

# Coupled Eulerian Wall Film-Discrete Phase model for predicting respiratory droplet generation during a coughing event

Nguyen Dang Khoa

Interdisciplinary Graduate School of Engineering Sciences, Kyushu University

Kuga, Kazuki

Faculty of Engineering Sciences, Kyushu University

Inthavong, Kiao

School of Engineering, Mechanical and Automotive, RMIT University

Ito, Kazuhide

Faculty of Engineering Sciences, Kyushu University

<https://hdl.handle.net/2324/7174458>

---

出版情報 : Physics of Fluids. 35, pp.112103-, 2023-11-09. American Institute of Physics : AIP  
バージョン :

権利関係 : This article may be downloaded for personal use only. Any other use requires prior permission of the author and AIP Publishing. This article appeared in "Physics of Fluids" and can be found via the link in the "Related DOI" on this page.



This is the author's peer reviewed, accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset.

PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0174014

Accepted to *Phys. Fluids* 10.1063/5.0174014

**1 Coupled Eulerian Wall Film-Discrete Phase model for predicting the**  
**2 respiratory droplets generation during the coughing event**

3

4 Nguyen Dang Khoa<sup>a)\*</sup>, Kazuki Kuga (久我一喜)<sup>b)</sup>, Kiao Inthavong<sup>c)</sup>, Kazuhide Ito (伊藤一  
 5 秀)<sup>b)</sup>

6

7 <sup>a)</sup> Interdisciplinary Graduate School of Engineering Sciences, Kyushu University, Fukuoka,  
 8 Japan

9 <sup>b)</sup> Faculty of Engineering Sciences, Kyushu University, Fukuoka, Japan

10 <sup>c)</sup> School of Engineering, Mechanical and Automotive, RMIT University, Melbourne, Australia

11

12 \* Corresponding authors

13 E-mail: [ndkhoa@kyudai.jp](mailto:ndkhoa@kyudai.jp) (NDK)

14 IGSES, Kyushu University, 6-1, Kasuga-koen, Kasuga, Fukuoka, 816-8580, Japan

15

16

## Abstract

Infectious respiratory diseases have long been a serious public health issue, with airborne transmission via close person-to-person contact being the main infection route. Coughing episodes are an eruptive source of virus-laden droplets that increase the infection risk of susceptible individuals. In this study, the droplet generation process during a coughing event was reproduced using the Eulerian wall film (EWF) model, and the absorption/expulsion of droplets was tracked using the discrete phase model (DPM). A realistic numerical model that included the oral cavity with teeth features and the respiratory system from the throat to the first bifurcation was developed. A coughing flow profile simulated the flow patterns of a single coughing episode. The EWF and DPM models were coupled to predict the droplet formation, generation, absorption, and exhalation processes. The results showed that the large droplet number concentration was generated at the beginning of the coughing event, with the peak concentration coinciding with the peak cough rate. Analysis of the droplet site of origin showed that large amounts of droplets were generated in the oral cavity and teeth surface, followed by the caudal region of the respiratory system. The size of the expelled droplets was 0.25–24  $\mu\text{m}$ , with the peak concentration at 4–8  $\mu\text{m}$ . This study significantly contributes to the realm on the site of origin and localized number concentration of droplets after a coughing episode. It can facilitate studies on infection risk assessment, droplet dispersion, and droplet generation mechanisms from other sneezing or phonation activities.

This is the author's peer reviewed, accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset.

PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0174014

*Accepted to Phys. Fluids 10.1063/5.0174014*

36

37 **Keywords:** Computational Fluid Dynamics, Eulerian Wall Film Model, Discrete Phase Model,  
38 Coughing, Droplet site origin and number concentration.

39

40

## 41 I. INTRODUCTION

42 Infectious respiratory diseases have long been a significant public health concern. This  
 43 includes instances of plagues, measles, tuberculosis, influenza, severe acute respiratory  
 44 syndrome coronavirus (SARS-CoV), Middle East respiratory syndrome coronavirus (MERS-  
 45 CoV), and the most recent SARS-CoV-2 (Churchyard et al., 2017; Piret & Boivin, 2021).  
 46 Person-to-person airborne transmission of respiratory viruses can occur via direct or indirect  
 47 contact, respiratory droplets, and droplet nuclei transmission (Dhand & Li, 2020; C. C. Wang  
 48 et al., 2021). Infected patients can expel pathogen carriers into the ambient environment via  
 49 respiratory activities such as breathing, talking, phonating, singing, sneezing, or coughing (Wei  
 50 & Li, 2016; Stadnytskyi et al., 2021). Once in the surrounding environment, viral-laden  
 51 droplets can remain airborne for an extended period and transported by indoor airflow to the  
 52 effective breathing zone of residents, and subsequently inhaled at various exposure levels, as  
 53 reported by previous studies that were comprehensively reviewed by Inthavong (Inthavong,  
 54 2020). During the expiratory phase, the infection risks are associated with the (1) droplet  
 55 number concentration, (2) size distribution, (3) content of infectious agents, and (4)  
 56 performance frequency (Morawska, 2006). Besides, more recent studies underscore the  
 57 dependence of disease transmission on infective dose threshold of the virus (SeyedAlinaghi et  
 58 al., 2022) and the viral shedding rate (Widders et al., 2020). Thus, quantitative studies are  
 59 required to determine the pathogen susceptibility targeting each activity.

60 The threat of coughing-related infections has gained public attention, being extensively  
61 studied over the past decades owing to its possibility for the eruptive release of many pathogens  
62 in a short period (Stadnytskyi et al., 2021). When coughing, the sequent build-up of expiratory  
63 flow velocity, reaching a Reynolds number of  $10^4$  (Bourouiba et al., 2014), expulses  
64 compressed air through the open mouth. Due to the high speed, droplets are produced in the  
65 oral cavity due to shear-induced surface-wave instabilities (Wei & Li, 2016; Pöhlker et al.,  
66 2021). The stripped droplet parcels follow the air stream and escape to the environment through  
67 the open mouth or are re-absorbed into the mucus layer. Virus-laden droplets are generally  
68 deposited in the respiratory tract after inhalation (H. Li et al., 2022; C. C. Wang et al., 2021).  
69 The mucus clearance process (i.e., coughing) can trigger the re-emittance of deposited virions  
70 or the local transmission of progeny viruses shed by infected cells (Schaefer & Lai, 2022).  
71 Therefore, the number concentration and size distribution of droplets from coughing have  
72 gained significant attention from the scientific community. A review of studies over the past 20  
73 years has indicated significant scatter (Yang et al., 2007; Chao et al., 2009; Morawska et al.,  
74 2009; Johnson et al., 2011; Lindsley et al., 2012; Zayas et al., 2012), which can be attributed  
75 to the heterogeneity of measurement techniques, sampling methods, or intersubject variability.  
76 More recently, facilitated by advanced techniques, the realm of measuring ejected cloud  
77 characteristics and generated droplet properties from oral activities in an indoor environment  
78 has been embarked upon to deliver a comprehensive understanding during the pandemic epoch

79 (Wang et al., 2020; Archer et al., 2022; Harrison et al., 2023; Bahramian & Ahmadi, 2023).  
80 Drawing upon the properties of generated droplets from experimental studies, computer-aided  
81 approaches have been expanded to explore further the deleterious effects of these droplets in  
82 the context of disease transmission. Among them, Computational Fluid Dynamics (CFD) has  
83 been universally adopted for the numerical investigation of the contagion risk of coughing.  
84 Most studies have investigated the cough-jet stream characteristics and fate of expiratory  
85 droplets in an enclosed environment (H. Li et al., 2021; Payri et al., 2021; Nie et al., 2022;  
86 Aljabair et al., 2023; Nishandar et al., 2023), or the distance-based exposure risks between  
87 residents (Calmet et al., 2021; Mariam et al., 2021; Hossain et al., 2023; X. Li et al., 2023). As  
88 can be seen, up to date, both experimental and numerical endeavors have extensively advanced  
89 our understanding of droplet size distribution and their behavior under varying microclimatic  
90 conditions within an enclosed environment. Nonetheless, the site origin and generation  
91 mechanism of these droplets in the respiratory tract have yet to be discussed in the listed studies.

92 Against this background, further numerical studies have been conducted on the interactions  
93 between high-speed, chaotic exhaled air and the liquid-layer lining the inner surface of the  
94 airway (i.e., the mucus layer) during the coughing episode. The two most common methods  
95 adopted are the volume of fluid (Paz et al., 2019; Rajendran & Banerjee, 2019; Pairetti et al.,  
96 2021; Yi et al., 2021) and Eulerian wall film (EWF) models (Paz, Suárez, Parga, et al., 2017;  
97 Paz, Suárez, & Vence, 2017; Ren et al., 2018, 2020, 2022; Anzai et al., 2022). These studies

98 provide an understanding of the respiratory droplet generation process, the effects of mucus  
 99 properties on cough clearance efficiency, and the impact of airway deformation. To facilitate  
 100 the assessment of the infection risks of virus-laden droplets, it is crucial to qualitatively and  
 101 quantitatively investigate the origin of respiratory droplets during expiratory events (i.e.,  
 102 coughing). Furthermore, the realistic and comprehensive characteristics of the target  
 103 respiratory airway model should be considered to ensure the accuracy of the cough-jet stream  
 104 and expelled droplet features.

105 In this study, the EWF model and Lagrangian discrete phase model (DPM) were coupled  
 106 to characterize the following: (1) fluid flow profiles of coughing; (2) number concentration,  
 107 size distribution, and locality of generated and expelled droplet particles during coughing; and  
 108 (3) absorption efficiency of stripped droplets. The results establish a link between the high viral  
 109 load of the infected respiratory tract and the possibility of such viral pathogens being released  
 110 into the environment by coughing. Subsequently, the infection risk can be determined for  
 111 different respiratory viruses.

## 112 II. MATERIALS AND METHODS

### 113 A. Numerical model geometry

114 The realistic airway model comprised a computed tomography (CT)-based trachea-  
 115 bronchus model and oral cavity produced by the open-source DAZ Studio software (DAZ  
 116 Productions, Inc.) shown in Fig. 1. During coughing, various oral shapes and sizes were



117 observed (Dbouk & Drikakis, 2020). In this study, the newly developed oral cavity model  
 118 mimicked the configuration of a slightly open mouth with dimensions of  $L = 4.7$  cm and  $H =$   
 119  $0.85$  cm (Fig. 1) to similarly match the data provided by experimental measurements from high-  
 120 speed imaging (Dbouk & Drikakis, 2020). The total area of the open mouth of  $3.76$  cm<sup>2</sup> was  
 121 within the range of  $4 \pm 0.95$  cm<sup>2</sup> as stated in a previous study (Seminara et al., 2020). In  
 122 addition, the teeth attributes were integrated to provide the most realistic traits of the oral cavity  
 123 (Fig. 1). The realistic trachea-bronchus model was created from CT scans, and details on the  
 124 process are available in the previous study by Ito (Ito, 2016). This trachea-bronchus model, in  
 125 combination with the nasal cavity, has been validated by our research group, providing reliable  
 126 results in diverse research themes (C. Wang et al., 2020; Yoo & Ito, 2022; Kuga et al., 2021,  
 127 2022, 2023; Murga et al., 2023; Khoa, Li, et al., 2023).

## 128 B. Grid design information

129 The discretization process was executed using the poly-hex core elements, which proposed  
 130 the CFD simulation with higher accuracy at a reduced computational cost (Zore et al., 2019).  
 131 The accuracy in the vicinity of the wall was enhanced by applying ten prism layers. This hybrid  
 132 mesh has been successfully used to predict airflow and particle transportation/deposition  
 133 simulation of the respiratory tract (Khoa, Phuong, et al., 2023; Khoa, Li, et al., 2023).  
 134 According to the mesh independence test, the mesh size of 15.5 million cells was selected for  
 135 subsequent simulation in this study, more detailed information can be found in Fig. S1

(Supplementary Material). This analysis strikes the balance between the computational burden and prediction accuracy.

### C. Numerical simulation of airflow pattern

The unsteady, incompressible, and isothermal fluid flow in the human respiratory tract was obtained by solving the Reynolds-averaged Navier–Stokes equations.

$$\frac{\partial \bar{U}_i}{\partial x_i} = 0 \quad (1)$$

$$\frac{\partial \bar{U}_i}{\partial t} + \frac{\partial \bar{U}_i \bar{U}_j}{\partial x_j} = -\frac{1}{\rho_g} \frac{\partial \bar{p}_g}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ (\nu + \nu_T) \left( \frac{\partial \bar{U}_i}{\partial x_j} + \frac{\partial \bar{U}_j}{\partial x_i} \right) \right] \quad (2)$$

where  $\bar{U}$  is the mean velocity;  $u'$  is the fluctuating components; and  $p_g$ ,  $\rho_g$ ,  $\nu$ , and  $\nu_T$  are the pressure, density, kinematic viscosity of the fluid, and turbulent viscosity, respectively.

This study selected the turbulent model of the shear stress transport (SST)  $k-\omega$ . This model has been used to predict adverse pressure gradient flow, strong curvature, and swirling flow in airway systems, as shown in previous experiments (Phuong & Ito, 2015; Elcner et al., 2016). The coughing flow profile was obtained from field measurements of Gupta for male subjects, as shown in Fig. 2A (Gupta et al., 2009). From the empirical equation, the coughing flow rate was allocated to four inlets according to the flow weighting of each lobe of the lung proposed in (Shelley et al., 2014), and reasonably applied in our study (Khoa, Li, et al., 2023), as shown in Fig. 2B. This procedure was implemented via a user-defined function (UDF) macro in ANSYS Fluent. The numerical boundary conditions for the coughing airflow simulation are

152 listed in Table I.

#### 153 D. Eulerian Wall Film simulation

154 In a coughing episode, an excessive fluid flow velocity is rapidly produced and subjected  
155 to turbulence and high shear stress at the interface between the airstream and thin liquid film  
156 (mucus/saliva). Under such conditions, Kelvin–Helmholtz instabilities occur, which cause  
157 waves with an escalating amplitude on the surface of a thin liquid film (Pöhlker et al., 2021).  
158 Droplets form from the crest of these waves in a multimodal mode and are carried by the flow.

