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Position Paper

Tracer gas is a suitable surrogate of exhaled droplet nuclei for studying airborne transmission in the built environment

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1 Introduction

Airborne transmission between persons is a valid and major respiratory transmission route for a number of infectious diseases (CDC 2007, 2017; Hodgson et al. 2012; Li et al. 2015). Worldwide there are approximately 3.0 million deaths annually caused by lower respiratory infections (WHO 2018). Airborne transmission has been shown to occur within an enclosed indoor space (Liu et al. 2017; Ai and Melikov 2018), between different rooms on a same floor (Wu et al. 2016), between different flats in the same building (Gao et al. 2009; Ai and Mak 2016; Mu et al. 2016) and even between adjacent buildings in high-density urban areas (Yu et al. 2004). Understanding the transmission characteristics, high-risk routes and influential factors is of great importance for formulating effective control measures, which would in turn contribute to reduced number of deaths and illness leaves as well as lowered health care costs. The whole process of airborne transmission between persons involves the generation of infectious droplets from an infected person, the spread of infectious droplet nuclei in the air and the inhalation of infectious droplet nuclei by an exposed person (Nicas et al. 2005; Tang et al. 2006; Wei and Li 2016). Human breathing, talking, coughing and sneezing can generate tens of thousands of droplets (Duguid 1946; Tellier 2006; Chao et al. 2009). Most of these droplets evaporate instantaneously to half of their initial size and become droplet nuclei (Nicas et al. 2005). These droplet nuclei spread in the air with the influence of factors like gravity, inertia, ventilation flow, human body boundary layer flow and respiratory flow (Melikov 2015; Nazaroff 2016). The spread of droplet nuclei in the air is usually evaluated by concentration distribution obtained using either experimental measurements or computational fluid dynamics (CFD) methods. The droplet nuclei are commonly simulated using a tracer gas or particles, which are termed as tracer gas simulation or particle simulation in this paper.

Compared with tracer gas simulation of the exhaled droplet nuclei, there are several deficiencies and difficulties associated with particle simulation. Firstly, in experimental contexts, the experimental space for particle simulation has to meet certain criteria so that the particles from other sources would not influence the measurements. Examples of these sources include particles in background and supply air and the resuspension of particles from surfaces of the space. Secondly, particle generators are normally stand-alone from a thermal manikin, where the influence of the presence of occupants and their thermal boundary conditions was not taken into account (Sze et al. 2009; Poon and Lai 2011; Pantelic and Tham 2013; Pantlic et al. 2015; Cao et al. 2015). Very few studies have successfully dosed aerosols through the breathing system of a thermal manikin. The major reason reported was that the integration of an aerosol generator into the breathing system of a manikin would easily result in the blockage of the breathing system, due to the narrow "respiratory tract" and the relatively low expiratory speed of aerosol particles (Ai and Melikov 2018). Thirdly, the aerosol generators reported in past studies could not simulate accurately the number and size distribution of human expiratory droplet nuclei (Sze et al. 2009; Poon and Lai 2011;

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Pantelic and Tham 2013; Cao et al. 2015; Pantlic et al. 2015), though most generators produce a range of particle sizes simultaneously (Sze et al. 2009). In addition, it is unknown to what extent the particles produced by these available generators are the same with expiratory droplet nuclei, in terms of quantity, size distribution, thermo-fluid properties and dynamics. Fourthly, the particle dynamics and fate are complicated (see Fig. 1), which is required in order to set up and perform the experiments properly and to analyze the data and explain the phenomena quantitatively. The movement of particles in turbulent flow is governed by gravitational force, thermophoretic force, Brownian force, and Saffman's lift force (Nazaroff 2004, 2016). In addition, particles could deposit on surfaces, re-suspend from surfaces, coagulate, change phase etc. (Nazaroff 2004, 2016). In numerical context, fully considering all dynamics and fates of particles in airflows in the built environment is impossible at the present. Knowledge on the relative importance of each force and fate in connection with particle size and particle volume loading in air is required in order to make reasonable assumptions and simplifications in numerical models. Fifthly, there are quite several uncertainties associated with the risk of cross infection, including the number concentration and size distribution of droplet nuclei generated by each respiratory process including coughing, sneezing and speaking, the frequency of the respiratory process, the infectivity of the virus concerned, the lifetime of the virus, the vulnerability of the exposed person. In addition, the droplet concentration and its size distribution can be influenced by many factors, such as body weight, gender, and age (Yang et al. 2007; Johnson and Morawska 2009; Zayas et al. 2012). It is reported that, generally for a same person, among the processes of mouth exhalation, nose exhalation, coughing and speaking, coughing produces the largest droplet concentrations (Lindsley et al. 2012; Morawska et al. 2013) and nose exhalation the least (Papineni and Rosenthal 1997). The error caused by these uncertainties may be comparable with that of tracer gas simulation of particles. Sixthly, some studies (Zhu et al. 2006; Rim and Novoselac 2009; Poon and Lai 2011; Yang et al. 2016; Liu et al. 2017) examined the dispersion of particles of different sizes, but most of them had no conclusion on the influence of particle size on the risk of cross infection, primarily because of the uncertainties mentioned above. In summary, the particle simulation cannot ensure an accurate modeling of the dispersion of expiratory droplet nuclei between persons, and the knowledge deficiency and the difficulties attached decrease the probability of obtaining reliable results.

