Rai, A.C., Lin, C.-H., and Chen, Q. 2014. "Numerical modeling of VOC emissions from ozone reactions with human-worn clothing in an aircraft cabin," *HVAC&R Research*, 20(8), 922-931.

Numerical modeling of VOC emissions from ozone reactions with human-worn clothing in an aircraft cabin

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Abstract

Volatile organic compounds (VOCs) are indoor air pollutants with many adverse health effects for humans. Ozone reactions with human surfaces (skin, hair, and clothing) are an important source of VOCs in the indoor air, especially in aircraft cabins because of their typically high ozone concentrations and occupant densities. Therefore, it is important to study the ozone-initiated VOC emissions from ozone reactions with passengers in an aircraft cabin and assess their resulting exposure. This investigation developed empirical models for computing the emissions of several major VOCs, including acetone, 4-oxopentanal (4-OPA), nonanal, and decanal, from ozone reactions with human-worn clothing. The empirical models were used to compute the contributions of human surfaces to these VOCs in an aircraft cabin mockup under different environmental conditions. The computed results were then compared with the corresponding experimental data obtained in the mockup. The models can provide rough estimates of ozone-initiated VOC concentrations. The empirical models were integrated into a CFD analysis, and the results showed that the levels of ozone-initiated VOCs were significantly enhanced in the breathing zones of the passengers. Therefore, to accurately assess passenger exposure to VOCs, their concentrations in the breathing zones should be used.

1. Introduction

Volatile organic compounds (VOCs) are an important class of indoor air pollutants. Exposure to VOCs has been associated with adverse health effects that include irritation of the eyes, nose, and throat; headaches; nausea; drowsiness; damage to the central nervous system; and even cancer (Jones, 1999; Mølhave, 1991). These compounds are emitted as gases from a variety of indoor materials such as paints, furniture, and building supplies, and these emissions are known as primary VOC emissions (Brown et al., 1994; Kostiainen, 1995). Another important source of VOCs in the indoor air are the gaseous and surface reactions of ozone with different indoor materials, which produce secondary VOC emissions. For example, Reiss et al. (1995) studied ozone reactions with interior latex paint in a tube flow reactor and found secondary carbonyl emissions. Morrison and Nazaroff (2000, 2002) investigated ozone reactions with carpets in an environmental chamber and found secondary emissions of saturated and unsaturated aldehydes. Those ozone-initiated VOC emissions are known to be particularly important in aircraft cabins because of the typically high ozone levels encountered in flights (Bhangar et al., 2008; Spengler et al., 2004; Weisel et al., 2013). Some researchers (Tamás et al., 2006; Weschler et al., 2007; Wisthaler et al., 2005) studied the ozone-initiated reactive chemistry

in an aircraft cabin mockup through a series of experiments. They concluded that humans themselves constitute the primary site for ozone-initiated chemistry, and occupants were found to be responsible for the generation of most of the VOCs identified in the cabin. Another investigation by Coleman et al. (2008) studied ozone reactions with samples of aircraft materials and clothing fabrics through controlled experiments in an environmental chamber. They also concluded that occupant clothing was the dominant contributor to ozone removal and VOC emissions under typical aircraft cabin conditions.

In additional to these experimental studies, several investigations have developed models for studying secondary VOC emissions. For example, Rim et al. (2009) developed a CFD model to study the chemical reactions of ozone with human surfaces, and the ensuing VOC emissions. They found that ozone is depleted and VOCs are enriched in the breathing zone of occupants, and they concluded that bulk air measurements might not accurately assess exposure to ozone and its initiated VOCs. Another recent investigation by Weisel et al. (2013) measured VOCs on 52 U.S. transcontinental or international flights and developed linear regression models based on the log transformed mean ozone concentration, percent occupancy, and plane type. Their models were able to explain 18–25% of the variance in concentrations of carbonyls. However, none of the published modeling investigations have accounted for the impact of environmental factors on secondary VOC emissions. Factors such as ozone concentration, humidity, and air change rate can have a big impact on ozone-initiated VOC emissions from human clothing (Coleman et al., 2008; Rai et al., 2014).

Therefore, this investigation developed models for computing secondary VOC emissions from ozone reactions with human-worn clothing on the basis of prevailing environmental conditions. Our objective was to compute the concentrations of common byproducts of ozone/human reactions in an aircraft cabin mockup, such as acetone, 4-oxopentanal (4-OPA), nonanal, and decanal. Our study also integrated the models into CFD to compute the ozone-initiated VOC concentrations in the breathing zones of passengers in an occupied airliner cabin mockup.

2. Research Method

To develop a suitable method for computing the secondary VOC emissions from ozone reactions with human-worn clothing, this investigation used measurements of emissions from soiled cotton T-shirts. Rai et al. (2014) conducted the measurements in an environmental chamber. The experimental method is briefly summarized here, and more details can be found in their paper. Figure 1 shows a schematic of the medium-scale environmental chamber with dimensions of 1.8 m × 1.7 m × 1.7 m. A steel box with dimensions of 0.2 m × 0.4 m × 1.2 m was placed in the center of the chamber. The box was used as a human simulator by maintaining its temperature at 31±1 °C and stretching a cotton T-shirt over it. The T-shirt was soiled with skin-oils by a human subject who slept in it, and it was the primary site for ozone reactions in the chamber. The chamber was ventilated with outdoor air enriched with ozone, which reacted with the T-shirt to generate secondary VOC emissions. The secondary emissions were measured under different ozone concentrations, relative humidity levels, air change rates, and degrees of soiling, in order to systematically study the impact of these conditions on ozone-initiated VOC emissions.

