

Report

Utilization of Computational Fluid Dynamics Simulation for Gas Exposure Chamber

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Received 22 December, 2021; revised 10 February, 2022; accepted 18 February, 2022

Testing devices and measuring physical parameters are often carried out in gas chambers. However, if the environmental conditions (e.g. gas concentration) inside the chamber is inhomogeneous, we may expect incorrect results of experiment. Confirmation of the gas distribution in various environmental conditions is an important problem in the design of the chamber. For checking the gas distribution, a theoretical approach using the computational fluid dynamics (CFD) simulation can be relatively-easily used. The article demonstrates the utilization of numerical calculations based on the CFD simulation for the analysis of gas uniformity in the virtual chamber.

Key words: gas, chamber, exposure

1. Introduction

Gas exposure chambers are often used for testing and experimenting gas measuring instruments under various exposure conditions¹⁻³). However, if the environmental conditions (e.g. gas concentration and temperature) inside the chamber are spatially uneven, incorrect results in testing and experimenting for gas measuring instruments may occur. Therefore, it is important to check whether the environmental conditions in the chamber are homogeneous in different exposure scenarios.

Two approaches to checking chamber homogeneity can be considered: 1) experimental, using passive type devices that do not interfere with the chamber operation;

2) theoretical, using the computational fluid dynamics (CFD) simulation. The experimental approach makes it possible to check the homogeneity of the chamber based on the variability of data from passive type devices installed in the chamber, while it can be relatively heavy work in terms of time and cost. On the other hand, the theoretical approach with CFD simulations is relatively easy to perform, which has been presented in this paper.

In the present work, distribution of gas in the exposure chamber is numerically simulated by using open source CFD toolbox, OpenFOAM version 8.

2. Computational fluid dynamics simulation

Nowadays computational fluid dynamics (CFD) provides the state-of-the-art capabilities of simulating the gas distribution in the exposure chambers. In this study, an Open source OpenFOAM toolbox⁴) was applied because it allows to easily implement a complex physical model.

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https://doi.org/10.51083/radiatenvironmed.11.2_61
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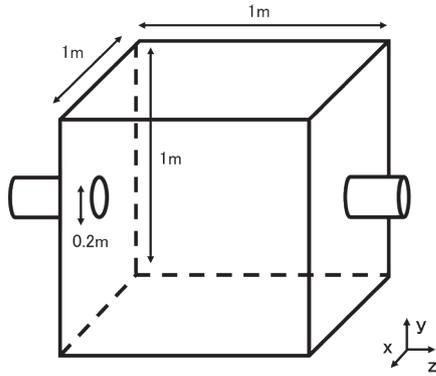


Fig. 1. Schematic of the virtual exposure chamber.

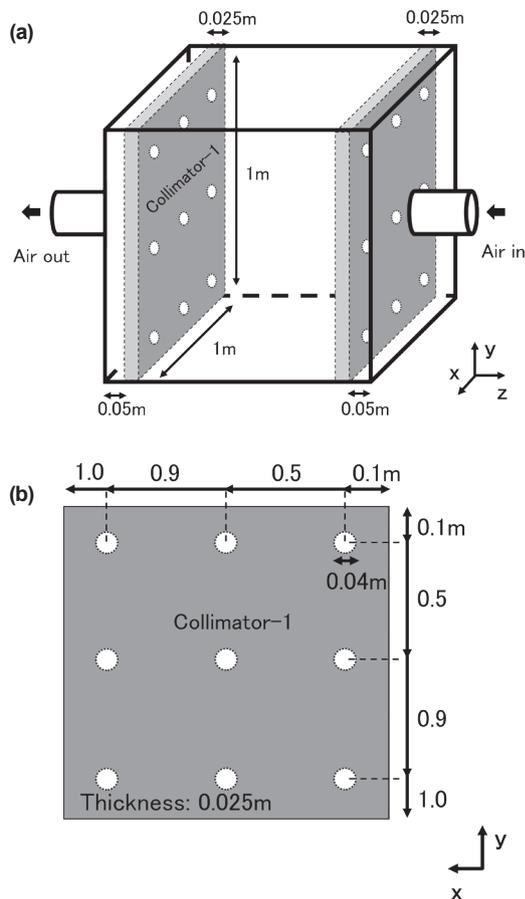


Fig. 2. The collimator-1 in this study (a: schematic of the virtual exposure chamber with the collimator-1; b: shape of the collimator-1).