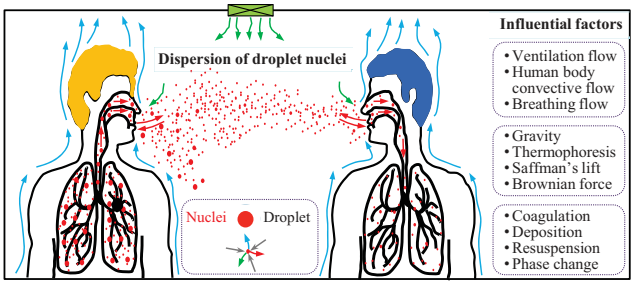

Fig. 1 The dynamic dispersion behavior of droplet nuclei in the air is influenced by the interaction of flows (ventilation flow, human body convective flow and breathing flow), the combination of forces (gravitational force, thermophoretic force, Saffman's lift force and Brownian force) exerted on a nucleus, and some other effects (e.g., coagulation, deposition on and resuspension from solid surfaces, and phase change)

The statement in this paper is that tracer gas is a suitable surrogate of exhaled droplet nuclei for studying airborne transmission in the built environment. Most studies on airborne transmission between occupants in different spatial scales in the built environment were based on tracer gas simulation (e.g., Qian et al. 2008; Bolashikov et al 2015; Lipczynska et al. 2015; Yang et al. 2015; Villafruela et al. 2016; Liu et al. 2017; Ai et al. 2019). The reasons for the popularity of tracer gas simulation should be attributed to not only the deficiencies and difficulties of particle simulation at the present stage, but also the well established tracer gas simulation techniques (Sherman 1990), their simplicity and good accuracy (described in Section 3). With the consideration that the main purpose of engineering studies of airborne transmission is to reveal the dispersion characteristics and its influential factors, to identify the major and high-risk dispersion routes, and to develop control measures, the proper use of tracer gas technique, and its pros and cons are reviewed in this paper.

2 Counter arguments

There are four major counter arguments as listed below:

- Particle dynamics differs from gases due to the effects of gravity, inertia and deposition at solid surfaces.
- Airflow with particles is a two-phase flow.
- The coagulation and resuspension of particles cannot be simulated by tracer gas.
- Particles have different aerodynamic diameters.

As the density of a particle is usually several orders of magnitude higher than air, a particle travelling in air is strongly influenced by its gravity and inertia (Hinds 1999; Nazaroff 2004). In addition, a particle could deposit and be collected by solid surfaces after deposition, which is one of the most important fates of a particle in the air (Nazaroff 2004). A tracer gas in the air does not have such dynamic characteristics, and it is therefore no doubt that the gravity, inertia and deposition of a particle cannot be modelled using a tracer gas. In addition, the material of a particle, namely fluid or solid, determines the fact that a mixture of

airflow and particles is typically a two-phase flow, where particles could departure from the main airstream and could even influence the airflow. Moreover, the coagulation and re-suspension are two important dynamic properties of particles (Thatcher and Layton 1995; Nazaroff 2004). The coagulation occurs when particles collide with one another and adhere together, which shifts the size distribution of particles in the air. The most important mechanism causing coagulation is Brownian motion, which increases the chance of collision between particles. The important influence of coagulation on the concentration of particles emitted from unvented natural gas combustion was reported by Dennekamp et al. (2001). Particles that have been deposited at solid surfaces may become re-suspended into the air by many mechanical activities including walking. A few studies have observed the increase of particle concentration indoors due to resuspension resulted by human activities (Thatcher and Layton 1995; Ferro et al. 2004). Obviously, both coagulation and resuspension of particles cannot be simulated using a tracer gas. Furthermore, the droplet nuclei exhaled by human beings have different aerodynamic diameters, which could range from zero to dozens of micrometer (μm). The key attributes of particles, such as source, dynamic behavior and fate, are all strongly related to particle size (Nazaroff 2004). However, the dispersion characteristics of droplet nuclei with different size bins cannot be investigated using a tracer gas.

