Review

Toward the development of an *in silico* human model for indoor environmental design

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Abstract: In modern society where people spend more than 90% of their time in indoor spaces, the indoor air quality (IAQ) created by buildings has the potential of greatly influencing quality of life. Because the time spent by workers/residents in indoor spaces has increased over time, the importance of IAQ issues in terms of public health is also increasing. Additionally, the quality of the indoor thermal environment also has great impact on human comfort and performance; hence, the development of a comprehensive prediction method integrating indoor air quality/thermal environment assessment and human physiological responses, is crucial for creating a healthy, comfortable, and productive indoor environment. Accordingly, the overarching objective of this study was to develop a comprehensive and universal computer simulated person (*i.e.*, *in silico* human model), integrating computational fluid dynamics (CFD), to be used in indoor environmental design and quality assessment. This paper presents and discusses the development of this computer-simulated person and its application to indoor environmental design.

Keywords: computer simulated person, *in silico* human, computational fluid dynamics, indoor environmental design

1. Introduction

In modern, industrialized society in which workers/residents spend more than 90% of their time indoors, the indoor air quality (IAQ) created by buildings greatly influences the quality of life. Because people now stay indoors more than in the past, IAQ issues are becoming increasingly important with regard to the health risks of building residents.1),2)

Indoor air pollution has been a serious issue for centuries, *e.g.*, carbon monoxide (CO) poisoning or casualties from combustion or heating gas in the past. In the past few decades, indoor air pollution has changed its status to become a social problem because of the growing prevalence of houses that are airtight, have effective thermal insulation, and are insufficiently ventilated.3) The deterioration of the atmospheric (exterior air) environment has aggravated the situation and contaminants originating outdoors could also diminish indoor air quality. Infiltration through ventilation systems has also been recognized as a dominant pathway for the transport of contaminants from outdoors to indoors.4) Indoor air pollution is caused by various pollutants, among them suspended particulate matter, biological aerosols including fungal spores and pollen, and chemical substances called volatile organic compounds (VOCs). The latter are emitted from new building materials used in new construction methods. The problems caused by multiple chemical sensitivities to air-phase VOCs have been recognized as building related illness, which is commonly called ‘sick building syndrome or sick house syndrome’ in Japan. This has become a significant social problem in Japan. Recent epidemiological studies indicate that exposure to particulate air pollution (*e.g.*, PM2.5 and PM10) is associated with increased risk of lung cancer, asthma, and chronic diseases, as well as increased risk of induced mortality and morbidity in humans.5)–8) When individuals are indoors, they can be exposed to particulate matter that originates from the outdoor environment and penetrates the indoor environment through ventilation. Health conditions

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related to particulate matter have also led to considerable attention being given to the effect of indoor air on the quality of life.

In recent years, computational fluid dynamics (CFD), which is based on the numerical simulation of airflow, temperature, and is used in the contaminant distribution field; has been used in air conditioning design and the analysis of indoor air quality.\textsuperscript{9–12} Numerical simulation is effective in analyzing the structure of the airflow, temperature, and contaminant distribution field, and can be used to design a precise method for control of indoor environmental factors, especially in a local domain. The thermal sensations experienced by humans are highly dependent on the local heat transfer characteristics of body surfaces. The exposure contaminant concentration and breathing air quality are also highly dependent on local contaminant concentration distributions around human body surfaces. The existence of the body itself has an effect, as metabolic heat production and breathing/aspiration can have large influences on the microclimate around the body. Furthermore, the local properties of this microclimate can also significantly affect airflow and contaminant distributions, as well as the local heat-transfer characteristics of the body. Thus, it is very important to analyze precisely the interaction (airflow, heat/moisture, and contaminant transfer) between the human body and its surrounding microclimate. Given this, interest in using a computer-simulated person (CSP) integrated with computational fluid dynamics (CFD) simulation for this purpose has been growing steadily in research and design fields. Although there has been much research on the development of various types of CSP for indoor environmental analysis, and while successful models have been reported for predicting the thermal sensation of residents in indoors, there is no previous study concerning the development of CSP in relation to a precise respiratory tract model for analyzing inhalation exposure in indoor environments.

The overarching objectives of this study were to develop a comprehensive and universal CSP (\textit{i.e.,} an \textit{in silico} human model) that would integrate thermo-regulation and respiratory tract models for indoor environmental quality assessment; and to develop an integrated numerical simulation procedure for airflow, temperature, and contaminant transport by CFD using the newly created CSP.

The significant results of this study pertain to the development of a numerical simulation method to predict the unsteady and non-uniform distributions of indoor environmental quality (IEQ), and an evaluation method for inhalation exposure concentration of a CSP with respiratory tract model. This study also resulted in the design and development of various methods for numerical prediction of IEQ distributions.

2. Outline of a Virtual Manikin for computational fluid dynamics

As mentioned, recent studies of the indoor environment focus on phenomena around the human body at the microclimate level, and therefore the need for more realistic and detailed geometries of human body models has been pointed out. A thermal manikin has been used in a number of experimental investigations to clarify the interaction between the human body and airflow field, temperature, and contaminant distributions around the human body, or in its breathing zone.\textsuperscript{13,14} In several studies, numerical models closely representing the actual shape of the human body have already been proposed for seated or standing female models (or androgynous models based on female body shapes), and these are available for indoor environment analysis applications.\textsuperscript{15–21} In a number of studies, Murakami \textit{et al.} used computational fluid dynamics (CFD) to calculate the flow, temperature, and contaminant field around geometries resembling the human body, and reported the investigation results of coupled simulation of convective and radiative heat transfer from the human body.\textsuperscript{15} However, models of other human body shapes such as with the proportions of a male or a child (or in other postures), have not been proposed. In addition, because existing models use relatively coarse meshes, the data gathered for various parts of the human body have provided inadequate detail.