159 The droplet generation mechanism can be predicted using the EWF model, in which thin  
160 liquid mucus layers were hypothesized to be aligned on the inner surface of the oral-tracheal  
161 model. The governing equation of the EWF model is as follows (ANSYS, Inc. 2022):

$$\frac{\partial \rho_l h}{\partial t} + \nabla_s \cdot (\rho_l h \bar{V}_l) = \dot{m}_s \quad (3)$$

$$\frac{\partial \rho_l h \bar{V}_l}{\partial t} + \nabla_s \cdot (\rho_l h \bar{V}_l \bar{V}_l + \bar{D}_V) = -h \nabla_s P_L + \rho_l h \bar{g}_s + \frac{3}{2} \bar{\tau}_{fs} - \frac{3\mu_L}{h} \bar{V}_l + \dot{q}_s \quad (4)$$

$$\bar{D}_V = \frac{\partial}{\partial s} \int_0^h v_l^2 dy \quad (5)$$

$$P_L = P_{gas} + P_h + P_\sigma \quad (6)$$

$$P_h = -\rho h (\bar{n} \cdot \bar{g}) \quad (7)$$

$$P_\sigma = -\sigma \nabla_s \cdot (\nabla_s h) \quad (8)$$

162 where  $\rho_l$  is the film density,  $h$  is the film height,  $V_l$  is the mean film velocity, and  $m_s$  is the  
163 mass source per unit wall area owing to droplet collection, film separation, film stripping, and

164 phase change. In Equation 4,  $D_V$  is the differential advection term computed based on the  
 165 quadratic film velocity with fluctuating velocity  $v_l(s,y,t)$ , in which  $s$  is the horizontal flow  
 166 direction and  $y$  is the vertical direction (Kakimpa et al., 2015). The term  $P_L$  is the mucus film  
 167 pressure,  $g_\tau$  is the gravity component,  $\tau_s$  is the shear force at the film–liquid interface,  $\mu_l$  is the  
 168 viscosity,  $q_s$  is the momentum source,  $\sigma$  is the surface tension,  $P_\sigma$  is the pressure exerted by the  
 169 surface tension,  $P_h$  is the gravity component normal to the wall, and  $n$  is the normal vector.

170 The reliability of applying the EWF model in anticipating the interaction between the  
 171 coughing stream jet and lining fluid is emphasized through supplementary simulations  
 172 conducted using a simplified airway model. The simulation results were subsequently  
 173 compared with experimental data, and additional information on this validation process is  
 174 elaborated upon in Fig. S2 (Supplementary Material).

175 In the context of our primary simulation, the EWF model was included with the fluid flow  
 176 at the beginning of the coughing episode. The simulation was applied to the total inner surface  
 177 of the numerical domain, including the teeth surface. In general, the mucus thickness varies  
 178 along the airway system. However, to simplify the simulation, a constant thickness of 30  $\mu\text{m}$   
 179 was used to represent the mucus layer in the throat, larynx, trachea, and bifurcation, based on  
 180 previous studies (Paz, Suárez, Parga, et al., 2017; Paz, Suárez, & Vence, 2017; Ren et al., 2022;  
 181 Anzai et al., 2022). For the oral cavity, the saliva thickness ranged from 11.3 to 68.9  $\mu\text{m}$ , as  
 182 proposed by the research of Assy (Assy et al., 2022). For the teeth surface, the saliva thickness

183 was assigned based on early experimental data (Collins & Dawes, 1987), which ranged from  
184 2.59 to 4.44  $\mu\text{m}$  following the mandibular, maxillary, left, or right position of teeth. The saliva  
185 and mucus layers were assumed to be water with a density of  $998.2 \text{ kg/m}^3$  and viscosity of  
186  $0.001 \text{ kg/m s}$ .

187 Shear-induced droplet generation was considered through the high velocity and turbulent  
188 flow, causing the instability of the lining mucus/saliva layers and leading to droplets peeling  
189 from the crests of the formed waves. This process was defined by the initial parameters given  
190 in Table II. Among them, the critical shear stress is the main factor that governs the number  
191 concentration of generated droplets. A parametric analysis was required prior to the main  
192 simulation to determine an appropriate value for the simulation, which is delivered in Fig. S3  
193 (Supplementary Material). Notably, this analysis was significantly influenced by the individual  
194 morphological characteristics considered in this study. Then, a value of 5 Pa was specified for  
195 the critical shear stress, which imposed the limit that any region subjected to shear stress greater  
196 than 5 Pa would trigger the shedding of mucus/saliva layers into droplets. In addition, a  
197 diameter coefficient, which specifies the droplet size range (ANSYS, Inc. 2022), was also  
198 determined by experiencing the parametric analysis with a value of 0.0003 (Fig. S4,  
199 Supplementary Material). Finally, the film time-step size was automatically assigned by  
200 ANSYS Fluent using adaptive time-stepping functions, which controlled the time-step size to  
201 be small enough to ensure that the maximum Courant number during the simulation was less

202 than 1. The continuous generation of mucus/saliva layers beneath the epithelial cells was  
203 neglected, which indicated no refill of mucus/saliva layers after being dispossessed.

#### 204 **E. Discrete Phase model simulation**

205 The EWF model was coupled with the DPM to track the trajectories of droplets stripped  
206 from the liquid film. Forces acting on the body were used to predict the droplet transportation,  
207 absorption, and exhalation characteristics of the oral-tracheal model. The Lagrangian discrete  
208 phase of the particle trajectories was computed by Equation 9.

$$\frac{d\vec{u}_p}{dt} = \vec{F}_D + \vec{F}_G + \vec{F}_s \quad (9)$$

209 where the subscript  $p$  is the droplet phase and  $\vec{F}_D$  is the drag force per unit particle mass  
210 derived from Stokes' drag law, expressed in Equation 10.

$$\vec{F}_D = \frac{18\mu}{\rho_p d_a^2} \frac{C_D Re_p}{24} (\vec{U} - \vec{u}_p) \quad (10)$$

211 where  $\mu$  is the air viscosity,  $\vec{U}$  is the fluid flow velocity,  $\vec{u}_p$  is the droplet velocity,  $d_a$  is  
212 the aerodynamic droplet diameter,  $\rho_p$  is the droplet density,  $C_D$  is the drag coefficient, and  $Re_p$   
213 is the particle Reynolds number.

214 The second term,  $\vec{F}_G$ , denotes the gravitational settling. The third term,  $\vec{F}_s$ , is Saffman's  
215 lift force due to shear on a unit mass basis. The lift force was adapted from a previous study by  
216 Li and Ahmadi (A. Li & Ahmadi, 1992), and is a generalization of the expression provided by  
217 Saffman (Saffman, 1965), expressed as Equation 11.

$$\vec{F}_s = \frac{5.188 v^{1/2} \rho d_{ij}}{\rho_p d_a (d_{lk} d_{kl})^{1/4}} (\vec{U} - \vec{u}_p) \quad (11)$$

218 where  $d_{ij}$ ,  $d_{lk}$ , and  $d_{kl}$  are deformation rate tensors.

219 The aerodynamic diameter and number of tracked droplets were determined based on the  
220 EWF simulation. The droplets were defined with a unit density ( $1000 \text{ kg/m}^3$ ), equal to that of  
221 pure water. The fate of the droplets was considered as exhaled via the mouth opening or was  
222 re-absorbed into the mucus layer; hence, the “escape” boundary condition was assigned to the  
223 mouth opening, and the “perfect trap” condition was applied as the wall boundary conditions.  
224 The evaporation and breakup of the droplets were negligible. The droplets were continuously  
225 generated during the simulation; therefore, the velocity, size, and spatial and temporal  
226 information of the droplets stripped from the mucus layer were recorded using the UDF macro  
227 for each time-step.

228 The generated, exhaled, and absorbed percentages, denoted as  $\eta_{G-i}$ ,  $\eta_{E-i}$ , and  $\eta_{A-i}$ , can be  
229 expressed by Equations 12, 13, and 14, respectively.

$$\eta_{G-i} = \frac{N_{G-i}}{N_G} \times 100\% \quad (12)$$

$$\eta_{E-i} = \frac{N_{E-i}}{N_E} \times 100\% \quad (13)$$

$$\eta_{A-i} = \frac{N_{A-i}}{N_A} \times 100\% \quad (14)$$

230 where  $N_{G-i}$ ,  $N_{A-i}$ , and  $N_{E-i}$  are the number of droplets generated, absorbed, and exhaled that  
231 belong to region  $i$ , which corresponds to the regions defined in Fig. 1.  $N_G$ ,  $N_A$ , and  $N_E$  are the  
232 total stripped, absorbed, and exhaled droplets after a single coughing episode (duration of 0.5

s), respectively. The size distribution of the coughed droplets was multimodal; accordingly, the droplet size bin was identified to establish the size distribution percentage of the generated, exhaled, and absorbed droplets ( $\eta_{G-s}$ ,  $\eta_{E-s}$ , and  $\eta_{A-s}$ ), given in Equations 15, 16, and 17, respectively.

$$\eta_{G-s} = \frac{N_{G-s}}{N_G} \times 100\% \quad (15)$$

$$\eta_{E-s} = \frac{N_{E-s}}{N_E} \times 100\% \quad (16)$$

$$\eta_{A-s} = \frac{N_{A-s}}{N_A} \times 100\% \quad (17)$$

where  $N_{G-s}$ ,  $N_{A-s}$ , and  $N_{E-s}$  are the number of droplets generated, absorbed, and exhaled, respectively, which decreases in the size bin, as listed in Table III.

The size distribution of exhaled droplets can be calculated by dividing the number of droplets within the specific size bin by the logarithm of the droplet size class interval ( $dN_E/d\log D$ ). Finally, the exhaled droplet size distribution was normalized with the total cough exhaled volume (1,000 cm<sup>3</sup>) to obtain the number concentration divided by the logarithm of the droplet size class interval ( $dC_{NE-s}/d\log D$ ).

### III. RESULTS

#### A. Coughing fluid flow characteristics

The results of the coughing fluid flow features are depicted in Fig. 3 at the start of the coughing episode at 0.01 s, cough peak flow rate (CPFR) at 0.077 s, and near the end of the coughing event at 0.4 s. Notably, the velocity magnitude and distribution herein are described



249 at the instantaneous times. At the onset of coughing (Fig. 3A), the culminated velocity occurred  
 250 at the bifurcation, trachea, glottis, and throat regions with a value of 3 m/s. At CPFR, the spatial  
 251 distribution of the jet stream remained, but the magnitude increased by almost 13-fold up to 40  
 252 m/s. In the final coughing stage, the coughing velocity rapidly decreased to less than 3 m/s in  
 253 identical acceleration regions.

254 In the oral cavity (Fig. 3B), the airstream accelerated in the throat region and impacted the  
 255 palate and bends following the curvilinear shape of the oral ceiling. The expulsive flow that  
 256 escaped the oral region was primarily distributed at the bottom of the mouth opening. Reserve  
 257 flow also formed in the basal region near the mouth opening, which contributed to the swirling  
 258 flow at the mouth opening (Fig. 3B). Due to the flow features toward the ceiling of the oral  
 259 cavity, the maxillary teeth are expected to endure the high-velocity flow during the cough. Fig.  
 260 3C shows the two-dimensional flow distribution for the maxillary teeth, which revealed that  
 261 the high-velocity fluid flow attacked the inner surface of the molars, premolars, canines, and  
 262 incisors.

#### 263 **B. Droplet generation mechanism during coughing**

264 The rapid increase in the flow rate due to coughing induces substantial shear stress on the  
 265 airway wall, closely linked to the droplet production criteria in the EWF model simulation. The  
 266 relationship between shear stress, mucus thickness, and stripped droplets is presented in Fig. 4,  
 267 which describes the instantaneous value of each variable. At 0.01 s (Fig. 4A), the low coughing

268 velocity resulted in a modest shear stress of less than 5 Pa on the airway wall, which failed to  
 269 meet the minimum threshold to produce droplets; hence, the droplets were not observed and  
 270 the mucus/saliva thickness remained in its original state. At CPFR (Fig. 4B), the cough ejection  
 271 velocity increased to 40 m/s, which induced significant shear stress on the wall surfaces.  
 272 Multiple airway surfaces experienced shear stress levels greater than 5 Pa, which fulfilled the  
 273 criterion for droplet generation off the thin liquid film on the oral-airway surfaces. Accordingly,  
 274 the mucus/saliva thickness decreased to almost 0  $\mu\text{m}$  and droplets simultaneously emerged in  
 275 the corresponding regions (Fig. 4B). The complex and uneven surface of the oral-airway model  
 276 produced an uneven distribution of the peak shear stresses. This completely removed the  
 277 mucus/saliva layers in several specific regions while the remaining areas preserved their initial  
 278 liquid film thickness. Droplet production decreased significantly at 0.15 s (Fig. 5C) due to the  
 279 mucus/saliva layers dissipating, following the former intense erosion process during CPFR.

