only the inspiration process is considered in our simulations. Furthermore, recent studies have shown that laminar flow is maintained for flow rates of magnitude lower than 10 L/min in a single nasal passage [25]. Assuming equal division of flow through the nostrils, we consider the flow with PIFR of 17 L/min as laminar, whereas for PIFR of 20 L/min, turbulent flow is considered. The walls of the nasal cavity are considered as no-slip and no-penetration boundaries.

![Profile of two breathing rates consisting of a sinusoidal inspiration cycle of 2 seconds.](image)

Each droplet cluster is considered to be a rigid sphere made up of 6 point beads. We consider different droplet sizes by varying the radius of the droplets in the range 0.25 - 0.75 mm. It is to be noted that the typical size of droplets secreted during breathing or coughing lie in the range of 0.1-0.45 mm [26]. The droplets are injected from a point slightly upstream of the nostrils, as shown in Fig. 1. The initial position of the droplets is randomly perturbed during each injection event and three independent runs are performed corresponding to each configuration in order to obtain statistically reliable results. The initial velocity of the sprayed droplets is set to be zero. As the simulation progress, the surrounding fluid quickly carries the droplets along the flow.
In the present study, we simulate continuous inhalation of the droplets during the inspiration phase. As such, a cluster of 50 droplets are injected in each nostril every 0.2 seconds, with a total of 800 droplets being injected by the end of inspiration. It should be noted that this type of continuous injection corresponds to the inhalation of droplets and suspended particles in the atmosphere, which are inhaled during the entire inhalation phase. In contrast, droplets from therapeutic drug delivery devices are typically introduced during a specific time window within the inhalation cycle [13]. The droplets are assumed to be deposited on the walls of the nasal cavity, when the minimum separating distance from the wall reduced below the grid spacing (Δ). This was implemented by setting the droplet velocity to zero, whenever the aforementioned condition is satisfied. Additionally, the particles are frozen when they reach the inlet or outlet faces of the computational domain.

In order to ensure that the results are independent of grid resolution, we progressively increase the number of cells/voxels and measure the relative change in flow velocity magnitude at a central point near the posterior nares, as tabulated in Table 1. It can be clearly observed that the results converge with grid refinement and the change in velocity reduces below 1%, when the grid spacing (Δ) is taken as 0.00025 m. In order to optimize the computational time, without compromising the solution accuracy, we chose the grid spacing of 0.00025 m for the rest of the simulations.

<table>
<thead>
<tr>
<th>No of voxels</th>
<th>Grid spacing (m)</th>
<th>Velocity magnitude (m/s)</th>
<th>% change</th>
</tr>
</thead>
<tbody>
<tr>
<td>470916</td>
<td>0.0004</td>
<td>1.631</td>
<td>-</td>
</tr>
<tr>
<td>704024</td>
<td>0.00035</td>
<td>1.662</td>
<td>1.94</td>
</tr>
<tr>
<td>1117678</td>
<td>0.0003</td>
<td>1.679</td>
<td>1.01</td>
</tr>
<tr>
<td>1932464</td>
<td>0.00025</td>
<td>1.693</td>
<td>0.75</td>
</tr>
</tbody>
</table>

Table 1: The relative change of velocity magnitude with grid refinement at a selected point near the posterior nares.
3. Results and Discussion

We initiate our analysis by discussing the general features of the flow field obtained from the computations. Figure 3 illustrates the temporal variation of the flow field for a PIFR of 17 L/min. The contours of velocity magnitude (\(|u|\)) at a sagittal plane for time instants 0.25, 0.5, 1.0 and 1.5 seconds are plotted in Figs. 3(a), (b), (c) and (d), respectively, superimposed with the velocity vectors. We recall here that the total duration of the inspiration cycle is 2.0 seconds. The geometry of the nasal cavity can be axially segregated into four regions, namely, vestibule, nasal valve, turbinate region and the nasopharynx. It can be clearly observed from Fig. 3 that the flow field keeps evolving throughout the entire inspiration period. The air after entering through the anterior nares undergo a change in flow direction in the vestibule, before reaching the nasal valve. Owing to the smaller cross-section, the flow field is accelerated, as represented by the regions of high velocity. After passing the nasal valve and entering the turbinate region, the area suddenly increases, leading to deceleration of flow. The airflow
is unevenly divided through the inferior, middle and superior meatus. Regions of high velocity can be observed in the middle meatus region. With increase in time, the inspiration flow rate increases and reaches the peak value at 1.0 second. Accordingly, the flow velocity attains the peak value at 1.0 second and thereafter continues to decrease. After passing through the turbinate region, the airflow from the two cavities merge and exit along the nasopharyngeal region.

