

Responses to Eric Jensen

Suggestions for authors:

5 1. It would be helpful if the authors would provide some information about the simulated microphysical properties of the convective tops extending into the stratosphere. Specifically, quantitative information about the simulated ice concentrations and size distributions would be helpful. I realize the simulations use bulk parameterizations, but the two-moment scheme should provide ice concentrations and some measure of the width of the assumed size distribution. Realistic treatment of ice microphysics is important because
10 the simulated convective hydration depends in part on the ice crystal size-dependent sedimentation and sublimation of ice in the lower stratosphere.

The microphysics scheme used here predicts the ice water content (IWC) and the number concentration for 4 solid hydrometeors: ice, snow, graupel and hail. The particle size of solid categories is assumed to be gamma distribution. For the detailed parameters used in the distribution please refer to Milbrandt et al. (2005a, 2005b). Here, in order to present the results in a succinct way, we calculated the effective radius (the ratio of the third to the second moment of a droplet size distribution) for each solid category predicted by the 1.0 km simulation and weighted them with the mass. The 2D histogram of this mass weighted effective radius is shown in Fig. R1 for 19:46 UTC, 25 Aug (the same time as Fig. 4), at the altitude of
15 ~15.5 km in domain A. At the other altitudes between 15 and 16, we find similar distributions (not shown).
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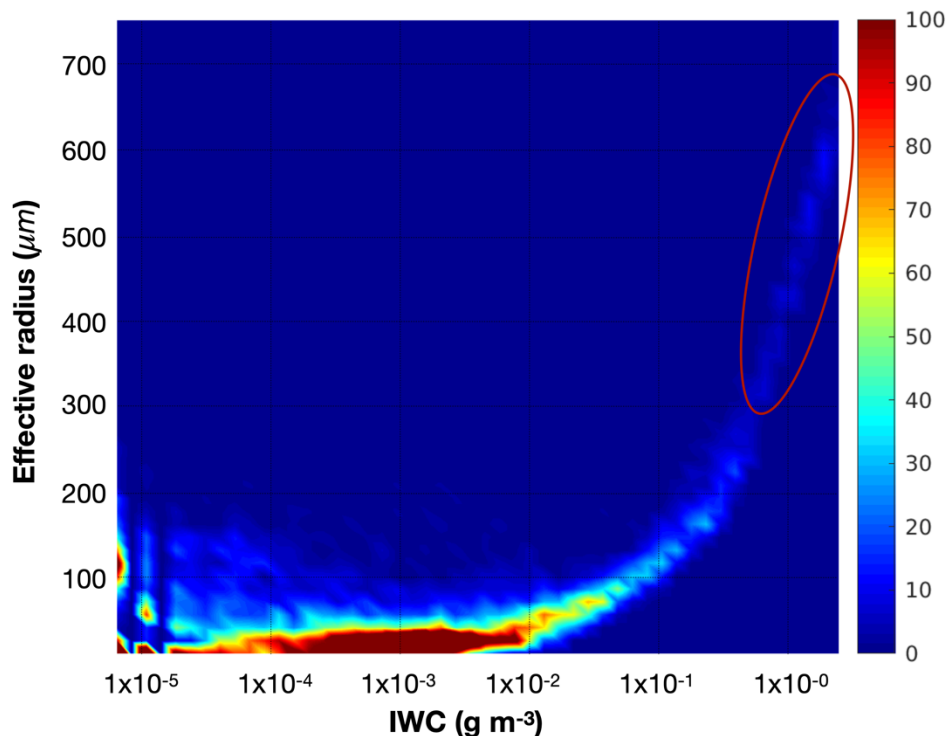


Figure R1: 2D histogram of cloud ice in domain A at the altitude of 15.5 km, 19:46 UTC 25 Aug. x-axis: ice water content in g m^{-3} ; y-axis mass weighted effective radius in micron. 50 bins are used in each axis to produce the histogram.

25 The cloud overshooting tops often contain high ice water content, e.g. $\text{IWC} > 0.5 \text{ g m}^{-3}$. In Fig. R1, we find that these air parcels containing high IWC are very few (light blue region circled). The mass weighted effective radius is between ~ 300 to $\sim 700 \mu\text{m}$ which suggests that there are large particles and they will fall faster. On the other hand, for the thin ice clouds, e.g. the ice plumes, with $\text{IWC} < 0.1 \text{ g m}^{-3}$, they occupy a

much larger area comparing to the overshooting tops as they are more frequently encountered (red color). The effective radius of these solid particles is small, mostly less than 30 μm as shown in Fig. R1.

5 For our current study, we don't have direct observation data of ice number concentration and ice water content during the convection time. Therefore, it will be difficult to validate the results of GEM. We considered this an interesting subject for a further study, e.g. to use other aircraft *in situ* observations for a different case for which we have good measurements near the convection. We add in the manuscript these descriptions:

10 *“The cloud ice properties are different in the overshooting tops and in the thin ice plumes. At the altitude of ~15.5 km (~ 1 km above the tropopause) within domain A at 19:42 UTC 25 Aug, the ice water content in the overshooting tops is relatively high with values from ~0.5 g m⁻³ up to ~2.8 g m⁻³. In the thin ice plumes the ice water content is generally lower than 0.1 g m⁻³. We calculated the effective radius for each solid category, e.g. ice crystals, rain, snow, graupel and hail. We find that in the cloud overshooting tops, the mass weighted effective radius for ice increases with the ice water content from ~300 to ~700 μm . On the other hand, the mass weighted effective radius for thin ice plume is usually lower than 30 μm . The area of cloud overshooting top occupies only 2.3% of the cloudy area but contains 68% of the total ice mass at this altitude.”*

20 2. Page 1, line 30: The authors cite Anderson et al. (2012) here for the influence of water vapor on stratospheric chemistry. I believe earlier references such as Solomon et al. (1986) would be more appropriate.

Done.

25 3. Page 2, lines 26–30: I would recommend citing Smith et al. (2017) here.

Done.

30 4. Page 3, lines 17–19: It is my understanding that global models generally do not include overshooting convection. If the authors are aware of whether (or how) global models treat overshooting convection, it would be helpful to provide some discussion here.

35 Many GCM and global NWP models employ the mass flux approach to represent deep convection. In this approach, the updraft characteristics are calculated using a steady state plume model. This includes solving an equation for the updraft vertical velocity as a function of the evolving buoyancy of the entraining plume. The cloud top will be defined as where the vertical velocity approaches zero. This level is always above the level of neutral buoyancy. Therefore, these schemes do represent in a very simplified manner overshooting convection. How high this convection reaches depends on the environmental characteristics as well as on many parameters of the convection scheme, namely on how entrainment and detrainment is calculated.

