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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Kinetic double-layer model of aerosol surface chemistry and gas-particle interactions (K2-SURF): degradation of polycyclic aromatic hydrocarbons exposed to O_3, NO_2, H_2O, OH and NO_3" *by* M. Shiraiwa et al.

Anonymous Referee #1

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The paper under review presents a detailed model treatment of the degradation of PAHs on the surface of aerosol particles. It focuses on PAH exposed to O3, NO2, H2O, OH and NO3 and combines parallel and sequential surface reactions between different gas phase species and species on the particle surface.

The paper fits nicely within the scope of ACP. It provides an up-to-date compilation of recent experimental studies on PAH degradation for different substrates and illustrates how the Poeschl-Rudich-Amman framework can be applied to a specific reaction system. The paper could be improved by adjusting the environmental conditions, so that

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they reflect more typical ambient conditions. This applies in particular to the chosen RH and the NO2 mixing ratio. I recommend this paper for publication after the comments below are addressed.

Comments: 1. p. 18030, l 15: Steady state assumption for O3, H2O and NO2: It is not clear why the steady state assumption is applied to these three species but not for PAH and NO3. Please include a justification for making this assumption. Furthermore it is not clear if the steady state assumption is applied for the model calculations presented in section 4 (Fig. 6 and 8 look like steady state is not assumed). Please clarify this point.

2. p. 18037, line 1: Wet conditions of 25% RH: While 25% RH means that there is some water vapor present, this is still pretty dry for atmospheric conditions. I certainly would not consider this as "typical ambient conditions at night time", as it is stated in section 4.3.3. The paper would benefit from adjusting the environmental conditions to be more representative of ambient atmospheric conditions. I suggest to change the cases with 25% RH to, say, 60% RH.

3. Section 4.1, and Fig. 6: It would be helpful to add one sentence why the PAH degradation is different on the soot surface compared to the organic surface.

4. Section 4.3.1 and section 4.3.2: The NO2 mixing ratio of 500 ppb is very large for atmospheric conditions. It would be interesting to see the results for much lower but atmospherically relevant NO2 mixing ratios, e.g. 50 ppb.

5. Section 3.1.2, description of Fig. 4: What was [H2O]gs for these calculations?

6. In Fig. 8 only γO3 is shown. It would be interesting to include γNO2 as well.

Minor comments: p. 18027, l. 1 and 2: Units for Dg should be in SI units.

p. 18027, l. 4: Sentence should read: "The diffusion effect . . ."

p. 18033, l. 4: Omit "as".

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p. 18034, l. 25: Should read “on the order of 10-8”.

Fig. 1: I suggest adding [NO3]s to this schematic figure.

p. 18037, l. 27: Should read “shorter”.

Interactive comment on Atmos. Chem. Phys. Discuss., 9, 18021, 2009.