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Numerical modeling of airborne transmission from airway mucosa of infected person to that of uninfected individual via indoor airflow

Kazuhide Ito[1*], *Kazuki* Kuga[1]

[1]Faculty of Engineering Sciences, Kyushu University, Japan

Abstract. To elucidate the mechanism of airborne transmission caused by virus-laden droplets/droplet nuclei, such as SARS-CoV-2, it is essential to clarify the transmission dynamics of infectious particles in indoor environments, from the respiratory tract of an infected person to that of an uninfected individual. In this study, assuming airborne transmission of SARS-CoV-2 in an indoor environment, we developed and conducted a seamless numerical analysis of (i) the size distribution of droplets/droplet nuclei using the Discrete Phase Eulerian Wall Film (DP-EWF) model, (ii) exhalation of droplets/droplet nuclei using the Computational Fluid and Particle Dynamics (CFPD) method, (iii) subsequent inhalation exposure of an uninfected person (via the respiratory tract), and (iv) time-series and heterogeneous changes in viral load (RNA copies/mL in mucus) in the respiratory tract predicted by a host cell dynamics (HCD) model that captures viral infection within the respiratory system. This comprehensive set of numerical analyses can accurately reproduce changes in viral load in droplets/droplet nuclei as a function of elapsed time since the onset of infection. Such insights contribute to a more accurate assessment of the risk of airborne infection in indoor environments.

1 Introduction

Although the pandemic caused by the novel coronavirus SARS-CoV-2 has peaked, it remains essential to consider the risk of airborne transmission in indoor and vehicle environments, including seasonal influenza and tuberculosis [1]. Managing airborne transmission and infection risk should be considered primarily from the perspective of both emission sources and ventilation control [2]. The primary emission source of airborne transmission indoors is the generation of virus-laden droplets through the coughing of an infected person(s) and their indoor release from the respiratory system. Understanding the mechanism of generation and emission of virus-laden droplets is crucial for developing methods to control infection risk. Once cough-generated virus-laden droplets released into the indoor environment are transported by advection and diffusion of the indoor airflow. Some of these droplets reach non-infected individuals, entering their respiratory systems and depositing on the mucosal epithelial tissue surface of the airway. The amount of inhalation exposure to virus-laden droplets depends on the characteristics of the indoor flow field and ventilation efficiency. Therefore, it is imperative to comprehend the series of transport mechanisms from the airway mucosa of an infected person to that of an uninfected individual via indoor airflow. Developing appropriate ventilation designs is crucial for controlling airborne transmission.

To address this issue, we have been developing a series of numerical analysis techniques to comprehensively and seamlessly analyze airborne transmission and infection dynamics from the generation of virus-laden droplets to infection. This involves integrating computational fluid dynamics (CFD) analysis and a computer-simulated person (CSP) with a respiratory tract model [3-5].

In the current study, focusing on the airborne transmission of SARS-CoV-2 in an indoor environment, we present a demonstrative seamless numerical analysis involving: (i) the size distribution of droplets/droplet nuclei generated in the respiratory tract due to coughing, analyzed using the Discrete Phase Eulerian Wall Film (DP-EWF) model, (ii) exhalation of droplets/droplet nuclei from the mouth and their dispersion in an indoor environment using the Computational Fluid and Particle Dynamics (CFPD) method, (iii) subsequent inhalation exposure of an uninfected person (via the respiratory tract) through transient breathing, and (iv) time-series and heterogeneous changes in viral load (RNA copies/mL in mucus) in the respiratory tract predicted by a host cell dynamics (HCD) model that captures viral infection within the respiratory system.