40 Other complex phenomena near the tropopause during the convection are not parameterized, e.g. the falling of cloud overshooting tops, gravity wave breaking and formation of jumping cirrus, as well as the trapping of ice within the supersaturated cloud overshooting tops which inhibits ice sublimation. We will discuss all these points in details in the later parts of the manuscript. They warrant also further investigations and eventually improvements of the way of parameterizing deep convection near the tropopause. We add in this

45 paragraph a brief discussion:

50 *“In the global NWP and GCM models, the deep convection is parameterized using mass flux approach. The complex phenomena near the tropopause during the convection are parameterized in a simplified manner, e.g. overshooting convection, or not parameterized, e.g. the falling of cloud overshooting tops (not sedimentation), gravity wave breaking and formation of jumping cirrus, etc.”*

5. As shown by previous cloud-resolving model studies (e.g. Dauhut et al., 2018) the magnitude of irreversible hydration in the lower stratosphere increases as the maximum heights of overshoots extending into the stratosphere increase. It would be helpful for the authors to discuss this issue within the context of the current simulations. In addition, it would be useful to see how the distribution of overshoot maximum heights depends on the model spatial resolution.

For the fully solved high resolution simulations, the maximum height of the cloud overshooting top depends on the model horizontal resolution. In our simulated case, the maximum heights are 16.64 and 16.96 km for 2.5 and 1.0 km simulation. For 0.25 km simulation, the early stage of the convection was simulated in the limited green box in Fig. 1 with a maximum height of 16.64 km. The irregularity here is probably due to the lack of the latter period of the convection for the 0.25 km simulation (in the other simulations, the maximum heights are often found in the later period). Nevertheless, we can conclude that the higher the model horizontal resolution is, the higher the cloud overshooting top will reach in the lower stratosphere. As for the 10 km simulation with parameterized convective cloud, as mentioned in the previous question, the height of cloud overshooting top depends on the environmental characteristics as well as on many parameters of the convection scheme, namely on how entrainment and detrainment is calculated. It will not be reasonable to compare directly the 10 km simulation with the other high resolution simulations, even though the maximal cloud top height of 10 km simulation (16.13 km) is lower than all the other high resolution simulations. We modified the manuscript and discussed this point later in the manuscript:

“It is not a surprise that the higher resolution NWP models tend to produce stronger direct vertical transports across the tropopause because, as shown in Subsection 3.1, the transport is closely related to the strength of overshooting and the breaking of the gravity waves. Similar to what was found by Weisman et al. (1997), we find in our GEM simulations that the simulated maximal vertical wind speed is inversely proportional to the horizontal grid-spacing of the NWP model. The stronger vertical wind speed in the convection updraft leads to higher cloud overshooting top. In our cases with high resolution simulation, the maximum cloud top altitude is 16.64 and 16.96 km for 2.5 and 1.0 km simulation respectively. We find that the stronger overshooting wind speed in the higher resolution simulations leads to favorable conditions for gravity wave breaking (see the discussions in Subsection 3.1) and thus more direct vertical transport. This agrees with Dauhut et al. (2018). In total, the direct vertical transport of water vapor contributes to 40% of the total transport at the tropopause level for the 2.5 km simulation and makes up to 89% for the 1.0 km simulation.”

6. Page 4, line 29: It is confusing (and possibly misleading) to refer to the aircraft flight paths as “trajectories”. It would be better to use terminology such as “flight path” or “aircraft altitude profile”.

Done.

7. Page 5, lines 1–10: Smith et al. (2017) also did a trajectory analysis to determine the convective systems responsible for the observed lower-stratospheric water vapor plumes. It would be helpful if the authors compared the results/conclusions from the trajectory analysis done here with Smith et al. (2017).

Smith et al. (2017) focused on the high water vapor content observed by the ER-2 aircraft between ~19:30 to ~19:50 UTC (the third dive in Fig. 2 in our manuscript) in the north-most part of domain B at the level near ~100 hPa. The source of the humid air parcels observed there are mostly traced back to the convection east to the Lake Superior between 26 Aug 2013 21:00 UTC and 27 Aug 2013 12:00 UTC (hereinafter named convection Day2). Our back trajectory calculation gives similar results as shown for a humid air parcel from the northeast of domain B (Fig. R2, dashed back tracking line) which is traced back to the area of convection Day2. We note that the simulated convection initiated at the end of 26 Aug is slightly north to the real convection observed by satellite image (a location error in the simulated convection). This

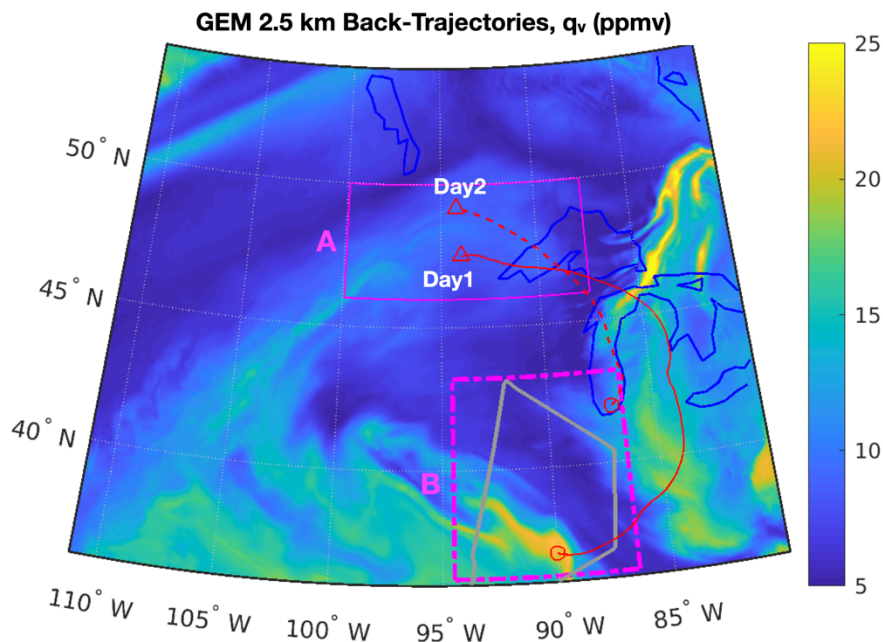
justifies the use of average of domain B, as opposed to individual location(s), for the evaluation so that humid areas linked to the convection Day2 are always included.

5 One of the foci of current paper is the average of water vapor content profile in the domain B. As explained above, this is designed to tolerate the spatial-temporal errors of the model simulations. For the southwest of domain B, the humid air parcels are mostly traced back to the convection that happened east to the Lake Superior between 25 Aug 17:40 UTC and 26 Aug 05:40 UTC (hereinafter named convection Day1). This is shown in Fig. R2 by the solid red back trajectory line. Having inspected these trajectory results, we found that the contribution for the average water vapor content in domain B by the convection Day1 (southwest) is more important than that of the convection Day2 (northeast). We therefore focused more on the convection Day1 in most parts of the manuscript, e.g. the convection shown in Fig. 3 as well as the budget analysis in section 3.4.

15 We added in the manuscript a brief discussion for the comparison with the results of Smith et al. (2017):

20 *“Using this technique, we find that the large water vapor anomalies observed by the aircraft in Domain B on 27 Aug 2013 originated from two deep convection events. The first one began at the end of 25 Aug and ended at the beginning of 26 Aug in Domain A (100° W to 87.5° W, 46° N to 50° N, ~860x445 km²) as illustrated in Fig. 1 (see more discussions below). This convection has major contribution to the water vapor content in the lower stratosphere of domain B. The second source is the convection began at the end of 26 Aug and ended at the beginning of 27 Aug in Domain A. This second convection increases the water vapor content in the northern part of domain A. This agrees with the results of Smith et al. (2017) in which the humid air parcels observed by the aircraft near 19:40 UTC (Fig. 1, northeast of domain B) are traced back to the convection began at the end of 26 Aug.”*

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30 Figure R2: background: water vapor mixing ratio at the altitude of ~15.5 km, 19:40 UTC 27 Aug; gray line: ER-2 aircraft path in 27 Aug; circles: starting points of back tracking from 19:40 UTC 27 Aug; triangles: ending points of back tracking: 22:40 UTC, 25 Aug for the parcel from the south of domain B (ended in the area of convection Day1); 21:00 UTC 26 Aug for the parcel from the northeast of domain B (ended in the area of convection Day2).

