Building and Environment 94 (2015) 12–20

Contents lists available at ScienceDirect

Building and Environment

journal homepage: www.elsevier.com/locate/buildenv

Estimation of the contribution of human skin and ozone reaction to volatile organic compounds (VOC) concentration in aircraft cabins

Kai Gao, Jiarong Xie, Xudong Yang*

Department of Building Science, Tsinghua University, Beijing 100084, PR China

ARTICLE INFO

Article history:
Received 8 May 2015
Received in revised form
18 July 2015
Accepted 20 July 2015
Available online 22 July 2015

Keywords:
Aircraft cabin
Volatile organic compounds (VOC)
Contribution
Ozonization
Human skin

ABSTRACT

The products derived from ozonolysis of organic compounds on the human skin may be an important source of volatile organic compounds (VOC) in aircraft cabins. This study aims to estimate the contribution of human skin and ozone reaction to VOC concentrations in aircraft cabins. Based on the measurements of ozone and VOC concentrations in five flights in March 2013, we estimated the contribution of human skin and ozone reaction to VOC concentration using the first-order kinetic formula. The results show that the prominent volatile products derived from ozonolysis contribution differed from each other, largely due to the difference of the O_3 concentrations among different flights. The results of sensitivity analysis show that the disturbance from substrate had evident effect on contribution from products of the squalene and ozone reaction, and the disturbance from substrate had little effect on the contribution from products of the linoleic acid and ozone reaction.

1. Introduction

The aircraft cabin environment is different from other indoor environments such as buildings in many respects. In aircraft cabin, people encounter a combination of environmental factors that include low humidity, reduced air pressure, and potential exposure to multiple air contaminants, such as ozone (O_3), particulate matters, volatile organic compounds (VOC), and biological agents [1–5]. Under the closed environment of cabin air, passengers are exposed to an ozone environment of low concentrations, which has been reported to be harmful for respiratory tract and cardiovascular system [6–9]. Recent investigations in a simulated aircraft cabin have shown that humans are significant sinks of ozone. Rai and Chen [10] simulated the ozone distribution in aircraft cabin by computational fluid dynamics (CFD), and found the ozone removal rate, deposition velocity, retention ratio, and breathing zone levels were well predicted in those cases. The CFD model predicted that the ozone concentration in breathing zone was 77–99% of the average cabin ozone concentration. This is a consequence of skin lipids that react with ozone to generate characteristic oxidation products. In the cabin, the human body is an important way for ozone removal [11–13]. Many researchers have studied indoor surface reactions, and identified gaseous and surface products. Related investigations have observed reactions between ozone and skin lipids on human hair [14] and on soiled clothing fabrics [15]. Collectively these studies benefited from earlier work by Fruekilde et al. [16], who demonstrated that ozone reacted with human skin lipids to produce acetone, 6-methyl-5-hepten-2-one (6-MHO), geranyl acetone, hexanal and nonanal, and that squalene, linoleic acid (LA) and oleic acid (OA) were the major precursors for these oxidation products [17,18]. Squalene-ozone surface reaction rates and products as well as heterogeneous reaction rates between ozone and linoleic acid or oleic acid thin film were investigated in earlier studies [17–19].

On-board measurements have also been taken in the aircraft cabin to obtain the actual levels of various air pollutants. Weisel et al. measured ozone and carbonyl compounds on 52 transcontinental U.S. or international flights between 2008 and 2010 [20]. Hexanal, heptanal, octanal, nonanal, decanal, and 6-MHO were detected at sub-to low ppb levels (<3 ppb). Guan et al. measured VOC types and concentrations in 107 randomly selected commercial flights from August 2010 to August 2013 [21]. A detection rate of 70% for hexanal, 53% for 6-MHO, above 90% for acetone, acetic acid, decanal and nonanal was found. 6-MHO, acetone and nonanal were on the target VOC list of cabin air based on Guan's report [22]. However, reporting the concentration data alone is not sufficient to determine VOC characteristics in aircraft cabins and identify possible emission sources. Ozone initiated

* Corresponding author.
E-mail address: xyang@tsinghua.edu.cn (X. Yang).

http://dx.doi.org/10.1016/j.buildenv.2015.07.022

reactions in the cabin may be an important source of VOC. Studies focusing on investigating the contribution of human and ozone reaction to VOC concentration in aircraft cabins could help to understand the nature of this important in-cabin pollutant source.

The objective of this study is to estimate the volatile products derived from ozonolysis of three components of human skin in aircraft cabins and how much they contribute to the aircraft cabin VOC concentrations. Five commercial flights were selected to test for the O_3 and VOC concentrations. The VOC concentration was estimated based on a VOC generation model with the measured concentrations of O_3 as input parameters. One possible application of this study result is the VOC source apportionment in the cabins. It could further provide guidance for actively control the gaseous pollutants in the cabins (e.g. by controlling the ozone concentrations) or reduce other emissions sources to meet the target concentration levels.