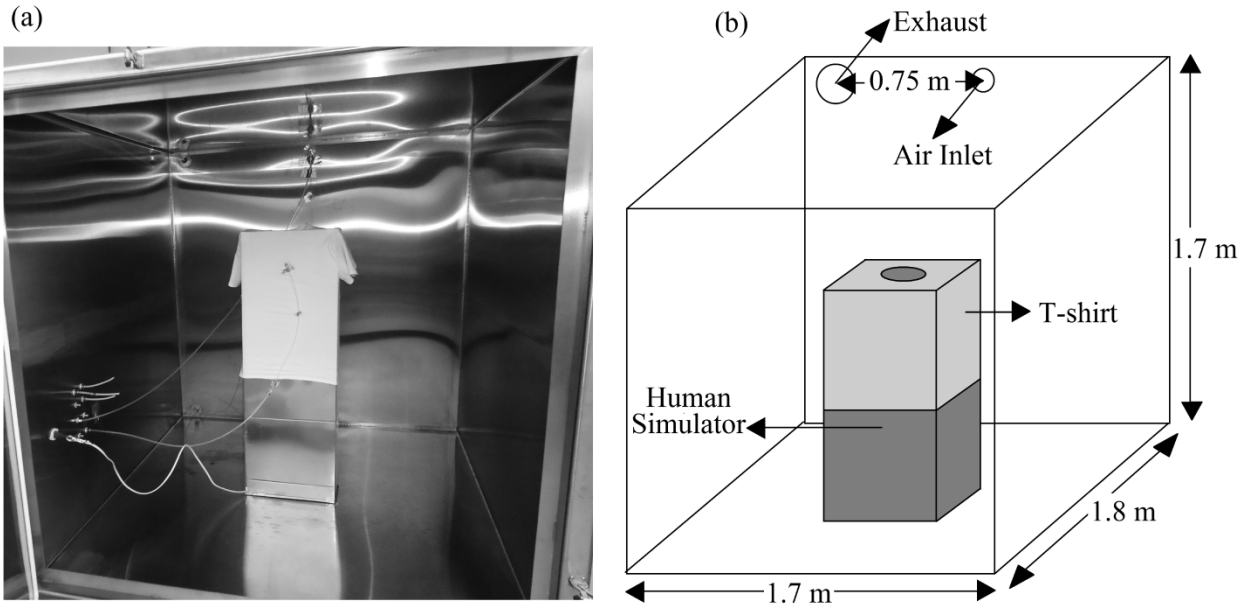

Fig. 1. Photograph and schematic of the environmental chamber used to study ozone reactions with a T-shirt on a human simulator.

The ozone concentration was monitored with a photometric ozone analyzer (Model 202, 2B Technology), which has a precision equal to the greater of 1.5 ppb or 2% of the reading. The air samples were collected on Tenax® TA filled tubes and DNPH (2, 4-Dinitrophenylhydrazine) cartridges using a sampling pump at the exhaust. The Tenax® TA samples were collected in duplicates at a sampling airflow rate of 100 ml/min for 2 hours (i.e., with a sampling volume of 12 L). These duplicate samples were analyzed by thermal desorption gas chromatography-mass spectrometry (TD-GC/MS) for nonanal, decanal, and 4-oxopentanal (4-OPA) according to ASTM-D6196 (American Society of Test and Materials, 2009a). The DNPH samples were collected at an airflow rate of 500 ml/min for 2.5 hours (i.e., with a sampling volume of 75 L), extracted with acetonitrile, and analyzed by high performance liquid chromatography (HPLC) for acetone as specified in ASTM-D5197 (American Society of Test and Materials, 2009b).

To compute the secondary VOC emissions from surface reactions of ozone, we used the molar yield equation (Weschler et al., 2007), which calculates VOC emissions directly from ozone consumption as follows:

$$J_{VOCi} = Y_i J_{ozone} \quad (1)$$

where J_{VOCi} and J_{ozone} are the molar fluxes of VOCi (i^{th} VOC) and ozone, respectively, on a particular surface; and Y_i is the molar yield of VOCi for that surface.

In the above equation, J_{ozone} can be computed as the product of the bulk air ozone concentration (C) and the measured/estimated ozone deposition velocity (v_d) for the surface, under the assumption of well-mixed conditions (Cano-Ruiz et al., 1993). Alternatively, J_{ozone} can be obtained by CFD analysis, which does not require the well-mixed assumption (Rai and Chen, 2012). We used the CFD analysis to obtain J_{ozone}. However, Y_i is generally unknown, and it depends on the environmental conditions under which ozone reacts with soiled clothing (Rai et al., 2014). Thus, it was reasonable to search for empirical equations connecting VOC yields to the environmental conditions for reactions with clothing. The equations can then be used to compute VOC yields and eventually their secondary emissions from Eq. (1). The procedure for determining these equations is discussed in the following subsection.

2.1 Selection of empirical equations

This investigation developed empirical equations for computing the yields of several major VOCs generated from ozone reactions with human-worn clothing based on the prevailing environmental conditions. The equations were developed from the chamber experiments discussed previously. From the experimental cases, we chose the ones that had been conducted with soiled T-shirts (a total of 12 cases) because human-worn clothing would normally be soiled with skin-oils. The chamber conditions for these cases are given in Table 1. Cases 1–10 were designed to systematically study the impact of ozone concentration, relative humidity, air change rate, and the soiling degree of the T-shirt by typically using Case 1 as the reference case and varying one factor at a time. For example, in Case 2 the ozone concentration was very large in comparison with that in Case 1, but the other conditions were roughly similar between the two cases. Therefore, by comparing the secondary VOC emissions in Cases 1 and 2, we were able to identify the influence of ozone concentration on secondary emissions. Similarly, Case 3 was used to identify the impact of humidity on secondary emissions. Cases 4–6 focused on the soiling degree of the T-shirt, and Cases 7 and 8 on the air change rate. Cases 9 and 10 simulated building conditions on a “poor air quality day” (a day with reasonably high indoor ozone concentration). The final two cases duplicated the conditions in Cases 1 and 7 in order to verify the repeatability of the results.

Table 1.
The experimental conditions in the chamber used for studying ozone reactions with clothing.

Case	Exhaust ozone concentration (ppb)	Relative humidity (%)	Hours the T-shirt was worn (h)	Air change rate (h^{-1})
1	40	12	6	0.5
2	148	20	6	0.5
3	54	44	6	0.5
4	70	23	2	0.5
5	57	24	12	0.5
6	53	27	6 hours by a different human subject	0.5
7	48	10	6	2.7
8	133	11	6	2.7
9	22	28	6	0.5
10	24	49	6	0.5
1D	44	11	6	0.5
7D	51	11	6	2.7

By analyzing the cases given in Table 1, Rai et al. (2014) found that air change rate (ACR), relative humidity (RH), and ozone concentration (C) were the major factors that influenced VOC yields. Therefore, we chose these factors as predictor variables for developing empirical equations connecting the VOC yields to the environmental conditions.

Among the predictors, humidity and ozone were used as continuous variables with linear (RH and C) and quadratic (RH^2 and C^2) terms because we had a range of conditions for these variables. ACR was used a dummy variable, and its value was set to zero or one for low or high ventilation conditions, respectively. We used ACR as a dummy variable because it was conjectured that ACR indirectly affected the yields of some VOCs by changing the airflow features and their resulting convective mass transport. For the cases given in Table 1, air change rates of 0.5 h^{-1} and 2.7 h^{-1} were used as low and high ventilation rates, respectively. Another possible approach to account for the influence of airflow features on VOC yields would be to use the friction velocity (u*) as a predictor variable, which would account for the effects of indoor airflow intensity at the reaction surface. Such an approach was used by Lai and Nazaroff (2000) to characterize the influence of airflow features on particle deposition. However, this approach requires the value of u*, which is very difficult to determine by either measurement or computation.

After the predictor variables had been selected, the yields of the major ozone-initiated VOCs were regressed on all the different linear combinations of these five variables (ACR, RH, RH^2, C, and C^2) for the 12 cases by using the SAS (Statistical Analysis System) statistical package. The resulting regression models (31 in total) were then categorized according to their

complexity (i.e., the number of predictor variables). From each of these categories, the best model was identified as the one with the largest value of R^2_{adj} (adjusted R^2). Figure 2 shows the relationship between R^2_{adj} and the number of predictors for each VOC, along with the models that were finally selected. The finally selected models were the ones having a relatively large value of R^2_{adj} together with least complexity.