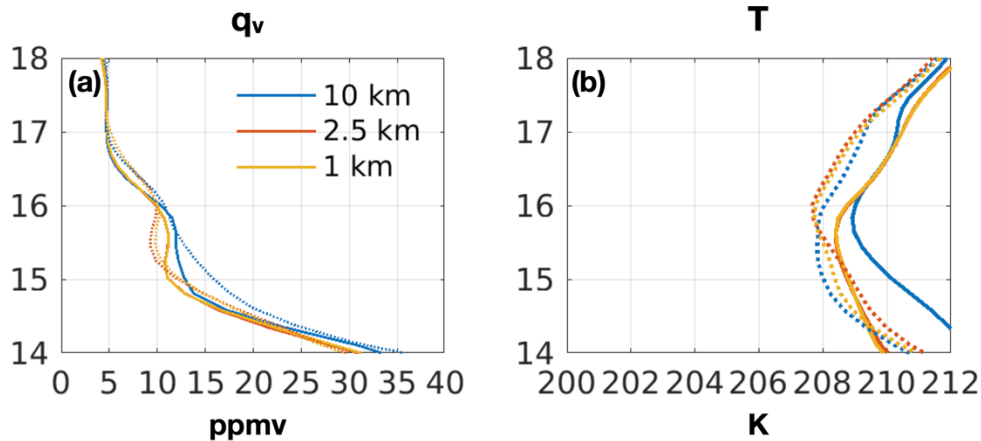
8. Figure 4 is presumably a longitude slice through Domain A. An x-axis should be provided. Also, does this slice correspond to a particular latitude, or are the authors averaging over latitude within Domain A?

The cross-section presented in Figure 4 is not along a longitude but along a skew line. We added a separated panel (e) in Figure 4 to show the location of this cross-section within the domain A.

5 9. Page 8, line 24: The authors discuss the simulated moisture enhancement in the lower stratosphere. How is this enhancement calculated? Is a difference taken between the post-convection moisture field and the pre-convection field?

10 Thanks, it's a good question. The profiles shown in Fig. 6a is for the average water vapor mixing ration during the 5 hours' evaluation time within domain A. The horizontal transport of water vapor should therefore have an impact on those profiles. In a more direct way, by comparing the averaged profiles before and after the convection in Fig. R3, we can see an enhancement of water vapor mixing ratio above the altitude of 16 km, but not between 15 and 16 km for the two high resolution simulations. This is mostly due to the horizontal transport of water vapor out of domain A through the western and southern borders. For the altitude between 15 and 16 km, the horizontal wind speed is fairly high (Fig. 5e). Therefore, the impact on the comparison of vertical profile is significant. On Fig. R4a, the water vapor mixing ratio field on the level of ~15.5 km is shown. At this time the convection just began. We find humid air in majority part of the domain A, except the westmost part. These humid areas are linked to the convection happened during the previous day (24 Aug). During the evaluation period on 25 Aug, the convection we focused on injected a large amount of water vapor into this altitude. Meanwhile, most of the humid air presented at the beginning of the evaluation time is moving out of the domain. This caused eventually a decrease of the average humidity within domain A as shown in Fig. R3a.

25 After rethinking about the statement here about the enhancement of water vapor, we considered that it is not suitable to mention it here because the conclusion could not be derived directly from Fig. 6a. A better way to evaluate the enhancement of water vapor is to calculate how much water vapor is transported vertically through the tropopause. This calculation is discussed in detail in the later section of the manuscript (section 3.4, budget analysis).



30 Figure R3: the mean profiles of water vapor volume mixing ratio (q_v) and temperature (T) for Domain A before (solid lines for 18:00 UTC, 25 Aug) and after (dotted lines for 23:00 UTC, 25 Aug) the convection.

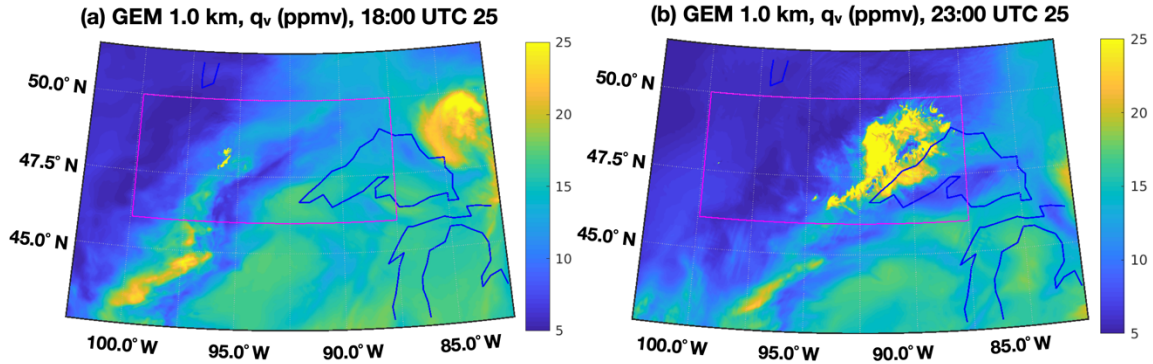


Figure R4: the water vapor mixing ratio field at the altitude of ~ 15.5 km before (a) and after (b) the convection on the day of 25 Aug. The magenta box represents the domain A.

5 The main purpose of Fig. 6a is to show that 10 km simulation produce clearly moister lower stratosphere than the two high resolution simulations. We modified the text as follow:

10 *“We further examine the water vapor fields simulated by GEM at different horizontal grid-spacings. Fig. 6a and 6b show the mean vertical profiles of water vapor volume mixing ratio and temperature within the afore-defined Domain A and 5-hour time window. All the simulations show irregular moisture profiles near 16 km, where the vertical trend of the humidity profiles bends and produces ‘bumps’ (elevated water vapor contents) above the tropopause (indicated by the circles in Fig. 6, hereinafter the tropopause is defined by the altitude where the mean lapse rate Γ within Domain A and 5-hour time window decreased to 2°C km^{-1} or less).”*

15 10. Page 9, lines 5–10: The authors discuss errors, uncertainties, and biases in the MLS H₂O retrieval. However, my understanding is that the 100-hPa retrievals that are most relevant for this paper are in good agreement with observations.