2 Methods

A schematic of the demonstrative analysis of airborne transmission and infection risk in an indoor environment using EWF analysis in a numerical airway model +

* Corresponding author: ito@kyudai.jp

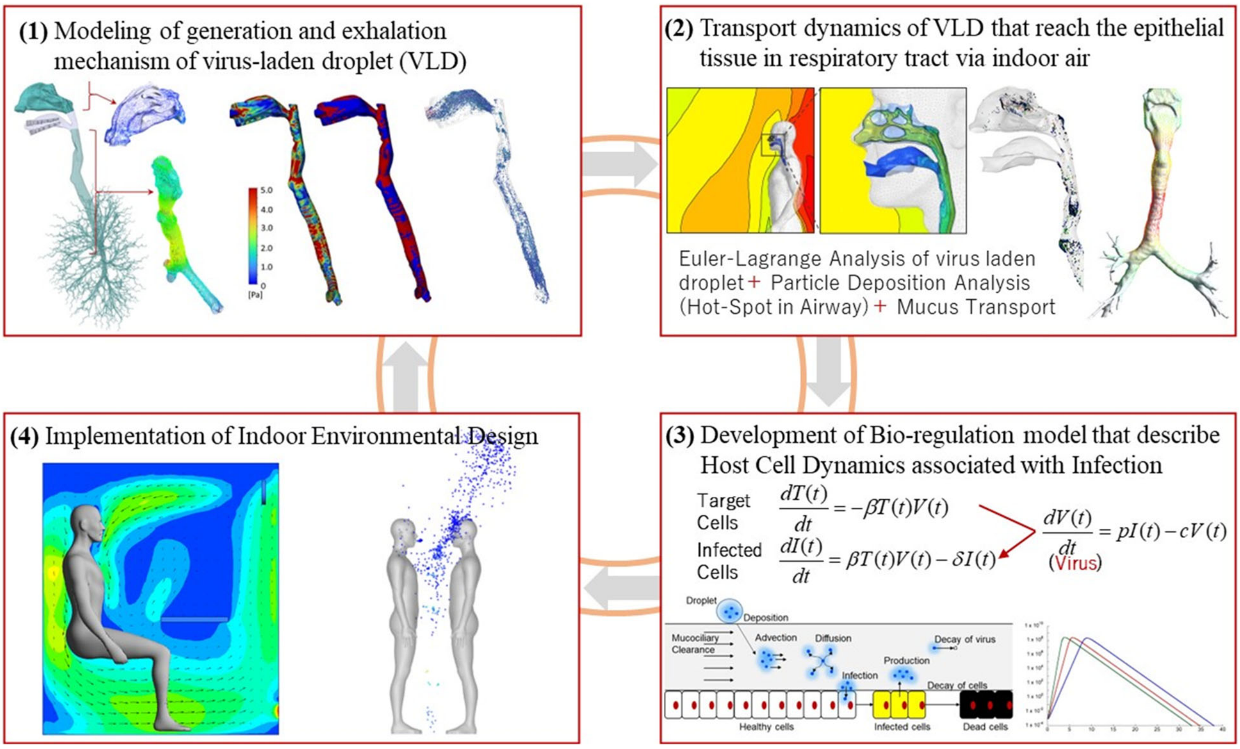

Figure 1 Outline of seamless numerical simulation for airborne transmission

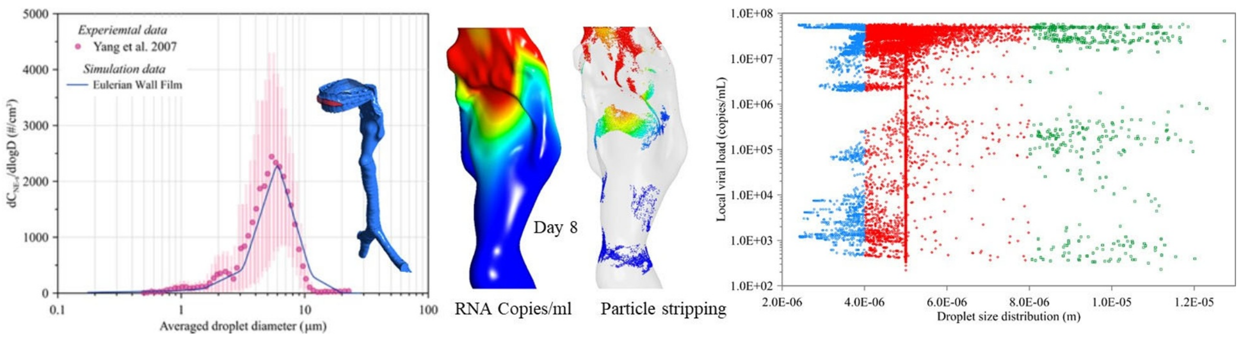

Figure 2 Number concentration of exhaled droplets/droplet nuclei and Virus concentration (RNA copies/mL) in each droplet [1, 2]

CFPD + computer simulated person (CSP) + HCD analysis is shown in Figure 1.