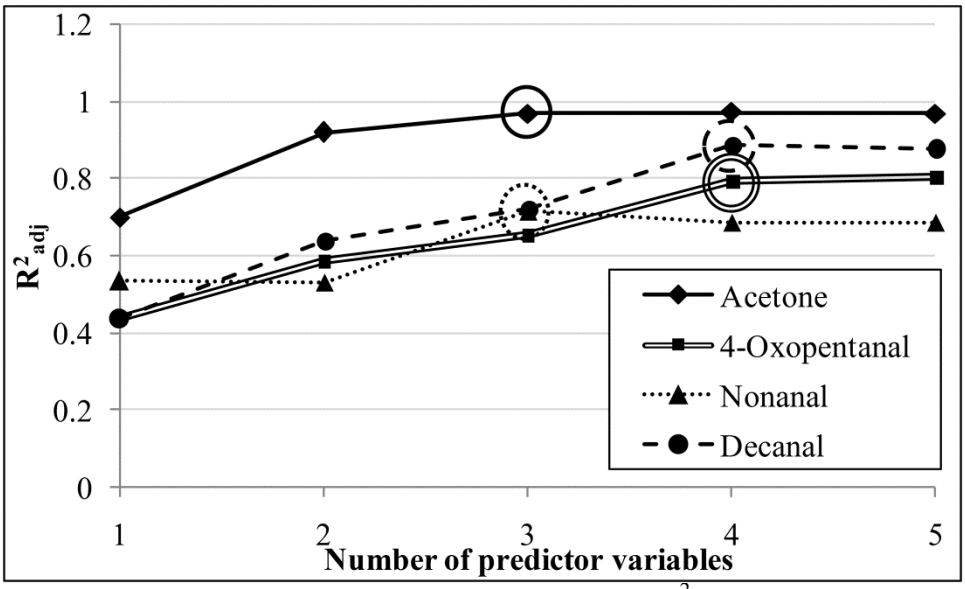

Fig. 2. Model selections for the different VOCs based on the R^2_{adj} criterion. The circles identify the final model selections.

The selected regressions models are as follows:

$$Y_{ace} = 1.85\times10^{-1} + 1.35\times10^{-1}\,ACR - 2.45\times10^{-3}\,C + 9.72\times10^{-6}\,C^2 \quad (2)$$

$$Y_{4\text{-}OPA} = -3.71?\ \ 0^{-2} + 3.94\times10^{-2}\,ACR + 1.14\times10^{-2}\,RH - 3.49\times10^{-4}\,C - 1.61\times10^{-4}\,RH^2 \quad (3)$$

$$Y_{non} = -4.32\times10^{-2} + 2.52\times10^{-3}\,RH + 2.25\times10^{-3}\,C - 1.16\times10^{-5}\,C^2 \quad (4)$$

$$Y_{dec} = ?\ \ .48\times10^{-1} + 1.53\times10^{-2}\,RH + 5.18\times10^{-3}\,C - 1.80\times10^{-4}\,RH^2 - 2.70\times10^{-5}\,C^2 \quad (5)$$

where Y_{ace}, $Y_{4\text{-}OPA}$, Y_{non}, and Y_{dec} are the molar yield of acetone, 4-OPA, nonanal, and decanal, respectively. Eqs. (2) to (5) are the models for estimating the secondary VOC emissions of acetone, 4-OPA, nonanal, and decanal, respectively, from ozone reactions with human-worn clothing. To use the above equations for computing VOC yields, the ozone concentration (C) must be inputted in ppb (on a molar basis). RH must be set to the value of the relative humidity without percentage. For example, if the relative humidity is 20%, the RH value must be set to 20. Finally, ACR value must be either zero or one depending on low or high ventilation conditions. It is recommended to use an ACR value of zero for buildings since they usually have low ventilation rates, and a value of one for high ventilation settings such as airliner cabins.

It should also be noted that the above equations for computing the yields of different VOCs are different despite the fact that the VOCs are essentially generated from the ozone reactions with human-worn clothing. These differences arise because the reactants and reaction mechanisms involved in generating these VOCs may be different. For example, nonanal and decanal are anticipated to be the reaction byproducts of ozone with the cotton fabric; whereas, acetone and 4-OPA were probably generated from ozone reactions with skin-oils (Rai et al., 2014).

The computed VOC emissions can then be incorporated into a simple mass balance analysis or used to provide boundary conditions for CFD analysis. The mass balance analysis can be used to estimate the contributions of human-worn clothing to bulk air concentrations of the VOCs, whereas the CFD analysis can provide a wealth of information about the concentration distributions. The next two subsections describe the mass balance and CFD modeling techniques, respectively; and a step-by-step description of the overall modeling procedure is illustrated in Figure 3.