20 Agreed. In response to the comments of the other reviewer, we updated the way of comparison between MLS data and GEM data by applying the averaging kernel of MLS to GEM profiles. This allows a more coherent comparison as suggested by another referee. The results are shown in the updated Fig. 6c, 6d (or the Fig. R5c and R5d here). For the pressure levels near 100 hPa, we observed moister air from both GEM simulations which might indicate the overestimation of water vapor from the model simulation. The 10 km simulation gives even higher water vapor mixing ratio than the 2.5 km simulation and MLS, which evidences the positive bias in the low resolution model. On the other hand, near the levels of 160 hPa, we can see significant differences between the model simulations and the MLS retrievals. At these lower levels, the MLS data might subject to the negative bias reported by Hegglin et al. (2013), Vömel et al. (2007) and Livesey et al. (2018). This makes the comparison more uncertain; hence the validation against aircraft data is used.

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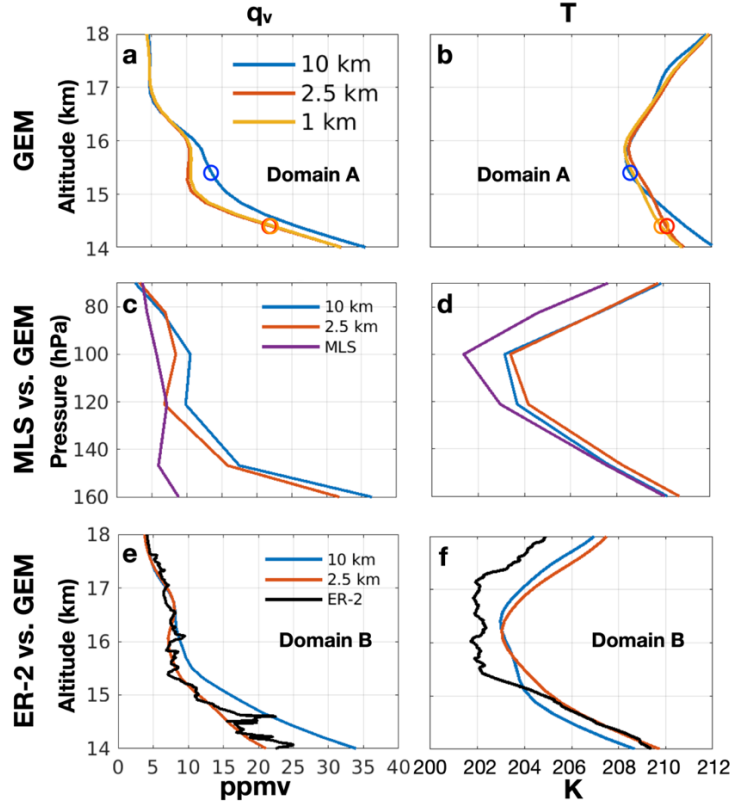


Figure R5: a), b) the mean profiles of water vapor volume mixing ratio (q_v) and temperature (T) for Domain A during the 5-hour period. The circles indicate the positions of the tropopause (mean $\Gamma < 2^\circ\text{C km}^{-1}$); c), d) mean profiles (q_v and T) after applying averaging kernels of MLS on GEM 2.5 km, 10 km simulation (100x100 km areas centred on 5 MLS footprints) and MLS profiles; e), f) the vertical profiles (q_v and T) within Domain B for GEM 10, 2.5 km simulations and for ER-2 aircraft *in situ* observations.

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We modified the text in the manuscript concerning the comparison between model simulations and MLS data:

10 “Figure 6c, 6d show the comparisons between the GEM simulations after applying averaging kernels of
 15 MLS and MLS retrievals (v4.2). Because of the scarcity of the collocated satellite data and also the afore-
 mentioned mismatch in time and location of the simulated convective system, we conduct the comparison
 with respect to area-averages rather than individual samples. The MLS measurements used here include
 20 five MLS footprints located between [38°N, 45°N] and [95°W 93°W], taken on 26 Aug 2013 around 19:00
 UTC, about 15 hours after the dissipation of the convection system (Fig. 7, red diamonds). We applied the
 averaging kernel of MLS on the mean profiles of GEM simulated humidity and temperature within the
 100x100 km regions centered on the MLS footprints. The comparison here suggests that both model
 25 simulations give higher estimations of water vapor content in the UTLS comparing to MLS retrievals,
 although the higher-resolution simulation better approximates the satellite observations. It is also found
 that GEM slightly overestimated the temperature comparing to MLS retrievals. This suggests that warmer
 temperatures in comparison to MLS could lead to slower ice crystal growth and thus less dehydration and
 thus higher gas-phase water. The spatial-temporal errors of the model simulation, e.g. shifted convection
 location or time, might also contribute to the discrepancies between the GEM and MLS profiles.
 Furthermore, the lower value of water vapor content from MLS near the level of 160 hPa may be subject
 to the aforementioned negative bias in the MLS data.”

11. Section 3.4: I believe this section could be better organized. There seems to be a fair amount of repetition, and the discussion seemed to meander. Perhaps this section could be more concise, and a sentence or two at the beginning outlining the analysis techniques would be helpful.

5 Please see the updated manuscript for the change of the section 3.4.

Responses to referee #2

Specific comments/questions:

5 Page 1, line 4: Maybe add here Riese et al. 2012. They showed also how small change in water vapor due to mixing processes change the radiative budget of the UTLS.

Reference added.

10 Page 2, line 24: Isentropic transport of water vapor due to planetary wave activity is also an important transport mechanism for transporting tropical tropospheric air into the lower extra-tropical stratosphere (see e.g. McIntyre and Palmer, 1983; Waugh, 1996; Homeyer and Bowman, 2012). I recommend to include this mechanism also in the manuscript to complete all transport pathways.

15 Thanks! It's added into the manuscript.

Page 2, line 33: I recommend to add the paper of Lee et al., 2019. They performed also high-resolution model simulation of an overshooting event in the Asian monsoon region and showed how the moistening occurred and how the hydrated air was transported in the lower stratosphere.

20 Reference added.

Page 4, line 34: In summer times the standard value in the extra-tropical lower stratosphere is more 5 ppmv (see Zahn et al. 2014 Figure 5). I would recommend to change the text from 4 to 5 ppmv.

25 Done.

Page 6, line 21: Here you state the time of Fig. 4 to be at 19:49. In the figure caption it is stated 19:46. Please correct one of these times.

30 Correction is done. The correct time is 19:46 UTC.

35 Where there any cloud instrumentation aboard the ER-2 for measuring cloud number concentration or IWC? If yes, did you check if there were still ice crystals present at flight altitude in the domain B. That would be interesting to see, because than the ice crystals would have been transported over a longer distance in the stratosphere. This transport is shown by the Lee et al. 2019 and it would be interesting to see, if it occurred also in your case.

40 Good point! We have checked the ice water content for the ER-2 flight within domain B. There are some areas we found the presence of ice with the IWC between 1×10^{-6} and 1×10^{-3} g/m³ at lower altitudes between 14 and 15.5 km below the tropopause level. Fig. R1b shows the ice water content observed by the aircraft. The horizontal locations of these ice are marked by red dots in Fig. R2 on the aircraft path (gray line). We traced the air parcels in the northern part of domain B from the altitude of 14 km back to 04:00 UTC when a more recent convection is happening in domain A. Particularly, the ice seen in the northeast part of domain B can be linked to the convection event as highlighted by the red rejectory. The back-tracing properties of this parcel are shown in Fig. R3. We can find that the formation of ice is near 04:00 UTC due to the convection (Fig. R3e). During the next 8 hours, the air parcel are slightly super-saturated (Fig. R3d). Therefore, the loss of ice is not due to the sublimation but the falling of ice to lower altitude. Near the time of 12:40 UTC, the relative humidity with regard to ice falls to below 1. All the remaining ice is quickly
50 sublimated within about half an hour. Nevertheless, the ice is then reforming near 13:40 UTC due to the

slow ascent of air with decreasing temperature and increasing relative humidity. The ice shown in Fig. R2 for the highlighted parcel is therefore not the ice originally formed during the convection, but formed later during the ascent of air about 6 hours before. We can also observe the impact of the dehydration due to the formation and the falling of ice near 15:40 UTC with a decrease of water vapor mixing ratio of ~ 20 ppmv.