### 280 C. Properties of generated droplets during coughing

281 The relationship between the coughing flow profile and droplet production was correlated  
 282 to understand the droplet generation process better. The instantaneous number of droplets  
 283 stripped from the mucus/saliva layers due to the coughing flow rate during the single coughing  
 284 episode ( $\sim 0.5$  s) is shown in Fig. 5A. The results demonstrate that the coughing flow rate  
 285 rapidly increased in the early stage of coughing. In contrast, droplet generation lagged and  
 286 didn't start until 0.04 s with an initial rapid rise. The number of droplets produced increased

287 rapidly in parallel with the coughing flow rate and formed a sharp slope, with the peak almost  
 288 coinciding with the CPFR (at approximately 0.077 s). After reaching their peaks, the cough  
 289 flow rate and number of stripped droplets exhibited a downward trend. The number of droplets  
 290 produced rapidly dropped to almost 0 at 0.25 s, in contrast to the cough flow that gradually  
 291 decreased to 0 taking 0.5 s. After the single coughing episode, 11,594,566 droplets were  
 292 generated (Table IV). The instantaneous position of the droplets during different times during  
 293 the cough are shown in Fig. 5B for time,  $t = 0.025, 0.04, 0.077$ , and 0.2 s, where the droplets  
 294 are colored by diameter. The results indicate an early appearance of droplets in the bifurcation  
 295 and throat regions (at 0.025 s). At 0.04 s, a dense population of droplets was observed in the  
 296 bifurcation and oral cavity, which corresponds to the airway curvature of the palate region in  
 297 line with the flow distribution in the oral cavity. At CPFR at  $t = 0.077$  s, the oral-airway model  
 298 is filled with a very high density of droplets due to the rapid droplet production (shown in Fig.  
 299 5A). At  $t = 0.2$  s, most of the droplets were re-absorbed into the mucus/saliva layers or  
 300 transported by the coughing flow toward the oral region and released into the external  
 301 environment via the mouth opening. Hence, fewer droplets are found in the airway compared  
 302 to the oral cavity. Furthermore, the droplet size was less than  $10\text{ }\mu\text{m}$  for the entire coughing  
 303 episode.

304 One advantage of this study is that it provides details on the origin of the stripped droplet  
 305 during the coughing event, illustrated in Fig. 5C. The oral region was identified as the primary

306 source of droplets (up to 46.8%) during the cough. In the remaining regions, the droplet  
307 production levels were similar (approximately 11.9–14.3%), slightly reducing towards the  
308 bifurcation region. The large amount of stripped droplets in the oral cavity is attributed to  
309 higher shear stresses (exceeding 5 Pa) than in other regions. Fig. 5D shows the total surface  
310 area ( $\text{cm}^2$ ) of each region subjected to shear stress of  $>5$  Pa, where the oral cavity exhibited the  
311 highest surface area. Therefore, more droplets were produced from the saliva film in the oral  
312 airway region.

313 The percentage of droplets generated per droplet diameter size bin can be estimated using  
314 Equation 15, as shown in Table IV. Most droplets produced were in the size interval of 4–8  $\mu\text{m}$   
315 (approximately 78.01%), followed by 2–4 and 8–16  $\mu\text{m}$ , respectively. The droplets in the size  
316 bin of  $<1$   $\mu\text{m}$  had a low percentage of 0.078–0.181%, while for the larger size bins ( $>16$   $\mu\text{m}$ ),  
317 the rate was only 0.169%.

#### 318 **D. Properties of exhaled droplets during coughing**

319 An analysis of the expelled droplet concentration for different droplet diameters was  
320 performed and compared with experimental measurements of Yang (Yang et al., 2007). In the  
321 experimental work, 54 volunteers of varying ages and genders coughed into a sampling bag  
322 with a well-controlled relative humidity; thus, the coughed droplets retained their original size.  
323 Fig. 6A shows the number concentration of droplets at the mouth opening plotted against the  
324 average droplet size and compared with Yang (Yang et al., 2007). The EWF model closely

325 matched the profile with the measured exhaled number concentration. There was a sharp  
326 increase in the number concentration for droplet sizes approximately at  $2\text{ }\mu\text{m}$  before reaching  
327 a peak concentration (approximately  $2,500/\text{cm}^3$ ) at  $4\text{--}8\text{ }\mu\text{m}$ . After the peak, a downward trend  
328 was observed, and the cutoff diameter where no droplets were expelled was  $>10\text{ }\mu\text{m}$ .

329 The source of droplets expelled to the environment is shown in Fig. 6B, where the oral  
330 cavity (including the teeth surface) was responsible for the largest amount of droplets exhaled  
331 into the environment (up to 75%). The amount gradually reduced for the geometry moving  
332 posteriorly toward the caudal airway; specifically, 12.3% originated from the throat, followed  
333 by the larynx (approximately 8.3%), trachea, and bifurcation (approximately 2.2%),  
334 respectively.

335 Most exhaled droplets, 73.1%, were between  $4\text{--}8\text{ }\mu\text{m}$  due to the highest percentage of  
336 droplets produced in this range (Table IV). For smaller droplets, the exhalation rates were  
337 12.8% and 8.9% for size bins of  $2\text{--}4\text{ }\mu\text{m}$  and  $8\text{--}16\text{ }\mu\text{m}$ , respectively. Despite the low production  
338 rate of droplets in the size bin of  $<1\text{ }\mu\text{m}$ , the appearance of these small droplets in the exhaled  
339 breath was 0.49–0.79%.

340 The spatial distribution of the droplets that escaped through the mouth during the coughing  
341 is illustrated in Fig. 6C, where the different droplet colors denote the source location. The  
342 results show that the oral cavity is the primary location of the expelled droplets, and the droplets  
343 exit through the entire space of the mouth opening. For the other airway regions (throat, larynx,

trachea, and bifurcation), the expelled droplets mainly dispersed through the lower half of the mouth opening. There was a small scattering of droplets in the upper half of the mouth opening. Despite the significant variation in the vertical distribution of droplets expelled, the horizontal distribution in the lower half was consistent. This distribution was due to the oral cavity shape and the exhaled jet stream found in the lower half of the mouth opening (shown in Fig. 3).

#### E. Absorbed efficiency of droplets during coughing

The total number of droplets absorbed onto the mucus/saliva layers was 10,128,559 (Table IV), accounting for approximately 87.3% of the total droplets produced by the cough. The primary absorption region was the oral cavity (including the teeth surface), with 47.8%. In contrast, in the remaining regions, the absorption efficiency significantly decreased by approximately four-fold in the 11.2–14.1% range. Most of the generated droplets re-absorbed into the oral region's saliva layer can be associated with the complex morphology of this region, which prevented the smooth movement of the droplets.

Fig. 7B shows the droplet absorption efficiency categorized by the region where the droplets originated from (e.g. slice color indicates the droplet source location). In general, droplets were immediately re-absorbed back into its own region where they were generated. For example, 87.5% of droplets produced in the oral cavity re-absorbed in its region, and that of the throat, larynx, trachea, and bifurcation, the re-absorption rate was 88.2%, 91.9%, 93.1%, and 100%, respectively.

363 The cough-jet stream began from the tracheal bifurcation, and the oral region had the  
 364 greatest exposure to all droplets originating from lower regions, including the throat (5.3%),  
 365 larynx (4.2%), trachea (1.8%), and bifurcation (1.3%). This geometry and flow feature explains  
 366 the lack of absorbed droplets from geometrically lower regions (e.g. upstream flow) than the  
 367 region itself since the jet flow transports the droplets from the bifurcation to the oral cavity.  
 368 Droplets with sizes of 4–8  $\mu\text{m}$  (Table IV) were the most re-absorbed due to the greater number  
 369 of generated droplets in this size bin. For the other size bins, the absorption rate was similar to  
 370 its generation rate.

371 Fig. 8 shows the deposition pattern on specific airway regions based on where the droplets  
 372 were produced. Deposition in the oral cavity showed that the focal absorption region occurred  
 373 in the palate regardless of the droplet origin. Most droplets in the throat tended to accumulate  
 374 in the upper and branching regions. In the larynx and trachea, there was a high rate of re-  
 375 absorption from itself. Only the droplets produced by itself were re-absorbed for the bifurcation,  
 376 and most were observed in the left bifurcation.

377 Generally, the cough-jet stream influenced droplet deposition in the oral airway, and the  
 378 droplet absorption patterns coincided with the high-velocity regions, as discussed in the  
 379 previous section.

#### 380 **F. Role of teeth surface in the simulation of droplet generation during coughing**

381 The results reveal the critical role of the oral cavity in droplet generation, emission, and

382 absorption. This raises the question of the contribution of the teeth surface to the areas of  
 383 interest in this study. In this section, the droplet generation, absorption and exhalation from the  
 384 oral cavity were divided into the teeth surface and the remaining portion of the oral airway  
 385 surface (shown in Fig. 9A). The total of 46.8% of droplets that were produced from the oral  
 386 cavity (from Fig. 5C), were found to originate evenly between the teeth surface and remaining  
 387 portion (approximately 23%).

388 The instantaneous shear stress at 0.04 s and 0.077 s is given in Fig. 10A. Shear stress >5  
 389 Pa was observed on the maxillary incisor surface in the early stage of the coughing event (0.04  
 390 s). A high shear rate was found on the inner surface of the maxillary teeth, including the incisors,  
 391 canines, and molars, at the CPFR (0.077 s). Consequently, many droplets were stripped from  
 392 the saliva layers along the inner side of the maxillary teeth surface (Fig. 10B). This  
 393 phenomenon is closely associated with the cough-jet stream, which impacted the upper jaw, as  
 394 discussed in the previous section.

395 For the expelled droplets (Fig. 9B), approximately 40% was derived from the teeth's surface.  
 396 This was attributed to the droplets that formed on the teeth surface, especially on the incisors,  
 397 which travelled a short distance without any obstacles to the mouth opening. For the re-  
 398 absorption capacity, the larger surface area of the remaining portion of the oral region caused  
 399 a larger number of droplets to re-absorb (approximately 27%). In comparison, 21% of droplets  
 400 re-absorbed onto the teeth surface.



Figure 11 presents both the quantitative analysis and spatial distribution of droplets absorbed on the teeth surface. Primarily, the quantitative analysis serves to delineate the proportion of total absorbed droplets on the teeth surface, which was generated from distinct regions within the model. The findings revealed that out of the total number of droplets absorbed on the teeth surface, 81.02% of absorbed droplets originated from this area. Subsequently, droplets emanating from the oral cavity constituted 14.79% of the total absorbed droplets on the teeth surface. The percentage gradually reduced for the posterior regions and reached 0.45% for the bifurcation, which implies a limited quantity of droplets stemmed from this region absorbed onto the teeth surface. In addition, the spatial distribution of the droplet deposition on the teeth surface indicates that most droplets tended to settle on the inner surface of the maxillary teeth or partially in the mandibular molars and canines, regardless of their origin.

#### IV. DISCUSSIONS

The coupled EWF-DPM model was applied to explore droplet generation and flow behavior during a single coughing event, where the origin and local number concentration of the generated, absorbed, and expelled droplets were determined. This study first analysed the coughing flow rate, which provides insight into the droplet generation process during coughing. The rapid development of airflow velocity along the airway and oral cavity subjected the surface walls to high shear stress, which caused the stripping of mucus/saliva layers into

420 droplets. The airstream accelerated through the narrow airway lumen (e.g., trachea, glottis, and  
421 throat regions), consistent with a previous study (Kou et al., 2018). Thus, the predicted fluid  
422 flow is recognized as a constant feature of coughing in terms of the velocity distribution but  
423 would vary in magnitude depending on the lumen diameter of individual airway structures. In  
424 the oral cavity, this study included the teeth geometry, which has been lacking in reported  
425 simulation studies of the fluid flow characteristics during coughing. Our results indicate a  
426 strong interaction between the cough-jet stream and maxillary teeth surface, which could  
427 influence droplet generation and absorption/exhalation.

428 The shear-induced droplet generation due to the high-speed velocity is one of the four  
429 generation mechanisms that mainly occurs in the main bronchus, trachea, and larynx regions  
430 (Pöhlker et al., 2021). The results revealed an essential connection between the shear stress and  
431 the number concentration of generated droplets, summarized as follows. The higher the  
432 coughing flow rate, the greater the shear stress, and the larger the number of droplets generated.  
433 This relationship indicates the uncertainty of the generated droplet number concentration owing  
434 to the coughing flow profile, particularly at the CPFR. For instance, the significant diversity  
435 between individuals and genders has been recorded for coughing parameters, such as the peak  
436 velocity, peak velocity time, and coughing duration by field measurements (Han et al., 2021).  
437 These variations are expected to affect droplet generation. In addition, the fidelity of the  
438 numerical domain needs to be considered. Earlier simulation studies used an idealized model

439 that proposed a smooth shear stress distribution on the wall surface (Anzai et al., 2022). The  
 440 study by Ren et al. (Ren et al., 2022) reported a nonuniform distribution of shear stress on a  
 441 realistic lower airway wall. The results showed heterogeneities in spatial distribution and  
 442 magnitude of shear stress compared with ours; consequently, the droplet generation differed.  
 443 Nevertheless, the coughing flow profile, realistic attributes, and intersubject variability  
 444 presented challenges, and the simulation results need to be benchmarked against the  
 445 experimental results.

446 For infection risk assessment, it is crucial to understand the origins of droplets during  
 447 expiratory activities within a specific area and to quantify the droplets generated from each  
 448 source (Morawska, 2006). For coughing, droplet-released sources are well established and  
 449 consist of the lungs, trachea, nasopharynx-larynx, and nasal and oral passages (Stadnytskyi et  
 450 al., 2021; Zhou & Zou, 2021). However, the exact location of droplet generation/exhalation  
 451 and their localized number concentration remain uncertain. Our droplet generation analysis  
 452 indicates that the most likely sources of droplets produced during coughing were the oral cavity  
 453 and teeth surface. Although common respiratory viruses primarily occur in the epithelial cells  
 454 of the respiratory system (Alexander-Brett & Holtzman, 2015), evidence suggests high viral  
 455 loads of SARS-CoV-2 in saliva samples from an asymptomatic cohort and the active replication  
 456 of infected cells in the oral cavity (Huang et al., 2021). In addition, previous clinical studies  
 457 have detected SARS-CoV-2 in patient saliva (To et al., 2020; Wölfel et al., 2020; Wyllie et al.,

2020). Thus, from our results, the high infection risk of SARS-CoV-2 may be associated with a high droplet concentration in the oral cavity. Apart from the oral cavity, the deposition site can be determined in the airway system of the potential host (C. C. Wang et al., 2021), but this depends on the aerosols or virus-laden droplet size. Droplets from the deposition regions may cause the re-emission of progeny viruses shed by infected cells (Schaefer & Lai, 2022). Therefore, the possibility of transmission droplets originating from the respiratory system was indicated by our analytical data, where considerable quantities of exhaled droplets were recorded from the throat, larynx, trachea, and bifurcation. The results showed that the generation sites of droplets tended to be in a particular position rather than evenly distributed.