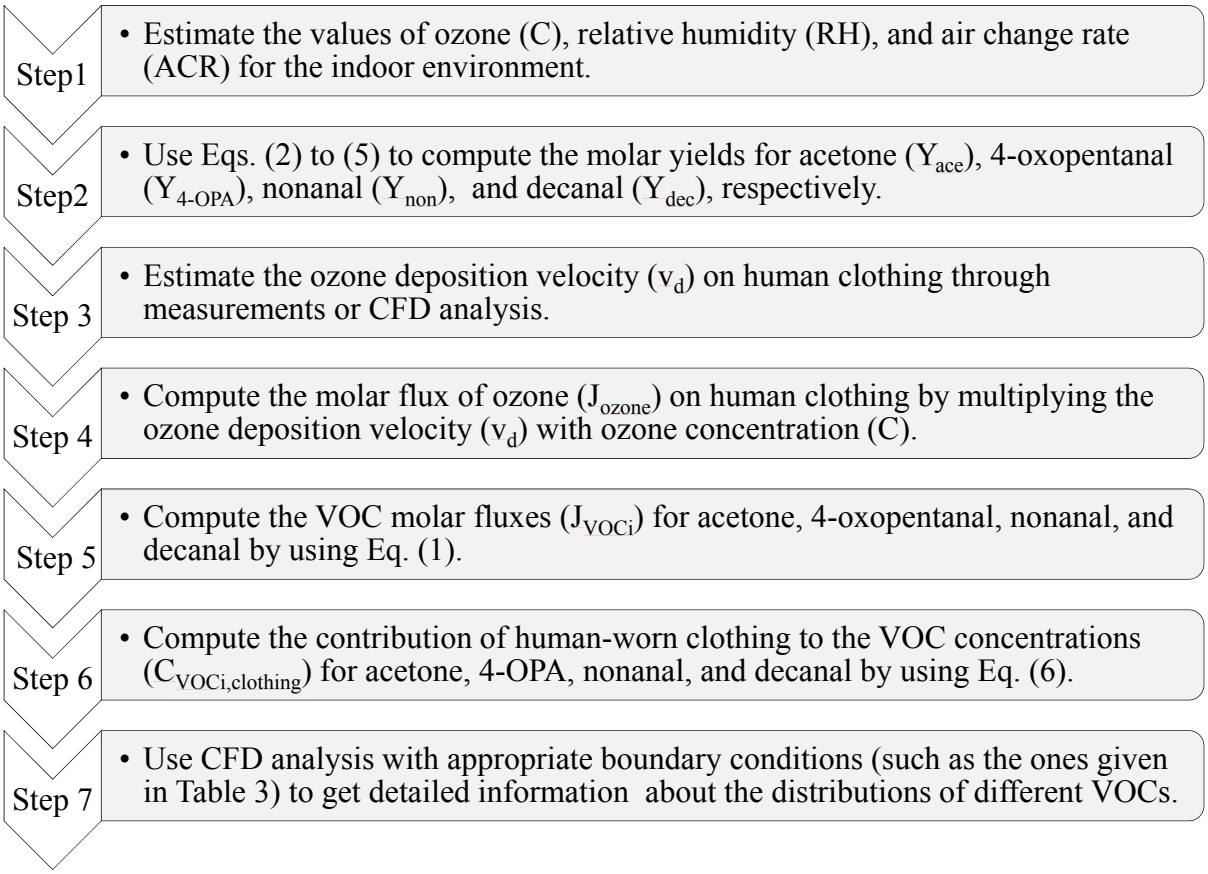

Fig. 3. A step-by-step description of the overall modeling procedure to compute ozone-initiated VOC emissions from ozone reactions with human-worn clothing.

2.2 Mass balance model

A simple mass balance can be used to compute the contributions of human-worn clothing to ozone-initiated VOCs indoors under the assumption of well-mixed conditions, as follows:

$$C_{VOCi,clothing} = \frac{J_{VOCi}.A_{clothing}}{V\lambda_v} \quad (6)$$

where $C_{VOCi,clothing}$ is the contribution of clothing to the concentration of VOCi, $A_{clothing}$ the clothing area, V the volume of the air in the indoor space, and λ_v the outdoor air change rate.

2.3 CFD model

If the air in a room cannot be assumed to be well mixed, CFD should be used to compute the velocity, temperature, ozone, and VOC distributions. This investigation solved the Reynolds-averaged Navier-Stokes equations for turbulenct flow in indoor spaces with the Re-Normalization Group (RNG) k-ε turbulence model (Yakhot and Orszag, 1986). The model can effectively predict the turbulent features of airflow in an aircraft cabin (Zhang et al., 2009). The ozone and VOC distributions were obtained by solving the corresponding species transport equations. For example, the transport equations for VOC_i take the following form:

$$\nabla.(\rho\vec{u}C_{VOCi}) = \nabla.((\rho D_{VOCi} + \frac{\mu_t}{Sc_t})\nabla C_{VOCi}) \quad (7)$$

where ρ is the air density, $\vec{u}$ the air velocity vector, C_{VOCi} the concentration of VOCi, D_{VOCi} the binary diffusion coefficient of VOCi in air, μ_t the turbulent viscosity, and Sc_t the turbulent Schmidt number. These equations were solved by the use of commercial CFD software FLUENT (FLUENT, 2009).

3. Case Setup

This investigation used a mockup of a Boeing-767 with three rows of seats as shown in Figure 4. The cabin was 4.9 m wide, 3.2 m long, and 2.0 m high in the center, with a total volume of 28.5 m^3. The cabin air was supplied by two overhead inlets and extracted by two outlets near the floor along the longitudinal direction. This mockup was used by some researchers for quantifying the ozone-initiated VOC emissions from different surfaces by adding them one at a time (Weschler et al., 2007; Wisthaler et al., 2005). For example, they first measured ozone-initiated VOC emissions in an empty cabin with carpet and seats only. Next, they stretched soiled T-shirts on the seat backs and repeated the VOC measurements. Finally, they conducted experiments with passengers in the cabin mockup. These arrangements enabled them to quantify the contributions to ozone-initiated VOC emissions from individual cabin surfaces, such as carpet and seats, soiled T-shirts, and passengers.

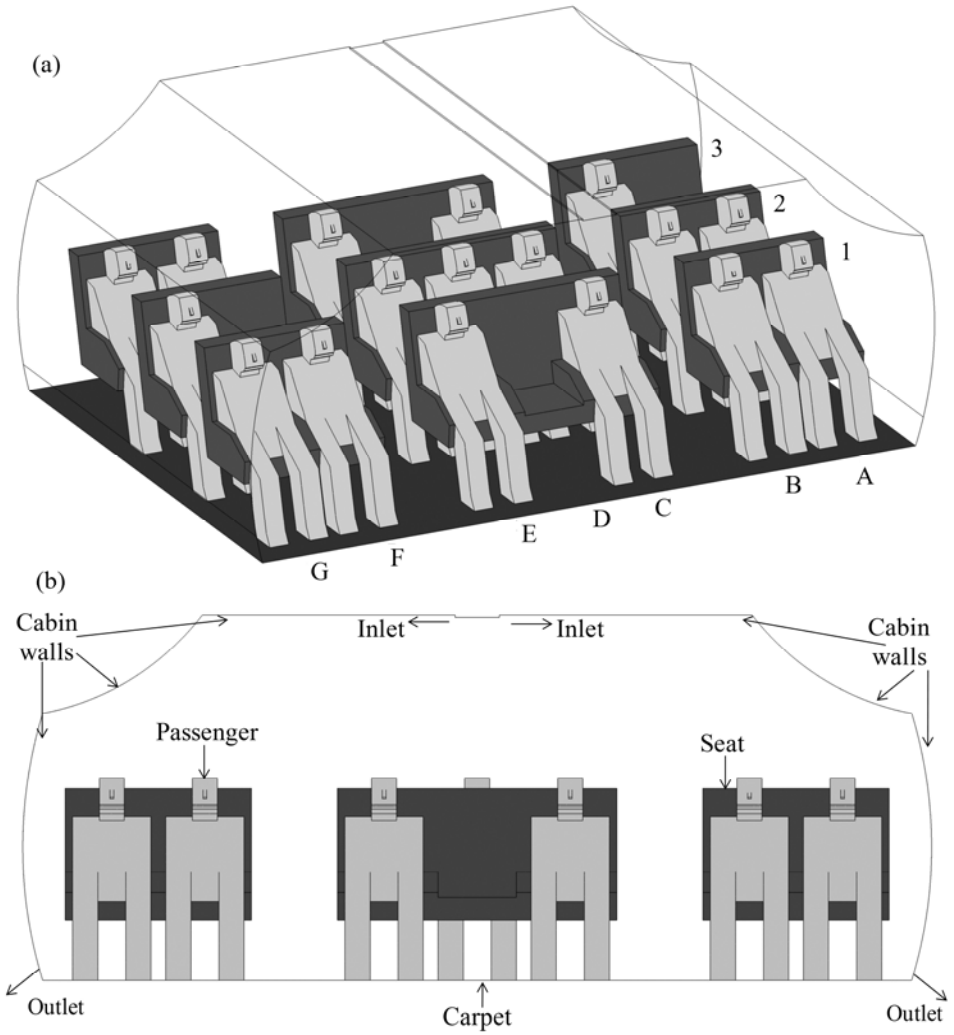

Fig. 4. The occupied cabin setup for Cases 2 and C: (a) the schematic of the case and (b) the boundary surfaces in the cabin mockup.