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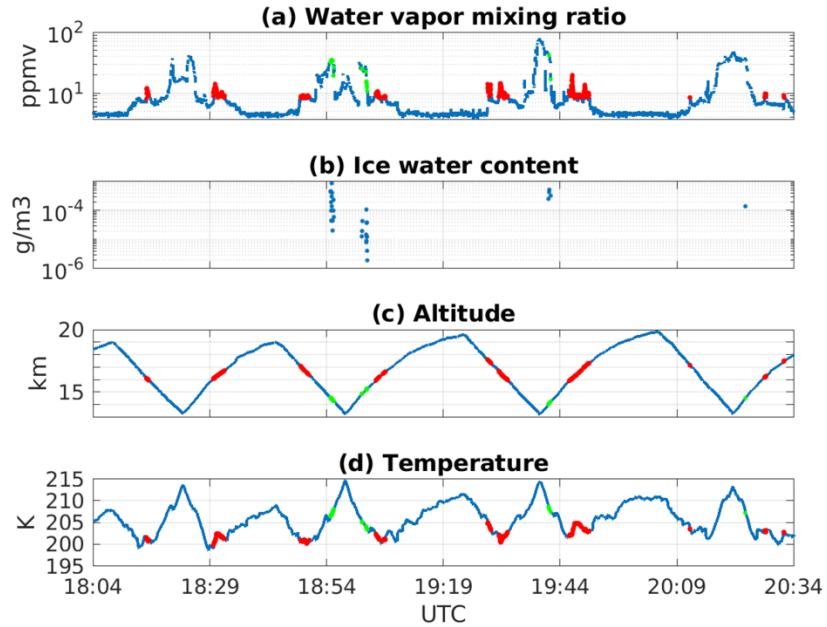


Figure R1: ER-2 aircraft observation of a) water vapor mixing ratio in ppmv in logarithmic scale, b) ice water content in g m^{-3} in logarithmic scale, c) altitude in km and d) air temperature in K, on 27 Aug 2013. The red dots highlighted the measurements with pressure lower than 115 hPa (tropopause) and water vapor volume mixing ratio greater than 8 ppmv. The green dots highlighted the measurements with the presence of ice.

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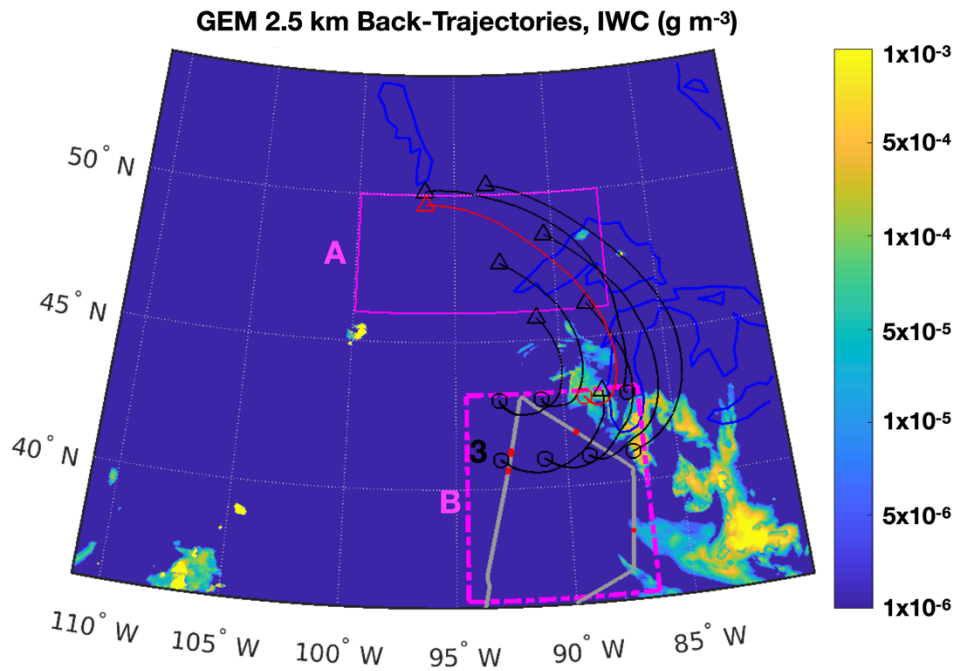


Figure R2: background: ice water content at the altitude of ~ 14 km, 1940 UTC 27 Aug; gray line: ER-2 aircraft path in 27 Aug highlighted by red dots for the areas with ice; circles: starting points of back tracking at 19:40 UTC 27 Aug; triangles: ending point of back tracking at 04:00 UTC 27 Aug.

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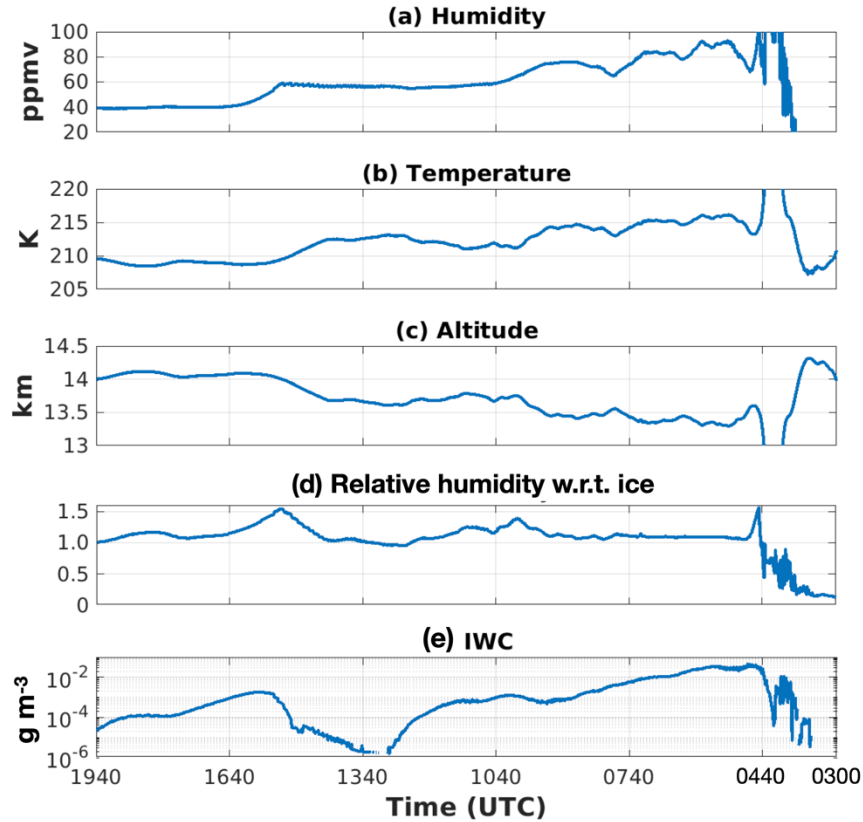


Figure R3: The changes of the properties of the highlighted air parcel in Fig. R2 along its back trajectory from 19:40 UTC to 03:00 UTC 27 Aug.