The site of origin affected the potential direction of the droplet cloud during a cough. Our results showed that exhaled droplets from the oral cavity escaped to the surroundings at all locations and angles from the mouth opening; hence, the droplets travelled further and dispersed widely. Meanwhile, exhaled droplets stripped from the respiratory airway exhibited a downward direction as they exited the mouth into the ambient environment. This phenomenon is expected to direct the droplets to the ground outside. Thus, our location-specific results can inform studies on the threat of coughing-related infections in indoor environments.

In addition to identifying the origin site, the local number concentration and size distribution of droplets exhaled during coughing were determined. Based on the literature review, these two parameters were estimated for a varied population and measurement

477 techniques. As summarized in Fig. S5 (Supplemental Material), the field measurement data  
478 were scattered broadly regarding the size distribution and number concentration. In particular,  
479 the peak number concentration was recorded in the 4–8  $\mu\text{m}$  range proposed by Yang and Chao  
480 (Yang et al., 2007; Chao et al., 2009). This peak shifted to 0.75–2  $\mu\text{m}$  in the experiment by  
481 Morawska and Johnson (Morawska et al., 2009; Johnson et al., 2011). The highest number  
482 concentration was recorded at a much smaller size, at 0.3  $\mu\text{m}$  measured by Lindsley and Zayas  
483 (Lindsley et al., 2012; Zayas et al., 2012). In addition, the number concentration among the  
484 references indicated significant variations. Therefore, our analysis was validated by recruiting  
485 one specific experimental data from Yang et al (2007). Both experimental and simulated data  
486 showed that a 4–8  $\mu\text{m}$  droplet size was formed and exhaled at a high number concentration  
487 during coughing. Within this size range, the expelled droplets would travel further into the  
488 environment and suspend for longer, enhancing the exposure risk of residents in a confined  
489 space (Jones & Brosseau, 2015; Dhand & Li, 2020; Bourouiba, 2021). Nevertheless, the  
490 lifetime and size of droplets have a complex relationship with many environmental factors,  
491 including temperature, humidity, and ventilation mechanisms (Jayaweera et al., 2020;  
492 Bahramian, 2023). Once inhaled by a susceptible person, fine aerosols (<5  $\mu\text{m}$ ) have a high  
493 possibility of escaping the defence mechanism of the upper airway and penetrating the lower  
494 airway, which is often associated with higher severity, morbidity, and fatality (Zuo et al., 2020;  
495 Sosnowski, 2021). A more significant amount of viral genomes of common respiratory viruses

496 have been revealed in fine aerosols ( $<5 \mu\text{m}$ ) compared with larger ones (Gralton et al., 2013;  
497 Yan et al., 2018). Information regarding the site origin and local number concentration was  
498 revealed by our analysis, which may not be possible in field measurements with volunteers  
499 owing to ethical and technical barriers.

500 Our simulation data showed that one issue that should be addressed in droplet generation,  
501 absorption, and exhalation studies is the inclusion of detailed oral cavity and teeth features.  
502 The oral cavity was a significant source of droplet expulsion; however, due to its complex  
503 anatomy with the existence of the teeth, the region provided a source for droplet absorption,  
504 thereby contributing to the mitigation of droplet emissions from caudal respiratory areas. By  
505 eliminating realistic features or simplifying the oral cavity, the high local concentrated  
506 absorption regions may shift to the larynx-throat region, according to our data and a previous  
507 simulation (Guo et al., 2020), allowing more droplets to be expelled. Thus, the realistic  
508 anatomy of the oral cavity alters the number concentration and spread angle of ejected droplets,  
509 thereby changing the dispersion and migration characteristics of the expelled droplets.

510 Throughout the discussion points, it is noteworthy that the data was obtained upon the  
511 assumption of one single cough event. Concerns may arise regarding whether introducing a  
512 successive coughing process would impact the results. In this context, the previous  
513 experimental research revealed the second cough characteristics with a homogeneous profile  
514 but weakened mechanical effectiveness, such as cough peak flow rate and expired volume

(Gupta et al., 2009; Hegland et al., 2013). This weakening was prolonged until the end of the cough epoch. Upon these conditions, outcome variation can be anticipated as following points:

(i) Within the coughing flow patterns, continuous accelerations are expected to occur during each coughing episode, with the highest magnitude in the first cough and a precipitous decline in the subsequent cough events.

(ii) Regarding the generated droplet number concentration, although a number concentration increase is conceivable, it would not be anticipated to yield a significant deviation from the current results. This expectation is rooted in the observation that the mucous membrane almost diminished after the initial coughing event, as indicated in Fig.4. Additionally, the WSS exerted on the respiratory wall may fall below the given CSS and be insufficient to trigger the droplet stripping.

(iii) In terms of droplet behaviors (absorbed or expelled), consecutive acceleration of fluid flow can result in the variation of the absorption rate due to the inertia, subsequently leading to the corresponding alternations in the escaped rate.

Henceforth, subjecting the current research to successive cough simulations while maintaining consistent initial conditions is expected to yield modest variations. Hence, it may be reasoned that the applicability of the results may be regarded as akin to the current findings under the assumption of a single cough process.

## V. CONCLUSIONS

Detailed information on the droplet generation, exhalation, and absorption behavior in a realistic oral-tracheal model was elucidated using the coupled EWF-DPM model. The main points of the analysis are summarised as follows:

- The EWF model reliably predicted the interaction between the free stream and liquid film lining by validating it against measured data. Coupled with the DPM model, the concentration profile of exhaled droplets from the mouth opening after a coughing episode could represent experimental data.
- The morphometry fidelity of the oral-tracheal model and the coughing flow rate affects the cough-jet stream and is expected to alter droplet generation, transportation/absorption, and exhalation.
- Shear stress at the liquid film-air interface is a critical factor governing the droplet generation properties. Therefore, appropriate values as the input criteria for the EWF and benchmarking against experimental data are required.
- The oral and teeth surface were primary locations for droplet generation. While other regions of the respiratory system showed a much lower droplet production rate. The rates gradually decreased toward the posterior regions.
- Most exhaled droplets were 4–8  $\mu\text{m}$  in diameter. Droplet sizes of  $<1 \mu\text{m}$  and  $>10 \mu\text{m}$  were also detected but were much fewer upon exhalation through the mouth opening.



553 • Including the teeth surface provided a more realistic simulation, directly influencing  
554 the droplet number concentration that could be expelled through the mouth opening.  
555 Our simulation can be a foundation for further studies on droplet cloud generation and the  
556 transmission of viral genomes in the environment from sneezing, speaking, singing, or  
557 phonation activities. It also provides quantitative and qualitative assessments of infection risk  
558 based on the site of origin, size distribution, and localised number concentration.

## 559 VI. FIGURES

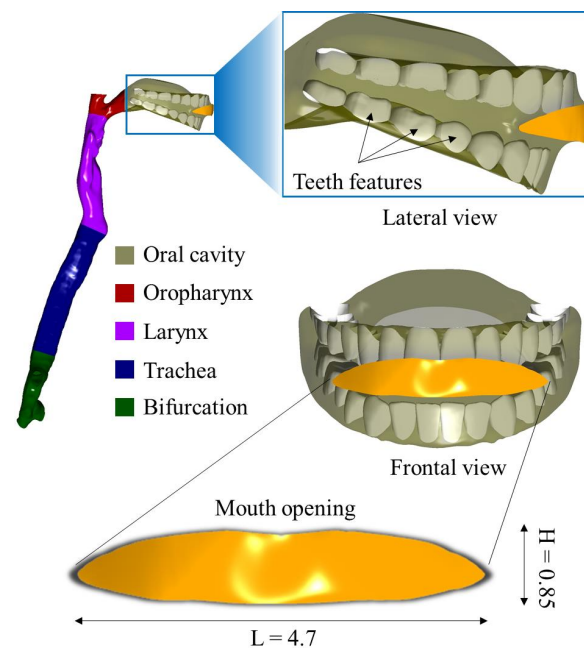


FIG. 1. Outline of the simulation model

This is the author's peer reviewed, accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset.

PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0174014

Accepted to Phys. Fluids 10.1063/5.0174014

562

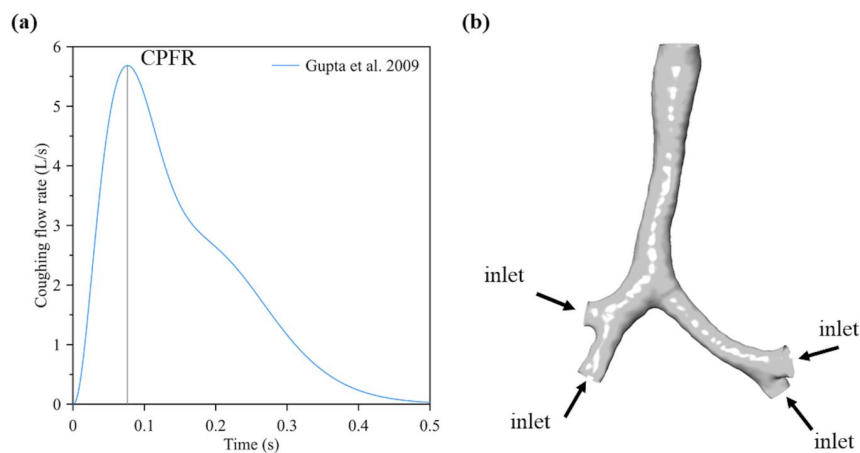


FIG. 2. (a) Coughing flow rate following the previous field measurement. (b) The description of inlet boundary conditions.

563

564

565

566

567

568

569

570

571

572

573

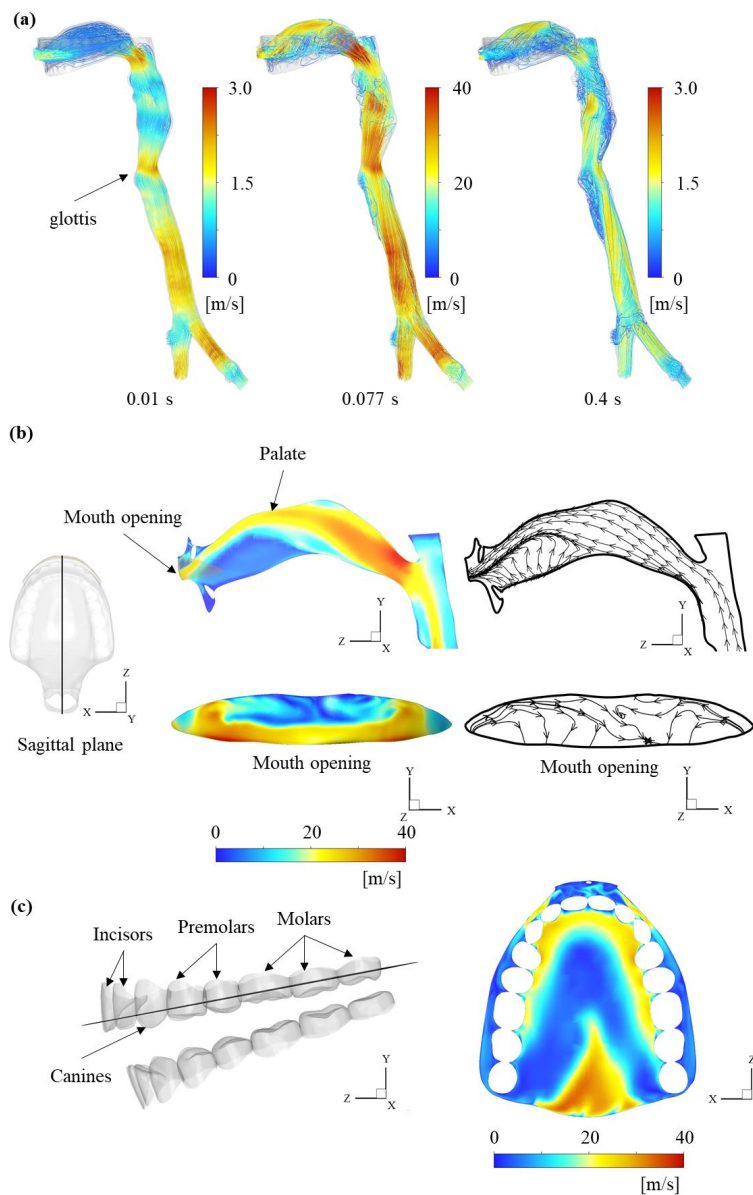


FIG. 3. (a) Instantaneous streamline velocity distribution at the specific time during coughing. (b) Instantaneous 2D flow features in the oral cavity and the mouth opening, and (c) in the vicinity of the maxillary teeth surface at the CPFR (0.077 s)

574

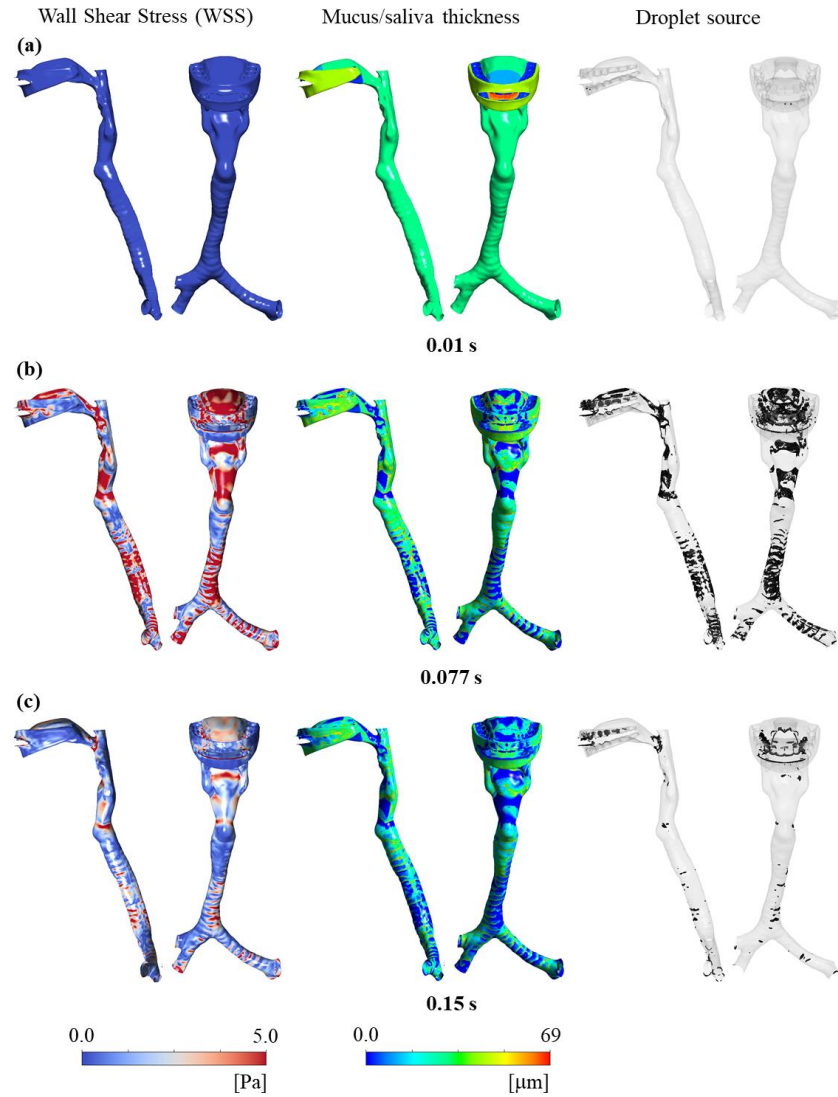


FIG. 4. The immediate distribution of wall shear stress (left), mucus/saliva thickness (middle), and initial position of stripped droplets (right) at (a) 0.01 s, (b) 0.077 s, and (c) 0.15 s.