Because one of our aims was to evaluate our model's performance in computing the secondary VOC emissions from human surfaces, we studied those cases that contained human-worn clothing or passengers, as given in Table 2. The environmental conditions for these cases are also summarized in Table 2. Case A was conducted with soiled T-shirts stretched on seat backs as surrogates for humans, whereas Cases B and C were conducted with real human subjects.

Table 2.
Description of the three cases used for studying ozone-initiated VOC emissions in a cabin mockup.

Case	Description	Ozone reaction surfaces	Average cabin ozone (ppb)	Relative humidity (%)	Air change rate (h^{-1})	
					Outdoor	Recirculated
A	Cabin with seats and T-shirts	Carpet, seats, and T-shirts	66	6.8	3.0	20.0
B	Occupied cabin	Carpet, seats, and passengers	75	10	8.8	12.2
C	Occupied cabin	Carpet, seats, and passengers	62	20	4.4	16.6

We have previously reported and validated detailed CFD modeling techniques for computing airflow, temperature, and ozone distributions in an identical occupied cabin mockup, but with a slightly higher air change rate (Rai and Chen, 2012). Therefore, in the current study we used similar meshing and solution techniques. The mesh consisted of 2.43 million elements with tetrahedral elements used for the bulk volume, and layers of extruded triangular prisms created on ozone reactive surfaces. The prism elements were used near the ozone reactive surfaces to accurately capture the boundary layer flow and ozone deposition. The y^+ values were kept very small (~5) near the ozone reactive surfaces, as required by the ozone deposition model (Sørensen and Weschler, 2002).

Table 3 presents the boundary conditions for ozone and different VOCs in the CFD model. The inlet ozone concentration was unknown, and a value for this concentration was assumed in order to obtain the correct cabin ozone concentrations as measured in Cases B and C. Correct concentrations in the cabin were essential for computing the flux of ozone (J_{ozone}) at reaction surfaces. The inlet VOC concentrations were calculated from those in the recirculated air because a portion of the exhaust air was recirculated. The outdoor air was assumed to have no VOCs. The VOC emissions from the cabin walls were assumed to be zero, and those from the carpet and seats were estimated from the measurements of Wisthaler et al. (2005), as the sum of both primary and secondary emissions. The primary VOC emissions from the human surfaces (clothing, skin, and hair) were neglected in accordance with the experimental measurements of Weschler et al. (2007). It was further assumed that all human surfaces had the same secondary emissions as the soiled cotton T-shirts, which were estimated from Eqs. (2)–(5). Because acetone is also present in human breath as a result of metabolic processes (Fenske and Paulson, 1999), this study set its flux at the nose of occupants on the basis of experimental estimates of Weschler et al. (2007).

Table 3.
The ozone and VOC boundary conditions used for this study.

Surfaces	Ozone	4-OPA, nonanal, and decanal	Acetone
Inlet	Case specific	Case specific	Case specific
Cabin walls	Zero flux	Zero flux	Zero flux
Carpet and Seats	Deposition model (Sørensen and Weschler, 2002)	Flux estimated from measurements	Flux estimated from measurements
Human surfaces (skin, hair, and clothing)	Zero concentration	Flux calculated with Eqs. (3), (4), and (5), respectively	Flux calculated with Eq. (2)
Passenger's nose	Zero concentration	Flux calculated with Eqs. (3), (4), and (5), respectively	Flux estimated from measurements
Outlets	Outflow	Outflow	Outflow

4. Results

The following subsections present (1) the comparisons between our model predictions and the corresponding experimental data for the three cases shown in Table 2, and (2) the results obtained by conducting CFD analysis for the occupied cabin cases.

4.1 VOC emissions

Case A was designed to study the contributions of the soiled T-shirts to ozone-initiated VOC emissions. In this case the VOC emissions were mainly composed of primary and secondary emissions from the carpet and seats plus secondary emissions from the soiled T-shirts (Wisthaler et al., 2005). The contributions of cabin surfaces (carpet and seats) to VOCs (both primary and secondary) were isolated by means of another experiment performed in the same cabin mockup without T-shirts. It should then have been possible to estimate the contribution of the T-shirts to the overall concentration of VOCi in the cabin by simply subtracting the contribution of the cabin surfaces from the total VOCi concentration measured in Case A. It should be noted, however, that because the T-shirts were stretched on the seat backs in Case A, about 55% of the seat surface was unavailable for VOC emissions. As a result, the VOCi emissions from the seats in Case A were probably 55% lower than in the similar case conducted without T-shirts. The above correction was incorporated in order to obtain the "measured" contributions of soiled T-shirts to the different VOCs in Case A.

Figure 5 shows the contributions of the soiled T-shirts to the concentrations of different VOCs as computed by the mass balance model and their corresponding "measured" data for Case A. The computed concentration of 4-OPA agreed well with the measurement. However, acetone, nonanal, and decanal concentrations were considerably over-predicted by the model.

The discrepancies between the model predictions and the measurements were caused primarily by the following factors. The regression models used to compute yields were developed on the basis of cotton T-shirts soiled by the same human subject in all but one of the cases, which means that the effects of fabric and of soiling by different human subjects could not be captured. The use of cotton T-shirts meant that VOC emissions were overestimated because soiled cotton fabric seems to have higher secondary emissions than the soiled wool or polyester fabrics, as demonstrated by Coleman et al. (2008). The measured relative humidity in the mockup was 6.8%, which was outside the humidity range (10%–49% RH) used to develop the model. When the above factors are taken into account, the model's performance does not seem to be poor.