In this study, a sophisticated numerical airway model was developed to reproduce the nasal cavity, oral cavity, and 16th bronchial branch. A mucus layer was set up on the wall surface of the airway to reproduce mucus transport and flow towards the pharynx. The DP-EWF model was applied to the mucus layer to analyze droplet generation, airway transport, and expulsion from the oral cavity into the indoor environment in response to shear stress on the mucosal surface caused by coughing.

The CFPD model was then applied to analyze the transport of droplets released into the indoor environment. For indoor environment models, two individuals are assumed: an infected person expelling virus-containing droplets and a non-infected individual who is the target of trans-oral airway infection.

The airway model of the non-infected person underwent an unsteady breathing cycle with alternating expiration and inhalation as a boundary condition. This analysis aimed to assess the amount of airway exposure to droplet particles reaching the respiratory tract and the nonuniform deposition distribution of droplet particles on the wall surface of the airway. Subsequently, by applying the Host Cell Dynamics (HCD) model using the droplet deposition distribution in the airway as the initial condition, viral multiplication (spatiotemporal distribution of RNA copies/mL) in the airway mucosa and mucosal epithelial cells was analyzed. This series of analyses was seamlessly conducted to quantitatively evaluate airborne transmission in indoor environments.

The prediction accuracy of the flow around the computer simulated person and the flow in the numerical airway model has been validated using the results of PIV experiments and various benchmark tests results, confirming that the numerical analysis can be performed with sufficient accuracy for engineering application [6]. All numerical models in this study were implemented on the ANSYS/Fluent platform. The quality control process for the series of numerical

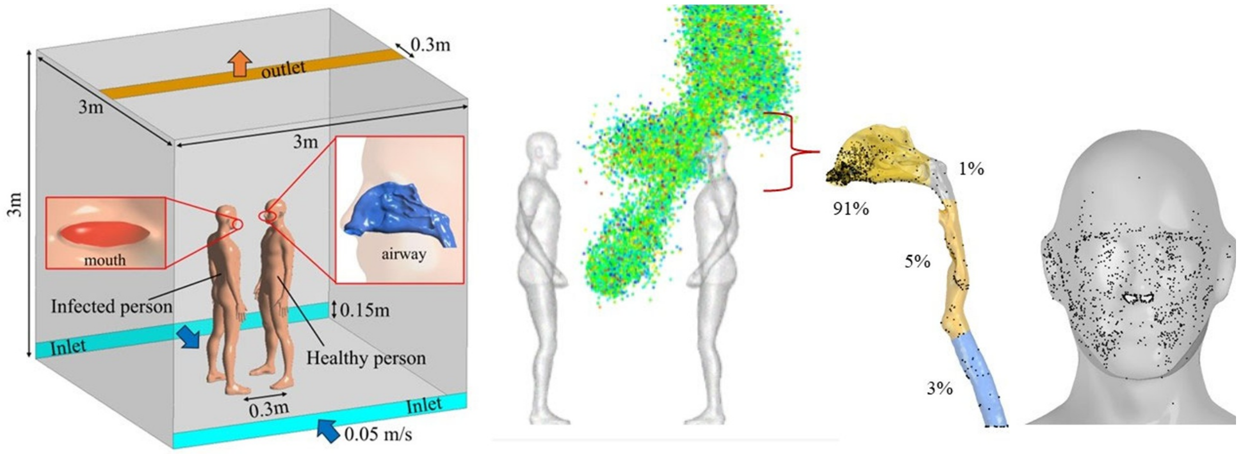

Figure 3 Trans-airway exposure analysis of non-infected individual (CFPD-CSP analysis)

