Answers to Reviewers' Comments on Kovacs *et al.*,
D region ion-neutral coupled chemistry within a whole atmosphere chemistry-climate model

Reviewer 1

Comment 1: p7, line 5 - a 5 year spin up period seems very long - similar dynamics-only experiments would likely require a considerably shorter spin up. Is the longer spin up chosen because of the very long lifetime of some of the key chemical reactions? This should be explained in the text

Answer 1: Explanation is given in the text. "The long spin up period was used in order to definitely allow enough time to reach steady-state and also to count for long lived species such as N_2O, CH_4." (page 7, line 18-19)

Comment 2: p12 Conclusions - given that the rSIC approach was trained using one period of data, and tested using just one period the authors should comment more on the wider applicability of the approach.

Answer 2: Comment is given in the text. "Note that the rSIC model contains temperature (and pressure) dependent rate coefficients (where available), therefore the chemical model can be used over a wide range of conditions." (page 12, lines 30-31)

Comment 3: p2, line 22 - this states the SIC model has 306 ion-molecule reactions but 307 are listed in the SM

Answer 3: Corrected in the text; 306 changed to 307. (page 1, line 16; page 2, line 22; page 3, line 5; page 4, line 15; page 8, line 8)

Comment 4: p2, line 29 - WACCM-D, WACCM-SIC, etc are defined in the abstract but I think they should be defined again in the main text.

Answer 4: Corrections made in the text. (page 2, line 29)

Comment 5: p4, line 12 - From the SM it is not clear which reactions are the 7 photoionization and 16 photodissociation reactions mentioned in the text (though some will be the ones marked PDE*) - this should be clarified.

Answer 5: Photoionization and photodissociation reactions are not listed in the SM as no fixed rate parameters are defined for them (they depend on the solar activity). They are listed separately in Table 2. This is made clear in the text (page 4, lines 15-17).

Comment 6: p8, line 2, and Figure 2 - the legend suggests the profiles from two WACCM experiments are plotted on the left hand panels, but the results appear identical and do not appear to correspond with the relative differences plotted on the right hand panels. Either alter the left hand panels to show the differences better or (if the log scaling and rage of values makes this impossible) indicate in the text that the differences can only be clearly seen n the right hand panels to clarify and to avoid the reader looking for a needle in a haystack on the left.

Answer 6: Corrections and clarification made in the text. It is not possible to show the differences better on the left panels. "Note that the differences can only be seen in the right hand panels of Figure 2." (page 8, lines 17-18)

Reviewer 2

Comment 1: A parametrization for HOx production due to ionization based on positive ion chemistry has been developed already by Solomon et al. (1981)… Why not use this version here as standard WACCM?

Answer 1: This is corrected and clarified in the text: "The HO_x species are produced via a complicated ion chemistry scheme that is based on (Solomon *et al.*, 1981)" (page 6, lines 30-32)

Comment 2: discussion of Figure 1: is this the change of rms error of one species, or of all species considered? If the first, which? What are the units on the y-axis?

Answer 2: Figure legend is corrected and clarified. RMS is for all species considered and they are dimensionless. (Figure 1 legend, page 20, line 4)

Comment 3: Results from the reduced scheme agree better with results using the full ion chemistry scheme than WACCM-D results… This suggests that the reactions included in WACCM-D but not in WACCM-rSIC are actually not important, and should not be called such without further justification.

Answer 3: The authors agree with this comment and the "important" term has been deleted from the sentence "as it can be seen in the SM, the ~~important~~ recombination reactions of NO^+ clusters forming NO". (page 10, lines 26-27)

Comment 4: Abstract, page 1, line 17: could you include the number of ion species in the reduced SIC scheme as well?

Answer 4: It is clarified now. "…a reaction scheme of 181 ion-molecule reactions of 27 positive and 18 negative ions" (page 1, lines 18-19)

Comment 5: Introduction, page 2, line 4, 12, and 17: the reference is Sinnhuber et al., 2012, or Sinnhuber, Nieder and Wieters, 2012.

Answer 5: Reference is corrected in the text. (page 2, lines 5, 12, 17)

Comment 6: Introduction, page 2, line 20: SIC is certainly "one of the" leading kinetic models of D region chemistry, though not "the" leading kinetic model of D region chemistry.

Answer 6: Corrected in the text. (page 2, line 20)

Comment 7: Methodology, page 3, line 6, caption of table in supplementary material: do you mean the "red" bold type? Please also make a note in the caption of the table.

Answer 7: Yes, it is the "red bold type". Corrected in the text. (page 3, line 7)

Comment 8: Methodology, page 3, line 10-11: Primary protons as well as secondary electrons will also collide with O2, leading to the same reactions as with N2, namely ionization, dissociation, and excitation (Porter et al., 1976). Also, ionization of O should play a role in the upper mesosphere and lower thermosphere, where O becomes one of the most abundant species. Is this not included in SIC? Please clarify.

Answer 8: Authors agree with the comment and necessary corrections have been made in the text: "In the initial step, primary proton collisions with molecular nitrogen or oxygen cause dissociative ionization and produce secondary electrons which also form atomic nitrogen or oxygen from molecular nitrogen or oxygen." (page 3, lines 11-12)

Comment 9: Methodology, pare 4, line 1: does the reduced mechanism contain all reactions of the important + necessary species, or a subset? E.g., is there an attempt to reduce/limit the number of reactions of the species included?

Answer 9: Yes, it contains all the reactions of the important and necessary species. Clarified: "…307 ion-neutral reactions in total of all the important and necessary species" (page 3, line 5)

Comment 10: Page 8, line 7, … neutral profiles are reproduced within a factor of 2 … in Figure 2, all neutral profiles are within the 5.

Answer 10: corrected: "within a factor of 5" (page 8, line 19)

Comment 11: Page 10, line 1-2: Earlier (line 6, line 21-22) you mention that the production of NOx due to ionization in the standard WACCM is parametrized to 1.25 NOx per ion pair; here you suggest that the NOx production is due to the five-ion chemistry scheme implemented in standard WACCM (for the lower thermosphere). Please clarify which is correct.

Answer 11: This is clarified in the text now: "According to (Jackman *et al.*, 2005) an ion pair produces 1.25 N atoms with branching ratios of 0.55 N(^{4}S) and 0.70 N(^{2}D). Then the nitrogen atoms will go through a complex ion chemistry that leads to the formation of NOx species." (page 6, lines 28-32)

Comment 12: Conclusions, page 12, line 13: You could include an additional statement like: Before and after the solar proton event, NO and NO2 from WACCM-rSIC agree much better with results from WACCM-SIC than the results of WACCM-D, because…

Answer 12: Additional sentence is given in the text. "Before and after the solar proton event, NO and NO_2 from WACCM-rSIC agree much better with results from WACCM-SIC than the results of WACCM-D, which is due to the absence of N_2 clusters of proton hydrates and of the O_2^+ ion in WACCM-D." (page 12, lines 23-25)