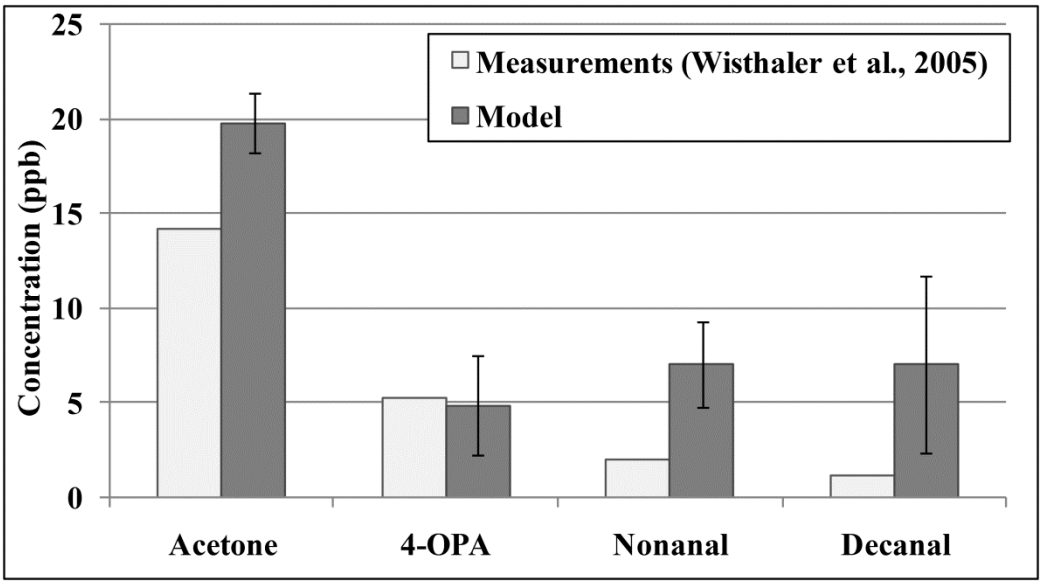

Fig. 5. Ozone-initiated VOCs from reactions with soiled T-shirts: comparisons of the predicted and measured data for Case A. (The measurement errors are unknown, and the model error bars represent the 95% confidence intervals.)

We also used the mass balance model to compute secondary VOC emissions from ozone/human-surface reactions in the occupied cabin mockup under high and low outdoor air change rate conditions (Cases B and C, respectively). As in Case A, the contributions of human surfaces were estimated from measurements by taking into account the portion of the seat backs that was covered by the passengers and unavailable for VOC emissions.

Figure 6 compares the computed contributions of ozone/human-surface reactions to VOC concentrations in the mockup with their corresponding experimental estimates at an air change rate of 8.8 h^{-1}. The computed VOC concentrations were higher than the measured data, especially for decanal. These discrepancies can be attributed to modeling deficiencies, as discussed above for Case A. In addition, different passengers in the cabin can be expected to have different secondary VOC emissions because of differences in clothing, skin-oil composition, and usage of terpene-containing personal care products (such as perfumes and other fragrances). However, incorporating those details was beyond the scope of the current investigation.

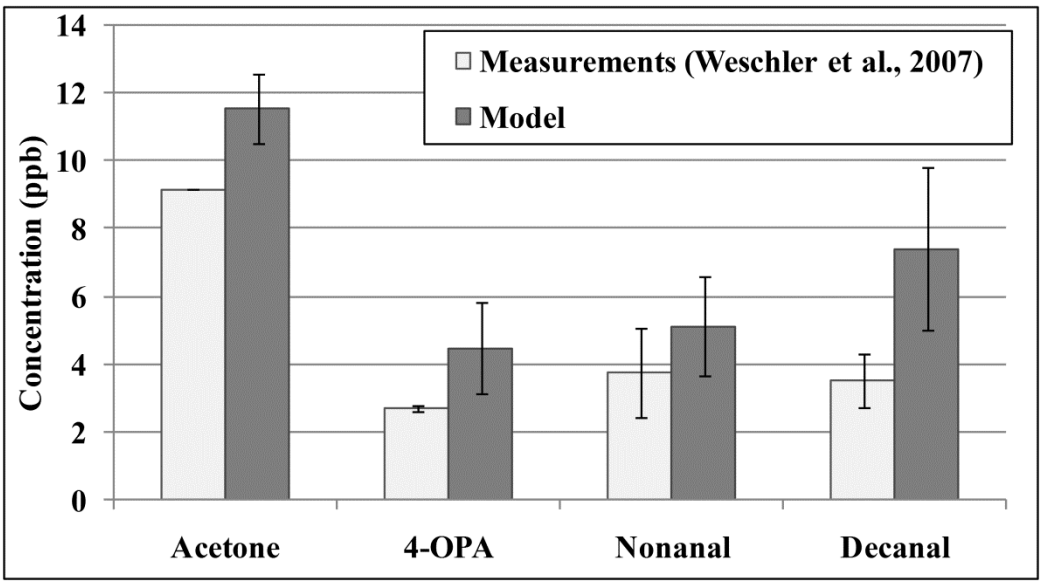

Fig. 6. Ozone-initiated VOCs from reactions with human surfaces: comparisons of the predicted and measured data for Case B. (The measurement error bars represent the range, and the model error bars represent the 95% confidence intervals.)

Figure 7 compares the contributions of human surfaces to the different VOCs in the cabin for Case C. The "measured" and predicted contributions of human surfaces to different VOCs in the cabin were higher in Case C than in Case B. Case B was conducted at 10% relative humidity, whereas in Case C the relative humidity was 20%. The VOC emission models (Eqs. (2) – (5)) are sensitive to changes in humidity, and they predicted a large increase in VOC emissions with increased humidity. A similar conclusion was obtained by Coleman et al. (2008) for laundered cotton fabrics. In reality, an increase in relative humidity may not have a significant influence on the secondary emissions from other clothing fabrics. Unfortunately, there is no information available in the literature that could be used to verify our hypothesis.

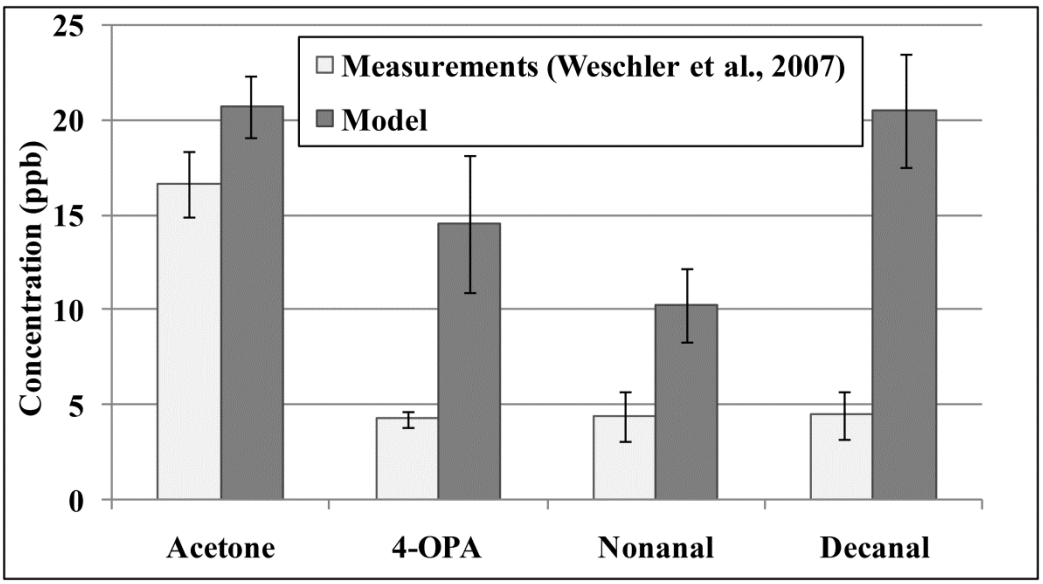

Fig. 7. Ozone-initiated VOCs from reactions with human-surfaces: comparisons of the predicted and measured data for Case C. (The measurement error bars represent the range, and the model error bars represent the 95% confidence intervals.)