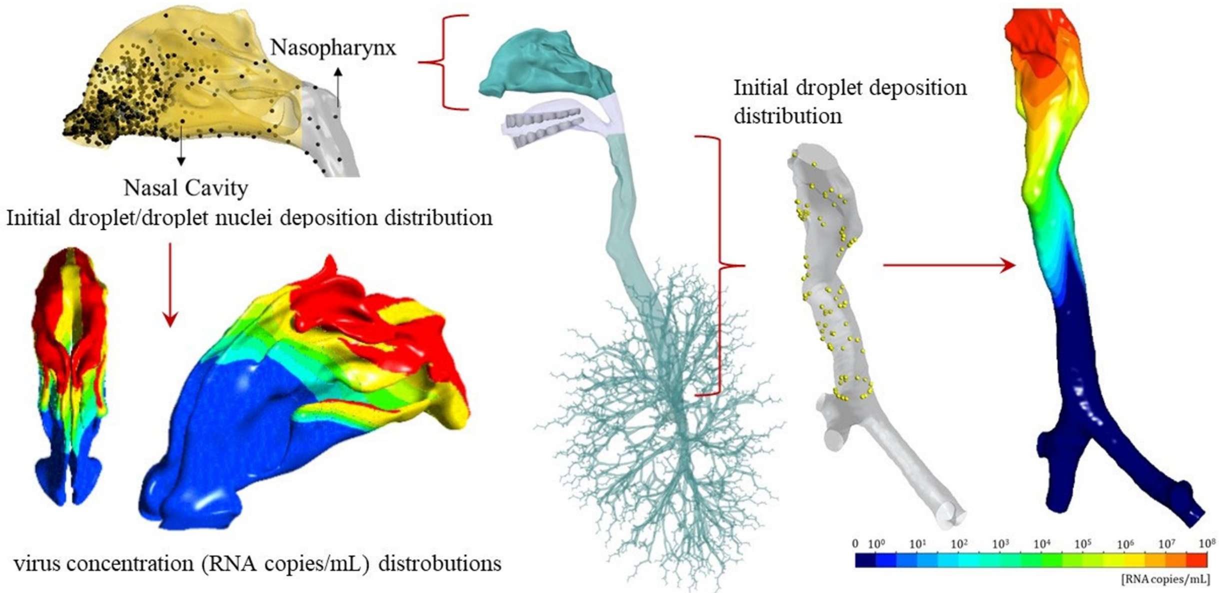

Figure 4 Time series of viral replication in respiratory trace (HCD analysis) [2, 3, 7, 9]

analysis properly followed the CFD benchmark guideline.

3 Results

Mucus transport and EWF models were applied as luminal wall surface boundary conditions in the numerical airway model. The airflow conditions, assuming coughing were analyzed to predict the number of droplets and droplet nuclei produced and exhaled from the airway, as depicted in Figure 2. The airway model, integrated with an oral model reproduced the dentition and mucus film thickness on its surface in detail. The results of this analysis reproduced the experimental results of the subjects. The majority of droplets generated in the airway were reattached to the airway walls, and the source of expelled droplets and droplet nuclei into the indoor environment was primarily via the oral cavity, with droplets derived from the mucus film on the dentition's surface being dominant.

The results of the trans-airway exposure analysis of non-infected individuals under conditions in which cough-derived droplets and droplet nuclei were released into the indoor environment are shown in Figure 3. Under the 1 m physical distance condition, approximately 5% of the total number of exhaled droplets was inhaled, resulting in the formation of a strong heterogeneous droplet deposition distribution in the airways.

The analysis of the viral load history and spatiotemporal distribution in the airways, using the HCD model with the droplet deposition distribution data in the airways as initial conditions, is presented in Figure 4. Under the current analysis conditions, the viral load peaked five days from the onset of droplet exposure, followed by a gradual decrease in the viral load, aligning with the results of the human challenge.

