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Concentration characteristics of ozone and product for indoor occupant surface chemical reaction under displacement ventilation

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ABSTRACT

Indoor chemical reaction occurring between ozone (O_3) and occupant surfaces (skin, hair, and clothing) is an important source of volatile organic compounds (VOCs) in the indoor air. This kind of chemical reaction can bring obvious impact on indoor air quality (IAQ) and building occupant health. Theoretical model describing indoor occupant surface chemical reaction between O_3 and Squalene, heat and mass transfer was established and verified by indoor environment experiment in this present study. Meanwhile, in order to obtain variation characteristics of ozone and product concentration in typical indoor space, four kinds of factors were taken into account and their influence on occupant surface chemical reaction under displacement ventilation was analyzed by means of numerical simulation, including air exchange rate (ACH), ozone concentration in supplied air, squalene concentration on occupant surface, chemical reaction rate. The results show that the rising of ACH is one favorite method for reducing the exposure concentration of product (secondary pollutant) under displacement ventilation. Moreover, as to ventilation system design and its commissioning, it's very necessary to reduce ozone concentration in supplied air by reasonable measures. In addition, lower squalene concentration on occupant surface and chemical reaction rate are very meaningful for improving IAQ during ventilation process.

1. Introduction

It is well known that outdoor air pollution and ventilation system pollution are two important factors influencing the supplied air quality, e.g. containing high ozone concentration, which may induce indoor ozone (O_3) concentration to increase. Meanwhile, rise of indoor ozone (O_3) concentration can induce chemical reaction, e.g. that occurring on occupant surfaces (skin, hair and clothing), which may significantly alter concentration of both reactants and products [1,2]. Moreover, the products, namely secondary air pollutants are often are more irritating than their precursors, which is secondary pollution emerging, shown in Fig. 1. For example, squalene is the most abundant unsaturated compound in human sebum and the major scavenger of ozone at the interface between room air and the human envelope. The reaction probability with squalene is 5×10^{-4} to 2×10^{-3}. Squalene of double bonds can be cleaved by ozone in the course of producing the volatile products, e.g. dicarbonyls, one of respiratory irritants [3]. Actually, mortality and morbidity associated with ambient ozone may be due, in part, to exposure to indoor ozone and its byproducts [4]. Therefore, indoor chemical reaction is one significant factor affecting air quality, which may further bring influence on occupants' health and comfort.

How to describe indoor chemical reaction accurately is one issue focused in the field of indoor air quality (IAQ). Özkaynak et al. established chemical reaction model by area method to predict indoor pollutant concentration [5]. Nazaroff and Cass put forward general chemical reaction model and adopted pseudo steady state approximation (PSSA) [6]. Weschler and Helen established single zone mass balance model based on fully mixed assumption and analyzed indoor single molecule and bimolecular reactions [7]. However, in order to overcome the limitation of single zone mass balance model, Dragou and Sorensen (2002) tried to analyze indoor chemical reaction process by computational fluid dynamics (CFD) [8,9]. Golam et al. (2002) analyzed indoor chemical reaction of OH radical and presented indoor chemical and exposed model (ICEM) [10]. In addition, as to city residential chemical reaction of the UK, Carslaw proposed chemical box model, which had been modified to include the degradation reactions of key indoor air pollutants [11]. It can be found that the basic features or rules of indoor chemical reaction may be obtain from the above models, but the chemical reaction process coupled with surface reaction needs to be quantified. Actually, indoor chemical reaction is impacted by reactant and product

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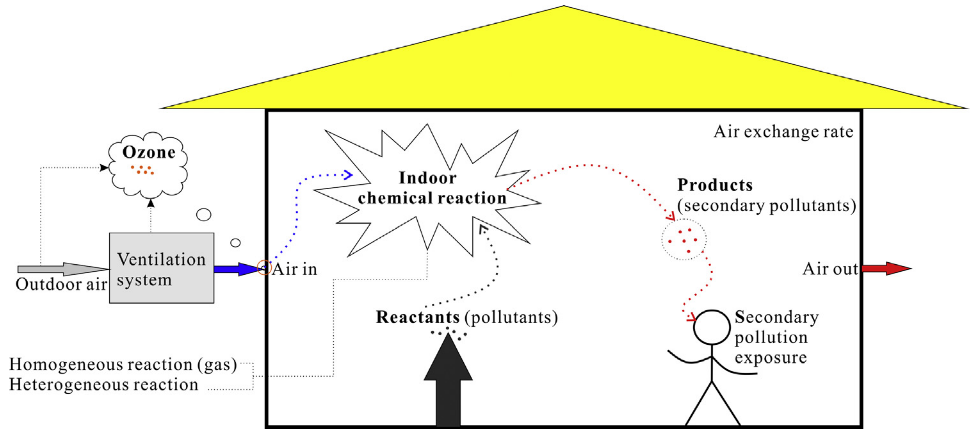

Fig. 1. Indoor chemical reaction induced by ozone.

concentration, their residence time and ventilation conditions. In the description of indoor chemical reaction, momentum and mass transfer should be considered in its theoretical model.