In this research, various grid data for computer-simulated persons, called Virtual Manikins in this study, were developed for indoor environmental prediction based on CFD simulation.\textsuperscript{22} In particular, the grid data for these Virtual Manikin geometries provide detailed designs for three kinds of human body proportions—a child-proportioned model, a male-proportioned model, and a female-proportioned model. The final purpose of this model development was to propose a grid library of Virtual Manikins that could be used with versatile, commercial CFD software.

Geometry and posture of the Virtual Manikins. Comprehensive posture, gender, and age types of Virtual Manikin were developed. These included models of (a) a seated child, (b) a standing
child, (c) a seated male, (d) a standing male, (e) a seated female, and (f) a standing female. The Virtual Manikin reproduces detailed geometries such as ears, nose, fingers, and toes. All Virtual Manikins are undressed and without hair, because those details could not be accurately modeled by CFD analysis.

Procedure for developing the Virtual Manikin geometry and grid information. Virtual Manikins imitate the average Japanese body proportions for a seven-year-old child, adult male, and adult female. The outlines of the human body are drawn using POSER software (Curious Labs, Inc.) and the data is then read out in DXF format. The overall shape of the human body is then adjusted using three-dimensional CAD software (Vector Works and A&A Co., Ltd.). The final geometry of the Virtual Manikins and the computational grids, are made using GRIDGEN (VINAS Co., Ltd.) which includes a generally available commercial mesh generator. The hands and feet of the Virtual Manikins are simplified in consideration of the computational load for CFD analysis.

The external shapes of the Virtual Manikins developed in this study are shown in Fig. 1, which gives a front view and a side view of the complete geometry. The essential information for each Virtual Manikin developed in this research is given in Table 1. One of the representative grid designs of a Virtual Manikin is shown in Fig. 2. The geometrical resolution is high and includes all relevant features of the human body, except hair and clothes. For instance, the surface areas of the standing and seated
**Table 1.** Surface area of the individual segments of the manikins

| Segments                        | Seated model | Standing model |
|---------------------------------|--------------|----------------|
|                                 | (a) Child    | (b) Male       | (c) Female    | (a) Child    | (b) Male       | (c) Female    |
| Area of whole body [m$^2$]      | 0.848        | 1.681          | 1.308         | 0.847        | 1.745          | 1.317         |
| Volume of whole body [m$^3$]    | 0.022        | 0.063          | 0.040         | 0.022        | 0.064          | 0.040         |
| Height of body [m]              | 1.048        | 1.351          | 1.236         | 1.289        | 1.736          | 1.584         |
| Smallest surface mesh size [mm$^2$] | 0.490    | 0.562          | 0.746         | 0.490        | 0.469          | 0.652         |
| Largest surface mesh size [mm$^2$] | 154.933 | 468.185        | 380.490       | 151.715      | 425.013        | 372.035       |
| Number of surface mesh          | 20,085       | 44,620         | 36,742        | 18,971       | 44,974         | 35,500        |
| Area of left and right foot [m$^2$] | 0.023  | 0.048          | 0.035         | 0.023        | 0.048          | 0.035         |
| Area of left and right leg [m$^2$]  | 0.063  | 0.112          | 0.091         | 0.060        | 0.111          | 0.088         |
| Area of left and right thigh [m$^2$] | 0.079  | 0.165          | 0.141         | 0.071        | 0.151          | 0.124         |
| Area of left and right hand [m$^2$] | 0.019  | 0.036          | 0.024         | 0.019        | 0.038          | 0.024         |
| Area of left and right arm [m$^2$]  | 0.030  | 0.061          | 0.040         | 0.030        | 0.071          | 0.040         |
| Area of left and right hand [m$^2$]  | 0.035  | 0.071          | 0.058         | 0.037        | 0.074          | 0.058         |
| Area of pelvis [m$^2$]           | 0.102        | 0.187          | 0.162         | 0.123        | 0.265          | 0.212         |
| Area of chest [m$^2$]            | 0.079        | 0.186          | 0.139         | 0.079        | 0.190          | 0.139         |
| Area of back [m$^2$]             | 0.073        | 0.155          | 0.084         | 0.068        | 0.127          | 0.084         |
| Area of face [m$^2$]             | 0.036        | 0.061          | 0.046         | 0.036        | 0.062          | 0.046         |
| Area of neck [m$^2$]             | 0.059        | 0.077          | 0.076         | 0.059        | 0.086          | 0.076         |

**Fig. 2.** Grid design around Virtual Manikin.

**Fig. 3.** Segments of the body.
child mesh size on the surface of the child model is allocated to the face (smallest mesh 0.49 mm²). About 20,000 cells are used for the whole body surface. The geometries of the nose, ears, mouth, and eyes on head are replicated with sufficient resolution for flow and heat mass-transfer analysis. The first mesh wall surface is set within the viscous sub-layer and the wall units (y⁺), which express the dimensionless normal distance from the surface. This satisfies the requirement for 1.0 or less over the whole surface of each airway model. The surface of each Virtual Manikin is divided into 17 segments (see Fig. 3), corresponding approximately to the original divisions of the thermal manikin.

