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Predicting Indoor Ozone and NOx Concentrations

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Summary: The purpose of this paper is to present a simple modeling of indoor chemistry involving outdoor ozone and nitrogen oxides and reactive compounds (mainly terpene and aldehydes) emitted indoors by selected building products. The model, designed with the FACSIMILE software, includes both ozone gas-phase chemistry and ozone surface chemistry on building products. Results of the model (ozone and nitrogen oxides indoor concentrations) are compared with results from a detailed field experiment conducted in the CSTB experimental house MARIA in July 2004. A satisfactory agreement between modeled and measured ozone and nitrogen oxides indoor concentrations is obtained.

Keywords: Indoor chemistry, modeling, ozone, NOx, building products

1 Introduction

The objective of this paper is to present a simple modeling of indoor chemistry involving outdoor ozone and nitrogen oxides (NOx) and target VOC and aldehyde compounds emitted indoors by selected building products. No specific indoor sources of ozone and NOx are considered. For this purpose, we used the FACSIMILE software which is frequently used for kinetic chemistry modeling. Recently, Pommer *et al.* [1] presented an experimental comparison of a kinetic model developed with the same software for the reaction of selected monoterpene with ozone and NOx occurring indoors.

2 Methods

The indoor chemistry model developed includes: 1) ozone and NOx gas-phase chemistry, 2) ozone and target volatile compounds chemistry, 3) ozone surface chemistry on three building products. Results from laboratory experiments of ozone reaction on three selected building products (carpet with SBR backing, pinewood board and polystyrene ceiling tiles) [2] are used as input data for the model. For each building products, we calculated the ozone adsorption rate, the formation yield of target aldehyde compounds and the reaction yield of target VOCs. Ozone reaction rates with target aldehyde compounds (formaldehyde, acetaldehyde, benzaldehyde, hexaldehyde) and with target VOCs (alpha-pinene, beta-pinene, limonene, terpinene, styrene) emitted by the building products, are taken from the literature. Outdoor ozone and NOx concentrations measured in July 2004 are also used as input data.

3 Results

The main results of the model (indoor concentrations of

ozone and NOx) are compared with experimental data collected during a 3 days detailed field experiment conducted in a test room of the CSTB experimental house MARIA in July 2004 [3]. During this experiment, the three selected products tested for their interactions with ozone were installed in the test room.

Figure 1 presents the comparison between modeled and measured indoor ozone concentrations. A good agreement is observed even if daytime modeled indoor ozone concentrations are slightly higher than measured concentrations. A good agreement between modeled and measured indoor concentrations is also observed for NOx.

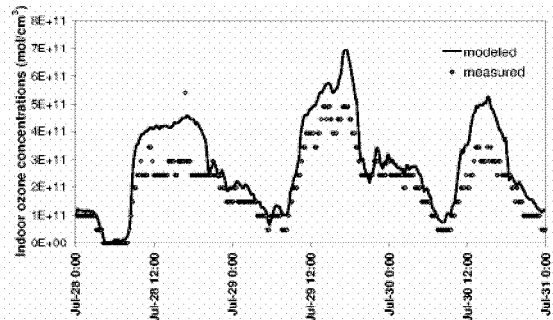


Fig. 1: Modeled and measured indoor ozone concentrations (mol/cm^3).

References

- [1] L. Pommer, J. Pick, C. Nilsson and B. Andersson. An experimental comparison of a kinetic model for the reaction of α -pinene and A3-carene with ozone and nitrogen oxides. *Indoor Air* 14 S8 (2004) 75-83. [2] M. Nicolas, O. Ramalho and F. Maupetit, Reactions between ozone and building products: Impact on primary and secondary emissions, *Proc. Indoor Air 2005*, pp. 2118-2122. [3] M. Nicolas, O. Ramalho and F. Maupetit, A preliminary field study of ozone chemistry, *Proc. Indoor Air 2005*, pp. 1739-1743.