We thank the reviewers for making very useful suggestions to improve the paper. Our point-by-point responses to the reviewers' comments and corresponding changes with line numbers are detailed below in blue text, and the changes are shown in the version of the manuscript with track changes.

Reviewer #1 comments (RC2):

General comments:

This is an interesting study on model simulations on Mg, Na and Fe (and their ions) in the mesosphere/thermosphere using an extended version of the WACCM-X model. In my opinion the study is suitable for ACP after some revisions have been made. Two more general aspects that will appear again in the specific comments below are:

(1) the differences between the Mg+ results presented here and the ones based on WACCM-Mg in Langowski et al. should be explicitly discussed and perhaps explained – if possible – by differences in the model set-up.

Response: This is a good suggestion. In the revised manuscript, we now describe the similarities and differences between our model results and the WACCM-Mg model and SCIAMACHY observations in Langowski et al. (2015). We have also added the model set-ups to facilitate the comparison with WACCM-Mg. The following briefly introduces the similarities and differences between the two models:

Similarities: As we stated in Section 2.1 (Line 52), "Validated metal chemistry modules for magnesium (Langowski et al., 2015), sodium (Marsh et al., 2013a), and iron (Feng et al., 2013) with updated rate coefficients from Plane et al. (2015), Bones et al. (2016) and Viehl et al. (2016), are added." Therefore, for Mg, our model is essentially the same as the Mg chemistry module in WACCM-Mg, and WACCM-X 2.0 and WACCM-Mg are extended from WACCM4 and have similar physical and chemical processes.

Differences: (1) The WACCM-X includes a self-consistent solution of global electrodynamics and extends the model top to more than 500 km, while the top of the WACCM-Mg model is about 140 km. (2) To make the model results more consistent with the observations by SCIAMACHY, the MIF adopted in the WACCM-Mg model by Langowski et al., 2015 was adjusted by scaling the Mg MIF to match the observed Mg^+ column density. (3) WACCM-Mg uses the specified dynamics version (SD-WACCM), which is nudged by the GEOS5 meteorological data set (including temperature, specific humidity, horizontal winds) below 60 km, while the model in the present paper is a free-running simulation that does not attempt to model specified lower atmosphere forcing.

The following table briefly summarizes the similarities and differences between WACCM-Mg and WACCM-X-Mg, taking Mg as an example.

	WACCM-Mg	WACCM-X-Mg
Model Framework	CESM1 (Based on WACCM4)	CESM2 (Based on WACCM4)
Metal Chemistry	Magnesium chemistry modules (Langowski et al., 2015)	Magnesium chemistry modules (Langowski et al., 2015)
Model top	$6x10^{-6}$ hPa (~140 km)	$4x10^{-10}$ hPa (500-700 km)
Ion transport	No	full ion transport
E dynamo	No	Yes
Specified Dynamics	Nudged by the GEOS5	Free-running
Meteoric Input Function (MIF)	Adjusted by scaling the Mg MIF to match the observed Mg^+ column density by SCIAMACHY.	Updated MIF considers more types of sources (Carrillo-Sánchez et al., 2016), but not adjusted to observations

Changes: Please see Lines 54-55, Lines 100-106 and Lines 113-116.

(2) I agree that there are similarities between the simulations presented here and the SCIAMACHY observations in Langowski et al. (which is very good!), but there are also quite significant differences (e.g., in [Mg+] peak altitude or absolute number densities) which are not mentioned at all. Please discuss the similarities and differences in an objective manner and also include the differences.

Response: Thank you for this suggestion to discuss the similarities and differences in greater detail. In the revised manuscript we now describe the difference between the Mg^+ number density and peak height in our model and the SCIAMACHY observations, and also provide possible reasons for the differences.

Changes: Please see Lines 100-106.

Specific comments:

Line 4: "The model with full ion transport significantly improves the simulation of global distribution 5 and seasonal variations of Mg+."

I don't think this is entirely correct. The WACCM-Mg simulations shown in Langowski et al. were in better agreement with SCIAMACHY observations in terms of number density than the WACCM-X simulations presented here.

Response: Thank you for pointing this out. We have modified the sentence in the revised manuscript to read: "The model with full ion transport significantly improves the simulation of global distribution and seasonal variations of Mg^+, although the peak density is slightly lower (by on average 5 km) compared with the SCIAMACHY measurements."

For the global and seasonal distribution of Mg^+, our model compares better with observations. Of course, as the reviewer points out, WACCM-Mg is more consistent in terms of number density. We provide possible reasons in the following point-by-point responses.

