

Interactive comment on “D region ion-neutral coupled chemistry within a whole atmosphere chemistry-climate model” by Tamás Kovács et al.

Anonymous Referee #2

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1 General comments

This paper is the second dealing with including a simplified D-region ion chemistry scheme in the WACCM model using a subset of SIC ion chemistry reactions. Compared to the development of WACCM-D discussed in the previous paper (Verronen et al., JGR, 2016), in this paper a more systematic approach is used in the reduction of the ion-chemistry reactions. WACCM-D already showed a significant improvement in some neutral mesospheric species compared to model versions without, or with parametrized, ion chemistry. This paper clearly demonstrates that using a systematic approach of reaction reduction yields a better reproduction of the key neutral species (NO_x, HO_x, ozone, HNO₃) during large ionization events in the mesosphere than WACCM-D, while at the same time reducing the number of ion reactions imple-

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mented even more. Both the description of the reduction process, as well as the list of full and reduced ion chemistry in the supplementary material, are of great interest to other modelers achieving similar. The paper is generally clearly and well written.

2 Specific comments

I was a bit surprised that for the comparison with standard WACCM, you include a parametrization for NO_x production, but not for the production of HO_x (page 6, lines 21-23). A parametrization for HO_x production due to ionization based on positive ion chemistry has been developed already by Solomon et al. (1981). This parametrization is widely used in models to study the impact of solar proton events and middle-energy electron events on the stratosphere and mesosphere (e.g. Jackman et al. 2000, 2001, 2005a, b; Rohen et al. 2005; Funke et al., 2011). It has also been included in WACCM to study solar proton events (e.g., Jackman et al., 2011). Why not use this version here as standard WACCM? The Solomon parametrization is based on HO_x production by positive protonized water cluster ions, an idea already developed in the 1970th and 1980th (Swider and Keneshea, 1973; Swider et al., 1978; Crutzen and Solomon, 1980; Solomon et al., 1981). It has been shown in a number of studies since then that this parametrization generally leads to a reasonable representation of HO_x production and ozone loss (see, e.g., Jackman et al. 2001; Funke et al. 2011). That a model not using a parametrization of the HO_x production by protonized water cluster ions underestimates HO_x production and subsequent mesospheric ozone loss during large solar proton events has been shown in a number of publications since the 1970th (see also page 9, line 23-24). However, I would assume that the reduced ion chemistry provides a better representation of the full ion chemistry than the Solomon parametrization which simplifies, e.g., the vertical range of HO_x production which depends on the availability of water vapor.

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Page 7, line 13 ff, 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,

Page 10-19: I found the discussion in this paragraph confusing. In particular you mention several times that “important reactions” are missing in the reduced SIC scheme as the reason for a disagreement between WACCM-rSIC and WACCM-D which apparently includes these “important” reactions. However, at the same time, results from the reduced scheme agree better with results using the full ion chemistry scheme than WACCM-D results (e.g., NO and NO₂ before and after the solar proton event: WACCM-rSIC really is in much better agreement with WACCM-SIC than WACCM-D there). 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 (e.g., reactions of hydrated O₂⁻ ions in line 11/12, and NO⁺ clusters in line 17).

3 Technical comments

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

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

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.

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.

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

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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.

Methodology, page 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?

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

Page 9, line 23/24: that models not including the effect of positive water cluster ions underestimate the HO_x production and ozone loss during solar proton events has been discussed since the 1970th, see specific comment above, and (Jackman et al., GRL, 2001) for one example.

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

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 . . .

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