All these counter arguments are correct. However, the importance of the particle dynamics mentioned above is strongly related to particle concentration and size distribution. For airborne transmission that is based on human expiratory droplet nuclei, they are less important and it is therefore believed that the tracer gas simulation is a suitable research method. The major reasons are listed below.

Firstly, the respiratory droplet nuclei were found to range in diameter from 0.25 to 42 μm, of which 97% between 0.5 to 12 μm and the most common between 1 and 4 μm (Duguid 1946). Settling times for a 3-m fall are 17 minutes for 10 μm and 62 minutes for 5 μm, while droplet nuclei with a diameter less than 3 μm essentially do not settle (Tellier 2006). The relaxation times for fine particles are much smaller than the typical time scales of indoor airflow; droplet nuclei with 10 μm in diameter take only 1.55 ms to reach 99.3% of their terminal speeds indoors. These three aspects may support the fact that the main driving force of the movement of the majority of expiratory droplet nuclei is airflow, rather than gravity (Nazaroff 2016). In addition, deposition at the solid surfaces is an important mechanism influencing the fate of droplet nuclei, only when the particle size is relatively large and the air exchange rate is small. It was reported that, for particles in the size range 0.5–1.0 μm, the deposition loss rate coefficient is 0.2–0.3 per hour for enclosed indoor environment (Thatcher et al. 2002; Nazaroff 2016). If, for example the air change rate is 3 h^{-1}, the airborne particles have a characteristic residence time of 20 minutes in the room air, during which the probability of deposition for 0.5–1.0 μm particles is only 0.067–0.1. Note that the air change rate of a high-risk space or during a high-risk period, such as at hospital wards during the outbreak of infectious diseases, can be much higher than 3 h^{-1}. Such a negligible deposition loss of fine particles was also supported by our CFD validation (Gao and Niu 2007) against a particle experiment (Chen et al. 2006), where 96% of 1.0 μm particles was found at ventilation exhaust, meaning that the deposition loss rate is only 4%.

Secondly, the particle loading is the key parameter determining if the particle-flow interaction is important (Elghobashi 1994). When the particle loading represented by volume fraction is higher than 10^{-6}, the influence of particles on turbulent flow would be important and the two-phase flow should be considered. The concentration of droplet nuclei generated by respiratory processes is generally much lower than this threshold loading. It was reported that 1.1–6.7 mg of saliva were collected on a mask during a single cough, and 18.7 mg were collected while counting from 1–100 (Zhu et al. 2006; Xie et al. 2009). A study by Chao et al. (2009) shows that the estimated total number of droplets at all sizes ranged from 947 to 2085 per cough and 112–6720 for speaking. Equivalently, the estimated droplet concentrations for coughing ranged from 2.4 to 5.2 cm^{-3} per cough and 0.004–0.223 cm^{-3} for speaking, which are much smaller than the threshold loading. However, as the frequency of respiratory processes is case dependent, the accurate loading of droplet nuclei is difficult to estimate. Many past CFD studies (Chen et al. 2006; Gao and Niu 2007; Gao et al. 2009; Zhao and Zhao 2016; Xu and Wang 2017; Mei and Gong 2019) using Eulerian method that treats the fluid phase and the particulate phase as continuum reported good agreements with experimental results, indicating that the simplification of one-way coupling for human expiratory droplet nuclei is reasonable.