For another thing, as to the all types of indoor chemical reaction, ozone reaction with occupant surface is typical one, which has been proved to exist universally in indoor space. Wisthaler used proton-transfer-reaction mass spectrometry (PTR–MS) to examine the products formed when ozone reacted with soiled T-shirts in a simulated aircraft cabin, found squalene oxidation products (acetone, 4-oxopentanal, and 6-methyl-5-hepten-2-one) [12]. Tamas et al. found people were responsible for almost 60% of the ozone removal occurring within the simulated aircraft and recirculation system [13]. Weschler et al. found one anticipates production of acetone, nonanal, decanal, 6-MHO, geranyl acetone, and 4-OPA, whenever human beings and ozone were simultaneously present [14]. Corsi et al. gave a proof of personal reactive clouds assessment based on reaction rates between ozone and five reactive organic compounds that were found in personal care products [15]. Pandrangi and Morrison quantified the cumulative ozone uptake, the ozone reaction probability and product yields of volatile aldehydes and ketones for human scalp hair [16]. Rim et al. found that breathing zone ozone levels could be substantially lower and ozone reaction products associated with human surfaces (ORPHS) levels considerably higher than room levels [17]. Nazaroff and Weschler found ozone reacted rapidly with skin lipids present on the exposed skin, hair and clothing of the cabin occupants. Meanwhile, ozone-initiated chemistry produced a series of carbonyls, di-carbonyls and hydroxyl-carbonyls [18]. Moreover, Wisthaler et al. had used proton transfer reaction-mass spectrometry (PTR-MS) for direct air analysis of volatile products resulting from the reactions of ozone with human skin lipids. Detected products included mono- and bi-functional compounds containing carbonyl, carboxyl, or α-hydroxy ketone groups [19]. In order to compute the emissions of several major volatile organic compounds from ozone reactions with human-worn clothing, Rai et al. established empirical models to determine the contributions of human surfaces to these volatile organic compounds in an aircraft cabin mockup under different environmental conditions. The results indicated that the levels of ozone-initiated volatile organic compounds were significantly enhanced in the breathing zones of the passengers [20]. In addition, as to the reaction probability, Pandrangi and Morrison determined the cumulative ozone uptake, the ozone reaction probability and product yields of volatile aldehydes and ketones for human scalp hair [21]. The mean values of integrated ozone uptake, initial and final follicle reaction probability values for eight washed and unwashed samples were $5.1 \pm 4.4\,\mu molO^3\,g^{-1}$, $(13 \pm 8) \times 10^{-5}$, $(1.0 \pm 1.3) \times 10^{-5}$, respectively. It can be found from the above studies that the pollution caused by ozone reaction with occupant surface can bring serious impact on indoor air quality, which should be focused and controlled.

As ventilation is applied to control this kind of pollution, concentration of ozone and product related with indoor occupant surface chemical reaction will vary with different factors, e.g. air exchange rate (ACH), ozone concentration in supplied air, squalene concentration in occupant surface, chemical reaction rate. Meanwhile, Displacement ventilation is a widely used type of ventilation and its supplied air with ozone is firstly flowing to human respiratory region, which may induce serious potential harm of second pollution emerging. For displacement ventilation, combined with established and verified theoretical model of indoor occupant surface chemical reaction and numerical simulation, the purpose of this present study is to determine the concentration variation characteristics of ozone and product related with indoor occupant surface chemical reaction, which may provide guide for lowering the harm of second pollution emerging by reasonable ventilation system design and commissioning.

2. Theoretical model of indoor occupant surface chemical reaction

Mass, momentum, turbulence and energy conservation of indoor air were taken into consideration under displacement ventilation conditions and occupant surface chemical reaction occurring. Meanwhile, the significant difference in temperature between bulk air and air layer near occupant surface can lead to natural convection, namely body force that acts throughout the volume of a body should be analyzed. Therefore, the buoyancy effects were applied to evaluate the above impact, which may bring buoyancy effects on turbulent dissipation rate (epsilon). For another hand, as to the region near to occupant surface, the influence of molecular viscosity on air flow was enhanced, namely low Reynolds number turbulence occurring. So there was low Reynolds number region in indoor air turbulent flow system. Accordingly, as to obvious difference between the Reynolds number (Re) in bulk air and that of air layer near occupant surface, the Low-Re k-ε model developed by Jones and Launder [22] was used to simulate turbulence flow in this case, which had many successful application in near wall flow. Therefore, the turbulence of air flow, heat and mass transfer through occupant surface were described by the Low-Re k-ε model and the buoyancy effects in this present study. The corresponding theoretical model of indoor air is as the following equation:

$$\frac{\partial}{\partial t}(\rho\phi) + \mathrm{div}(\rho U\phi) = \mathrm{div}(\Gamma_\phi \mathrm{grad}\phi) + S_\phi \quad (1)$$