5 Similarly, in the GEM simulation even in a higher altitude above the tropopause we still found this formation of ice although with smaller ice water content (in the order of $\sim 1 \times 10^{-5}$, see updated Fig. 8). The origin of the humid air parcel is often linked to the convection that happened before. In the case of Fig. 8, it is the convection started from 25 Aug in the simulation. Since the formation of ice in higher altitudes above tropopause is much less significant than in lower altitudes. Contrary to the dehydration effect in Fig. R3 near 15:40 UTC, we didn't find a significant impact of dehydration in high altitudes (e.g. Fig. 8).
 10 Therefore, this will not change our conclusion by linking the water vapor injected in domain A with the simulated/observed water vapor in domain B for the altitudes above the tropopause.

Some new texts are added into the manuscript, the Fig R2 and R3 will be added to the SI materials:

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“One particular note for Fig. 8 is the formation of ice shortly after 19:40 UTC 27 Aug when the humid air parcel slowly ascends with decreasing temperature and increasing relative humidity with regard to ice. At these altitudes, the ice water content is relatively low ($\sim 1 \times 10^{-5} \text{ g m}^{-3}$). The ice particles will gradually fall to a lower altitude and eventually be sublimated again. This process will partly dehydrate the upper layer of the atmosphere where the ice is forming, and later hydrate the lower atmospheric layer through ice sublimation. However, this dehydration has minor impact for the air parcels above the tropopause. We observe that the water vapor mixing ratio of the air parcel at the 15.5 km altitude (i.e., the upper layer) increased slightly after 19:40 UTC (Fig. 8a). This might be the results of the mixing with the adjacent air in the northeast side of the parcel which is more humid (pointed by the black arrow in Fig. 7). Due to the limited impact of dehydration through ice formation above the tropopause, our interpretation of linking the stratospheric water vapor injected in domain A and water vapor simulated/observed in domain B is therefore not affected in a significant way by the ice formation process.”

5 For the atmospheric layer under the tropopause between the altitude of 13.5 and 14.5, the horizontal wind speed increases significantly. The back-tracking results show that the humidity and ice field in the northern part of Domain B are linked to the convection initiated at the beginning of 27 Aug in domain A. The locations of ice water content in domain B from the simulation partly agree with what are observed by the aircraft in Fig. 2b. Based on the back tracing results, we noticed that the ice in Domain B is not originally formed during the convection, but later during the slow ascent of the humid air parcel. This is similar to the hydration/dehydration process discussed above but at a lower altitude below the tropopause. The ice formed at this lower altitude is more abundant (in the order of $1 \times 10^{-3} \text{ g m}^{-3}$). The impact of dehydration (ice formation and falling) at this level is significant which can be seen in Fig. SI.3 near 15:40 UTC with an amplitude of about 20 ppmv. The readers are referred to the supplementary materials for more discussions on this topic (Fig. SI.2, SI.3).”

15 • Page 9, lines 5-10: Maybe it is worth a mention that the averaging kernels of limb sounders like MLS smear out the strong vertical gradient in water vapor at the tropopause (Hegglin et al., 2013).

Added to the manuscript.

20 • Page 9: The comparison between GEM and MLS is not really done in a balanced way. The difference is partly larger ($> 100\%$) than the biases which are reported in the literature. These strong differences can be hardly explained by just mentioned the possible bias of MLS water vapor. It could also be a result of the model simulation. For example, warmer temperatures in comparison to MLS could lead to slower ice crystal growth and thus less dehydration and thus higher gas-phase water, which could be transported into the lower stratosphere.

25 Thanks, this is a very good point! We modified the text as follow:

30 “We applied the averaging kernel of MLS on the mean profiles of GEM simulated humidity and temperature within the $100 \times 100 \text{ km}$ regions centered on the MLS footprints. The comparison here suggests that both model simulations give higher estimations of water vapor content in the UTLS comparing to MLS retrievals, although the higher-resolution simulation better approximates the satellite observations. It is also found that GEM slightly overestimated the temperature comparing to MLS retrievals. This suggests that warmer temperatures in comparison to MLS could lead to slower ice crystal growth and thus less dehydration and thus higher gas-phase water. The spatial-temporal errors of the model simulation, e.g. shifted convection area, and time, etc., might also contribute to the discrepancies between the GEM and MLS profiles. Further, the lower value of water vapor content from MLS near the level of 160 hPa may be subject to the aforementioned negative bias in the MLS data.”

40 The averaging kernels of MLS are applied to the GEM profiles for a more suitable comparison. The Fig. 6c and 6d are modified accordingly.

Can you please comment on the following questions and suggestions?

- Which Version of MLS data are you using (this would be also nice to mention in the text)?

45 The version used in this study is v4.2. We added this information to the manuscript.

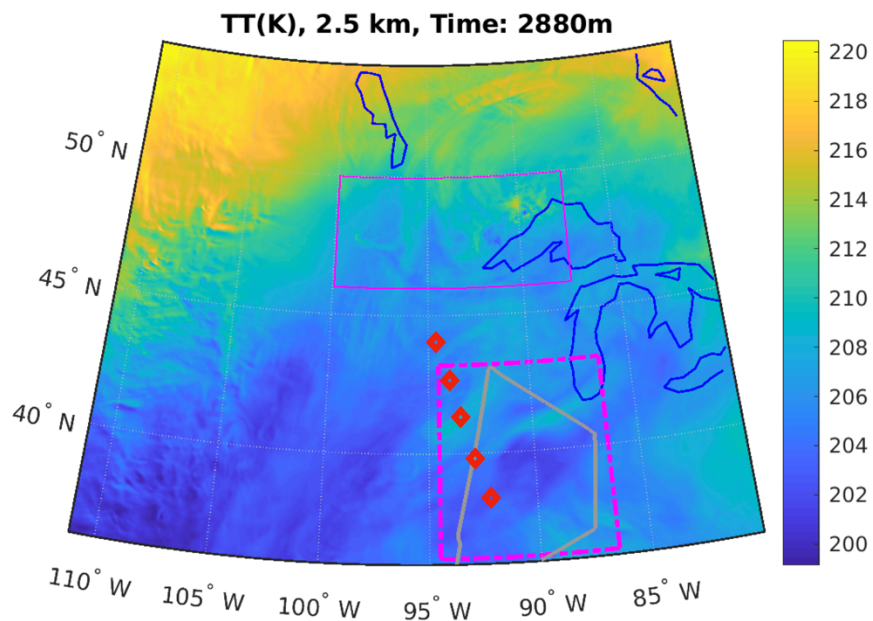
- Did you apply the averaging kernels of MLS onto the GEM profile? Otherwise a fair comparison is barely possible. Why not using the exact location of MLS and applying the averaging kernels?

