Interactive comment on “Lagrangian simulation of ice particles and resulting dehydration in the polar winter stratosphere” by Ines Tritscher et al.

Anonymous Referee #2

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The manuscript ‘Lagrangian simulation of ice particles and resulting dehydration in the polar winter stratosphere’ by Tritscher et al. extends the Chemical Lagrangian Model of the Stratosphere (CLaMS) with a new nucleation and sedimentation scheme for ice PSCs, in addition to existing parameterizations for STS and NAT. The new model version simulates the nucleation, growth, sedimentation, and evaporation of ice PSC particles along individual trajectories and simulates the related dehydration within the ice sedimentation module of CLaMS. The model development can significantly advance the scientific knowledge on polar stratospheric cloud formation. It further enlarges the range of applicability of the CLaMS model to Antarctic polar vortex conditions.

CLaMS results for the Arctic winter 2009/2010 and for the Antarctic winter 2011 are compared to PSC observations from the Cloud-Aerosol Lidar with Orthogonal Polar-
The simulations reasonably reproduce the timing and extent of PSC occurrence inside the vortex in the Arctic winter 2009/2010 and the Antarctic winter 2011, and therefore support the applicability of the stratospheric ice nucleation scheme recently suggested by Engel et al. (2013) to regional and even global scales. This is an important new result that merits publication. Deviations between model results and satellite observations as well as shortcomings of the nucleation schemes (used in CLaMS) are mentioned however this point could be discussed in a more detail to elucidate gaps or open questions in PSC science.

The manuscript represents a substantial contribution to scientific progress on polar stratospheric processes and is well within the scope of Atmospheric Chemistry and Physics. The scientific approach and applied methods are valid and clearly outlined and the results of the manuscript are discussed in a balanced way. The overall presentation is well structured and clear and the language fluent and precise. The quality of figures and text is excellent.

In sum, the paper is an important contribution to polar science and well suited for publication in ACP after the major concerns have been fully addressed by the authors.

Major concerns

(1) In addition to the general agreement of the model and the observations, which is impressive, the deviations of the model and the observations could be addressed in a more comprehensive way in order to highlight and fill gaps in scientific knowledge on PSC microphysics.

This discussion can help to answer the following questions: Are implemented nucleation schemes for NAT and ice sufficient to explain all observations? How could the nucleation schemes be corrected or extended to better cover dehydration and denitrification measured by MLS? Shortcomings in the implemented NAT nucleation pathways
lead to deviations in NAT particle size distributions and therefore to biases in the representation of denitrification in the model. Which processes or modifications could reduce those deviations? Similarly deficits in the ice nucleation schemes lead to smaller coverage of ice PSCs in the model and related reduced dehydration. Which processes could reduce shortcomings of the implemented ice nucleation schemes with respect to coverage with ice PSCs? This discussion could help to increase the scientific relevance of the paper and extend science beyond the state of the art. The results of the discussion should clearly be summarized in the abstract.

(2) A quantification of the deviation of the model results with respect to observations will strengthen the discussion of model agreement / disagreement with observations and will help to quantify uncertainties in the observations. In particular, quantitative deviations in stratospheric water vapor and nitric acid distributions between MLS und ClaMS could be added in a new the panel in Figures 5 and 10. Further a quantitative discussion of the agreement of model results and PSC observations by CALIOP and MIPAS could help to increase the value of the so far more qualitative discussion. Adding contour lines of TNAT and Tice to Figures 3, 7 and 8 could give further insights in data quality from observations and model. Could delta TNAT (or delta Tice) instead of temperatures be shown in Figures 3, 7 and 8 lowermost panel to get independent information on PSC phase or ambient conditions?

(3) The abstract could be rephrased to specifically highlight the results of the study with respect to ice PSCs and dehydration. The first 3 sentences of the abstract are too general and do not cover the content of the manuscript and therefore could be shifted to the introduction. If needed in the abstract, a more specific motivation could be given why Lagrangian simulations of ice PSCs and sedimentation are important. The scope of the abstract is to present the scientific results of this study. Comments with respect to previous work or campaigns (without explanation) could be omitted or shifted in the introduction unless it is urgently needed for a specific result. Quantitative descriptions of model agreement with observations should be given and disagreement could be
discussed in sight of missing processes. Comments (1) and (2) will help to enhance the quality of the abstract, which as rather descriptive at the moment.

Minor comments

P2 l19 Which knowledge gaps exist? Be more specific.
P2 l27 Which gaps, weaknesses and uncertainties exist? Be more specific.
P5 l36 Water equilibrium depends in water partial pressure and ice crystals concentrations/surface areas.
P6 l25 Are the temperature fluctuations used for the NAT nucleation pathway, too?
P10 l8 More information on MLS data and uncertainties could be given.
P11 l14 What causes the MIPAS NAT observations/interference < 15km altitude? Polar cirrus are not measured by MIPAS.
P11 l18 Could you comment on the CALIOP and CLAMS results of total PSC, ice and NAT areas below 13 km altitude?
P11 l26 Could you comment/quantify the agreement/disagreement between ClaMS and CALIOP?
P11 l26 Could you comment on the deviations in EnhNAT between ClaMS and CALIOP (Figure 3).
P11 l29 What causes the spread in CALIOP data (Figure 3, lowermost row) with respect to ClaMS results?
P12 l33 NAT PSCs do not follow due to data gaps, maybe rephrase.
P12 l35 Could you comment on the disagreement in PSC occurrence below 15 km altitude between CLAMS and CALIOP and MIPAS?
P13 l1 Explanation of results from Figure 7 are missing. Again there are similarities
but also differences in the NAT and ice PSC occurrence in the upper panel and in the scatter in the lowermost panel in Figure 7.

P14 General agreement is reasonable or good. Please now explain in detail deviations between model results and observations in sight of current PSC formation schemes. Which processes are not understood or not covered in the model that help to resolve the deviations?

Figure 5 and 10
Could a new the panel be added in Figures 5 and 10 that quantifies the agreement/deviations between MLS and CLaMS?

Figure 3, 7 and 8
Could the TNAT contour lines be given in Figure 3, 7 and 8? This could help to decide on a bias in NAT occurrence by CLaMS or the observations.
Could the Tice contour lines be given in Figure 3, 7 and 8? This could help to decide on a bias in NAT occurrence by CLaMS or the observations.
Could delta TNAT (or delta Tice) instead of temperatures be shown in Figures 3, 7 and 8 lowermost panel to get independent information on PSC phase and to be independent on altitude/H2O and HNOP3 partial pressures?

Ice manuscript. . . .