575

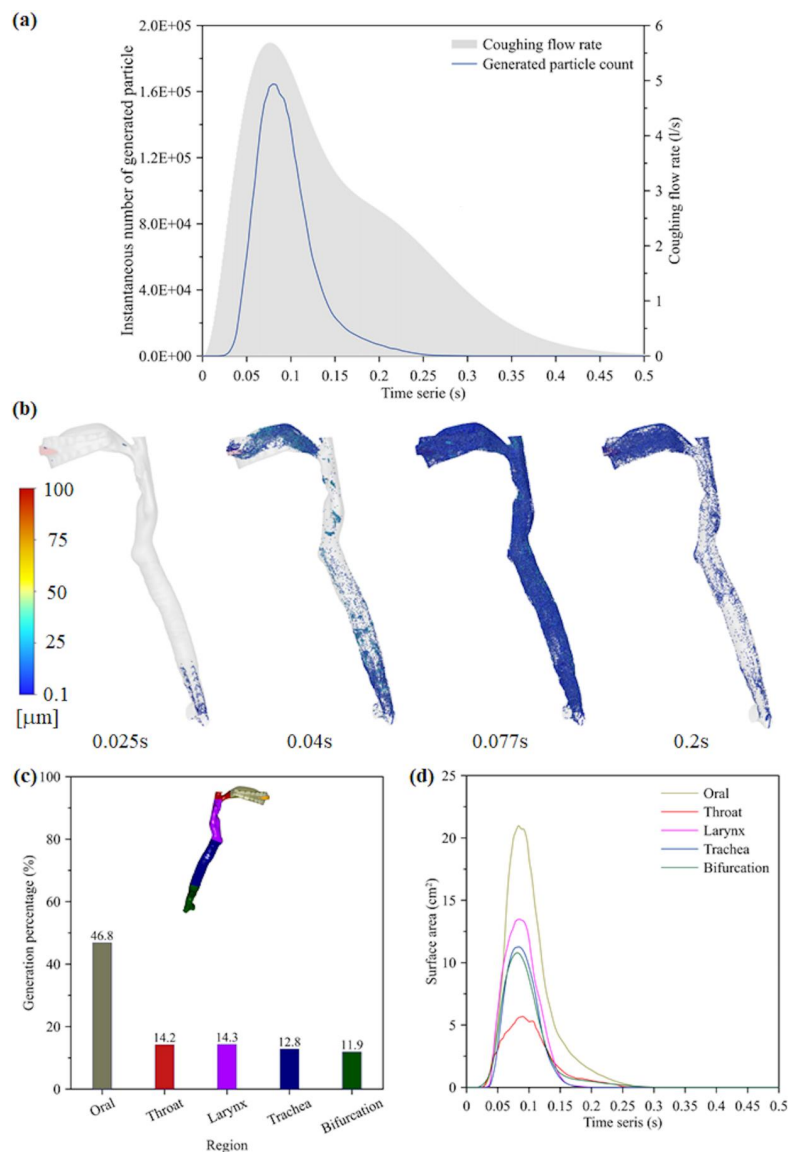


FIG. 5. (a) The instantaneous number of generated droplets during the cough event associated with the coughing flow rate. (b) Instantaneous positions of droplets at different times during the cough. (c) The percentage of droplets produced from their origin. (d) The surface area of each airway region that experienced wall shear stresses greater than 5 Pa.

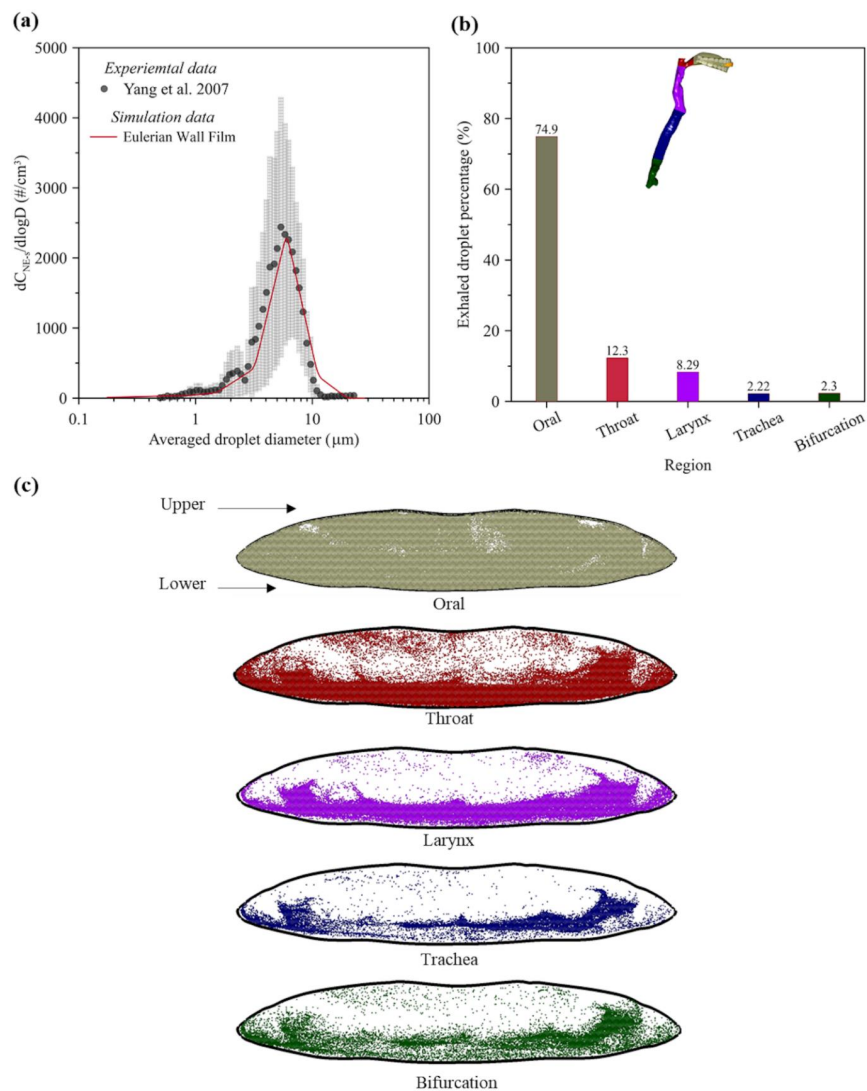


FIG. 6. (a) Validation of total concentration of exhaled droplets after one single cough event. (b) The percentage of exhaled droplets following their site origin. (c) Spatial distribution of exhaled droplets on the mouth opening after a single coughing episode.

576

577

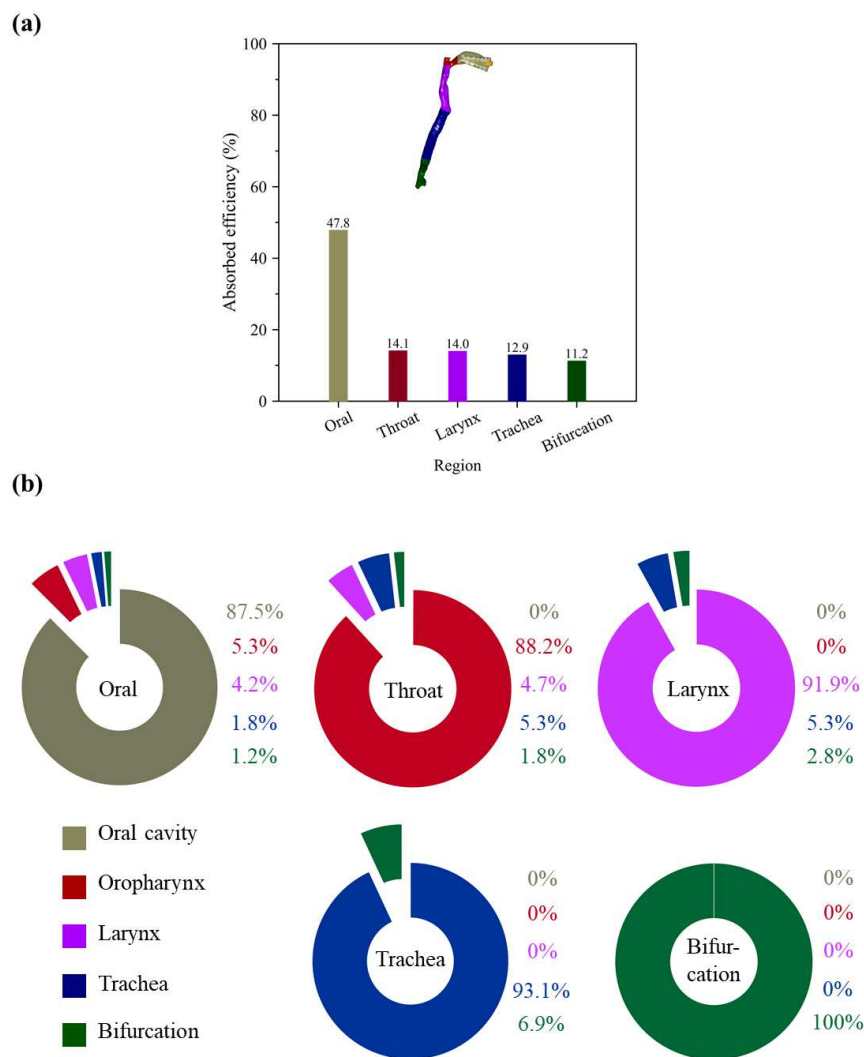


FIG. 7. (a) Total absorbed efficiency of the generated droplets on the inner surface of the airway region. (b) The absorption efficiency rate for different droplet source locations.

578

579



This is the author's peer reviewed, accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset.

PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0174014

Accepted to Phys. Fluids 10.1063/5.0174014

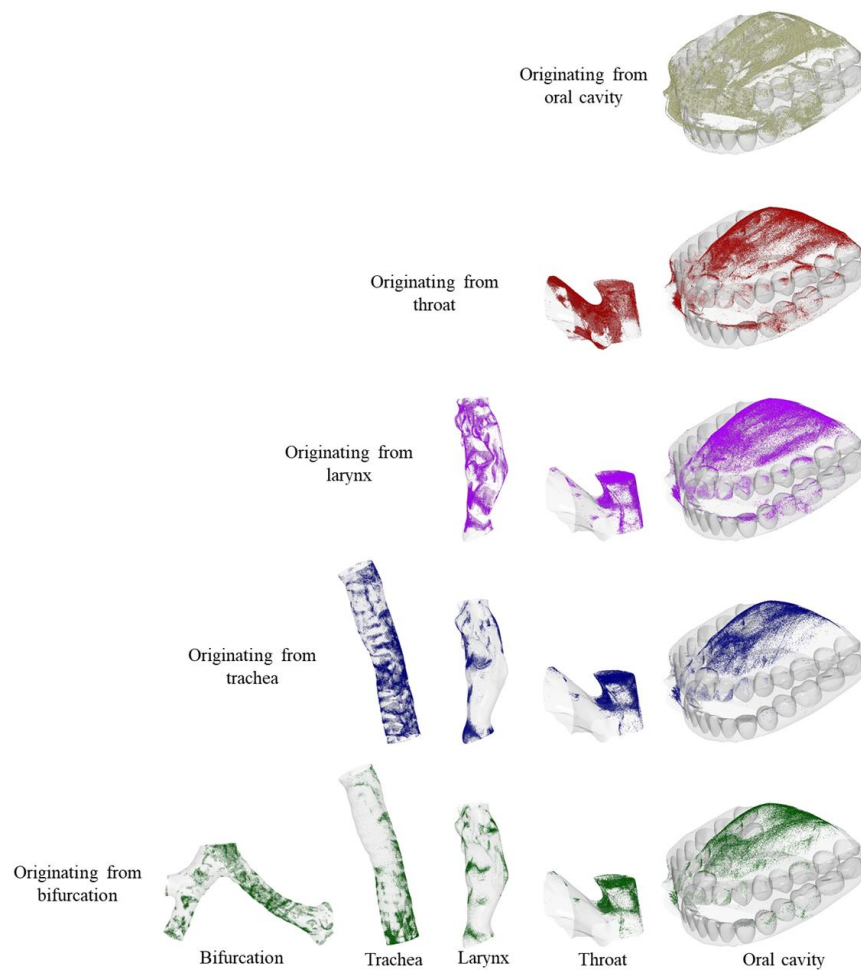


FIG. 8. Visualization of the absorbed droplets in local regions of the oral-tracheal model (column) derived from a specific location (row).

