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Validation of different Eulerian and Lagrangian solvers of aerosol dispersion in indoor spaces

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SUMMARY:
The corona pandemic accelerated a lot of studies about aerosol dispersion and different aerosol-generating tasks ranging in intensity from sneezing to breathing. Both measurements and numerical simulations were used to understand the behaviour of aerosols. For numerical simulations, Computational Fluid Dynamic (CFD) simulations were used; however, the set-up of cases varied between studies. Different solvers, methods, turbulence models and steadiness are used depending on the scope and aim of each study. The aim of this study is to compare different set-ups and solvers and validate them against measurements conducted in the Senselab at the Delft University of Technology. The purpose is to find the best approach that balances between accuracy and computational cost to use afterwards in ventilation design decision-making. Consequently, we set up several numerical cases with different levels of complexities (e.g.: eulerian-eulerian to eulerian-lagrangian, including/excluding temperature and relative humidity, steady/unsteady). We then compare those cases to the experiments of a breathing manikin in the Senselab. The performance of each case is determined depending on how well it predicts aerosol dispersion and the run time cost.

Keywords: CFD, validation, aerosols

1. INTRODUCTION

After health organisations acknowledged the fact that SARS-CoV-2 is airborne, it became clear that the focus should be on understanding aerosol dispersion in indoor spaces. Laboratory experiments (Ho et al., 2021; Ortiz et al., 2021) and Computational Fluid Dynamic (CFD) simulations (Dbouk and Drikakis, 2020; Foster and Kinzel, 2021) were conducted to study the behaviour of aerosols from an infected individual in an indoor space. Studies used CFD simulations to deal with different aspects of the aerosol dispersion topic, such as assessing cross-infection between a source (infected person) and a receptor (healthy person) (Wu and Weng, 2021) and modelling the generation of aerosols from the alveoli into the air (Xu et al., 2020). These studies led to a rising awareness about pathogen-source-based design (Shen et al., 2021) where the design of a room is based on the presence of infectious individuals. This design approach would require iterating several CFD simulations that ideally would not be computationally expensive and accurate enough to predict the performance of diverse proposed designs. However, these studies all present different technical set ups that depend on the goal of the study and the level of detail needed. This makes it difficult to conclude on an approach to support design ventilation solutions. The aim of this study is to compare different solvers that model breathing in a room with no ventilation and validate them against measurements conducted in the Senselab at the Delft University of Technology. Through this comparison, we will conclude on the most suitable approach tested so far. This represents the first step towards a simulation framework that allows for room design exploration in future studies.

2. METHODS

2.1. Case set-up

The measurements used as validation are the work of Liu (2021) and take place in the experiment room of the SenseLab. The set-up is a manikin head, placed on a stick, exhaling from the back of the room. The exhaled cloud is visualised with six lasers and recorded with a high-speed camera. The dimensions of the room are 6.5 × 4.2 × 3.0 m and define the computational domain used for the simulations. The aim of the simulations is to replicate the measurements of Liu (2021). In the simulations, we include a 3D model of a head in the room's domain. Only exhalation puffs are modelled with a certain time interval between two consecutive puffs based on the behaviour of the breathing manikin. Therefore, the interval time between two puffs is 1.75 seconds, and we set the inlet velocity at the mouth to zero; whereas an exhaled puff lasts 2.1 seconds and we set the inlet velocity as a sinusoidal function based on Eq. (1) presented in Faleiros et al. (2022):

$$Q_{out}(t) = \frac{1}{2}\bar{Q}_{out}\,\omega_{out}T_{resp}\sin\left[\omega_{out}(t-t_{in})\right] \quad (1)$$

where Q_{out} [l/s] is the mean expired flow rate, f_{out} [min^{-1} and ω_{out} [s^{-1}] are the linear and angular frequencies, t_{in} [s] is the half period of inhalation, and T_{resp} [s] is the respiration period. We present the results at 2.8 seconds which is the peak of the exhalation function and at 3.8 seconds to visualise fields after the puff.