At the final stage of model development, detailed data on the Virtual Manikin will be disclosed on our website. For this purpose, we prepared two kinds of grid libraries for the Virtual Manikin, aiming at use with a general commercial CFD code. The first includes grid data that give only the surface geometry and mesh divisions of the human body (Tori-gone surface mesh). The second includes grid data to distribute four triangular prism meshes of width of less than 1 mm in a direction normal to the surface of the human body, in addition to the surface geometry and mesh divisions. (These Virtual Manikin data can be downloaded freely for academic purposes at the website: www.phe-kyudai.jp)

In this study, the average Japanese body proportions were adopted to generate Virtual Manikin geometries because the detailed statistical information concerning the human body shape and the physiology as functions of age and gender can be used. These Virtual Manikins might be appropriate for reproducing the forms of other Asians, but would not be expected to represent a universal human body shape; hence, it is important to consider this limitation when these Virtual Manikins are used under various indoor environmental conditions.

3. Outline of a Virtual Airway for computational fluid dynamics

Breathing is one of the most essential processes in the human body. The basic functions of breathing are to exchange gases (supply oxygen from ambient air and remove carbon dioxide from the blood) and to exchange heat and moisture through the mucous surfaces of the airway. During an average lifetime, human beings experience significant exposure to indoor air and countless contaminants/particles via inhalation. In order to understand the inhalation exposure phenomenon, a detailed respiratory tract model is crucial for numerical simulation. Against this background, we developed a Virtual Airway model for inhalation exposure analysis and for understanding the transfer of heat, moisture, and contaminants inside the respiratory tract.

Original respiratory tract data were obtained using a Toshiba 64 multi-detector row computed tomography (MDCT) scanner. The subject was a nonsmoking Asian male volunteer, with a body mass index (BMI) of approximately 22. The CT scans produced 785 slices of the respiratory tract. The images were stored as standard Digital Imaging and Communications in Medicine (DICOM) data, a format commonly used for the transfer and storage of medical images. Figure 4 shows the combined CT images of the human upper airway.

The original set of CT images was converted into a file format compatible with Mimics (Materialise). This is 3-D imaging software, which generates and modifies 3-D surface models from medical images. Generation of a surface model from the 2-D contour data began with the translation of the segmented, modified, and smoothed contour points into a data series that was loaded into the ANSYS preprocessing software packages GAMBIT and TGrid. GAMBIT and TGrid were used to modify the surface mesh and then to create a volume mesh of the model, respectively. Surface geometries of the respiratory tract were also exported as STL format. Figure 5 shows views of the human airway model after going through this process. This respiratory tract model is composed of an upper airway (nasal and oral cavity, pharynx, and larynx) and a lower airway (trachea and bronchial tree). This respiratory tract model possessed the height and volume of about 34.8 cm and 173 cm³, respectively. One of the representative grid designs of respiratory tract models is shown in Fig. 6. The surface geometries of Virtual Airway model were composed by the combination of triangulated mesh.

4. Development of in silico human model by integrating Virtual Manikin and Virtual Airway

We created a comprehensive model that integrates Virtual Manikin with Virtual Airway by generating a continuous grid design in order to analyze the effect of the indoor environment around the human body, on the inside of the respiratory tract via the nostrils and oral cavity. In this study, we call this model a Computer Simulated Person (CSP).
Figure 7 shows an outline of the comprehensive CSP and the grid design in the region of the head and of the nostril surfaces. This model has continuous grid design; hence, mass and energy conservation were automatically secured with accurate CFD analysis. In our numerical simulation, the creation of approximately 10 million meshes was ensured.

**Unsteady breathing cycle model.** In order to analyze the interaction between indoor air quality and its impact on human health through inhalation exposure, an unsteady breathing cycle model was integrated into the CSP. This was done for two purposes: to provide high-accuracy prediction of heat loss (sensible and latent heat) from respiration by applying the breathing operation, and to estimate contaminant exposure during continuous inhaling and exhaling. In order to reproduce the unsteady breathing cycle and breathing flow rate, an unsteady breathing cycle model based on experimental data by Gupta et al., was applied on the virtual airway as the inlet boundary condition at the nostril surfaces. This breathing cycle model was defined through

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Fig. 4. Selective CT images of human upper airways.

Fig. 5. Schematic of Virtual Airway.

Fig. 6. Representative grid design of numerical airway model.

Fig. 7. Grid design of computer simulated person and details of nasal area.
MV (volume per minute) [L/min], RF (respiration frequency) [times/min], and TV (tidal volume) [L/1 breathing cycle] by using $H$ (body height) [m], $W$ (body weight) [kg], and BSA (body surface area) [m$^2$] in the following equations:

$$MV = 5.225 \times BSA$$  \hspace{1cm} [1]

$$TV = \frac{MV(RF_{in} + RF_{out})}{2RF_{in}RF_{out}}$$  \hspace{1cm} [2]

$$RF_{in} = 55.55 - 32.86H + 0.2602W$$  \hspace{1cm} [3]

$$RF_{out} = 77.03 - 45.42H + 0.2373W$$  \hspace{1cm} [4]

A linear relationship between $MV$ and BSA was assumed per previous experimental data. Regarding the relationship between $RF$ and $H$, $RF$ decreased with the increased lung volume caused by increase of height, in the case of fixed $MV$. In addition, the $RF$ of the male tends to depend on $W$ and increase of $W$ causes increase of $RF$ as well as decreased time for one breathing cycle. Moreover, the breathing flow rate $Q$ determined by $\alpha_x \sin(\beta_x t)$ and $\alpha_x$ as well as $\beta_x$, were defined by the following equations:

$$Q = \alpha_x \sin(\beta_x t)$$  \hspace{1cm} [5]

$$\alpha_x = \frac{\beta_x TV}{2}$$  \hspace{1cm} [6]

$$\beta_x = \frac{\pi RF_x}{30}$$  \hspace{1cm} [7]