Thirdly, coagulation due to particle-particle interaction is important for very fine particles with several sources, when particle concentrations are high (Nazaroff 2004) and air exchange rate is low (Rivas et al. 2015). Kumar et al. (2011) reported that, depending on the duration of interests, particle coagulation may be neglected for particles larger than 0.01 μm, as the coagulation is too slow to substantially affect the number concentrations. According to Hinds (1999), coagulation rate is proportional to the square of the number concentration. Assuming a diameter of 1.0 μm and a concentration of 10 particles per cm^3, 1% loss of particle number concentration by coagulation requires about 500 days (Gao et al. 2009). Particle re-suspension from a solid

surface is influenced by many parameters, such as particle size, surface material, and human activities. However, for fine particles, such as $PM_{2.5}$, resuspension is very difficult and even human activities have a minor influence on it (Thatcher et al. 1995). Considering also the low deposition rate of fine particles, the resuspension effect may also be neglected.

Fourthly, though the different aerodynamic diameters cannot be examined using a tracer gas, the most important and major portion of airborne droplet nuclei exhaled by human beings falls in the range of less than 5–10 μm, especially within 2–3 μm. In addition, a tracer gas certainly cannot simulate large particles like 10 μm in diameter. However, in this paper, we would like to claim that a tracer gas is suitable to simulate the commonest range of expiratory droplet nuclei that is less than 5–10 μm. Justification of this claim is described in detail in Section 3.

3 Arguments

Tracer gas is a suitable surrogate of exhaled droplet nuclei for studying airborne transmission in the built environment, mainly because of the following reasons:

- If a disease is found to be transmitted via airborne route, it is mostly the fine droplet nuclei generated by human respiratory processes that are the vehicles of pathogens.
- Studies show that the movement of fine particles less than 3–5 μm can be well represented with tracer gas simulation.
- Tracer gas simulation is of lower complexity and less demand on user knowledge and thus it is easier to obtain reliable results.

Argument No. 1: if a disease is found to be transmitted via airborne route, it is mostly the fine droplet nuclei generated by human respiratory processes that are the vehicles of pathogens

A study of ferrets found that transmission of influenza from infected to susceptible ferrets occurred despite the ferrets being separated by a long, straight air duct or by "S" or "U"-shaped ducts (Andrewes and Glover 1941). As large respiratory droplets could not move around the bends of the ducts whereas the smaller droplet nuclei could, this study may well indicate that fine airborne droplet nuclei were the major vehicles of pathogen, and that they could remain suspended in air for a prolonged period and be transported over an extended distance by airflows. Another study pointed out that the majority of droplets from human respiration activities are less than 5–10 μm in diameter (Nicas et al. 2005), and this size range is used to differentiate between airborne transmission and droplet transmission. Another earlier study by Duguid (1946) reported that 97% of human respiratory droplet nuclei ranged in diameter from 0.5 to 12 μm and the commonest range between 1 and 4 μm (see Fig. 2). In addition, the size of viruses is mostly from 0.02 to 0.3 μm. For examples, an individual SARS coronavirus ranges from 0.075 to 0.16 μm, and an influenza virus is of a similar size (Morawska 2006). Lindsley et al. (2010) measured influenza virus in droplet nuclei generated by coughing patients and reported that 42% of detected viruses were found in droplet nuclei less than 1 μm and 23% in droplet nuclei of 1–4 μm, which suggested that most viruses are contained within droplet nuclei in the very fine size range. Yang et al. (2011) confirmed that a substantial fraction of the detected influenza A viruses was associated with fine particles smaller than 2.5 μm. It is known that fine particles travel readily between persons and penetrate and deposit deeply in the respiratory tract. Based on a semi-empirical model (Yeh et al. 1996), particles around 3 μm have the highest deposition efficiency in the respiratory tract (Nazaroff 2016).

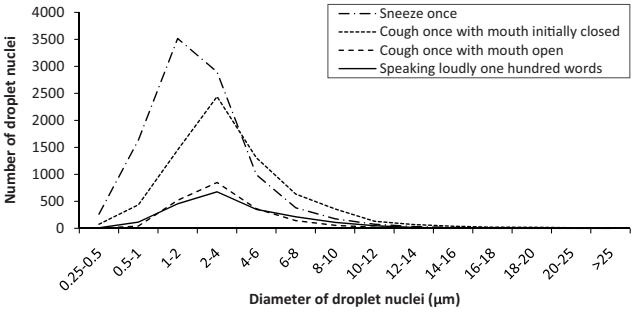

Fig. 2 Size distributions of droplet nuclei produced by different types of expiratory activities, where 97% of the nuclei were between 0.5 and 12 μm and most of them were around 1–4 μm (Duguid 1946, reproduced with permission © 1946 Cambridge University Press)

Argument No. 2: studies show that the accuracy of tracer gas simulation of fine particles can be good enough

A few studies compared the dispersion of tracer gas and particles, which show that the accuracy of tracer gas simulation of fine particles can be good enough. These studies are briefly described below. Results of two studies are also summarized in Fig. 3.