580

581



This is the author's peer reviewed, accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset.

PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0174014

Accepted to Phys. Fluids 10.1063/5.0174014

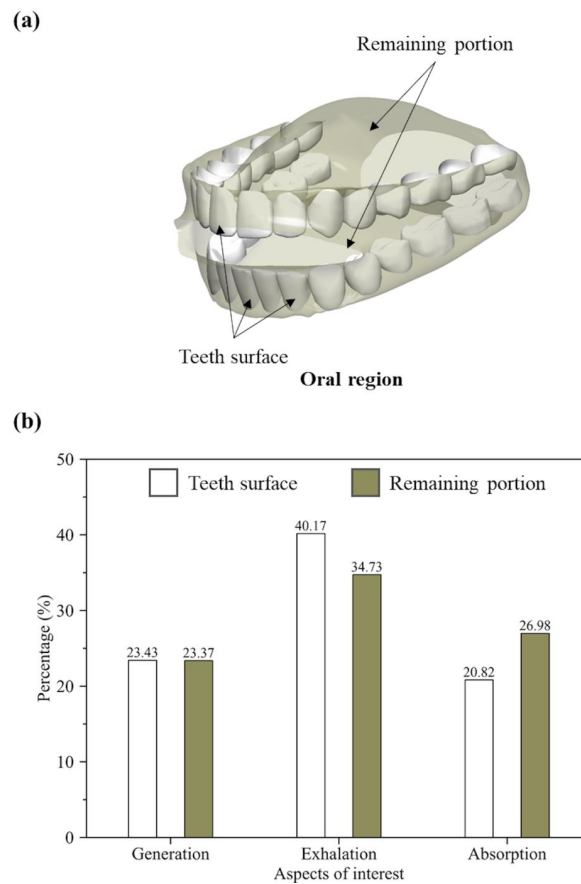


FIG. 9. (a) Outline of the oral cavity, including teeth surface and the remaining regions. (b) The total percentage of generation, exhalation, and absorption of droplets collapsed for the teeth surface and remaining portion.

582

583

584

585

586

This is the author's peer reviewed, accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset.

PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0174014

Accepted to Phys. Fluids 10.1063/5.0174014

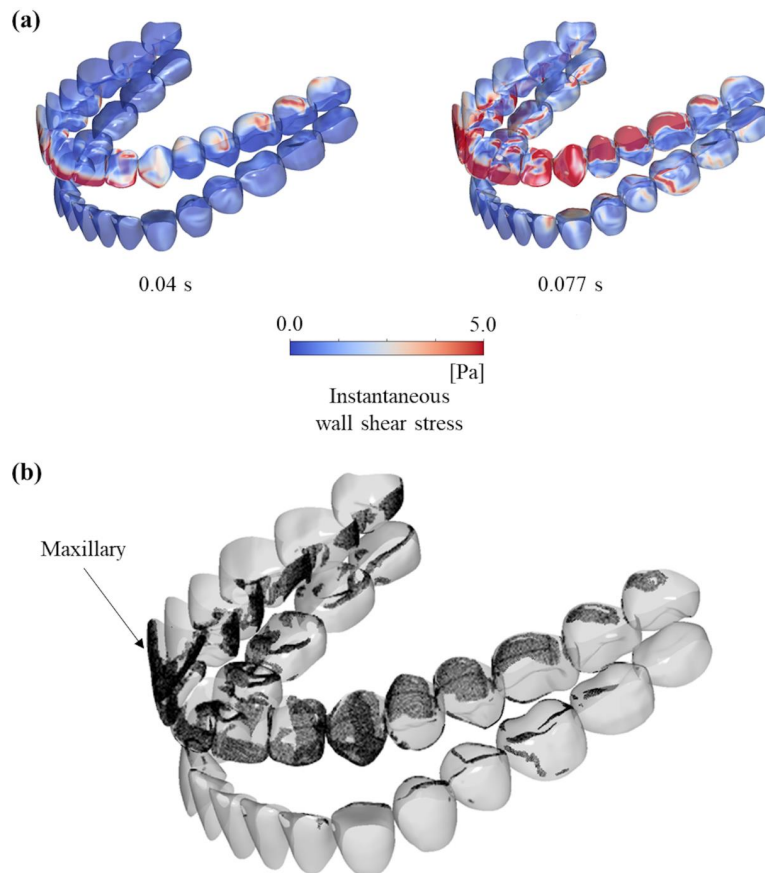


FIG. 10. (a) The instantaneous wall shear stress distribution on the teeth surface at 0.04 s (left) and 0.077 s (right). (b) Generated location and distribution of droplets on the teeth surface during coughing.

587

588

589

590

591

This is the author's peer reviewed, accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset.

PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0174014

Accepted to Phys. Fluids 10.1063/5.0174014

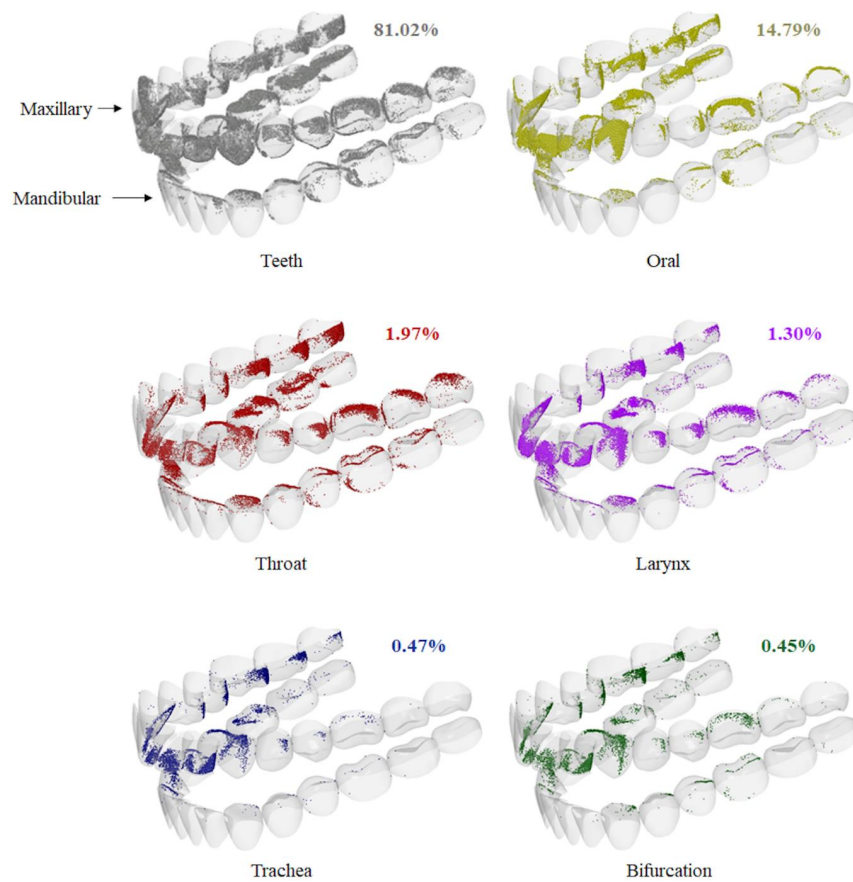


FIG. 11. 3D visualization of deposited droplets on the teeth surface colored by where the droplet was produced.

592

593

594

595

596

597 **VII. TABLES**

598 TABLE I. Numerical boundary conditions for the coughing airflow simulation.

Parameter	Information
Algorithm	SIMPLE (Semi-Implicit Method for Pressured Linked Equations)
Convection scheme	Second order upwind
Density (kg/m <sup>3</sup> )	1.185
Viscosity (kg/m s)	1.81x10 <sup>-5</sup>
Averaged cough peak flow rate (L/s)	5.75
Averaged cough exhaled volume (cm <sup>3</sup> )	1,000
Total simulation time (s)	0.5
Time step size (s)	0.001

599

600 TABLE II. Initial parameter for Eulerian Wall film model.

Parameter	Value
Critical shear stress – CSS (Pa)	5
Diameter coefficient	0.0003
Mass coefficient	0.25
Surface tension (N/m)	0.0589

601

602

603

604

605

606

607

608

609

610

This is the author's peer reviewed, accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset.

PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0174014

Accepted to Phys. Fluids 10.1063/5.0174014

611 TABLE III. Classification of droplet size bin.

Droplet size bin ( $\mu\text{m}$ )	Averaged size ( $\mu\text{m}$ )
0.1 – 0.25	0.175
0.25 – 0.5	0.375
0.5 – 0.75	0.625
0.75 – 1.0	0.875
1.0 – 2.0	1.5
2.0 – 4.0	3.0
4.0 – 8.0	6.0
8.0 – 16.0	12.0
16.0 – 24.0	20.0
24.0 – 32.0	28.0

612  
613  
614  
615  
616  
617  
618  
619  
620  
621  
622  
623  
624  
625  
626  
627  
628  
629  
630  
631  
632

This is the author's peer reviewed, accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset.

PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0174014

Accepted to Phys. Fluids 10.1063/5.0174014

TABLE IV. Generated, exhaled, and absorbed efficiency of droplets during the coughing event following the droplet size bin.

Droplet size bin( $\mu\text{m}$ )	Generated	Exhaled	Absorbed
	percentage- $\eta_{G-s}$ <sup>a</sup>	percentage- $\eta_{E-s}$ <sup>b</sup>	percentage- $\eta_{A-s}$ <sup>c</sup>
	(%)	(%)	(%)
0.1 – 0.25	0.078	0.49	0.044
0.25 – 0.5	0.133	0.79	0.078
0.5 – 0.75	0.149	0.65	0.108
0.75 – 1.0	0.181	0.50	0.157
1.0 – 2.0	1.94	2.60	1.94
2.0 – 4.0	11.81	12.82	11.58
4.0 – 8.0	78.01	73.06	78.47
8.0 – 16.0	7.53	8.93	7.47
16.0 – 24.0	0.15	0.15	0.15
24.0 – 32.0	0.019	0.01	0.003
<b>Total percentage</b>	100	100	100
<b>Total number count</b>	11,594,566 ( $N_G$ )	938,206 ( $N_E$ )	10,128,559 ( $N_A$ )

<sup>a,b,c</sup> The percentage was calculated using Equations 15, 16 and 17

## 648 **VIII. SUPPLEMENTARY MATERIAL**

649 The supplementary material contains details and discussions regarding the optimization  
650 processes for the total mesh counts and the initial parameters for the EWF model, such as  
651 critical shear stress –  $CSS$  and diameter coefficient –  $F$ . In addition, detailed boundary  
652 conditions and results, which serve to reinforce the reliability of employing the EWF model to  
653 simulate the interaction between the free-stream flow and the lining fluid on the surface, are  
654 provided.

## 655 **IX. LIMITATIONS**

656 This study focused on a specific oral-tracheal model, which did not cover the individual-  
657 related variability. Besides, it is notable that the initial parameters for the EWF model including  
658 critical shear stress –  $CSS$  and diameter coefficient –  $F$  were emphasized by the individual  
659 structure and numerical boundary conditions of this study. In addition, a rigid airway model  
660 was assumed, which is the opposite of the elastic nature of the respiratory tract and ignores  
661 glottis deformation during coughing.

## 662 **ACKNOWLEDGMENTS**

663 This study was partially funded by Japan Science and Technology (JST), CREST Japan (JP  
664 20356547), FOREST program from JST, Japan (JPMJFR225R) and JSPS KAKENHI (JP  
665 22H00237, JP 22K18300, JP 20KK0099, JP 22K14371), and MEXT as "Program for  
666 Promoting Researches on the Supercomputer Fugaku" (JPMXP1020210316).

## 667 REFERENCES

- 668 Alexander-Brett, J., & Holtzman, M. J. (2015). Virus Infection of Airway Epithelial Cells. In  
669 *Mucosal Immunology* (pp. 1013–1021). Elsevier. [https://doi.org/10.1016/B978-0-12-](https://doi.org/10.1016/B978-0-12-415847-4.00053-7)  
670 [415847-4.00053-7](https://doi.org/10.1016/B978-0-12-415847-4.00053-7)
- 671 Aljabair, S., Alesbe, I., & Alkhalaf, A. (2023). CFD modeling of influenza virus diffusion  
672 during coughing and breathing in a ventilated room. *Journal of Thermal Engineering*,  
673 127–137. <https://doi.org/10.18186/thermal.1243491>
- 674 Ansys® Academic Fluent, Release 2022 R2, Theory Guide, Eulerian Wall Films, ANSYS, Inc.
- 675 Anzai, H., Shindo, Y., Kohata, Y., Hasegawa, M., Takana, H., Matsunaga, T., Akaike, T., &  
676 Ohta, M. (2022). Coupled discrete phase model and Eulerian wall film model for  
677 numerical simulation of respiratory droplet generation during coughing. *Scientific*  
678 *Reports*, 12(1), 14849. <https://doi.org/10.1038/s41598-022-18788-3>
- 679 Archer, J., McCarthy, L. P., Symons, H. E., Watson, N. A., Orton, C. M., Browne, W. J.,  
680 Harrison, J., Moseley, B., Philip, K. E. J., Calder, J. D., Shah, P. L., Bzdek, B. R.,  
681 Costello, D., & Reid, J. P. (2022). Comparing aerosol number and mass exhalation rates  
682 from children and adults during breathing, speaking and singing. *Interface Focus*, 12(2),  
683 20210078. <https://doi.org/10.1098/rsfs.2021.0078>
- 684 Assy, Z., Jager, D. H. J., Brand, H. S., & Bikker, F. J. (2022). Salivary film thickness and  
685 MUC5B levels at various intra-oral surfaces. *Clinical Oral Investigations*, 27(2), 859–  
686 869. <https://doi.org/10.1007/s00784-022-04626-3>
- 687 Bahramian, A. (2023). Influence of indoor environmental conditions on airborne transmission  
688 and lifetime of sneeze droplets in a confined space: A way to reduce COVID-19 spread.  
689 *Environmental Science and Pollution Research*, 30(15), 44067–44085.  
690 <https://doi.org/10.1007/s11356-023-25421-x>
- 691 Bahramian, A., & Ahmadi, G. (2023). Effect of sneeze flow velocity profiles on the respiratory  
692 droplets dispersion in a confined space: An experimental and computational fluid  
693 dynamics study. *Physics of Fluids*, 35(6), 063330. <https://doi.org/10.1063/5.0151254>
- 694 Bourouiba, L. (2021). The Fluid Dynamics of Disease Transmission. *Annual Review of Fluid*  
695 *Mechanics*, 53(1), 473–508. <https://doi.org/10.1146/annurev-fluid-060220-113712>
- 696 Bourouiba, L., Dehandschoewercker, E., & Bush, J. W. M. (2014). Violent expiratory events:  
697 On coughing and sneezing. *Journal of Fluid Mechanics*, 745, 537–563.  
698 <https://doi.org/10.1017/jfm.2014.88>
- 699 Calmet, H., Inthavong, K., Both, A., Surapaneni, A., Mira, D., Egukitza, B., & Houzeaux, G.  
700 (2021). Large eddy simulation of cough jet dynamics, droplet transport, and inhalability  
701 over a ten minute exposure. *Physics of Fluids*, 33(12), 125122.  
702 <https://doi.org/10.1063/5.0072148>
- 703 Chao, C. Y. H., Wan, M. P., Morawska, L., Johnson, G. R., Ristovski, Z. D., Hargreaves, M.,



This is the author's peer reviewed, accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset.

PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0174014

Accepted to Phys. Fluids 10.1063/5.0174014

- 704 Mengersen, K., Corbett, S., Li, Y., Xie, X., & Katoshevski, D. (2009). Characterization  
705 of expiration air jets and droplet size distributions immediately at the mouth opening.  
706 *Journal of Aerosol Science*, 40(2), 122–133.  
707 <https://doi.org/10.1016/j.jaerosci.2008.10.003>
- 708 Churchyard, G., Kim, P., Shah, N. S., Rustumjee, R., Gandhi, N., Mathema, B., Dowdy, D.,  
709 Kasmar, A., & Cardenas, V. (2017). What We Know About Tuberculosis Transmission:  
710 An Overview. *The Journal of Infectious Diseases*, 216(suppl\_6), S629–S635.  
711 <https://doi.org/10.1093/infdis/jix362>
- 712 Collins, L. M. C., & Dawes, C. (1987). The Surface Area of the Adult Human Mouth and  
713 Thickness of the Salivary Film Covering the Teeth and Oral Mucosa. *Journal of Dental*  
714 *Research*, 66(8), 1300–1302. <https://doi.org/10.1177/00220345870660080201>
- 715 Dbouk, T., & Drikakis, D. (2020). On coughing and airborne droplet transmission to humans.  
716 *Physics of Fluids*, 32(5), 053310. <https://doi.org/10.1063/5.0011960>
- 717 Dhand, R., & Li, J. (2020). Coughs and Sneezes: Their Role in Transmission of Respiratory  
718 Viral Infections, Including SARS-CoV-2. *American Journal of Respiratory and Critical*  
719 *Care Medicine*, 202(5), 651–659. <https://doi.org/10.1164/rccm.202004-1263PP>
- 720 Elcner, J., Lizal, F., Jedelsky, J., Jicha, M., & Chovancova, M. (2016). Numerical investigation  
721 of inspiratory airflow in a realistic model of the human tracheobronchial airways and a  
722 comparison with experimental results. *Biomechanics and Modeling in Mechanobiology*,  
723 15(2), 447–469. <https://doi.org/10.1007/s10237-015-0701-1>
- 724 Galton, J., Tovey, E. R., McLaws, M.-L., & Rawlinson, W. D. (2013). Respiratory virus RNA  
725 is detectable in airborne and droplet particles: Viral RNA in Airborne and Droplet  
726 Particles. *Journal of Medical Virology*, 85(12), 2151–2159.  
727 <https://doi.org/10.1002/jmv.23698>
- 728 Guo, Y., Wei, J., Ou, C., Liu, L., Sadrizadeh, S., Jin, T., Tang, L., Zhang, Y., & Li, Y. (2020).  
729 Deposition of droplets from the trachea or bronchus in the respiratory tract during  
730 exhalation: A steady-state numerical investigation. *Aerosol Science and Technology*,  
731 54(8), 869–879. <https://doi.org/10.1080/02786826.2020.1772459>
- 732 Gupta, J. K., Lin, C.-H., & Chen, Q. (2009). Flow dynamics and characterization of a cough:  
733 Flow dynamics and characterization of a cough. *Indoor Air*, 19(6), 517–525.  
734 <https://doi.org/10.1111/j.1600-0668.2009.00619.x>
- 735 Han, M., Ooka, R., Kikumoto, H., Oh, W., Bu, Y., & Hu, S. (2021). Measurements of exhaled  
736 airflow velocity through human coughs using particle image velocimetry. *Building and*  
737 *Environment*, 202, 108020. <https://doi.org/10.1016/j.buildenv.2021.108020>
- 738 Harrison, J., Saccente-Kennedy, B., Orton, C. M., McCarthy, L. P., Archer, J., Symons, H. E.,  
739 Szczepanska, A., Watson, N. A., Browne, W. J., Moseley, B., Philip, K. E. J., Hull, J.  
740 H., Calder, J. D., Costello, D., Shah, P. L., Epstein, R., Reid, J. P., & Bzdek, B. R. (2023).  
741 Emission rates, size distributions, and generation mechanism of oral respiratory

- droplets. *Aerosol Science and Technology*, 1–13.  
https://doi.org/10.1080/02786826.2022.2158778
- Hegland, K. W., Troche, M. S., & Davenport, P. W. (2013). Cough expired volume and airflow rates during sequential induced cough. *Frontiers in Physiology*, 4.  
https://doi.org/10.3389/fphys.2013.00167
- Hossain, M., Chinenye-Kanu, N., Faisal, N. H., Prathuru, A., Asim, T., & Banik, S. (2023). Numerical Prediction of the Effect of Thermal Plume of a Standing Human on the Airborne Aerosol Flow in a Room: Assessment of the Social Distancing Rule. *Aerosol Science and Engineering*, 7(1), 96–106. https://doi.org/10.1007/s41810-022-00165-2
- Huang, N., Pérez, P., Kato, T., Mikami, Y., Okuda, K., Gilmore, R. C., Conde, C. D., Gasmi, B., Stein, S., Beach, M., Pelayo, E., Maldonado, J. O., Lafont, B. A., Jang, S.-I., Nasir, N., Padilla, R. J., Murrah, V. A., Maile, R., Lovell, W., ... Byrd, K. M. (2021). SARS-CoV-2 infection of the oral cavity and saliva. *Nature Medicine*, 27(5), 892–903. https://doi.org/10.1038/s41591-021-01296-8
- Inthavong, K. (2020). From indoor exposure to inhaled particle deposition: A multiphase journey of inhaled particles. *Experimental and Computational Multiphase Flow*, 2(2), 59–78. https://doi.org/10.1007/s42757-019-0046-6
- Ito, K. (2016). Toward the development of an *in silico* human model for indoor environmental design. *Proceedings of the Japan Academy, Series B*, 92(7), 185–203. https://doi.org/10.2183/pjab.92.185
- Jayaweera, M., Perera, H., Gunawardana, B., & Manatunge, J. (2020). Transmission of COVID-19 virus by droplets and aerosols: A critical review on the unresolved dichotomy. *Environmental Research*, 188, 109819. https://doi.org/10.1016/j.envres.2020.109819
- Johnson, G. R., Morawska, L., Ristovski, Z. D., Hargreaves, M., Mengersen, K., Chao, C. Y. H., Wan, M. P., Li, Y., Xie, X., Katoshevski, D., & Corbett, S. (2011). Modality of human expired aerosol size distributions. *Journal of Aerosol Science*, 42(12), 839–851. https://doi.org/10.1016/j.jaerosci.2011.07.009
- Jones, R. M., & Brosseau, L. M. (2015). Aerosol Transmission of Infectious Disease. *Journal of Occupational & Environmental Medicine*, 57(5), 501–508. https://doi.org/10.1097/JOM.0000000000000448
- Kakimpa, B., Morvan, H. P., & Hibberd, S. (2015). Solution Strategies for Thin Film Rimming Flow Modelling. *Volume 5C: Heat Transfer*, V05CT15A026. https://doi.org/10.1115/GT2015-43503
- Khoa, N. D., Li, S., Phuong, N. L., Kuga, K., Yabuuchi, H., Kan-O, K., Matsumoto, K., & Ito, K. (2023). Computational fluid-particle dynamics modeling of ultrafine to coarse particles deposition in the human respiratory system, down to the terminal bronchiole. *Computer Methods and Programs in Biomedicine*, 237, 107589.

This is the author's peer reviewed, accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset.

PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0174014

Accepted to Phys. Fluids 10.1063/5.0174014

- 780 <https://doi.org/10.1016/j.cmpb.2023.107589>
- 781 Khoa, N. D., Phuong, N. L., Tani, K., Inthavong, K., & Ito, K. (2023). In-silico decongested
- 782 trial effects on the impaired breathing function of a bulldog suffering from severe
- 783 brachycephalic obstructive airway syndrome. *Computer Methods and Programs in*
- 784 *Biomedicine*, 228, 107243. <https://doi.org/10.1016/j.cmpb.2022.107243>
- 785 Kou, G., Li, X., Wang, Y., Lin, M., Zeng, Y., Yang, X., Yang, Y., & Gan, Z. (2018). CFD
- 786 Simulation of Airflow Dynamics During Cough Based on CT-Scanned Respiratory
- 787 Airway Geometries. *Symmetry*, 10(11), 595. <https://doi.org/10.3390/sym10110595>
- 788 Kuga, K., Ito, K., Chen, W., Wang, P., Fowles, J., & Kumagai, K. (2021). Secondary indoor air
- 789 pollution and passive smoking associated with cannabis smoking using electric
- 790 cigarette device—demonstrative in silico study. *PLOS Computational Biology*, 17(5),
- 791 e1009004. <https://doi.org/10.1371/journal.pcbi.1009004>
- 792 Kuga, K., Kizuka, R., Khoa, N. D., & Ito, K. (2023). Effect of transient breathing cycle on the
- 793 deposition of micro and nanoparticles on respiratory walls. *Computer Methods and*
- 794 *Programs in Biomedicine*, 236, 107501. <https://doi.org/10.1016/j.cmpb.2023.107501>
- 795 Kuga, K., Sakamoto, M., Wargocki, P., & Ito, K. (2022). Prediction of exhaled carbon dioxide
- 796 concentration using a computer-simulated person that included alveolar gas exchange.
- 797 *Indoor Air*, 32(8).
- 798 Li, A., & Ahmadi, G. (1992). Dispersion and Deposition of Spherical Particles from Point
- 799 Sources in a Turbulent Channel Flow. *Aerosol Science and Technology*, 16(4), 209–226.
- 800 <https://doi.org/10.1080/02786829208959550>
- 801 Li, H., Kuga, K., & Ito, K. (2022). SARS-CoV-2 Dynamics in the Mucus Layer of the Human
- 802 Upper Respiratory Tract Based on Host–Cell Dynamics. *Sustainability*, 14(7), 3896.
- 803 <https://doi.org/10.3390/su14073896>
- 804 Li, H., Leong, F. Y., Xu, G., Kang, C. W., Lim, K. H., Tan, B. H., & Loo, C. M. (2021). Airborne
- 805 dispersion of droplets during coughing: A physical model of viral transmission.
- 806 *Scientific Reports*, 11(1), 4617. <https://doi.org/10.1038/s41598-021-84245-2>
- 807 Li, X., Mak, C. M., Ai, Z., Ma, K. W., & Wong, H. M. (2023). Numerical investigation of the
- 808 impacts of environmental conditions and breathing rate on droplet transmission during
- 809 dental service. *Physics of Fluids*, 35(4), 043332. <https://doi.org/10.1063/5.0144647>
- 810 Lindsley, W. G., Pearce, T. A., Hudnall, J. B., Davis, K. A., Davis, S. M., Fisher, M. A., Khakoo,
- 811 R., Palmer, J. E., Clark, K. E., Celik, I., Coffey, C. C., Blachere, F. M., & Beezhold, D.
- 812 H. (2012). Quantity and Size Distribution of Cough-Generated Aerosol Particles
- 813 Produced by Influenza Patients During and After Illness. *Journal of Occupational and*
- 814 *Environmental Hygiene*, 9(7), 443–449.
- 815 <https://doi.org/10.1080/15459624.2012.684582>
- 816 Mariam, Magar, A., Joshi, M., Rajagopal, P. S., Khan, A., Rao, M. M., & Sapra, B. K. (2021).
- 817 CFD Simulation of the Airborne Transmission of COVID-19 Vectors Emitted during