![Figure 4: Snapshots of the flow field along a coronal plane at the instant of peak flow \((t = 1.0\) second). (a) and (b) corresponds to PIFR of 17 and 20 L/min, respectively.](image)

On increasing the PIFR value to 20 L/min, the flow velocity is augmented over the entire nasal cavity. Figures 4 (a) and (b) compares the velocity magnitude \(|u|\) at a coronal plane, located in the turbinate region, for PIFR of 17 and 20 L/min, respectively. As expected, the local flow velocity is significantly higher in the meatus region for PIFR of 20 L/min.

We then investigate, both qualitatively as well as quantitatively, the pattern of droplet deposition upon the walls of the nasal cavity. The parameters investigated in our simulations are the droplet size and the breathing rate. Figures
Figure 5: Sagittal (side) and transverse (top) views of the nasal cavity showing droplets deposited on the walls of the nasal cavity for droplets of radius (a) 0.25 mm and (b) 0.75 mm, respectively. Each red dot represent a particle and a droplet is made up of a rigid cluster containing 6 particles. The PIFR is set at 17 L/min.

(a) and (b) present a qualitative picture of droplets deposited on the nasal walls, with radius of 0.25 mm and 0.75 mm, respectively. The PIFR value is fixed at 17 L/min. A close examination of the deposition patterns reveal many interesting features. The droplets with smaller size penetrate more into the posterior region of the nasal cavity. Additionally, the deposition is spread over a larger nasal wall area. In contrast, a preferential tendency to deposit in the anterior region of the nasal cavity is observed for larger sized droplets. A strong concentration of droplets can be observed near the nasal valve region.
Figure 6: Number of droplets deposited on the walls of the nasal cavity for droplets of radius (a) 0.25 mm, (b) 0.5 mm and (c) 0.75 mm, respectively. The y axis is directed along the flow from the nostrils towards the nasopharynx. The PIFR is set at 17 L/min.

In order to obtain a quantitative estimate of droplet deposition, we divide the entire nasal surface into 10 slabs along the flow direction (y axis). The thickness of each slab is around 9.5 mm. The variation of number of droplets deposited with increasing size of the droplets is depicted in the form of histograms in Fig. 6. It can be clearly perceived from Fig. 6 that droplets with smaller size spread over the entire nasal lining. On the other hand, larger droplets demonstrate enhanced deposition near the anterior region with significantly lesser penetration downstream of the cavity.

We then explore the effect of breathing rate on the pattern of droplet deposition. Figure 7 presents a qualitative picture of droplets deposited on the nasal cavity for PIFR value of 20 L/min. Owing to the enhanced breathing rate, the nature of droplet deposition is notably altered. The penetration of the droplets into the turbinate region is much higher, when the flow rate is increased. The majority of the droplets are agglomerated near the middle turbinate region. For smaller droplets, a scattered distribution of the droplets is attained, whereas, the larger droplets remain clustered in a narrow region. Furthermore, a reduced deposition of droplets near the nasal valve region is observed, which is in contrast to the deposition shown in Fig. 5.

A quantitative analysis of the deposition pattern at PIFR value of 20 L/min is shown in Fig. 8. The histograms clearly demonstrate that the higher flow rate leads to enhanced penetration of the droplets into the posterior regions of
Figure 7: Sagittal (side) and transverse (top) views of the nasal cavity showing droplets deposited on the walls of the nasal cavity for droplets of radius (a) 0.25 mm and (b) 0.75 mm, respectively. Each red dot represents a particle and a droplet is made up of a rigid cluster containing 6 particles. The PIFR is set at 20 L/min.