The averaging kernel was not applied in the original version. We added the comparison applying the averaging kernel in the updated version (see answer above). This does not change the comparison results or any conclusion.

- 5
- Why are the profiles of water vapor (panel a/c/e) and also temperature (panel b/d/f) so different? They should both represent air masses moving from domain a to domain b as shown by the trajectories. It seems that the situation is strongly variable. Can please discuss in the text about the standard deviation of the mean profiles to get a better feeling on the variability.

10 One factor causing the differences in profiles is that there is a slow but persistent vertical movement of air as shown both in Fig. 8c in the manuscript and Fig. R3c in this response document. This will change the form of the profiles. For example, the ‘bump’ in humidity profile in Fig. 6a is at the level of 16 km, while it moves to 16.7 km in Fig. 6e which is coherent with the slow ascending motion. Other factors such as the large circulation, radiative heating/cooling and the significant differences in latitude which results a warmer tropopause temperature in the north (domain A) and a cooler one in the south (domain B) (Fig. R4).

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20 Figure R4: the temperature field at the altitude of 16 km, at 23:00 UTC 25 Aug. Magenta solid line zone: domain A (profile a/b); magenta dash-dot line zone: domain B (c/f); red diamonds: MLS footprints (c/d).

- For better understanding of the deviation between GEM and MLS, I would also recommend to add the location of the MLS profile also into the map in Figure 7.

25 Done

30 Figure 8: You show some parameters of an individual trajectory in this figure. The water vapor amount with ~20 ppmv is quite high and the temperatures are cold between 203-206K, which could create conditions with supersaturation wrt ice. and therefore, additional ice formation. Do you see any signs of ice formation in the lower stratosphere along these trajectories? This could be important, because it could partly dehydrate the previously hydrated air masses.

For this particular air parcel, the formation of very thin ice does happen during the ending hours. More discussion is added into the manuscript for the dehydration effect by the formation of the ice (see the answer above). The ice water content and relative humidity are added to the Fig. 7 in the manuscript.

- 5 • Page 10-11: For me it is not clear, which part of the equation 5 account for ice sublimation/transport? Because in the equation only q , which stands for water vapor, is considered. Can you please better explain how you estimated the change due to advection and ice sublimation as stated in lines 16-20.

10 We clarify that the equation is used for analyzing and understanding the direct transport. In the manuscript, we try to use the Reynolds decomposition to investigate the importance of injection due to gravity wave breaking with regard to the direct transport only. We argue that for the high-resolution simulation, the majority of the direct transport is linked to the gravity wave breaking. Ice sublimation is therefore not taken into account in Eq. 5.

- 15 • Page 12-14: Where does the sublimation occurs in the high-resolution models? Is it directly in the overshoot or are the ice crystals first mixed into the lower stratosphere by wave breaking and small-scale mixing and then sublimate? Which brings me to a further question, if ice crystals are transported along the trajectories in the lower stratosphere? Perhaps, you can add this information also into the manuscript.

20 In the high-resolution simulations, ice was firstly brought to the lower stratosphere within the cloud overshooting tops. There the ice cannot be sublimated efficiently. During the fall of the overshooting top the gravity wave breaking happens, a fraction of ice in the overshooting top will be brought into lower stratosphere in an irreversible way (no downward movement to bring then back to troposphere, only relying on sedimentation). Further, the humid air transported into the lower stratosphere might be supersaturated depending on the temperature of the reached altitude. This will be a second contribution to the ice plume. These plumes will gradually be sublimated through mixing with dryer air or be sediment to a lower altitude. In our simulation at 1.0 km grid-spacing, these plumes will not last for a long time (generally less than 1 hour) before they disappeared completely near the convective zone. We added the description for ice staying in lower stratosphere in the manuscript:

30 *“Ice plumes are also formed near the areas where the gravity wave breaking happens. Two sources are found: the direction transport of ice and the formation of ice under supersaturation condition within humid plumes. The sizes of ice plumes are generally smaller than those of the water vapor plumes, because ice will be completely sublimated/sediment within a short period of time, generally within one hour.”*

- 35 • Page 13/14: What does a negative sublimation tendency mean? I would guess it is additional ice formation or particle growth. Or is it both?

40 The notion ‘sublimation’ presented in the manuscript denotes the dynamical effect of both ice sublimation and vapor deposition. The negative value signifies that the vapor deposition is faster than the ice sublimation, hence dehydration. We realize that the use of ‘sublimation’ in might cause confusion. Additional explanation is added to clarify the definition of sublimation:

45 *“Ice sublimation (hydration) and vapor deposition on ice (dehydration) are two opposing microphysical processes competing for dynamical balance. We use hereinafter ‘sublimation’ to denote the combined effect of these two processes. The positive value signifies that the ice sublimation is faster than the vapor deposition, and the negative value signifies the other way around.”*

- 50 • Page 14: I agree with your conclusion that ice sublimation occurs less pronounced in the high-resolution model because of existence of ice crystals mostly in the overshooting core. In the relative humidity

distribution (Figure 12 b) I would expect higher fraction of IWC in the sub-saturated region ($R_{hi} < 1$) for the low resolution compared to the high resolution, if there is a much higher sublimation rate. Do you have an explanation for the agreement of IWC distribution in sub-saturation for all three model setups?

5 In 10 km simulation (Fig. 11d and 11g), we can find that the majority of the ice at this altitude is located in an area of slight supersaturation ($r_{hi} \sim 1.09$). This means that the majority of the ice is not sublimating, but slowly growing by vapor deposition. This can be seen in Fig.11a that in the cloudy area the vapor deposition is happening although with slow rates (light blue area). The areas where we find high ice sublimation rates are near the northern edges of the cloudy area due to the mixing with the dry stratospheric air. These areas have an important contribution for the mean sublimation rate in the domain A, and their relative humidity tends to be sub-saturated, although their ice mass fraction in domain A is not significant. This can be one of the reasons why in Fig.12b the majority of the ice is slightly supersaturated rather than sub-saturated.

15 Another important factor is the way GEM calculates the dynamic and physical processes. At a given time step, GEM calculates the dynamic processes first (advection, etc.) and then the physical processes (microphysics, etc.). After the dynamic calculations, the sub-saturation should be very pronounced on the edge of the cloudy area, but the properties are not saved until the physical processes are finished which reduces quickly the sub-saturation due to the sublimation. Considering that in the 10 km simulation the time step is set to 5 min which is long enough to reduce the sub-saturation produced by the mixing with dry stratospheric air (dynamics).

Technical comments/suggestions:

25 Page 8, line 8: Citation should be Vömel et al.

Done

Page 14, line 9: It is more common to use the term supersaturated instead of oversaturated.

30 Done

Figure 2: Can you please include the date of the ER-2 measurements into the figure caption.

Done

35 Figure 4: The comprehensibility of the vertical wind speed in panel d would be better, if you choose a color scale centered with the color white at the value of 0 and with positive/negative values in two different colors (e.g. red and blue).

40 Done

Figure 5: Same suggestion above for panel c and d.