Line 15: “and Friedman et al. (2013) investigated a descending thermospheric K layer up to 155 km at Arecibo“

This statement is a little vague. Did the layer descend from altitudes above 155 km downwards to 155 km? The combination of “descending” and “up to” makes the sentence difficult to understand.

Response: The sentence is rephrased to the following: “and Friedman et al. (2013) investigated a thermospheric K layer that descended from altitudes above 155 km at Arecibo, Puerto Rico.”

Line 33: “However, no previous studies appear to have examined the full transport of metal ions in a self-consistent global chemical-dynamical model.”

I’m not sure what “self-consistent” really means here. “Self-consistent” is used several times throughout the manuscript and at least in some cases with a different meaning. Can you explain, what it means here?

Response: what we mean here by “self-consistent” is that WACCM-X contains atmospheric dynamics (of the whole atmosphere up to ~500 km), chemistry (including the injection of the three metals from meteoric ablation), and ion transport, all solved numerically in a single model. In previous modelling work on ion transport of metallic species, most of the background physical quantities are input from empirical models rather than solved self-consistently. For example, neutral winds have been specified by the HWM empirical model and the thermospheric composition and temperature by NRLMSISE.

Line 43: “affects” -> “effects” ?

Response: Corrected.

Line 47: “WACCM-X is developed in the present study”

I suggest replacing “developed” by “extended”, because WACCM-X did already exist before.

Response: Changed.

Same sentence: “combined with interactive chemistry”

Please mention briefly in what sense the chemistry is interactive. Often the chemistry is not “fully” interactive.

Response: “Interactive chemistry” in the model is relative to “specified chemistry”, which refers to the full coupling of chemistry and atmospheric physics – in particular, heating through exothermic chemical reactions, and cooling through radiative emission from chemical species. As stated in Line 51 “The key chemistry and dynamical features are based on CAM4 and WACCM4 and are described in detail in Marsh et al. (2013).” WACCM4, as described in Marsh et al. (2013), includes fully interactive chemistry.

Marsh, D. R., Mills, M. J., Kinnison, D. E., Lamarque, J., Calvo, N., & Polvani, L. M. (2013). Climate Change from 1850 to 2005 Simulated in CESM1(WACCM), Journal of Climate, 26(19), 7372-7391.

Line 53: “and winds is treated in the same way as most active chemical species”

Which species are treated in a different way? Why?

Response: In WACCM, most chemical species are treated as advected tracers. However, a few species, including NO^+, O_2^+ and N_2^+, are short-lived so that transport is less important, and they are treated as being in photochemical steady-state in the model.

Perhaps “as most” -> “as for most” ?

Response: changed to “…as the transport of most …”

Line 56: “including a self-consistent electrodynamics module“

Can you mention briefly, what “self-consistent” means here?

Response: The term “self-consistent” is used here in the same way as before – the atmospheric physics, dynamics and chemistry is all treated in a single model”

According to Liu et al. (2018), the electric field (and along with it the E×B drift) at low and mid-latitudes in WACCM-X 2.0 is solved according to the electric dynamo equations, using neutral winds and electric conductivities resolved by the model. In earlier version of the model (WACCM-X 1.0), the electric field (and E×B drifts) had to be specified by an empirical model.

Liu, H.-L., Bardeen, C. G., Foster, B. T., Lauritzen, P., Liu, J., Lu, G., … Wang, W. (2018). Development and validation of the Whole Atmosphere Community Climate Model with

thermosphere and ionosphere extension (WACCM-X 2.0). Journal of Advances in Modeling Earth Systems, 10, 381– 402. https://doi.org/10.1002/2017MS001232

Line 61: “constant F107=124“

I suggest to replace “F107” by “F10.7”. Also: The 10.7 cm flux is not dimensionless. Please add sfu (solar flux units) to the numerical value.

Response: Thank you for pointing this out. Now it is rephrased to the following: “(constant F10.7=130 sfu (solar flux units) and Kp=1)”.

Line 95: “At middle latitudes .. , the peak altitude of Mg+ is 10 km higher in the summer hemisphere,”

Higher compared to which region? The same latitudes in the winter hemisphere? Or the rest of the latitudes? Please specify.

Response: We have modified the sentence in the revised manuscript to: “The peak altitude of Mg^+ in the summer hemisphere at middle latitudes (~40±10°) is ~10 km higher than at other latitudes, in accord with observations (Langowski et al., 2015).”

Line 104: “To address this, we also present the simulation results at the same local time (10:00 LT) in Figure 2, and they are in better agreement with SCIAMACHY observations.”