Here, $\alpha_x$ indicates the maximum flow rate [L/min], and $\beta_x$ implies $RF_x$ [times/min]. Because inhalation and exhalation time periods are different, subscript $x$ can be replaced by ‘in’ for inhalation and ‘out’ for exhalation. Under normal circumstances, the pulmonary ventilation rate $m_{res}$ [kg/s] is primarily defined as a function of $M$ (the rate of metabolic heat production) [W/m$^2$] and $K_{res}$ (proportionality constant) (= 1.43 $\times$ 10$^{-8}$ [kg/J]).

$$m_{res} = K_{res}BSA \cdot M$$  \hspace{1cm} [8]

Here, $m_{res}$ is defined as the effective breathing airflow rate for lung/blood-flow gas exchange and is given by Eq. [9],

$$m_{res} = Q_{res}' + m_{pds}$$  \hspace{1cm} [9]

where $Q_{res}'$ denotes the breathing airflow rate at the nostril or oral surface [kg/s], and $m_{pds}$ is the physiological dead space rate [kg/s]. Generally, $m_{pds}$ is calculated using the Bohr equation as a function of the partial pressure of CO$_2$ in the breathing air and in the artery (~150 [mL/breath]).

By using Eqs. [8] and [9], the following relationship between metabolic rate $M$ and breathing airflow rate was derived:

$$Q_{res}' = K_{res}BSA \cdot M + m_{pds}$$  \hspace{1cm} [10]

Finally, $MV$, a parameter in the breathing model of Gupta $et$ $al.$ in Eq. [1], can be improved using $M$ and $K_{res}$, as given by Eq. [11].

$$MV = (0.08260M + 1.271) \times BSA$$  \hspace{1cm} [11]

Here, $RF$ was assumed to be independent on the change in $M$ and the breathing airflow rate $Q_{res}'$ was determined based on this breathing model supposing an adult male. Figure 8 shows a breathing cycle adopted into the CSP. In applying the breathing cycle to the CSP, we assumed the nose was the respiratory organ, and the velocity of time-dependent change was applied to the nostril surfaces (surface area: left = 1.288 cm$^2$, right = 1.329 cm$^2$) as the inlet boundary condition. Under the condition of standard metabolic rate, the length of one breathing cycle is 4.05 s, with the length of inhaling time set to 1.9 s and exhaling to 2.15 s. Although inhaling time is shorter than exhaling time, the maximum flow rates of inhaling and exhaling are 0.3 L/s and 0.27 L/s, respectively, which lead to higher velocity inhaling than exhaling at the nostril surface. In this study, a simulation with a boundary condition of an unsteady breathing cycle was performed under unsteady conditions, and the calculation time step was set to meet the Courant-Friedrichs-Lewy (CFL) condition.

**Human thermoregulation model.** The human body controls the skin surface temperature by heat exchange with surrounding environment. To understand the unsteady and non-uniform thermal environments formed in the indoor environment and the thermal sensation of residents, development of a thermoregulation model that could predict the skin
surface temperature with high accuracy is of substantial importance. Many thermoregulation models have been suggested by researchers. Representative high-accuracy, multi-node type thermo-regulation models include the 65MN model, JOS model, Stolwijk model, and Fiala model.\textsuperscript{29–32}

Here, a fundamental unsteady thermoregulation model called the two-node model, proposed by Gagge \textit{et al.},\textsuperscript{33} was integrated with the CSP, and coupled analysis with convection, radiation, and humidity analysis, using CFD simulation was conducted. CSP has precise and detailed mesh design on the skin surface. By applying the two-node model concept to each skin surface mesh, various distributions such as temperature and sensible and latent heat flux on the human body could be calculated.

The two-node model is a basic model of unsteady thermoregulation, and it is defined by the following basic heat balance equation:

\begin{equation}
M = Q_{sk} + Q_{res} + S = (Q_{cv} + Q_{r} + E_{sk}) + (C_{res} + E_{res}) + S_{cr} + S_{sk}
\end{equation}

The two-node model consists of two parts, the core and the skin, each a ‘node’ or division of the human body. The heat balance equation of the core and skin compartments can be defined by Eqs. \[13\] and \[14\].

\begin{equation}
S_{cr} = (M - C_{res} - E_{res}) - K(T_{cr} - T_{sk}) - c_{p,bl}m_{bl}(T_{cr} - T_{sk})
\end{equation}

\begin{equation}
S_{sk} = K(T_{cr} - T_{sk}) + c_{p,bl}m_{bl}(T_{cr} - T_{sk}) - E_{sk} - (Q_{cv} + Q_{r})
\end{equation}

Here, \(Q_{sk}\) denotes the total rate of heat loss from the skin [W/m\(^2\)], and \(Q_{res}\) is defined as the total rate of heat loss through respiration [W/m\(^2\)]. \(Q_{cv}\) and \(Q_{r}\) denote the rates of convective and radiative heat loss from the skin [W/m\(^2\)], respectively; \(E_{sk}\) is defined as the total rate of evaporative heat loss from the skin [W/m\(^2\)]; and \(C_{res}\) and \(E_{res}\) indicate the rates of convective and evaporative heat loss from respiration [W/m\(^2\)], respectively. The terms \(S_{cr}\) and \(S_{sk}\) are the rates of heat storage in the core and skin compartments [W/m\(^2\)], respectively, and \(K\) denotes the effective heat transfer coefficient between core and skin compartments [W/m\(^2\)K]. The specific heat of the blood is indicated by \(c_{p,bl}\) [kJ/kgK], and \(m_{bl}\) is the blood flow rate [kg/m\(^2\)s].