Bivolarova et al. (2017) investigated the influence of ventilation rate, free convection flow produced by a thermal manikin, and the presence of objects on the distribution of tracer gas (N_2O) and particles (0.07, 0.7 and 3.5 μm) in a full-scale room. Three scenarios were examined, including an empty chamber, an office room with an occupant sitting in front of a table, and a single-bed hospital room. The concentrations of gas and particles were measured in the bulk room air, in the breathing zone of the manikin, and in

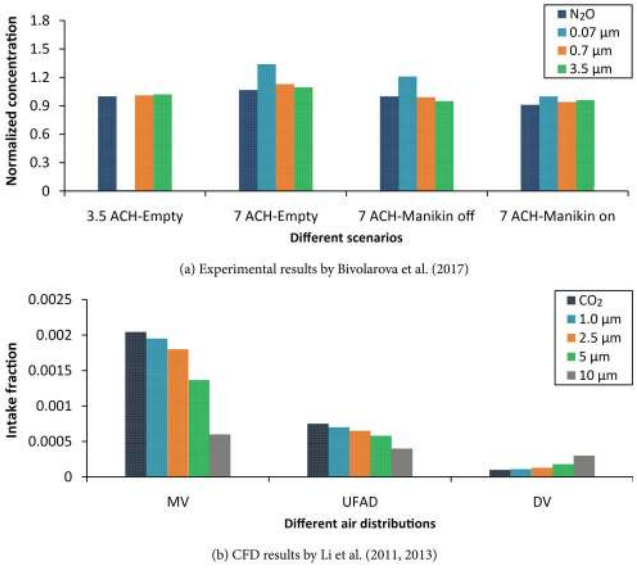

Fig. 3 Comparison of the dynamic dispersion behaviors of tracer gas and particles with different diameters: (a) experimental results by Bivolarova et al. (2017) (reproduced with permission © 2017 John Wiley & Sons A/S), where "3.5 ACH-Empty" denotes that the air change per hour was at 3.5 and the test chamber was empty, "Manikin off" denotes that one manikin without heat release was presented in the test chamber, and "Manikin on" means that the heating function of the manikin was switched on so that it simulated the heat release of an average person; (b) CFD results by Li et al. (2011, 2013) (reproduced with permission © 2011 Taylor & Francis and © 2012 John Wiley & Sons A/S, respectively), where "Intake fraction" is defined as the proportion of pollutant mass exhaled from the infected person that is then inhaled by the exposed person, and "MV", "UFAD" and "DV" denote mixing ventilation, under floor air distribution, and displacement ventilation, respectively

the exhaust air. It was found that, within the breathing zone of the sitting manikin, the tracer gas was a reliable predictor for the exposure to all the three investigated particles, regardless of the change of ventilation rate and room surface area.

Zhang et al. (2009) experimentally and numerically investigated contaminant transport in a section of half occupied, twin-aisle cabin mockup, where a tracer gas (SF_6) and particles (0.7 μm) released at the same location were used to simulate a gaseous and a particulate contaminant. The results show that the distributions of the gaseous and particulate contaminants were similar in most part of the cabin (except for the region near ceiling), suggesting that, in occupied zone, such very fine particles behave like a passive tracer gas.

Noakes et al. (2009) experimentally compared tracer gas technique and tracer particle technique for evaluating the behavior of bioaerosols in hospital isolation rooms with mixing air distribution at 10 ACH (air change per hour). Both the tracer gas (N_2O) and particles (including 3–5 μm) were released from a heated cylinder simulating a patient in bed. The results show that both N_2O tracer gas and 3–5 μm particles compared well with bioaerosol data, suggesting both techniques gave a good representation of the behavior of bioaerosols.

Gao and Niu (2007) modelled the particle dispersion and deposition in a room with typical office settings including a thermal manikin, a computer, a desk, ceiling lights etc. The room was conditioned by a mechanical ventilation system. Tracer gas simulation was performed for comparison purpose. The particle dynamics were treated by Eulerian approach in combination with a drift-flux model. It was found that the movements of particles not larger than 2.5 μm were like a tracer gas. Human exposure to this level of particles was also very close to a tracer gas, when the two were released at the same location.