4.2 Distributions of different VOCs in the cabin mockup

The previous subsections described modeling results for the concentrations of ozone-initiated VOCs from reactions with human surfaces under the assumption of well-mixed conditions. However, the well-mixed assumption might not be suitable because ozone/clothing reactions occur in rising thermal plumes, and the VOCs are expected to be enriched in the breathing zone. Hence, the actual exposure of passengers to VOCs could be higher than that calculated from a simple mass balance analysis under the well-mixed assumption. By using CFD modeling of VOC distributions, we can determine their concentrations in the breathing zone and make better risk assessments.

Figure 8 shows the distribution of 4-OPA normalized by its exhaust concentration along the longitudinal plane through the center of the cabin in Case B. It can be seen that 4-OPA was enriched in the breathing zone of the occupant. The normalized distributions of nonanal and decanal were similar to the distribution of 4-OPA, and those compounds were also enhanced in the breathing zone. The distribution of acetone was qualitatively similar to that of OPA, but its concentration was much higher near the breathing zone since it was also emitted in human breath.

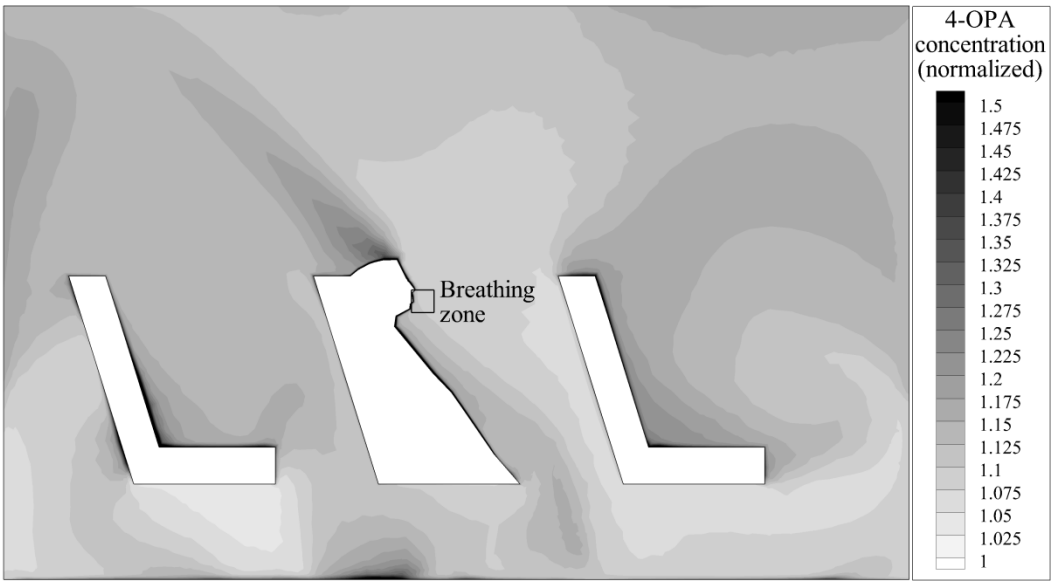

Fig. 8. The 4-OPA distribution in the longitudinal section through the center of the occupied cabin mockup with an outdoor air change rate of 8.8 h^{-1} for Case B.

The normalized 4-OPA distribution in Case C was qualitatively similar to that in Case B, as shown in Figure 9. The normalized concentration in Case C was significantly lower than in Case B. This difference occurred because the exhaust concentration in Case C was much higher than that in Case B as a result of the lower outdoor air change rate, which was used for normalization.

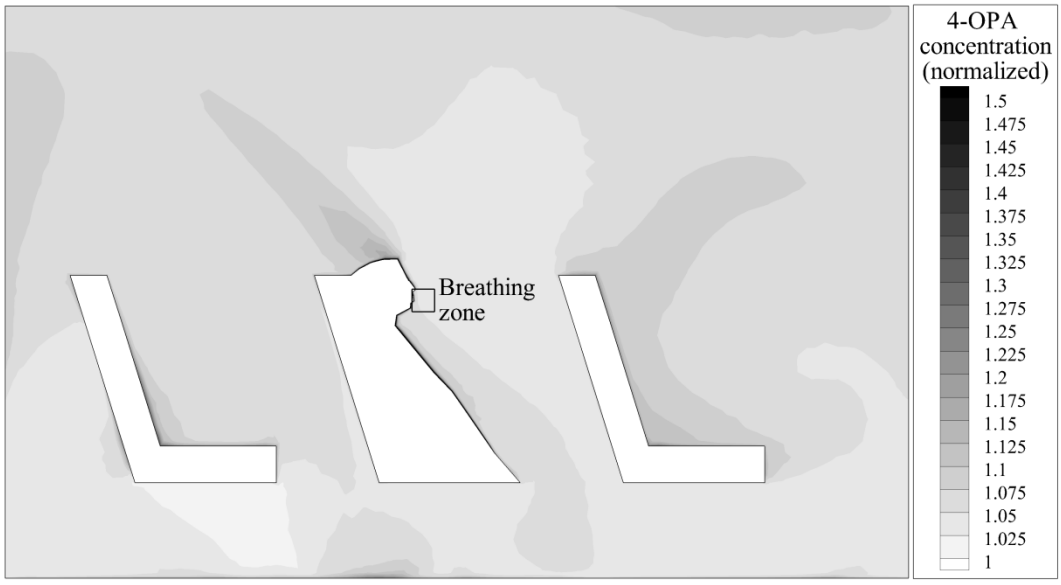

Fig. 9. The 4-OPA distribution in the longitudinal section through the center of the occupied cabin mockup with an outdoor air change rate of 4.4 h^{-1} for Case C.

To quantify the enhancement of VOC concentrations in the breathing zone, this investigation computed the VOC ratio (r_{VOCi}), which was defined as the VOC concentration in

the breathing zone divided by its exhaust concentration. Figure 10 shows the r_{VOCi} for the different VOCs under the two air change rates for the middle row in the cabin mockup. The $r_{acetone}$, $r_{4\text{-}OPA}$, $r_{nonanal}$, and $r_{decanal}$ were 1.51±0.18, 1.22±0.05, 1.22±0.06, and 1.21±0.05, respectively, in Case B; and 1.26±0.10, 1.11±0.03, 1.11±0.03, and 1.10±0.03, respectively, in Case C. The r_{VOCi} values were higher in Case B than in Case C because the exhaust concentrations were much lower in Case B as a result of the higher air change rate. The $r_{acetone}$ was much higher than $r_{4\text{-}OPA}$, $r_{nonanal}$, and $r_{decanal}$ because acetone is also present in human breath and was consequently enriched in the breathing zone, as discussed previously.