Moreover, if data such as the specific heat of the core and skin compartments (\(c_{cr}\) [kJ/kgK], \(c_{sk}\) [kJ/kgK]); fraction of body mass concentrated in the skin compartment (\(\alpha_{sk}\ [\%]\)); body mass (\(m\) [kg]); and surface area of the human body (\(A_D\) [m\(^2\)]) are already known; then the changes in heat storage rate for the core and skin compartments can be defined by Eqs. \[15\] and \[16\], using the time-dependent changes in the core and skin temperatures (\(T_{cr}, T_{sk}\)).

\begin{equation}
S_{cr} = \frac{(1 - \alpha_{sk})m \cdot c_{cr}}{A_D} \times \frac{dT_{cr}}{dt}
\end{equation}

\begin{equation}
S_{sk} = \frac{\alpha_{sk} \cdot m \cdot c_{sk}}{A_D} \times \frac{dT_{sk}}{dt}
\end{equation}

By applying the forward difference, the core and skin temperatures of the next time step \((t + \Delta t)\) are calculated.

\begin{equation}
T_{cr}^{(t+\Delta t)} = T_{cr}^{(t)} + \frac{A_D \cdot S_{cr}}{(1 - \alpha_{sk})m \cdot c_{cr}} \Delta t
\end{equation}

\begin{equation}
T_{sk}^{(t+\Delta t)} = T_{sk}^{(t)} + \frac{A_D \cdot S_{sk}}{\alpha_{sk} \cdot m \cdot c_{sk}} \Delta t
\end{equation}

By applying Eqs. \[13\] and \[14\] to Eqs. \[17\] and \[18\], the core and skin temperatures of the next time step can be calculated explicitly.

When the human body is thermally neutral, it was reported that the core temperature \((T_{cr,n})\) is 36.8 [°C] and the skin temperature \((T_{sk,n})\) is 33.7 [°C]. Furthermore, changes in the blood flow rate and sweating occur as the result of the temperature differences between the surrounding environment, and the core and skin compartments. Table 2 shows the physiological signals that occurred as a result of these differences of temperature.

Based on these signals, the blood flow rate \((m_{bl})\) can be defined by Eq. \[19\].

\begin{equation}
m_{bl} = \left( \frac{6.3 - 200 \cdot WSIG_{cr}}{1 + 0.1 \cdot CSIG_{sk}} \right) \div 3600
\end{equation}

By applying the blood flow rate as changed by environmental conditions, the fraction of the body mass concentrated in the skin compartment (\(\alpha_{sk}\)) can be calculated by Eq. \[20\]. If the human body is thermally neutral, the fraction of body mass concentrated in the skin compartment is assumed 0.1.\textsuperscript{33}

\begin{equation}
\alpha_{sk} = 0.0418 + \frac{0.745}{(3600m_{bl} + 0.585)}
\end{equation}

The skin wetness is defined with the consideration that the skin surface is partly wet and partly dry (no intermediate conditions). This fraction of fully wetted surface to the whole surface can be calculated as the skin wetness. The skin wetness \((w)\) is defined by Eq. \[21\]:

\begin{equation}
w = \frac{E_{sk}}{E_{max}} = \frac{E_{res} + E_{df}}{\alpha_c(P_{sk,s} - P_a)} = \frac{m_{res} \cdot h_{sy} + E_{df}}{\alpha_c(P_{sk,s} - P_a)}
\end{equation}
According to an expression proposed by Fanger,26) by sweating feature, and humidity inevitable. By analyzing the tract; hence, a certain level of uncertainty was simple circular cylinder geometry of the respiratory Equation [23] was derived from the assumption of complicated geometry and realistic unsteady calculation, the convective heat loss $C_{res}$ and evaporative heat loss $E_{res}$ in Eq. [23] could be directly calculated and the prediction accuracy thereby improved. Time-dependent changes of $C_{res}$ and $E_{res}$ due to change in the inhaled-air temperature $T_a$ and humidity $P_a$ could be calculated using the integrated unsteady simulation of the CSP (with Virtual Airway and transient breathing cycle model). This result was given as real-time feedback to the two-node model. The prediction accuracy of the $C_{res}$ and $E_{res}$ was improved, compared with the results estimated by assumption of simple circular cylinder geometry (shown in Eq. [23]).

**Physiologically based pharmacokinetic (PBPK) model.** As mentioned before, the CSP with integrated thermoregulation model (two-node model) allows for an analysis of the interaction between the indoor environmental quality and human physiological responses continuously and simultaneously via the skin surface and respiratory tract. Furthermore, in order to estimate the comprehensive risk of inhalation exposure in indoor environments, a physiologically based pharmacokinetic (PBPK) model, harmonized with the computational fluid dynamics simulation of the numerical Virtual Airway model, was integrated into the CSP.34–39 The PBPK model incorporated into the tissue surface boundary condition of the Virtual Airway of the CSP can estimate the airway tissue dosimetry caused by IAQ problems.

For decades, pharmacokinetic models have been successfully applied to address issues of extrapolation between contaminants, dose, dose-rate/dose-response, or types of exposure to drugs or chemicals. PBPK models have become a staple for chemical risk

### Table 2. Thermal control function of the human body

| Signal   | Definition                                                                 | Thermal sensation      | Thermal control function          |
|----------|---------------------------------------------------------------------------|------------------------|-----------------------------------|
| $WSIG_{tr}$ | $T_{tr} - T_{tr,n}$ ($T_{tr} > T_{tr,n}$)                                | Warm signal from the core | Expansion of blood vessels        |
| $CSIG_{tr}$ | $T_{tr,n} - T_{tr}$ ($T_{tr} < T_{tr,n}$)                                | Cold signal from the core | Contraction of blood vessels (low), shivering |
| $WSIG_{sk}$  | $T_{sk} - T_{sk,n}$ ($T_{sk} > T_{sk,n}$)                                | Warm signal from the skin | Sweating                          |
| $CSIG_{sk}$  | $T_{sk,n} - T_{sk}$ ($T_{sk} < T_{sk,n}$)                                | Cold signal from the skin | Contraction of blood vessels (high) |
| $WSIG_{b}$   | $T_b - T_{b,n}$ ($T_b > T_{b,n}$)                                        | Warm signal from the body | Expansion of blood vessels        |
| $CSIG_{b}$   | $T_{b,n} - T_b$ ($T_b < T_{b,n}$)                                        | Cold signal from the body | Shivering                         |