Li et al. (2011, 2013) simulated the spatial distribution of human respiratory droplet nuclei and the risk of cross infection between two face-to-face persons in a typical office room under different ventilation methods. Both particles (1, 2.5, 5, and 10 μm) and a tracer gas (CO_2) were examined. The results show that both the spatial distribution and co-occupant's exposure of particles not larger than 2.5 μm are very close to the tracer gas.

A study by Beato-Arribas et al. (2015) concluded that the distributions of CO_2 tracer gas and aerosolized Bacilus Subtilus bacteria are similar in a single isolation hospital mock-up at 12 ACH. A CFD study by Gao et al. (2009) showed that the dispersion characteristics and concentration distributions of CO_2 tracer gas and 1.0 μm particles are very close in a building with multiple stories.

In summary, these studies indicate that tracer gas simulation is accurate enough to study the dispersion of particles not larger than 3–5 μm. This size range is the dominant part of human expiratory droplet nuclei in terms of quantity.

Argument No. 3: tracer gas simulation is of lower complexity and less demand on user knowledge and thus it is easier to obtain reliable results

As an alternative, tracer gas simulation is a well established research method both in experimental and numerical contexts. Experimentally, tracer gas simulation has been widely performed in different spatial scales, from a single room up to an urban area. For a single-room scale, tracer gas experiments do not have a special requirement on the cleanness of the experiment room, and the characteristics and area of the surfaces of the room do not obviously influence the experimental results. For an urban-area scale, there are very strong tracer gas sources to generate a large amount of tracer gas that allows the measurement at locations a few kilometers away from the source. Both the dosing system

and the sampling system have been developed to a very high accuracy of control. The dosing system can be perfectly integrated with a breathing thermal manikin to include the influence of the presence of manikin body and its thermal boundary layer. The mixture of a tracer gas with air is a one-phase flow, which has nearly the same properties of air. There are no complicated dynamic processes, such as evaporation, condensation, coagulation, resuspension and phase change. Similarly, numerical simulation of tracer gas dispersion is much easier than particle simulation in terms of mathematical model complexity and practitioners' knowledge. In numerical context, a tracer gas is considered to be a passive scalar and only one more mass transport equation requires to be solved. The sensitivity of the influential parameters and constants (such as density, mass fraction, Schmidt number, and diffusion coefficient) related to this equation are easy to be tested. There are no assumptions and simplifications required for modelling the dispersion of tracer gas. Because of the lower complexity and less demand on user knowledge, it is easier for tracer gas simulation to obtain reliable results. This is especially important from the viewpoint of engineering practice.

4 Conclusion and future possibilities

Tracer gas is a suitable surrogate of exhaled droplet nuclei for studying airborne transmission in the built environment, because (a) if a disease is found to be transmitted via airborne route, it is mostly the fine droplet nuclei generated by human respiratory processes that are the vehicles of pathogens, and fine droplet nuclei have aerodynamics more close to a gas, (b) studies show that the movement of fine particles less than 3–5 μm can be well represented with tracer gas simulation, and (c) tracer gas simulation is of lower complexity and less demand on user knowledge and thus it is easier to obtain reliable results. Note that dispersion and deposition of droplet nuclei in the respiratory tract were not discussed in this paper.

As reviewed, tracer gas simulation and particle simulation of droplet nuclei have different error sources. Few studies have evaluated quantitatively the error of particle simulation. It would be interesting to assess whether or not the error of tracer gas simulation is smaller than the error of particle simulation, when compared to the real-life dispersion of exhaled droplet nuclei. In addition, few studies have compared the dispersion characteristics of different tracer gases, and it is still unknown how different are the experimental results obtained by using different tracer gases (i.e., different densities, diffusion coefficients and Schmidt numbers). Further studies are required.

Particle simulation of exhaled droplet nuclei may be necessary when the deposition becomes the dominating factor such as when the airflow passes through narrow passages (e.g., window or door gaps). In addition, particle simulation would potentially become an effective method for airborne transmission studies in the built environment, if (a) a particle generation system is developed for experimental studies to a level that the number and size distribution of the generated particles can be accurately controlled, (b) in experimental settings the factors including the background concentration that influence the measurement accuracy and repeatability can be conveniently eliminated, and (c) numerical models are advanced to be able to take into account the major dynamics and fates of particles.

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