

## ***Interactive comment on “Modeling the possible role of iodine oxides in atmospheric new particle formation” by S. Pechtl et al.***

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The authors present interesting modelling results regarding the role of OIO homomolecular homogeneous nucleation in atmospheric new particle formation. This work compares the relative importance of homogeneous OIO versus the ternary H<sub>2</sub>SO<sub>4</sub>-NH<sub>3</sub>-H<sub>2</sub>O nucleation under a number of different case scenarios of relevance in clean marine and semi-polluted environments. It also provides further evidence for localised iodine coastal emissions as responsible for the observed particle bursts. This paper fits very well into the scope of ACP and I recommend publication after minor revisions.

Specific comments:

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- As a general comment, and given the general title “ role of iodine oxides in atmospheric new particle formation”, have the authors considered other possible channels, specifically that of IO + OIO to I<sub>2</sub>O<sub>3</sub> following recent evidence that the reaction occurs at a fast rate?. It would be desirable to make a sensitivity study on the possible contribution of this channel to the particle formation perhaps considering as a condensable unit or via further polymerization (i.e. to higher order iodine oxides) or subsequent oxidation by atmospheric O<sub>3</sub>.

- Also, the authors do not seem to have considered the kinetics of the OIO self-reaction in Table 1. This reaction has now been shown to occur relatively fast. Also, the thermal stability of the I<sub>2</sub>O<sub>4</sub> product and its possible role as a condensable vapour is not commented.

- The authors consider the branching ratio to OIO from the IO self-reaction to be equal or more than 80

- In their model runs the authors assume rather large mixing ratios of OIO, even a daytime. To the best of this referee’s knowledge, the molecule has never been reported to be measured during daytime above instrumental detection limits of around 4 pmol mol<sup>-1</sup>. Even assuming the ‘hot spot’ theory, model results show that it would not reach significant concentrations when considering the IO + OIO and OIO + OIO reactions. It would be desirable to introduce these reactions in the model to check whether significant particle formation rates are still obtained from the OIO homomolecular homogeneous nucleation and subsequent growth by condensable vapors such as OIO.

- Following the previous point, throughout the paper it is assumed that the daytime OIO mixing ratio is some 3 to 4 times higher than that of IO. This is in contradiction with up to date reported observations and it could be explained by the abovementioned reactions.

- Unlike for IO and OIO, I<sub>2</sub> is not considered at the levels recently measured by in-situ

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instruments in hot-spot like scenarios (up to 90 pmol mol<sup>-1</sup>) (See Saiz-Lopez et al., 2005 in ACPD), which may have a considerable effect on the rate of formation of iodine condensable units.

- Finally, ultrafine particle bursts have only been observed during daytime and they are significantly enhanced by strong solar irradiance at low water periods. For instance, in a low tide event at noon, can we expect homogeneous OIO nucleation to be responsible of the observed particle formation if we considered its reaction with IO and with itself?

Minor points:

Page 9908, line 24 ‘.. formation of new nuclei itself’ - delete ‘itself’

Page 9909, line 6 ‘..thorough understanding how’ - insert ‘of’

Page 9909, line 23 ‘..were used as source for..’ - change to ‘sources’

Page 9910, line 12 ‘was published..’ - change to ‘were published’

Page 9910, line 15 ‘..the question whether..’ - insert ‘of’

Page 9912, line 16 ‘..the assymmetric dimer..’ - change to ‘asymmetric’

Page 9912, line 26 ‘The nucleation modul..’ - change to ‘module’

Page 9914, line 1 ‘The negligance..’ - replace with ‘omission’ or ‘insignificance’

Page 9914, line 24 ‘..and realtive humidity..’ - change to ‘relative’

Page 9915, line 25 ‘Nucleation interactively interacts..’ - delete ‘interactively’

Page 9918, line 17 ‘..continuously versus..’ - replace with ‘with those’

Page 9919, line 4 ‘..in the range of some..’ - needs to be more specific, quantify ‘some’

Page 9919, line 17 ‘We used these..’ - change to ‘this’

Page 9920, line 2 ‘only up to about 3 ppt’ - change to ‘up to about 10 ppt’ Note that this

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change arise following re-analysis of data using an up-to-date cross-section

Page 9922, line 2 ‘..what is below..’ - change to ‘which’

Page 9922, line 4 ‘..during day result from..’ - change to ‘daytime’

Page 9922, line 12 ‘within some minutes..’ - needs to be more specific, quantify ‘some’

Page 9922, line 16 ‘obeservations’ - change to ‘observations’

Page 9922, line 25 ‘In case of the..’ - insert ‘the’

Page 9923, line 7 ‘which is a nearly..’ - change to ‘..nearly a’

Page 9923, line 7 ‘Under worse conditions..’ - delete ‘under’ / replace ‘worse’ with ‘alternative’  
‘..hot spots in further..’ - change to ‘at’

Page 9923, line 12 ‘..some ten seconds’ - does this mean approx. 10 s or tens of seconds?

Page 9923, line 17 ‘..detectable in some distance..’ - change to ‘at’ / quantify ‘some’

Page 9923, line 19 ‘..conserved for while..’ - delete ‘for while’

Page 9926, line 3 ‘..contribute noteworthy..’ - replace with ‘significantly’

Page 9928, line 1 ‘Sensitivity studies..’ - change to ‘sensitivity’

Page 9928, line 10 ‘..IO self-recation..’ - change to ‘reaction’  
Page 9915, line 15 ‘..self-reaction of OIO to..’ - change to ‘self-reaction of IO to..’

Page 9929, line 29 ‘ photolysis..’ - insert ‘to’

Page 9930, line 1 ‘..even in case..’ - insert ‘the’

Page 9930, line 3 ‘..apparently is not..’ - change to ‘are’

Page 9930, line 5 ‘..OIO likely has a ..’ - change to ‘has a likely’

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Page 9930, line 5 ‘..at least some ten..’ - does this mean approx. 10 s or tens of seconds?

Page 9930, line 19 ‘In case..’ - insert ‘the’

Page 9931, line 17 ‘..nuclei noticably..’ - change to ‘noticeably’

Page 9931, line 26 ‘.. quite stable..’ - replace with ‘relatively’

Page 9931, line 28 ‘.., what has never..’ - change to ‘which’

Page 9932, line 21 ‘.. should be adressed..’ - change to ‘addressed’

Page 9940, Table 4 caption ‘..molecules per cm2 and second..’ - change to ‘per’

Page 9944, Fig. 4 caption ‘Scetch..’ - change to ‘Sketch’

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