Here, $E_{sk}$ is defined as the total rate of evaporative heat loss from the skin [W/m²]; $E_{max}$ denotes the maximum rate of evaporative heat loss from the skin [W/m²]; $E_{res}$ is the rate of the evaporative heat loss by sweating [W/m²]; and $\alpha_i$ indicates the evaporative heat transfer coefficient [W/m²·kPa]. Here, $P_{sk,s}$ is the saturated water vapor pressure at the skin [kPa]; $P_a$ is defined as the water vapor pressure in the ambient air [kPa]; $m_{res}$ denotes the rate at which sweat is generated [kg/m²·s]; and $h_f$ indicates the heat of vaporization of water [= 2430 kJ/kg at 30 °C].

$E_{dif}$ is defined as the rate of the natural diffusion of water from the skin [W/m²]. If regulatory sweating is not occurring, skin wetness $w$ is approximately 0.06, and by applying this value, the rate of the natural diffusion of water from the skin $E_{dif}$ can be calculated by Eq. [21].

The rate at which sweat is generated is changed by physiological signals, and this process is defined by Eq. [22]. Here, $WSIG_{sk,local}$ indicates a warm thermal signal at one section of the skin.

\[
m_{res} = 4.7 \times 10^{-5} WSIG_b \exp\left(\frac{WSIG_{sk,local}}{10.7}\right) [22]
\]

According to an expression proposed by Fanger,26) sensible and latent heat loss by respiration is normally calculated using the following, simplified Eq. [23]:

\[
Q_{res} = C_{res} + E_{res}
\]

\[
= 0.0014 M (34 - T_a) + 0.00017 (5867 - P_a) [23]
\]

Equation [23] was derived from the assumption of simple circular cylinder geometry of the respiratory tract; hence, a certain level of uncertainty was inevitable. By analyzing the flow pattern, temperature, and humidity field inside the virtual airway with complicated geometry and realistic unsteady
assessments by the US EPA (Environmental Protection Agency) and the WHO International Program on Chemical Safety (IPCS). This is primarily because they account for differences of contaminants in physiological and other processes associated with absorption, distribution in the body, metabolism, and elimination.

In this study, integrated modeling of a CSP with numerical Virtual Airway, which had been adapted to predict air flow and contaminant distribution around the human body, was developed to include PBPK modeling in the respiratory tract. By creating an integrated numerical simulation model (CFD–CSP–PBPK), critical contaminant-specific differences in anatomy and physiology that could not be determined with simplified empirical or compartmental representations of the respiratory system, can now be accounted for. Figure 9 denotes the schematic diagram of this CFD-CSP-PBPK model and Fig. 10 shows the conceptual detail and governing equations of the PBPK-CFD hybrid analysis.

Here, we focused on formaldehyde as the inhaled contaminant in an indoor environment and developed a two-compartment PBPK model. This PBPK model consisted of clearance via a saturable pathway (formaldehyde dehydrogenase; \( K_{m1} \) [µg/m³], \( V_{max1}C \) [µg/m³/s]). This is a first-order pathway assumed to represent the intrinsic reactivity of formaldehyde with tissue constituents \( (K_f \ [s^{-1}]) \), and a first-order binding of formaldehyde to DNA responsible for DNA-protein crosslink formation \( (K_b \ [s^{-1}]) \). The governing equations of the PBPK model are shown in Eqs. [24] and [25].

\[
\frac{\partial C_t}{\partial t} = \left( \frac{V_{max1}C}{K_{m1} + C_t} \right) - K_f C_t - K_b C_t + D_t \nabla^2 C_t \quad [24]
\]

\[
\frac{\partial C_b}{\partial t} = -K_f C_b - K_b C_b - \left( \frac{Q_b}{V_b} \right) C_b + D_b \nabla^2 C_b \quad [25]
\]

where \( C_t \) and \( C_b \) [µg/m³] are the respective soluble vapor concentrations of formaldehyde in the epithelium + mucus, and subepithelium compartments, respectively.

![Fig. 9. Schematic diagram of the CFD-CSP-PBPK model.](image)

![Fig. 10. Details of concept and governing equations of the PBPK-CFD hybrid analysis.](image)
The formaldehyde concentration in the air $C_a$ [µg/m³] and that in tissue $C_t$ and $C_b$ [µg/m³] have different concentration units (the former volume [m³] represents air and the latter [m³] represents tissue). As a result, the following relationship between the concentration on the air-side (lumen in the Virtual Airway) and that on the tissue-side is generally applied.

$$C_t = P_{t:air} C_a$$

Here, $P_{t:air}$ is the partition coefficient [m³(air)/m³(tissue)]. In order to solve Eq. [26], we adopted the following explicit scheme as the lumen-tissue interface. The suffix $n$ and $n+1$ in Eqs. [27] and [28] denote the iterative time step of the CFD.

$$C_{a,0}^{n+1} = \frac{1}{1 + P_{t:air}} (C_{a,0}^n + C_{t,0}^n)$$

$$C_{t,0}^{n+1} = \frac{P_{t:air}}{1 + P_{t:air}} (C_{a,0}^n + C_{t,0}^n)$$

where $n$ in Eqs. [27] and [28] denotes the step of iterative calculation. Finally, at the air-tissue interface, Eq. [29] was coupled to the lumen convection-diffusion equation by matching of diffusion flux by:

$$D_a \frac{\partial C_a}{\partial n} = D_l \frac{\partial C_t}{\partial n}$$

where $n$ in Eq. [29] denotes the surface normal direction.