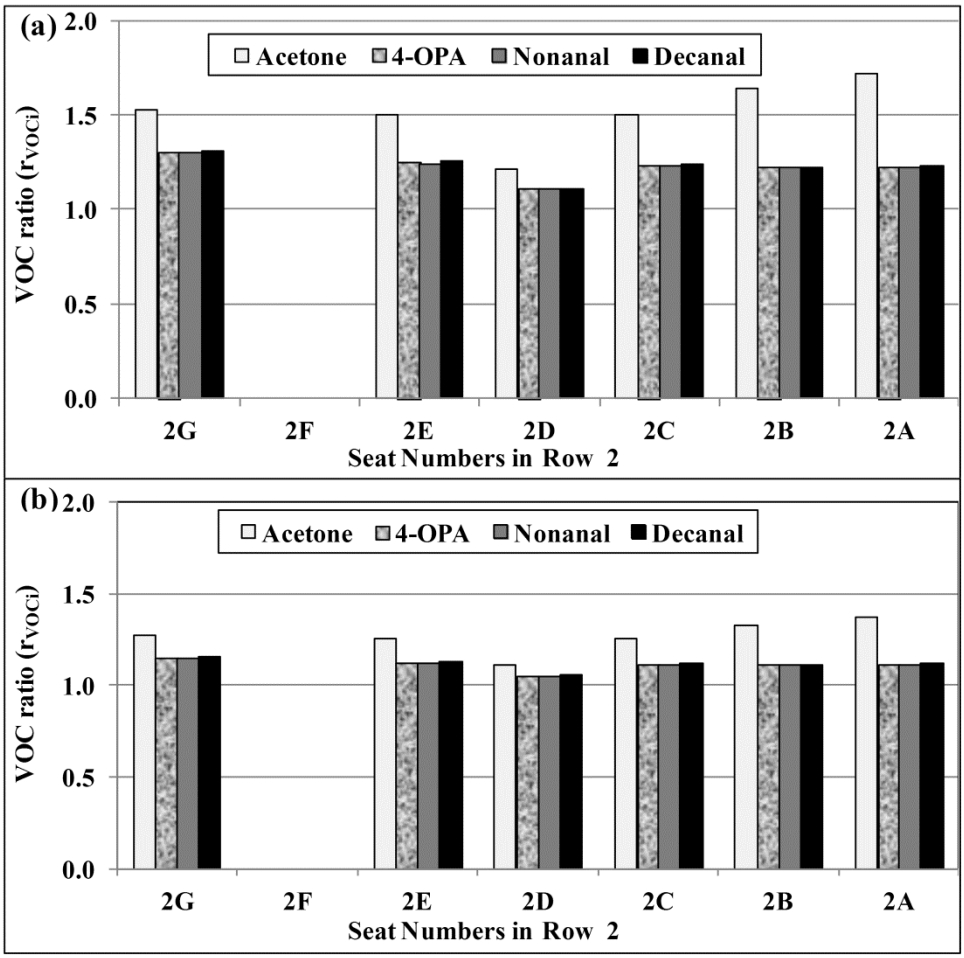

Fig. 10. VOC ratio for different passengers seated in the middle row of the occupied cabin mockup under an outdoor air change rate of (a) 8.8 h^{-1} (Case B) and (b) 4.4 h^{-1} (Case C).

Our results are qualitatively similar to those obtained by Rim et al. (2009), who also used CFD to evaluate exposure to ozone and its initiated byproducts associated with human surfaces in a ventilated room; however, there exist quantitative differences. Rim et al. (2009) found that the r_{VOCi} ranged from 2.9–6.0 for air change rates between 8.8–17.6 h^{-1} using ceiling air supply. However, our results showed that the r_{VOCi} ranged from 1.10–1.51 at an air change rate of 21 h^{-1} (sum of fresh and recirculated air change rates) in an aircraft cabin. These differences exist possibly because of differences in airflow distributions between a room and an aircraft cabin environment.

Overall, the ozone-initiated VOCs were found to be significantly enhanced in the breathing zones as compared with their corresponding exhaust concentrations, and thus the exhaust air measurements would have underestimated the inhalation dosage of the passengers. Hence, to accurately estimate passengers' exposure to such VOCs, their concentrations in the breathing zones should be used instead of those at the exhausts.

5. Discussion

This investigation demonstrated a method for estimating the contributions of human surfaces to the concentrations of several ozone-initiated VOCs in an aircraft cabin mockup. The method developed is a general one, and it can be extended to compute secondary emissions from a variety of materials under given indoor conditions. The model development shows that experimental data obtained through chamber measurements constitutes the most important component of the model. The experimental dataset used in our investigation was rather small (only 12 cases), and it did not address the effects of clothing fabric or variations in soiling from different human subjects. These limitations were the major reasons for the discrepancies that were observed between the model predictions and experimental data. The model's performance and scope may be enhanced by conducting additional experiments with different types of indoor surfaces under a wide range of conditions. Nevertheless, the model is useful for estimating concentrations of ozone-initiated VOCs in indoor spaces.

6. Conclusions

This investigation studied ozone-initiated secondary emissions of acetone, 4-oxopentanal (4-OPA), nonanal, and decanal from reactions with human-worn clothing in an aircraft cabin mockup. The study was conducted by developing empirical models to compute the secondary VOC emissions from the prevailing environmental conditions (such as ozone concentration, humidity, and air change rate) based on experiments conducted in an environmental chamber.

These models were then used to compute the contributions of human surfaces (skin, hair, and clothing) to the ozone-initiated VOCs in an aircraft cabin mockup. The model predictions showed very good trends qualitatively, but with quantitative discrepancies when compared with the corresponding experimental data obtained in the mockup. A major reason for the discrepancies is that a limited dataset from the chamber was used for developing the model. Nevertheless, the models are promising and can be improved with more experimental data.

When the VOC emission models were integrated into a CFD model, much higher concentrations of the various VOCs were identified in the breathing zone of the passengers than in the mockup exhausts. The reason for this difference is that the VOC concentrations are not uniform, and the ozone/human-surface reactions occurring in the thermal plumes from passengers can enhance their concentrations. Therefore, it is more accurate to assess the passengers' exposure risk by using the concentrations of the ozone-initiated VOCs in the breathing zone than those in the exhausts.

Acknowledgements

This study was partially supported by the National Basic Research Program of China (the 973 Program) through Grant No. 2012CB720100 and the Center for Cabin Air Reformative Environment (CARE) at Tianjin University, China. This investigation was also partially funded by the U.S. Federal Aviation Administration (FAA) Office of Aerospace Medicine through the National Air Transportation Center of Excellence for Research in the Intermodal Transport Environment at Purdue University under Cooperative Agreement 10-C-RITE-PU. Although the FAA sponsored this project, it neither endorses nor rejects the findings of the research. This information is presented in the interest of invoking comments from the technical community about the results and conclusions of the research.

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