This series of numerical analyses allows seamless prediction of heterogeneous and transient virus concentrations (RNA copies/mL) in each droplet/droplet nuclei. In addition, the airborne transmission and infection risk can be assessed based on transient virus concentrations (RNA copies/mL) at the respiratory hot spot, with an expected improvement in prediction accuracy compared to simple infection risk assessments such as the Wells-Riley model.

4 Discussion

This study presented a series of numerical techniques for quantitatively analyzing airborne transmission and infection risks in indoor environments, accompanied by demonstrative examples of seamless numerical analyses within a simplified indoor room model were validated separately.

By applying the seamless integrated analysis model proposed in this study, it is possible to quantitatively evaluate the infection risk based on changes in RNA copies/mL in the epithelium tissue of respiratory tract. By integrating the HCD with the EWF model, changes in RNA copies/mL in droplets/droplet nuclei generated in the airways can also be predicted.

Although individual models and parameters were validated separately, the entire series of analyses was not directly validated by experiments. For issues that are difficult to validate directly experimentally, numerical analysis offers the advantage of performing unlimited parametric analyses without ethical constraints.

The study's limitations are as follows: (i) the micro-movement of the human body was not reproduced, (ii) there is a need for discussion on droplet/droplet nuclei production when given non-cough expiratory air velocity profiles, and (iii) there is a need for discussion of the impact of changes in indoor ventilation systems. These aspects should be addressed in future studies.

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Table S1 CFD

$$\frac{\partial \overline{U_i}}{\partial x_i}=0 \quad (1)$$

$$\frac{\partial \overline{U_i}}{\partial t}+\frac{\partial \overline{U_i U_j}}{\partial x_j}=-\frac{1}{\rho_g}\frac{\partial \overline{p_g}}{\partial x_i}+\frac{\partial}{\partial x_j}\left[\left(\nu+\nu_T\right)\left(\frac{\partial \overline{U_i}}{\partial x_j}+\frac{\partial \overline{U_j}}{\partial x_i}\right)\right] \quad (2)$$

Table S2 Lagrangean Particle Tracking

$$\frac{d\vec{u}_p}{dt}=\vec{F}_D+\vec{F}_G+\vec{F}_S \quad (3)$$

$$\vec{F}_D=\frac{18\mu}{\rho_p d_a^2}\frac{C_D \mathrm{Re}_p}{24}\left(\vec{U}-\vec{u}_p\right) \quad (4)$$

$$\vec{F}_S=\frac{5.188\nu^{1/2}\rho d_{ij}}{\rho_p d_a\left(d_{lk}d_{kl}\right)^{1/4}}\left(\vec{U}-\vec{u}_p\right) \quad (5)$$

Table S3 HCD model

$$\frac{\partial \overline{V_L}}{\partial t}+\frac{\partial \overline{U_i}\overline{V_L}}{\partial x_i}=D_v\frac{\partial^2 \overline{V_L}}{\partial {x_i}^2}+\frac{p\prime}{V_m}I_i-c\overline{V_L} \quad (6)$$

$$\frac{\partial T_i}{\partial t}=-\beta T_i V_L \quad (7)$$

$$\frac{\partial I_i}{\partial t}=\beta T_i V_L-\delta I_i \quad (8)$$

Table S4 EWF model

$$\frac{\partial \rho h}{\partial t}+\nabla_s\cdot\left(\rho h\vec{U}_f\right)=\dot{m}_s \quad (9)$$

$$\frac{\partial \rho h\vec{U}_f}{\partial t}+\nabla_s\cdot\left(\rho h\vec{U}_f\vec{U}_f+\vec{D}_A\right)= -h\nabla_s P_f+\rho h\vec{g}_\tau+\frac{3}{2}\vec{\tau}_f-\frac{3\mu_f}{h}\vec{U}_f+\dot{\vec{q}}_s \quad (10)$$

$$P_f=P_{gas}+P_h+P_\sigma \quad (11)$$

$$P_h=-\rho h(\vec{n}\cdot\vec{g}) \quad (12)$$

$$P_\sigma=-\sigma\nabla_s\cdot(\nabla_s h) \quad (13)$$

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