OpenFOAM has extensive capabilities, including models for transport, turbulence, thermodynamics, chemical reactions, particle flows, surface films etc. While it is open source architecture where complete source code is available to all users, it can be customized and extended at no cost. The 2D and 3D figures with simulated results can be presented using ParaView⁵⁾ software.

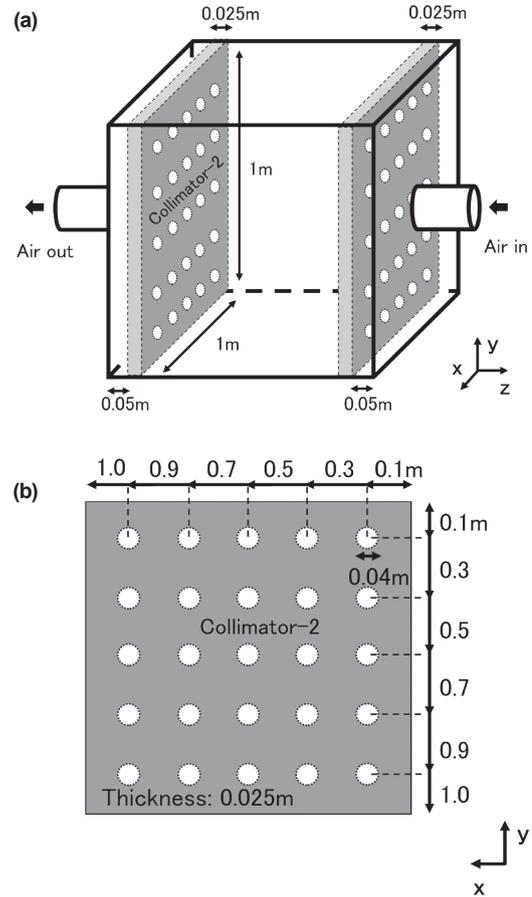


Fig. 3. The collimator-2 in this study (a: schematic of the virtual exposure chamber with the collimator-2; b: shape of the collimator-2).

3. Demonstration of the calculation

3.1. Calculation condition

To illustrate CFD modeling, a virtual concentration (i.e. a passive scalar) was used as an indicator of diffusion in the fluid. Passive scalar is a scalar quantity that is not actively involved in the flow physics of the CFD simulation. The equation governing transport of the passive scalar is expressed as follows:

$$\partial C / \partial t + \nabla \cdot (UC) - \nabla^2 \cdot (DC) = 0 \quad (1)$$

where C is the passive scalar concentration, U is the velocity, D is the diffusion coefficient and t is the time⁶⁾. In the present work, the virtual gas exposure chamber for CFD simulation was set to the size of 1 m × 1 m × 1 m (1 m³), as shown in Figure 1, with reference to the structure of actual radioactive gas exposure chambers located on the National Institutes for Quantum Science and Technology (QST) and Hiroaki University^{7, 8)}. Two different configurations with collimators, as shown in Figure 2 (collimator-1) and Figure 3 (collimator-2), were used to calculate the gas distribution in the virtual chamber. The simulations were performed by using air

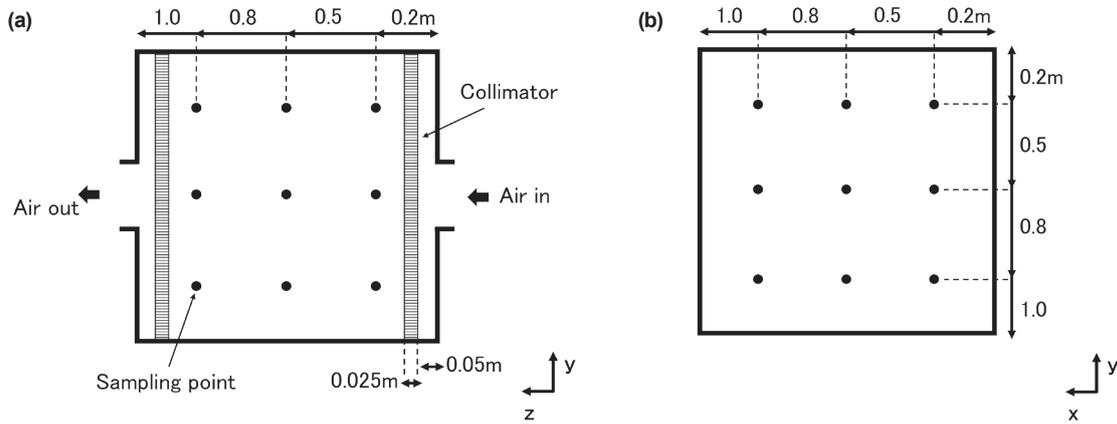


Fig. 4. Sampling points for data on the passive scalar concentration (a: y-z plane; b: x-y plane).