2.2. CFD simulations set-up

In this study, we compute the airflow field, particle concentration, temperature, and relative humidity. We use the Reynolds-Averaged Navier-Stokes equations with the k-ε turbulence model (Launder and Spalding, 1983). We run different solvers using OpenFOAM8 (*The OpenFOAM Foundation* 2021) to model one puff.

2.2.1. The Eulerian-Eulerian cases

In the first case, we run a Eulerian-Eulerian case where aerosols' concentration is computed with a passive scalar transport equation. We inject the passive scalar concentration at the manikin mouth into the computational domain in steady state. We add a transport passive scalar equation to the simpleFoam solver. The first case does not include temperature and relative humidity.

Second, we run the previous case with temperature and relative humidity. We use the Boussinesq approximation to model buoyancy-driven flow. We also assume no generation of heat and thus the governing equation of temperature is a second passive scalar transport equation. Finally, relative humidity is calculated based on the water vapour concentration that is modelled as the third passive scalar transport equation in the simulation.

2.2.2. The Eulerian-Lagrangian cases

For the Eulerian-Lagrangian cases, we first model aerosols as particles in space without implementing temperature and relative humidity. We use DPMFoam which is an unsteady state solver.

To model the kinematic cloud for the aerosols particle, we adapted the cloud developed by Holzmann (2020) based on Han et al. (2013) for a breathing case instead of a sneezing case. Finally, we add temperature and relative humidity to the DPMFoam solver.

2.3. Validation

For the validation, we conduct a quantitative comparison between the simulations and Liu (2021)'s measurements. Quantitatively, we can validate the air velocity at the points where it was sampled along with temperature and relative humidity when applicable. Instead, comparing the airflow pattern has proven to be more challenging (see Fig. 1) and thus, we will validate by comparing the duration that aerosols suspend in the air and the distance they travel in space.

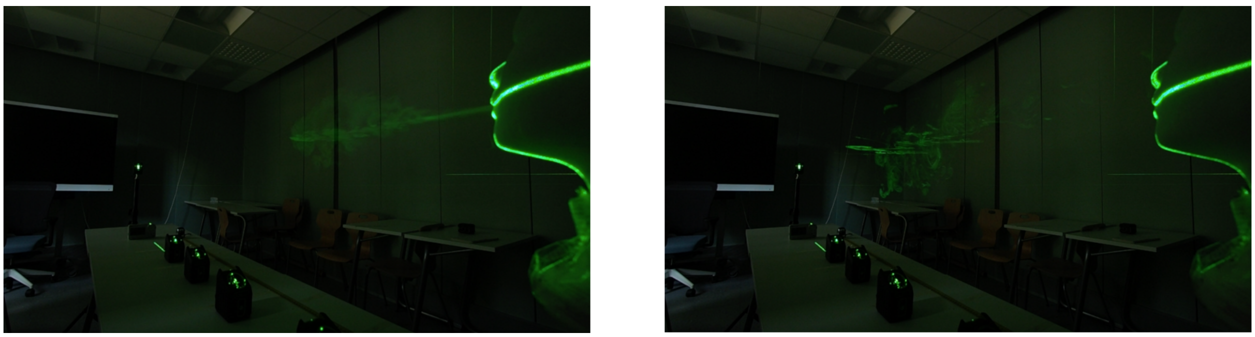

Figure 1. Airflow patterns of a breathing manikin with no ventilation. The left image shows the peak of a puff. The right image shows the puff a second later. Source: Liu (2021).

3. RESULTS

We present in this abstract the first case where we model the Eulerian-Eulerian case without temperature and relative humidity. In Fig. 2, the velocity field shows the peak in velocity in the near-field of the head. We can also see the two vortices that form under and above the main stream of the exhaled breath. In Fig. 3, the velocity field shows how the velocity from the puff moves further away from the head. The two vortices become larger as the intensity of the velocity decreases. For the aerosol concentration field, we see the accumulation and travelled distance of the exhaled aerosols. The results of the remaining simulations and the validation will be provided elsewhere.