Yes, in some respect these results are in better agreement with the SCIAMACHY observations, but the number densities are even lower and the discrepancy to the number densities observed by SCIAMCHY is even bigger. In addition, the Mg+ peak altitude is still about 10 km lower than in the SCIAMCHY data set. These differences should also be explicitly discussed in my opinion, not only the aspects that fit well.

Response: Thank you for this suggestion. For the global and seasonal distribution of Mg^+, our model results are in better agreement with the SCIAMACHY observations. In terms of number density and peak altitude, there is a larger discrepancy with the SCIAMCHY observations. We have now added a description of the difference between the modelled Mg^+ number density and peak height and the SCIAMACHY observations, and also give possible reasons for the differences.

Changes: Please see Lines 100-106 and Lines 113-116.

Line 107: “which is absent in the previous models.”

It is unclear – at least to me - what “previous models” refers to. Previous studies by other groups, WACCM-MG?

Response: This has been changed to refer specifically to Langowski et al. (2015), which reported in Section 7.2: "The Mg^+ peak altitude is close to 95 km and shows no strong variation with latitude and time."

Line 110: "the Mg+ column density exhibits relatively high distributions at"

I suggest replacing "high distributions" by "high values". "High distributions" doesn't really make sense here.

Response: Changed as suggested.

Section 3.1: Please explain the differences between the extended WACCM-X used in this study and WACCM-Mg used Langowski et al.. The WACMM-Mg results agreed much better with SCIA in terms of [Mg+]. Any idea why? In my opinion these differences are an important aspect that should be addressed in the paper.

Response: As we stated in Section 2.1 (Line 52), "Validated metal chemistry modules for magnesium (Langowski et al., 2015), sodium (Marsh et al., 2013a), and iron (Feng et al., 2013) with updated rate coefficients from Plane et al. (2015), Bones et al. (2016) and Viehl et al. (2016), are added." Therefore, for Mg, our model is basically consistent with the chemical scheme in WACCM-Mg, and both WACCM-X 2.0 and WACCM-Mg are based on WACCM4 and have similar physical and chemical processes.

The biggest difference are that WACCM-X includes global electrodynamical transport of the metallic ions (equation (2) in the manuscript), and extends the model top to more than 500 km (the top of WACCM-Mg model is about 140 km).

The major reason why the Mg^+ densities from WACCM-Mg are in better agreement with SCIAMACHY is because the MIF adopted by Langowski et al. (2015) was scaled to match the observed Mg^+ column density. Another possible reason is that WACCM-Mg used specified dynamics (SD-WACCM), where the meteorological fields (including temperature, specific humidity and winds) below 60 km are nudged by the GEOS5 meteorological data set. In contrast, WACCM-X-Mg is a free-running simulation.

Another difference is that we have used an updated MIF in the present study which considers more sources of interplanetary dust particles (Carrillo-Sánchez et al., 2020), compared with the MIF used by Langowski et al. (2015). Because the model simulates Na, Fe, and Mg simultaneously, and the present paper mainly focuses on the global transport processes of metal ions, we have not scaled the MIF to make the simulations conform to the observations.

Carrillo-Sánchez, J. D.; Gómez-Martín, J. C.; Bones, D. L.; Nesvorný, D.; Pokorný, P. Benna, M.; Flynn, G. F.; Plane, J. M. C. (2020) Cosmic dust fluxes in the atmospheres of Earth, Mars, and Venus, *Icarus*, *335*, art. no. 113395

Also section 3.1: There are of course similarities between your Mg+ results and the SCIAMACHY observations, but there are also significant differences. The Mg+ peak altitude in your simulations is about 10 km lower than in the SCIAMACHY data. Also, the modelled number densities are about a factor of 2 lower than in the SCIAMACHY data set. These differences should also be explicitly mentioned in the paper and possible reasons discussed. I'm not asking for new simulations, just an objective description of the agreement between model and measurement results.

Response: See above.

Fig. 2: Here, the low bias compared to SCIAMACHY is even more pronounced than in Fig. 1. Any idea why?

Response: The pronounced discrepancy in Fig. 2 is probably due to the diurnal variation of ion electro-dynamical transport. Figure 4e in the revised manuscript shows the diurnal variation of Mg^+ number density near the dip equator as a function of local time. This shows that Mg^+ drifts down towards the main layer at 10 LT, where removal of Mg^+ is more rapid.

Fig. 3: Units below colour bar is wrong/incorrect. Please correct.

Response: Changed the unit of column density to 10^9 atoms cm^{-2}.

Also, the MgII VCDs shown here are significantly lower than the ones determined from the SCIAMACHY observations (compare to Fig. 16 (right) in Langowski et al.).

