Atmos. Chem. Phys. Discuss., 5, S682–S683, 2005
www.atmos-chem-phys.org/acpd/5/S682/
European Geosciences Union

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Evaluation of the pathways of tropospheric nitrophenol formation using a multiphase model" *by* M. A. J. Harrison et al.

Anonymous Referee #2

Received and published: 4 May 2005

Review of manuscript "Evaluation of the pathways of tropospheric nitrophenol formation using a multiphase model" by M.A.J. Harrison, M. R. Heal, and J. N. Cape

The article gives a possible interpretation of pathways of formation of nitrophenols in the troposphere. The model based on the CAPRAM 2.3 (Herrmann et al al., 1999, 2000) reaction scheme has been used to evaluate the contribution of gas and aqueous phase formation channels of mono-nitrophenols in the atmosphere. A simple model for the conversion of aromatic compounds has been implemented. In fact, the mechanism of formation of nitrophenols in the aqueous phase has been considered in the cur-

rent model through the consecutive reaction of NO3 and NO2 with phenol. However, different studies showed the possibility of alternative formation pathways such as the reaction initiated by OH radical followed by the addition of a molecule of NO2 (Barzaghi and Herrmann, 2002). The authors considered in the presented model the reaction of OH with phenol only as loss process. This assumption might have an effect on the observed aqueous phase concentrations. Recently, a review on nitrophenols in the atmosphere has been published (Harrison et al., 2005) and several other mechanisms of nitration in solution have been reported. The possible influence and impact on the product yields of nitrophenols predicted with this model should be discussed in view of the possible other source reactions. Further, to test the effect of the liquid phase on the production of nitrophenols the authors used two different scenarios where the products ratios were estimated on the basis that no literature values were available. However, several product studies have been published in the literature and different product ratios have been reported (Niessen et al., 1988; Machado and Boule, 1995; Barletta et al., 2002; Vione et al. 2001; Barzaghi and Herrmann, 2002) under different experimental conditions. Barzaghi and Herrmann (2002) obtained a ratio of 1:1 in the case of nitration driven by NO3 radical in presence of NO2. More realistic scenarios should be considered. The manuscript title should make clear that (i) only benzene and phenol are considered as aromatics and (ii) only radical nitrations are treated.

Recommendation: Publish after modification according to the above.

Interactive comment on Atmos. Chem. Phys. Discuss., 5, 1115, 2005.