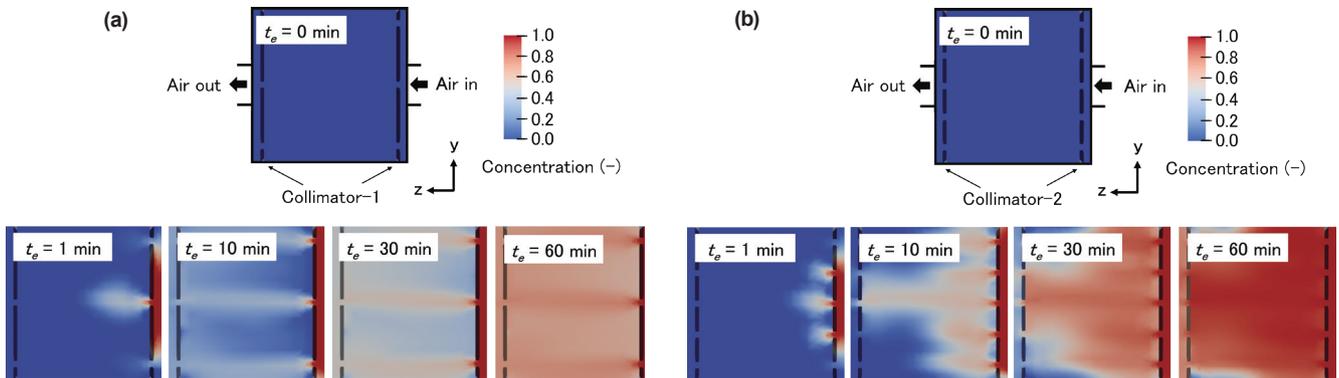


Fig. 5. The passive scalar concentration in the elapsed time (Slice in the middle of the x axis) (a: with the collimator-1; b: with the collimator-2).

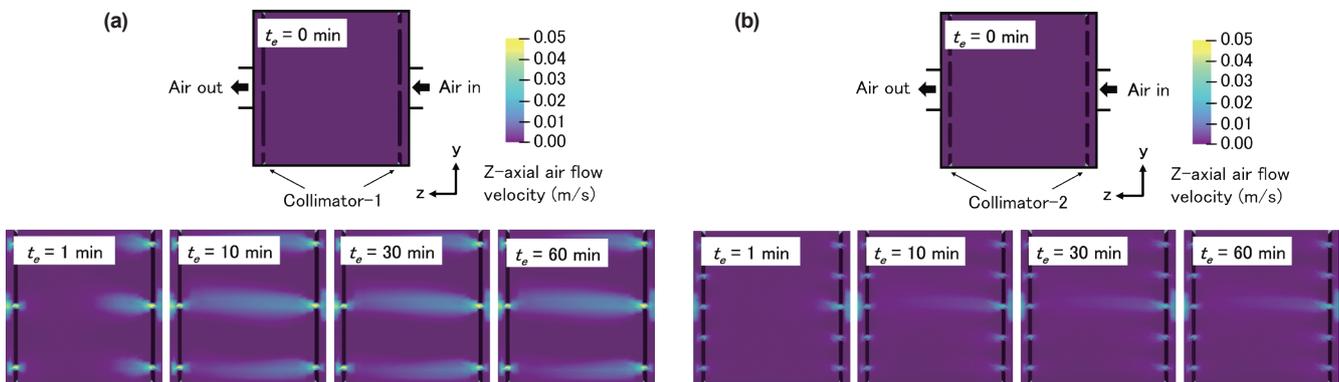


Fig. 6. The z-axial air flow velocity in the elapsed time (Slice in the middle of the x axis) (a: with the collimator-1; b: with the collimator-2).