- 818 Respiratory Mechanisms: Revisiting the Concept of Safe Distance. *ACS Omega*, 6(26),  
819 16876–16889. <https://doi.org/10.1021/acsomega.1c01489>
- 820 Morawska, L. (2006). Droplet fate in indoor environments, or can we prevent the spread of  
821 infection? *Indoor Air*, 16(5), 335–347. [https://doi.org/10.1111/j.1600-](https://doi.org/10.1111/j.1600-0668.2006.00432.x)  
822 0668.2006.00432.x
- 823 Morawska, L., Johnson, G. R., Ristovski, Z. D., Hargreaves, M., Mengersen, K., Corbett, S.,  
824 Chao, C. Y. H., Li, Y., & Katoshevski, D. (2009). Size distribution and sites of origin of  
825 droplets expelled from the human respiratory tract during expiratory activities. *Journal*  
826 *of Aerosol Science*, 40(3), 256–269. <https://doi.org/10.1016/j.jaerosci.2008.11.002>
- 827 Murga, A., Bale, R., Li, C.-G., Ito, K., & Tsubokura, M. (2023). Large eddy simulation of  
828 droplet transport and deposition in the human respiratory tract to evaluate inhalation  
829 risk. *PLOS Computational Biology*, 19(3), e1010972.  
830 <https://doi.org/10.1371/journal.pcbi.1010972>
- 831 Nie, Z., Chen, Y., & Deng, M. (2022). Quantitative evaluation of precautions against the  
832 COVID-19 indoor transmission through human coughing. *Scientific Reports*, 12(1),  
833 22573. <https://doi.org/10.1038/s41598-022-26837-0>
- 834 Nishandar, S. R., He, Y., Princevac, M., & Edwards, R. D. (2023). Fate of Exhaled Droplets  
835 From Breathing and Coughing in Supermarket Checkouts and Passenger Cars.  
836 *Environmental Health Insights*, 17, 117863022211482.  
837 <https://doi.org/10.1177/11786302221148274>
- 838 Pairetti, C., Villiers, R., & Zaleski, S. (2021). On shear layer atomization within closed  
839 channels: Numerical simulations of a cough-replicating experiment. *Computers &*  
840 *Fluids*, 231, 105125. <https://doi.org/10.1016/j.compfluid.2021.105125>
- 841 Payri, R., Martí-Aldaravi, P., Quintero, P. M., & Marco-Gimeno, J. (2021). LARGE EDDY  
842 SIMULATION FOR THE PREDICTION OF HUMAN COUGHING. *Atomization and*  
843 *Sprays*, 31(9), 49–73. <https://doi.org/10.1615/AtomizSpr.2021037129>
- 844 Paz, C., Suárez, E., Parga, O., & Vence, J. (2017). Glottis effects on the cough clearance process  
845 simulated with a CFD dynamic mesh and Eulerian wall film model. *Computer Methods*  
846 *in Biomechanics and Biomedical Engineering*, 20(12), 1326–1338.  
847 <https://doi.org/10.1080/10255842.2017.1360872>
- 848 Paz, C., Suárez, E., & Vence, J. (2017). CFD transient simulation of the cough clearance  
849 process using an Eulerian wall film model. *Computer Methods in Biomechanics and*  
850 *Biomedical Engineering*, 20(2), 142–152.  
851 <https://doi.org/10.1080/10255842.2016.1206532>
- 852 Paz, C., Suárez, E., Vence, J., & Cabarcos, A. (2019). Analysis of the volume of fluid (VOF)  
853 method for the simulation of the mucus clearance process with CFD. *Computer*  
854 *Methods in Biomechanics and Biomedical Engineering*, 22(5), 547–566.  
855 <https://doi.org/10.1080/10255842.2019.1569637>

- 856 Phuong, N. L., & Ito, K. (2015). Investigation of flow pattern in upper human airway including  
857 oral and nasal inhalation by PIV and CFD. *Building and Environment*, 94, 504–515.  
858 <https://doi.org/10.1016/j.buildenv.2015.10.002>
- 859 Piret, J., & Boivin, G. (2021). Pandemics Throughout History. *Frontiers in Microbiology*, 11,  
860 631736. <https://doi.org/10.3389/fmicb.2020.631736>
- 861 Pöhlker, M. L., Krüger, O. O., Förster, J.-D., Berkemeier, T., Elbert, W., Fröhlich-Nowoisky,  
862 J., Pöschl, U., Pöhlker, C., Bagheri, G., Bodenschatz, E., Huffman, J. A., Scheithauer,  
863 S., & Mikhailov, E. (2021). *Respiratory aerosols and droplets in the transmission of*  
864 *infectious diseases* (arXiv:2103.01188). arXiv. <http://arxiv.org/abs/2103.01188>
- 865 Rajendran, R. R., & Banerjee, A. (2019). Mucus transport and distribution by steady expiration  
866 in an idealized airway geometry. *Medical Engineering & Physics*, 66, 26–39.  
867 <https://doi.org/10.1016/j.medengphy.2019.02.006>
- 868 Ren, S., Cai, M., Shi, Y., Luo, Z., & Wang, T. (2022). Influence of cough airflow characteristics  
869 on respiratory mucus clearance. *Physics of Fluids*, 34(4), 041911.  
870 <https://doi.org/10.1063/5.0088100>
- 871 Ren, S., Li, W., Wang, L., Shi, Y., Cai, M., Hao, L., Luo, Z., Niu, J., Xu, W., & Luo, Z. (2020).  
872 Numerical Analysis of Airway Mucus Clearance Effectiveness Using Assisted  
873 Coughing Techniques. *Scientific Reports*, 10. [https://doi.org/10.1038/s41598-020-](https://doi.org/10.1038/s41598-020-58922-7)  
874 [58922-7](https://doi.org/10.1038/s41598-020-58922-7)
- 875 Ren, S., Shi, Y., Cai, M., Zhao, H., & Zhang, Z. (2018). ANSYS-MATLAB co-simulation of  
876 mucus flow distribution and clearance effectiveness of a new simulated cough device.  
877 *International Journal for Numerical Methods in Biomedical Engineering*, 34(6).  
878 <https://doi.org/10.1002/cnm.2978>
- 879 Saffman, P. G. (1965). The lift on a small sphere in a slow shear flow. *Journal of Fluid*  
880 *Mechanics*, 22(2), 385–400. <https://doi.org/10.1017/S0022112065000824>
- 881 Schaefer, A., & Lai, S. K. (2022). The biophysical principles underpinning muco-trapping  
882 functions of antibodies. *Human Vaccines & Immunotherapeutics*, 18(2), 1939605.  
883 <https://doi.org/10.1080/21645515.2021.1939605>
- 884 Seminara, G., Carli, B., Forni, G., Fuzzi, S., Mazzino, A., & Rinaldo, A. (2020). Biological  
885 fluid dynamics of airborne COVID-19 infection. *Rendiconti Lincei. Scienze Fisiche e*  
886 *Naturali*, 31(3), 505–537. <https://doi.org/10.1007/s12210-020-00938-2>
- 887 SeyedAlinaghi, S., Karimi, A., Mojdeganlou, H., Pashaei, Z., Mirzapour, P., Shamsabadi, A.,  
888 Barzegary, A., Afroughi, F., Dehghani, S., Janfaza, N., Fakhfour, A., Khodaei, S.,  
889 Mehraeen, E., & Dadras, O. (2022). Minimum infective dose of severe acute respiratory  
890 syndrome coronavirus 2 based on the current evidence: A systematic review. *SAGE*  
891 *Open Medicine*, 10, 205031212211150. <https://doi.org/10.1177/20503121221115053>
- 892 Shelley, D. A., Sih, B. L., & Ng, L. J. (2014). *An integrated physiology model to study regional*  
893 *lung damage effects and the physiologic response*. 19.

This is the author's peer reviewed, accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset.

PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0174014

Accepted to Phys. Fluids 10.1063/5.0174014

- 894 Sosnowski, T. R. (2021). Inhaled aerosols: Their role in COVID-19 transmission, including  
895 biophysical interactions in the lungs. *Current Opinion in Colloid & Interface Science*,  
896 54, 101451. <https://doi.org/10.1016/j.cocis.2021.101451>
- 897 Stadnytskyi, V., Anfinrud, P., & Bax, A. (2021). Breathing, speaking, coughing or sneezing:  
898 What drives transmission of SARS-CoV-2? *Journal of Internal Medicine*, 290(5),  
899 1010–1027. <https://doi.org/10.1111/joim.13326>
- 900 To, K. K.-W., Tsang, O. T.-Y., Yip, C. C.-Y., Chan, K.-H., Wu, T.-C., Chan, J. M.-C., Leung,  
901 W.-S., Chik, T. S.-H., Choi, C. Y.-C., Kandamby, D. H., Lung, D. C., Tam, A. R., Poon,  
902 R. W.-S., Fung, A. Y.-F., Hung, I. F.-N., Cheng, V. C.-C., Chan, J. F.-W., & Yuen, K.-Y.  
903 (2020). Consistent Detection of 2019 Novel Coronavirus in Saliva. *Clinical Infectious*  
904 *Diseases*, 71(15), 841–843. <https://doi.org/10.1093/cid/ciaa149>
- 905 Wang, C. C., Prather, K. A., Sznitman, J., Jimenez, J. L., Lakdawala, S. S., Tufekci, Z., & Marr,  
906 L. C. (2021). Airborne transmission of respiratory viruses. *Science*, 373(6558),  
907 eabd9149. <https://doi.org/10.1126/science.abd9149>
- 908 Wang, C., Yoo, S.-J., Tanabe, S., & Ito, K. (2020). Investigation of transient and heterogeneous  
909 micro-climate around a human body in an enclosed personalized work environment.  
910 *Energy and Built Environment*, 1(4), 423–431.  
911 <https://doi.org/10.1016/j.enbenv.2020.04.011>
- 912 Wang, H., Li, Z., Zhang, X., Zhu, L., Liu, Y., & Wang, S. (2020). The motion of respiratory  
913 droplets produced by coughing. *Physics of Fluids*, 32(12), 125102.  
914 <https://doi.org/10.1063/5.0033849>
- 915 Wei, J., & Li, Y. (2016). Airborne spread of infectious agents in the indoor environment.  
916 *American Journal of Infection Control*, 44(9), S102–S108.  
917 <https://doi.org/10.1016/j.ajic.2016.06.003>
- 918 Widders, A., Broom, A., & Broom, J. (2020). SARS-CoV-2: The viral shedding vs infectivity  
919 dilemma. *Infection, Disease & Health*, 25(3), 210–215.  
920 <https://doi.org/10.1016/j.idh.2020.05.002>
- 921 Wölfel, R., Corman, V. M., Guggemos, W., Seilmaier, M., Zange, S., Müller, M. A., Niemeyer,  
922 D., Jones, T. C., Vollmar, P., Rothe, C., Hoelscher, M., Bleicker, T., Brünink, S.,  
923 Schneider, J., Ehmann, R., Zwirgmaier, K., Drosten, C., & Wendtner, C. (2020).  
924 Virological assessment of hospitalized patients with COVID-2019. *Nature*, 581(7809),  
925 465–469. <https://doi.org/10.1038/s41586-020-2196-x>
- 926 Wyllie, A. L., Fournier, J., Casanovas-Massana, A., Campbell, M., Tokuyama, M., Vijayakumar,  
927 P., Warren, J. L., Geng, B., Muenker, M. C., Moore, A. J., Vogels, C. B. F., Petrone, M.  
928 E., Ott, I. M., Lu, P., Venkataraman, A., Lu-Culligan, A., Klein, J., Earnest, R., Simonov,  
929 M., ... Ko, A. I. (2020). Saliva or Nasopharyngeal Swab Specimens for Detection of  
930 SARS-CoV-2. *New England Journal of Medicine*, 383(13), 1283–1286.  
931 <https://doi.org/10.1056/NEJMc2016359>



- 932 Yan, J., Grantham, M., Pantelic, J., Bueno De Mesquita, P. J., Albert, B., Liu, F., Ehrman, S.,  
933 Milton, D. K., EMIT Consortium, Adamson, W., Beato-Arribas, B., Bischoff, W., Booth,  
934 W., Cauchemez, S., Ehrman, S., Enstone, J., Ferguson, N., Forni, J., Gilbert, A., ...  
935 Tellier, R. (2018). Infectious virus in exhaled breath of symptomatic seasonal influenza  
936 cases from a college community. *Proceedings of the National Academy of Sciences*,  
937 *115*(5), 1081–1086. <https://doi.org/10.1073/pnas.1716561115>
- 938 Yang, S., Lee, G. W. M., Chen, C.-M., Wu, C.-C., & Yu, K.-P. (2007). The Size and  
939 Concentration of Droplets Generated by Coughing in Human Subjects. *Journal of*  
940 *Aerosol Medicine*, *20*(4), 484–494. <https://doi.org/10.1089/jam.2007.0610>
- 941 Yi, H., Wang, Q., & Feng, Y. (2021). Computational analysis of obstructive disease and cough  
942 intensity effects on the mucus transport and clearance in an idealized upper airway  
943 model using the volume of fluid method. *Physics of Fluids*, *33*(2), 021903.  
944 <https://doi.org/10.1063/5.0037764>
- 945 Yoo, S., & Ito, K. (2022). Validation, verification, and quality control of computational fluid  
946 dynamics analysis for indoor environments using a computer-simulated person with  
947 respiratory tract. *JAPAN ARCHITECTURAL REVIEW*, *5*(4), 714–727.  
948 <https://doi.org/10.1002/2475-8876.12301>
- 949 Zayas, G., Chiang, M. C., Wong, E., MacDonald, F., Lange, C. F., Senthilselvan, A., & King,  
950 M. (2012). Cough aerosol in healthy participants: Fundamental knowledge to optimize  
951 droplet-spread infectious respiratory disease management. *BMC Pulmonary Medicine*,  
952 *12*(1), 11. <https://doi.org/10.1186/1471-2466-12-11>
- 953 Zhou, M., & Zou, J. (2021). A dynamical overview of droplets in the transmission of respiratory  
954 infectious diseases. *Physics of Fluids*, *33*(3), 031301.  
955 <https://doi.org/10.1063/5.0039487>
- 956 Zore, K., Parkhi, G., Sasanapuri, B., & Varghese, A. (2019). 21th Annual CFD Symposium,  
957 August 8-9, 2019, Bangalore. *Annual CFD Symposium*, 0–11.
- 958 Zuo, Y. Y., Uspal, W. E., & Wei, T. (2020). Airborne Transmission of COVID-19: Aerosol  
959 Dispersion, Lung Deposition, and Virus-Receptor Interactions. *ACS Nano*, *14*(12),  
960 16502–16524. <https://doi.org/10.1021/acsnano.0c08484>

## 962 CONFLICT OF INTEREST STATEMENT

963 The authors declare that they have no competing financial interests or personal  
964 relationships that could have influenced the work reported in this paper.

## 965 DATA AVAILABILITY

This is the author's peer reviewed, accepted manuscript. However, the online version of record will be different from this version once it has been copyedited and typeset.

PLEASE CITE THIS ARTICLE AS DOI: 10.1063/5.0174014

*Accepted to Phys. Fluids 10.1063/5.0174014*

966        The data supporting this study's findings are available from the corresponding author upon  
967        reasonable request.