Response: We have updated Figure 3 using different color ranges. Compared with the Mg^+ VCDs simulated by WACCM-Mg (Fig. 16 (right) in Langowski et al. (2015)), the VCDs in Fig. 3e in our paper are comparable in value. Compared with the SCIAMACHY observations (Fig. 9 in Langowski et al. (2015)), although the VCDs in Fig. 3e are slightly lower in value (by 20%), there is good agreement with the observed global distribution and seasonal variation.

Line 173: "Figure 7 and 8 compares" -> " Figures 7 and 8 compare" ?

Response: Corrected.

Line 186: “In contrast, the reduced densities of the molecular ions (and electrons) at night means that their increased lifetimes become comparable to transport lifetimes.“

Is the logic behind this sentence entirely correct? Please check.

Response: The sentence is rephrased to the following: “In contrast, the reduced densities of the molecular ions (and electrons) at night means that their increased lifetimes become comparable to the transport time-step.”

Fig. 6: The Mg+/Na+ ratios exhibit an interesting interhemispheric difference for solstice conditions. Please comment on it and perhaps provide a qualitative explanation, if possible.

Response: Thank you for pointing this out. We have now provided the following explanation at Lines 178-190: “Figure 6 shows that whereas the Mg^+/Fe^+ ratios (left panel) show relatively little latitudinal variation compared with the variation with altitude (mostly caused by the mass difference of the ions), the Mg^+/Na^+ ratios (right panel) show marked interhemispheric differences at the solstice periods. The reason for this is the difference in the ion-molecule chemistry of Na^+, compared with Mg^+ (and Fe^+). The Na^+ ion has a closed electronic shell (it is isoelectronic with the inert gas Ne), and so does not react with O_3, in contrast to Mg^+ and Fe^+ (Plane et al., 2015). Formation of MgO^+ by the fast reaction with O_3 is the main route to neutralization of Mg^+ above 90 km (Whalley et al., 2011). During summer at mid- to high-latitudes (> 30º), O_3 above 90 km is heavily depleted through a combination of longer diurnal photolysis and reaction with the elevated levels of H produced from H_2O which upwells over the summer pole (Plane et al., 2015). In contrast, the O_3 density in the lower thermosphere is more than an order of magnitude higher in the winter polar vortex. The result is that lower thermospheric Mg^+ ions at latitudes higher than ~30º are relatively long-lived in summer, and can be transported vertically throughout the thermosphere. This leads to the higher Mg^+/Na^+ ratios in the summer hemisphere, as shown in Figure 6. The converse operates at latitude higher than 30º in the winter hemisphere, where the relatively high O_3 tends to neutralize lower thermospheric Mg^+. Because Na^+ and Mg^+ have very similar masses, their ratios above 100 km are fairly constant with height.”

Whalley, C. L., J. C. Gomez Martin, T. G. Wright, and J. M. C. Plane (2011), A kinetic study of Mg+ and Mg-containing ions reacting with O_3, O_2, N_2, CO_2, N_2O and H_2O: implications for magnesium ion chemistry in the upper atmosphere, Physical Chemistry Chemical Physics, 13, 6352-6364.

Line 190: “the full life cycle of multiple meteoric”

I’m not sure what this really means: “the full life cycle”. Is the formation of meteoric smoke particles included as well?

Response: The "full life cycle" in this paper is a phrase used to emphasise that our model simulates all relevant processes of metal species in the atmosphere (of which we are aware), including the injection rate of each element into the atmosphere as a function of time and latitude (the meteoric input function (MIF)), the metal chemistry, the transport of metal atoms and ions, and removal of the metallic species as particles.

To treat the polymerization of the metal reservoir species into meteoric smoke particles (MSPs), each metal chemistry module is assigned a "dimerization" reaction, where formation of the dimer represents permanent removal. For more information, please refer to Section 5.2 of Plane et al., (2015).

Plane, J. M. C., Feng, W., and Dawkins, E. C.: The mesosphere and metals: chemistry and changes, Chemical Reviews, 115, 4497–541, https://doi.org/10.1021/cr500501m, 2015.

Line 195: "(1) A clear seasonal cycle is found in the monthly averaged global distributions of Mg+, in good agreement with the SCIAMACHY measurements"

I agree the seasonal cycle is in good overall agreement with the SCIAMACHY measurements. However, several other aspects show significant differences (e.g. peak altitude, absolute values etc.). The differences should also be mentioned.

Response: Thank you for pointing this out. The sentence is rephrased to the following: "A clear seasonal cycle is found in the monthly averaged global distributions of Mg^+, in good agreement with the SCIAMACHY measurements (Langowski et al., 2015), although the peak height and peak density are about 5 km and 35% lower than the observations, respectively."