5. Integrated CFD and CSP analysis

In this study, sensitivity analysis was carried out to demonstrate the effectiveness of analysis using integrated CFD and CSP. A virtual space was created with the simple geometry of $3 \times 3 \times 3$ m for CFD simulation, and an adult male CSP was located in the center of the inside space (see Fig. 11). This room model had an inlet on the front wall with inflow of uniform velocity, and an outlet on the back wall with a free-slip-outflow condition. With this setting, the space had uniform, horizontal flow from front to back of the CSP.

The total number of computational cells in the room model was set to about 2 million. In addition, 8 million cells were allocated in the numerical airway model. A triangular surface mesh was used to reproduce the complex geometry of the human body. To resolve the boundary layer around the CSP, four layers of prism cells were created on its surface with a height of less than 1.0 mm between layers. The tetrahedrons formed an unstructured grid that was then arranged from the outside of the boundary layer to the other sidewalls in the analytical model room. Under this numerical condition, the wall units ($y^+$), which express the dimensionless normal distance from the surface, met the requirement of 1.0 or less over the whole surface of the CSP. The unsteady respiratory cycle and thermoregulation model were integrated into the CSP.

CFD simulations were performed to calculate airflow, temperature, humidity, and contaminant transport profiles under transient breathing conditions. This low-Re k-ε model (Abe–Kondoh–Nagano model) has been adopted for the various types of flow field analysis (from laminar to turbulent) and confirmed the good prediction accuracy for flow and thermal field analysis intended for the near-wall. The low-Reynolds-number, affects both the attached and detached flows. A no-slip boundary condition was applied for the wall surfaces in the target analytical space, and inside the Virtual Airway model. The second-order upwind was used for the convection term, and a SIMPLE (semi-implicit method for pressure-link equations) algorithm was applied.

The inlet boundary condition of the room model was set to $U_{in} = 0.1$ m/s for inflow air velocity, $T_{in} = 25 ^\circ C$ for air temperature and $\phi_{in} = 50\%$ RH for relative humidity. In order to discuss the inhalation exposure, representative and hypothetical contaminant generation points were assumed in the room model. Here, contaminant generation point in front of the head of the CSP was assumed (as shown in
Fig. 12). In the case of the CFD-CSP-PBPK hybrid analysis, a hypothetical contaminant that originated from this point (in Fig. 12) was assumed to be formaldehyde.

Concerning the flow field analysis in the respiratory tract, a transient breathing cycle model was adopted as a boundary condition at the openings on the nostril surface. This meant that the flow boundary condition at the nostril surface (as inlet opening) was defined by an unsteady breathing cycle model and this was shared with the boundary condition of the nostril surface of the CSP in the room model. This means that the air-flow pattern at the nostril (nesting plane) was used as a fixed breathing model and that this inflow/outflow boundary condition was shared with the analysis in the respiratory tract, and for the indoor environment around the CSP. Unsteady and non-uniform temperature and contaminant concentration were analyzed simultaneously, in accordance with the CSP simulation, and were two-way coupled between the CSP and the numerical airway model.

6. Results and discussion

The air-flow patterns around the CSP are shown in Fig. 13. The temperature and humidity distributions around the CSP are also shown in Fig. 13. The non-uniform distributions of temperature and humidity caused by the existence of the CSP, and the metabolic heat generation from the thermoregulation model integrated into the CSP, were confirmed. Figure 14 provides the simulation result of the CSP coupled with virtual airway analysis. Although the core temperature inside the human body was uniformly distributed, a non-uniform skin-surface temperature distribution was confirmed because of heterogeneous distributions of flow, temperature, and humidity around the human body. An especially strong non-uniformity of sensible and latent heat flux was observed around the head of the CSP. This was mainly caused by the transient flow, temperature, and humidity patterns in the breathing zone due to the unsteady breathing cycle model.

Figure 15 shows a time series of flow patterns in the vicinity of the breathing zone. The inhalation and exhalation modes of the respiration model integrated into the CSP were periodically changed and the flow pattern around the breathing zone also changed. Figure 16 shows the air velocity, temperature and humidity distribution inside the virtual airway (upper airway). The effect of the unsteady breathing cycle was clearly observed in the time-dependent changes of the flow, temperature, and humidity distribution. Moreover, the non-uniform distribution of the temperature and humidity was due to inhomogeneous distribution of velocity.

Figure 17 provides the distribution of contaminant concentrations around the CSP. Hypothetical contaminant generated in front of the head of the CSP was transported by convection and diffusion, and non-uniform contaminant concentration distributions around the CSP were formed in the target space. The concentration in this figure was normalized to the concentration of the generating source. In this case analyzed, relatively highly concentrated contaminant reached the breathing area and entered the CSP airway.

Figure 18 provides a time series of contaminant concentration distributions inside the Virtual Airway (upper airway) with the unsteady breathing cycle, and Fig. 19 shows a time series of contaminant-adsorption flux-distributions on the epithelium tissue surfaces inside the Virtual Airway.41) Time-dependent changes of the concentration distribution in respiratory tract were confirmed, under the effect of the unsteady breathing cycle. We observed increasing concentration and adsorption flux on epithelium tissue surfaces with contaminant inhalation when $t = 1–2s$, and decreasing concentration with contaminant exhalation when $t = 2–3s$. Clear, non-uniform, contaminant-concentration distributions in the respiratory tract were confirmed. In this analysis, contaminant adsorption flux distributions on the surface of epithelial tissue inside the respiratory tract, denoted tissue dose distributions. Hence, the highest region of adsorption flux represented the hot spot of inhalation exposure by way of the respiratory tract. Through the integrated numerical simulation of CFD and CSP, the precise concentration of the exposure-contaminant in the respiratory tract, taking into
account the non-uniformity of indoor environmental conditions, could be predicted. This integrated CFD-CSP numerical simulation will contribute to optimization of indoor environmental design to minimize the adverse health impact of indoor contaminants, and to maximize the thermal comfort of residents.

