Building and Environment 46 (2011) 711–718

Contents lists available at ScienceDirect

Building and Environment

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

# Coupled CFD analysis of size distributions on indoor secondary organic aerosol derived from ozone/limonene reactions

Kazuhide Ito [a,*], Hiroshi Harashima [b]

[a] Interdisciplinary Graduate School of Engineering Science, Kyushu University, 6-1 Kasuga-koen, Kasuga, Fukuoka 816-8580, Japan
[b] Obayashi Co. Ltd., Fukuoka, Japan

ARTICLE INFO

*Article history:*
Received 11 June 2010
Received in revised form
17 September 2010
Accepted 7 October 2010

*Keywords:*
Indoor environment
CFD
Chemical reaction
Secondary organic aerosol (SOA)

ABSTRACT

Recently, theoretical analysis and experiment have been initiated to investigate the generation of secondary organic aerosols (SOA) by chemical reactions in indoor air. In particular, it has been confirmed that SOA are generated by the reaction of ozone with various terpenoids. The overarching goal of this work was to better understand ozone, VOC (volatile organic compounds) and generated SOA distributions within rooms. We carried out cylindrical test chamber experiments to measure SOA generation from the chemical reaction of ozone and limonene and discussed numerical models to describe it. In this paper, we propose a method for predicting the particle size distribution of SOA generated by ozone and limonene chemical reactions in air. In particular, we discuss an analytical method that involves a sectional modeling approach governing equations of SOA. Although the changes in particle size distribution in a 40-section model were reproduced to a certain extent, rigorous modeling for the generation and growth of SOA and an increased number of sections are needed for improvement of prediction accuracy.

© 2010 Elsevier Ltd. All rights reserved.

## 1. Introduction

The quality problem regarding the overall indoor air environment is called IAQ (indoor air quality) and this area has been attracting increasing attention with the increasing health consciousness of residents. In the field of IAQ, it has been pointed out that a specific chemistry exists and causes various chemical reactions and intermediate products and final products are produced as results of chemical reactions. These products have the potential to exert far greater health and physiological effects than compounds prior to reactions [1,2]. In particular, it is confirmed that secondary organic aerosols (SOA) are generated by the reaction of ozone with various terpenoids and theoretical analysis and investigations have begun to evaluate that SOA are generated by chemical reactions in indoor air [3–8]. There is concern that SOA are a serious source of secondary pollution in indoor environments [9].

Many studies have reported associations with ozone-initiated chemistry and subsequent SOA generation in indoor environments. Weschler demonstrated that ozone chemistry produces various products which include primary and secondary ozonides, peroxyhemiacetals, $\alpha$-hydroxy ketones, and peroxyacyl nitrates. Secondary organic aerosols are important stable products resulting from chemical reaction with ozone. They are formed from low-vapor-pressure oxidation products that partition between the gas phase and the surface of pre-existing aerosols or nucleate to form new aerosols. The reaction of ozone with various terpenoids in indoor settings has been shown to contribute tens of $\mu g/m^3$ to the indoor concentration of sub-micron particles under appropriate conditions [9]. Nazaroff et al. analyzed and reported detailed SOA data from a series of small-chamber experiments in which terpene-rich vapors from household products were combined with ozone under conditions analogous to product use indoors [10–12].

Concerning the numerical prediction of SOA generation and subsequent particle size distribution/change in indoor environments, there are numerous factors that affect the transportation phenomena and reasonable models and numerical procedures to characterize these are needed.

We have already carried out cylindrical test chamber experiments to investigate SOA generation resulting from the chemical reaction of ozone and D-limonene in terpenoid chemical substances and have discussed numerical models to describe this phenomenon [13]. We have also reported the results of coupled CFD analysis of flow field and the concentration distributions of ozone and limonene [14].

In this study, we focus on the initial nucleation/generation of SOA and subsequent size distribution and discuss the analytical method by the sectional modeling approach. We also carry out sensitivity

* Corresponding author. Tel.: +81 92 583 7628; fax: +81 92 583 7627.
*E-mail address:* ito@kyudai.jp (K. Ito).

0360-1323/$ – see front matter © 2010 Elsevier Ltd. All rights reserved.
doi:10.1016/j.buildenv.2010.10.003