The differing nature of droplet deposition can be explained by considering the relative importance of droplet size and flow rate. Owing to the small, but finite size of the droplets, the trajectories of the moving droplets can deviate from the flow streamlines. Increasing the size of the droplets leads to higher deviation from the streamlines, leading to enhanced deposition. Furthermore, the deviation from the streamlines is more pronounced, when the airflow abruptly changes...
Figure 8: Number of droplets deposited on the walls of the nasal cavity for droplets of radius (a) 0.25 mm, (b) 0.5 mm and (c) 0.75 mm, respectively. The $y$ axis is directed along the flow from the nostrils towards the nasopharynx. The PIFR is set at 20 L/min.

direction or encounters an obstruction. As a consequence, higher droplet deposition is observed near the nasal valve region, owing to the sharp curvature of the nasal geometry. It is to be noted here that the droplets in our simulations consist of a cluster of particles, convected as a rigid body by the flowing air. Increasing the breathing rate leads to stronger convection by the air, leading to deeper penetration into the cavity. Additionally, the curvature of the airflow in the turbinate region causes the droplets to diverge from the streamlines, thereby engendering higher deposition in this region. It is to be noted that the overall deposition of droplets is diminished at the higher flow rate, irrespective of the size of the droplets, which can be attributed to the stronger inertia of the airflow in the nasal passageway.

Figure 9: Effect of droplet size on the penetration efficiency for the two PIFR configurations.
Lastly, we examine the infiltration of the droplets into the nasopharyngeal region after passing through the nasal airway. The amount of penetration is quantified in terms of a parameter called ‘penetration efficiency’, defined as,

\[
\text{Penetration efficiency (\%) = } \frac{\text{No of droplets reaching nasopharynx}}{\text{Total number of droplets inhaled}}. \tag{2}
\]

The variation of penetration efficiency with droplet size and flow rate is elucidated in Fig. 9. It can be clearly perceived from Fig. 9 that increasing the droplet size leads to a sharp decrease in the number of droplets reaching the nasopharynx. In other words, smaller drops have a higher probability to infiltrate the nasal passageway. A higher breathing rate assists the penetration capability, which in turn allows more droplets to reach the nasopharynx. In the context of pathogen loaded inhaled droplets, a higher penetration efficiency indicates stronger potential for droplets to move into the trachea and engender disorders in the lower respiratory tract and the lungs.

4. Summary

Numerical simulations have been performed to investigate the airflow dynamics and droplet transport during inhalation through an averaged human nasal cavity. The study focuses on the effect of droplet size and breathing rate on the deposition patterns inside the nasal lining. The simulations reveal that for a lower value of peak inspiration flow rate (17 L/min), the penetration of droplets into the posterior regions of the airway is diminished. For smaller droplet sizes, a wide distribution pattern over the entire nasal surface area is observed. On the contrary, larger droplets tend to accumulate near the anterior region of the nasal cavity. The deposition patterns at higher PIFR rates (20 L/min) indicate enhanced penetration into the turbinate and nasopharyngeal regions. Furthermore, a notably diminished deposition of droplets occurred near the nasal valve region. As expected, increasing the droplet size lead to enhanced deposition in the nasal cavity. However, the overall deposition of droplets is reduced at higher flow rate, irrespective of the size of the droplets.
In the context of the current Covid-19 pandemic, droplet inhalation and deposition have gained immense interest in the scientific community, owing to potential applications for spray based remedial technologies. At the same time, Covid-19 infection is transmitted by droplets that once inhaled can make their way to the trachea. The present study provides valuable insight into the dynamics of droplet transport and deposition in the nasal cavity and demonstrates the constructive role of CFD based tools for aiding prognosis and treatment of respiratory disorders. However, there remains ample scope for improving and extending the current study. The droplets considered in our study are considerably larger than typical ‘aerosol’ like microdroplets, which have a higher probability of remaining suspended in the ambient air. The size of the droplets is limited by the grid resolution considered in our study. It will be worthwhile to study the deposition patterns for micrometer sized droplets, in order to obtain a more holistic picture of droplet transport in the nasal cavity. The inclusion of more detailed mechanisms of droplet adsorption at the nasal walls can be explored. Additionally, evaporation in the ambient medium leads to shrinkage of the droplets, which may radically alter the dynamics of the deposition process. A more extended study is currently underway to elucidate the complex interplay of these diverse operating parameters.

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