Figure 20 shows the representative simulation results of the time-averaged formaldehyde concentration profile inside the airway tissue, targeting the nasal cavity and nasopharynx, and these results denote the tissue dosimetry in the local domains within the respiratory tract. By applying CFD-CSP-
PBPK hybrid analysis for estimating the inhalation exposure of formaldehyde, it was revealed that over 96% of the formaldehyde adsorption flux was concentrated in the nasal cavity and nasopharynx. If the inhalation concentration of formaldehyde at the nostril was assumed to be 100 µg/m³ ($C_a$), the epithelial tissue surface concentration in the nasal cavity was estimated to be 690 µg/m³ ($C_t$). The formaldehyde concentration in the tissue was confirmed to be gradually decreased by saturable metabolic clearance, first order reaction, and blood perfusion inside the tissue.

7. Conclusions and implications

The purpose of ventilation is to provide and maintain acceptable indoor air quality by replacing
polluted air with fresh air. Not only to better maintain good indoor air quality, but also to save energy for ventilation, there is a need for indoor environmental design that considers imperfect mixing and the non-uniform distribution of airflow and contaminants in a room. To satisfy both trade-off requirements, numerical simulation in the design stage should be carried out using a computer-simulated person (CSP) as representative and sensor, to provide a locally controlled object within indoor environments of heterogeneous quality.

In this paper, we introduced the outline of a comprehensive CSP (i.e., an \textit{in silico} human model), for indoor environmental design, and aimed to provide demonstration examples of integrated simulation of indoor environmental quality and its

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\textbf{Fig. 17.} Distribution of contaminant concentration around CSP ($y = 1.5\, \text{m}$, Concentration of generation point $= 1.0$).

\textbf{Fig. 18.} Time series of contaminant concentration distributions inside Virtual Airway (in case of contaminant generation point $\#5$, one breathing cycle).

\textbf{Fig. 19.} Contaminant adsorption flux distribution on the epithelium tissue surfaces inside Virtual Airway.
We also presented a method of analyzing contaminant exposure using a comprehensive CSP model. We found that applying an unsteady breathing cycle, and non-uniform contaminant concentration distribution in the indoor space, could affect the analysis result of the contaminant exposure. Furthermore, we demonstrated some simulation results of a CFD-CSP-PBPK hybrid analysis for estimating inhalation exposure of formaldehyde.

Generally, a universal CFD code is used for unstructured mesh design. Therefore, in consideration of the increased calculation load, the comprehensive and universal Computer Simulated Person is hereby made available for use in various research fields. Moreover, the CSP could be applied as an environment estimation tool for exposure analysis of indoor air quality. With the development of accurate evaluation methods for indoor spaces, the analysis target is moving from indoor scale to personal scale. Our results demonstrate that it is possible to apply analysis methods using CSP to estimate environmental design at a personal scale.

Understanding the exposure to airborne gas-phase and aerosol-phase contaminants, and their effects on indoor occupants, is critical for identifying effective preventative measures to limit exposure and improve indoor air safety conditions. In this study, a comprehensive numerical prediction method was developed based on new mathematical models, for use in characterizing airborne contaminant exposure and deposition of contaminants during inhalation. An advanced integrated computational platform involving CFD and CSP modeling was developed for use in predicting the risks associated with airborne contaminant exposure. CFD simulation combined with CSP modeling is expected to be able to provide fundamental information about airborne contaminant dispersion in indoor environments and to reduce significantly occupational diseases and socio-economic burdens associated with poor indoor air quality.

As already stated, people spend the majority of their time in indoor environments, and hence the indoor air quality has a crucial impact on the health of residents. The precise design that optimizes the trade-off problem involving energy conservation, thermal comfort, and health will be of increasingly greater importance in indoor environments. The respiratory system is the principal interface between the human body and the indoor environment, and is a portal for various airborne contaminants in the indoor air. An important goal in research on the...
indoor environment is an enhanced understanding of the mechanisms responsible for human perception and physiological response to different exposures. In predicting inhalation exposure risk, CSP is useful as a surrogate for biological bodies (in vivo). There are many restrictions on using real human subjects (i.e., conducting in vivo experiments) in this type of research. An important advantage of CSP modeling is that no ethical restrictions apply to CSP use (i.e., conducting in vitro experiments). In future research, this CSP model will be applied to analysis of inhalation toxicology, inhalation exposure, and development of drug delivery systems (DDS) by way of respiratory traces within the human body. The development of the CSP model is also expected to offer potential for making significant contributions to research in a wide range of engineering and medical science fields.

A computer simulation model should be validated by experimental data and/or theoretical solutions. Furthermore, the exact boundary conditions and suitable parameter settings are critically important for precise numerical simulations. CSP is not a technology in which everything is concluded on the computer; hence, the establishment of close cooperation with the medical field (i.e., in vivo and in vitro studies of human physiology) is important for its future development.

We believe that the Computer Simulated Person, in silico human models, have great potential for contributing to essential understanding of the interactions between the human body and surrounding indoor environment, in addition to in vivo and in vitro studies specifically about health.

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