2. Experiments and methods

2.1. The VOC mass balance in the cabin and VOC produced by chemical reaction

The aircraft cabin is assumed to be a single zone or several zones divided by cabin classes (first, business, and economy), the air and VOC in each zone is completely mixed. Each zone is independently considered with its own model inputs, and no interactions are assumed between different zones.

Concentration of VOC in cabin air meets the mass balance of:

$$V\frac{dC_{I,j}}{dt} = C_{S,j}Q_j - C_{R,j}Q_j + E_{so,j} - E_{si,j} \tag{1}$$

where,

V: The volume of the cabin (m^3);
$C_{I,j}$: Concentration of one specific VOC in breathing zone air at time j ($\mu g/m^3$), j = 0 is assumed when the aircraft door is closed;
$C_{S,j}$: Concentration of the VOC in supply air at time j ($\mu g/m^3$);
$C_{R,j}$: Concentration of the VOC in re-circulated air at time j ($\mu g/m^3$);
Q_j: The total airflow rate at time j (m^3/s);
$E_{so,j}$: The emission rate of VOC source at time j ($\mu g/s$);
$E_{si,j}$: The sorption rate of VOC at time j ($\mu g/s$).

On the whole, the VOC sources in cabin can be divided into various categories, such as human, material, service, chemical reaction, bleed air, etc. Here we separate the chemical reaction item with all others, thus the $E_{so,j}$ item can be written as:

$$E_{so,j} = E_{ch,j} + E_{ot,j} \tag{2}$$

where,

$E_{ch,j}$: The equivalent VOC emission rate (the production rate of VOC) of chemical reaction at time j ($\mu g/s$);
$E_{ot,j}$: The emission rate of other sources except for chemical reaction at time j ($\mu g/s$).

According to our previous study [23], VOC sorption by carpet and seating can be neglected during the flight due to high air change rate in the cabin, i.e. $E_{si,j} = 0$.

With Equations (1) and (2) and $E_{si,j} = 0$, we have:

$$V\frac{dC_{I,j}}{dt} = C_{S,j}Q_j - C_{R,j}Q_j + E_{ch,j} + E_{ot,j} \tag{3}$$

Under the fully mixing condition, VOC concentration in re-circulated air is equal to concentration in breathing zone air, thus $C_{R,j} = C_{I,j}$. Equation (3) can be written as:

$$V\frac{dC_{I,j}}{dt} = C_{S,j}Q_j - C_{I,j}Q_j + E_{ch,j} + E_{ot,j} \tag{4}$$

By discretizing Equation (4) with a time step, the VOC concentration at time j is written as:

$$V\frac{dC_{I,j}}{dt} = C_{S,j}Q_j - C_{I,j}Q_j + E_{ch,j} + E_{ot,j} \tag{5}$$

where,

Δt is time step used in discretization (s).

The VOC concentration caused by chemical reaction, $C_{ch,j}$ ($\mu g/m^3$), is:

$$C_{ch,j} = E_{ch,j-1}\frac{\Delta t}{V} \tag{6}$$

The contribution rate of ozone reaction with human skin component to VOC concentration in aircraft cabin, X_j, is defined as the following:

$$X_j = \frac{C_{ch,j}}{C_{I,j}} \tag{7}$$

The measured VOC concentration in aircraft cabin C_j can be viewed as the mean of $C_{I,j}$ within certain time period.

We assume $\Delta t = 10s$ in Equation (5), the general concentration rate in the sampling period can be obtained by Equation (8),

$$X = \frac{\sum_{i=1}^{n} \frac{E_{ch,j-1+i}\times\Delta t}{V}}{n \times C_j} \tag{8}$$

where n is the result of sampling time divided by Δt, here n = 30.

The loss rate of skin constituents due to ozonization $d[sk]_s/dt$ can be described by Equation (9).

$$\frac{d[sk]_s}{dt} = -k[O_3]_s[sk]_s \tag{9}$$

where,

$[sk]_s$: The surface concentration of lipids on human skin, mol/m^2;
$[O_3]_s$: The surface concentration of ozone, mol/m^2;
k: The second-order surface rate constant, $m^2 \cdot mol^{-1} \cdot s^{-1}$;
t: The time interval, s.

Assuming $k_1 = k[O_3]_s$, in excess ozone the rate law can be written as pseudo-first-order with respect to skin by Equation (10):

$$\frac{d[sk]_s}{dt} = -k_1[sk]_s \tag{10}$$

where,

k_1: The pseudo-first-order reaction rate constant, s^{-1}.

Given that the loss rate of lipids of human skin is equal to the formation rate of products [19], which is the equivalent VOC emission rate that can be obtained from Equation (11):