Atmos. Chem. Phys. Discuss., 2, S391–S393, 2002
www.atmos-chem-phys.org/acpd/2/S391/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Modelling of the photooxidation of Toluene: conceptual ideas for validating detailed mechanisms" *by* V. Wagner et al.

Anonymous Referee #3

Received and published: 11 September 2002

General comments

The paper describes a computer simulation of the toluene photo-oxidation system, based on (known and speculative) reactions extracted from the MCMv3 Master Chemical Mechanism, and gives an overview of the status of toluene modelling. A comparison with available experimental (smog-chamber) studies allows the authors to detect the insufficiencies in the available chemical mechanism of this aromatic compound. The shortcomings are mainly due to the lack of information on some specific (toluene) reaction routes, which to date are still (very) speculative. In their model, OH production is far too low and the ozone concentration at the end of the experiment is over predicted.

The authors give a clear picture of what is needed concerning future research on aromatics and how important the interaction between experimentalists, modellers and theoreticians is.

The paper is well structured, and major findings are presented in a clear and concise way. Overall I find this is an excellent and useful piece of work.

Specific comments

a) The authors might still find important information in the theoretical publications by Tonachini's group (at present not considered in the manuscript). If so, any (new) relevant theory-validated reaction for the ring-opening route in benzene should be taken into consideration in this work, and analogous pathways developed for toluene implemented in TOL_MCM3a.

The references are the following:

Ghigo and Tonachini (1999), From benzene to muconaldehyde: investigation on some tropospheric oxidation channels, J. Am. Chem. Soc. 121, 8366-8372

and

Motta et al. (2002), Oxidative degradation of benzene in the troposphere. Theoretical mechanistic study of the formation of unsaturated dialdehydes and dialdehyde epoxides, J. Phys. Chem. A 106, 4411-4422.

b) Concerning Olario's private communication (page 1223): there is now a published paper for more specific referencing:

Olariu et al. (2002), FT-IR study of the ring-retaining products from the reaction of OH radicals with phenol, o-, m-, and p-cresol, Atmos. Environ. 36, 3685-3697.

Technical corrections

1. page 1220 line 3: delete hyphen in word "intermediates" 2. page 1221 line 5:

ACPD

2, S391–S393, 2002

Interactive Comment

NOx, put x in subscript 3. page 1222 line 5: delete space between hyphen and word "opening" in "ring-opening" 4. page 1224 line19: same as above for "nitro-aromatics", delete space after hyphen 5. page 1238 line 20: "...the system passes..." and not "the systems passes.."

Interactive comment on Atmos. Chem. Phys. Discuss., 2, 1217, 2002.