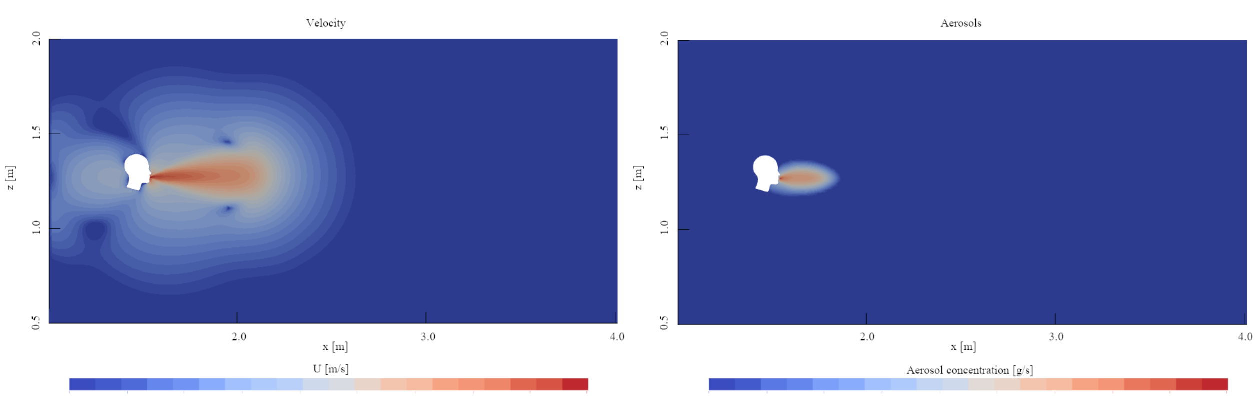

Figure 2. The velocity (on the left) and aerosol concentration (on the right) fields at 2.8 seconds.

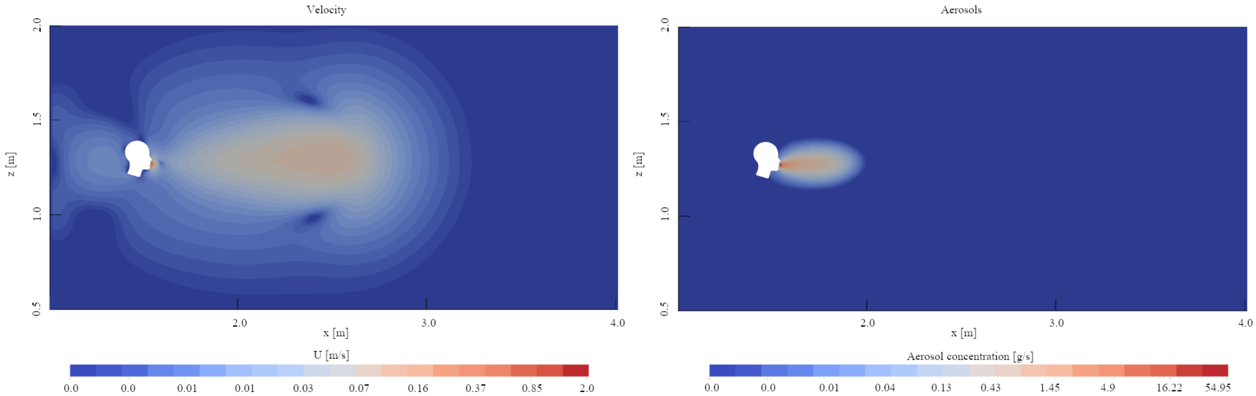

Figure 3. The velocity (on the left) and aerosol concentration (on the right) fields at 3.8 seconds.

4. CONCLUSIONS

The aim of this study is to compare and validate different solvers to model the behaviour of aerosols in a room with no ventilation. The goal is to find the most efficient approach to model aerosols in a space to quickly optimise the design of a given room. For future work, we still need to implement additional solvers to explore more options to model breathing and choose the most appropriate solver to optimise design solutions. Moreover, we need to validate with more measurements around the room using velocity and temperature sensors in addition to the images from cameras.

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