($C = 1$ (-)) with volumetric flow rate at 30 LPM. Air was forced through the inlet on the right side of the chamber and blown out through the outlet on the left side of the chamber. Drawing these structures were performed by a CAD software. As initial conditions, the gravitational acceleration and temperature inside the chamber was set to zero and 300 K, respectively. The boundary conditions

of collimators and walls in the chamber were set to be adiabatic. The spatial mesh size was set to be $0.05 \times 0.05 \times 0.05$ m for the whole region and $0.0125 \times 0.0125 \times 0.0125$ m for the collimator and hole regions, with correction of arc shape. A web-based preprocessor for OpenFOAM was used to create calculation files under the above conditions⁹). The passive scalar concentration

was obtained for the elapsed time (t) from 0 to 60 min, with the 1 second step. In order to assess of concentration distribution inside the chamber, the Relative Standard Deviation ($RSD = S_A / C_A$) was used in this study, where C_A and S_A are the passive scalar average concentration and standard deviation, respectively. The RSD was calculated using data comes from 27 sampling points which were chosen selectively, as shown in Figure 4.

3.2. Calculation result

Using calculated data, heat maps of the passive scalar concentration and the z -axial air flow velocity against elapsed time (t_e) under two conditions, i.e., with the collimator-1 and with the collimator-2, are presented in Figures 5 and 6, respectively. As a result of the simulation, differences in the space-time evolution of passive scalar concentrations between collimator-1 and collimator-2 were observed. In the case of the collimator-1 the passive scalar concentration at the air inlet on the right was transported towards the z -axis within 10 minutes and then propagated in the volume of the chamber, while the passive scalar concentration through the collimator-2 at the air inlet on the right was propagated upward in 10 minutes and then transported in the z direction. The differences can be explained by two reasons: 1) the air flow velocity through the collimators, because the air flow velocity through the collimator-1 was faster than that through the collimator-2 and 2) the number of holes for air passage on the collimators, i.e. the collimator-2 had more air passage holes than the collimator-1.

The values of average concentration and RSD at each sampling point are shown in Figure 7. It can be observed that the values of RSD with the collimator-1 were initially lower than those with the collimator-2, while both values reached $C_A < 0.1$ in 60 minutes. The average gas concentration in the chamber with the collimator-2 changed significantly with time compared to the chamber with the collimator-1 and reached $C_A > 90\%$ of the saturation within 60 minutes. According to these results, it is suggested that the design and selection of collimator are one of the important factors for gas distribution inside the chamber.

4. Future Work

In general, direct measurements, which is the best solution, should be conducted for checking the distribution of the gas in the exposure chamber. However, direct measurements are not reasonable from a cost-effectiveness and time-efficient perspective when it is obvious that the distribution of the gas in the exposure chamber is homogeneous (e.g, when the convection velocity in the exposure chamber is large). In such a case, the CFD simulation proposed in this study looks

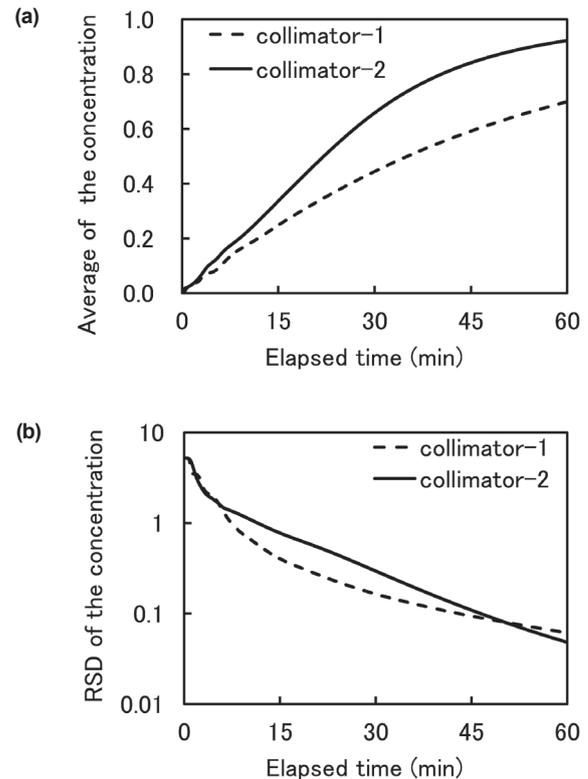


Fig. 7. Average and RSD for the passive scalar concentration at 27 sampling points (a: average; b: RSD).

promising especially. We plan to conduct further research in terms of the possibility of using CFD simulations in various situations, including the development and improvement of a simple small radioactive gas chamber¹⁰. Such efforts are eventually expected to contribute the optimal selection of gas chamber design parameters (e.g. size, inlet and outlet velocity) depending on the desired level of uniformity.

Disclosure

The authors declare that they have no conflicts of interest.

Author Contribution

Kazuki Iwaoka performed the study and wrote the manuscript. All authors contributed extensively in the discussion of the work and the review of the manuscript.

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