Done

45 Figure 12, caption: "relative humidity" instead of "relatively humidity"

Done

Simulation of convective moistening of extratropical lower stratosphere using a numerical weather prediction model

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Abstract. Stratospheric water vapor (SWV) is a climatically important atmospheric constituent due to its impacts on the radiation budget and atmospheric chemical composition. Despite the important role of SWV in the climate system, the processes controlling the distribution and variation of water vapor in the upper troposphere and lower stratosphere (UTLS) are not well understood. In order to better understand the mechanism of transport of water vapor through the tropopause, this study uses the high resolution Global Environmental Multiscale model of the Environment and Climate Change Canada, to simulate a lower stratosphere moistening event over North America. Satellite remote sensing and aircraft *in situ* observations are used to evaluate the quality of model simulation. The main focus of this study is to evaluate the processes that influence the lower stratosphere water vapor budget, particularly the direct water vapor transport and the moistening due to the ice sublimation. In the high-resolution simulations with horizontal grid-spacing less than 2.5 km, it is found that the main contribution to lower-stratospheric moistening is the upward transport caused by the breaking of gravity waves. In contrast, for the lower-resolution simulation with horizontal grid-spacing of 10 km, the lower-stratospheric moistening is dominated by the sublimation of ice. In comparison with the aircraft *in situ* observations, the high-resolution simulations predict well the water vapor content in the UTLS, while the lower resolution simulation over-estimates the water vapor content. This overestimation is associated with the overly abundant ice in the UTLS along with too-high sublimation rate in the lower stratosphere. The results of this study affirm the strong influence of overshooting convection on the lower-stratospheric water vapor and highlight the importance of both dynamics and microphysics in simulating the water vapor distribution in the UTLS region.

1. Introduction

Stratospheric water vapor (SWV) strongly influences the Earth radiation budget (IPCC, 2013) and stratospheric chemistry (e.g., Anderson et al., 2012). Global climate models (GCMs) generally project an increase of SWV during global warming, which may lead to cooling of the stratosphere and further warming of the troposphere and surface (Forster and Shine, 1999, 2002; Solomon et al., 2010; Riese et al. 2012) and thus constitutes a potentially important climate feedback mechanism (Dessler et al. 2013; Huang 2013; Huang et al. 2016; Banerjee et al. 2019). Dessler et al. (2013) estimated the SWV feedback to be +0.3 W/(m² K). Especially emphasized in these previous studies is the

importance of SWV in the extratropical lowermost stratosphere, which has the most significant impact on the energy budget at the top of the atmosphere.

5 Despite its importance, the processes that control the distribution and variation of water vapor in the upper troposphere and lower stratosphere (UTLS) are not well understood. Large discrepancies are found between the “A-Train” satellite observations and the GCMs of the Phase 5 of the Coupled Model Inter-comparison Project (CMIP5) (Jiang et al. 2012). This study shows that the ratio of water vapor content in the GCMs to that from satellite observations can be as large as 2 to 5 in the mid-latitude UTLS region. Such discrepancies cast significant uncertainty in the SWV radiative feedback simulated by the GCMs (Huang et al. 2016). Global reanalyses also suffer from SWV biases, including the 10 Modern- Era Retrospective Analysis for Research and Applications (MERRA), its newer release MERRA2 and the Interim Reanalysis of the European Centre for Medium-Range Weather Forecasts (ECMWF) (Jiang et al., 2015). One of the motivations of this study is therefore to investigate the possible causes of such overestimation of water vapor in the UTLS in GCM and numerical weather prediction (NWP) models.

15 The mechanisms controlling the transport of water vapor into the stratosphere are different for the tropical and mid-latitude regions. In the tropical region, water vapor enters the stratosphere primarily through the slow ascent associated with the Brewer-Dobson Circulation (BDC) (Brewer, 1949). The cold temperature of the tropical tropopause layer (TTL) regulates the humidity of the air and therefore is responsible for the moistening of the stratosphere. However, it remains uncertain how factors such as the temperature in the TTL, strength of the BDC, and the vertical and 20 horizontal mixing are weighted to determine SWV distribution and variation (Fueglistaler et al., 2014). In extratropical region, there are several mechanisms that can influence the distribution and variation of the water vapor in the lower stratosphere (Weinstock et al., 2007). Water can be transported to the lowermost extratropical stratosphere by poleward transport from the TTL, [by isentropic transport due to planetary wave activity from the tropical troposphere](#), and by deep convection in the extratropics. Among these mechanisms, the vertical transport by mid- 25 latitude convection, although demonstrated to be impactful by studies using *in situ* and remote sensing measurements, remains poorly understood (Poulida et al., 1996; Hegglin et al., 2004; Dessler and Sherwood, 2004; Ray et al., 2004; Hanisco et al., 2007; Weinstock et al., 2007; Homeyer et al., 2014, 2017; Sun and Hang 2015, [Smith et al., 2017](#)).

30 A few studies have attempted to simulate the injection of water into the lower stratosphere using high-resolution NWP models. These studies found that the transport of water vapor into the stratosphere occurs through gravity wave breaking near overshooting tops (e.g., Wang, 2003; Wang et al., 2009, 2011; Homeyer et al., 2017; Dauhut et al. 2018, [Lee et al., 2019](#)). The overshooting tops form as strong updrafts within convective cells penetrate the stable stratification at the tropopause. They act as obstacles to the lower stratospheric flow and generate gravity waves. In favorable conditions (Baines, 1995; Sachsperger et al., 2016), the gravity waves break near the cloud overshooting 35 tops, dissipate wave energy through strong turbulence and cause sudden “jumps” of air flow up to more than 2 km height. This upward wind with strong turbulence transports a substantial amount of water vapor and ice into higher altitude in the stratosphere. The mechanism of gravity wave breaking is well demonstrated, e.g., by Figure 7 in Wang

(2003). An associated phenomenon is the so called “jumping cirrus” (Fujita 1982), which provide evidences that ice particles are brought into, and potentially hydrate, the lower stratosphere. The mechanism of cross-tropopause transport of humidity associated with gravity wave breaking is generally well simulated using idealized forcing for a short duration over a limited domain (Wang, 2003; Wang et al., 2009, 2011; Homeyer et al., 2017; Dauhut et al., 2018). In order to evaluate model results against satellite and aircraft measurements it is necessary to develop an experimental framework in which high resolution simulations can be performed over an extended period in which observations are available.

In this study, we use a high-resolution NWP model, Global Environmental Multiscale (GEM), to simulate an observed lower stratospheric moistening event over North America from 26 to 27 Aug 2013 (Smith et al. 2017). The first objective is to evaluate the model capability to successfully simulate the vertical transport of water vapor through mid-latitude tropopause and reproduce the observed increase of lower stratospheric humidity during and after the deep convection event. The second objective is to evaluate, using all available satellite and aircraft measurements, the simulated water vapor fields at different horizontal resolutions, ranging from low resolution with parameterized deep convection to high resolutions with explicitly simulated convection. The third objective is to compare processes, such as direct water vapor transport versus ice sublimation, that influence the lower stratosphere water vapor budget. *In the global NWP and GCM models, the deep convection is parameterized using mass flux approach. The complex phenomena near the tropopause during the convection are parameterized in a simplified manner, e.g. overshooting convection, or not parameterized, e.g. the falling of cloud overshooting tops (not sedimentation), gravity wave breaking and formation of jumping cirrus, etc.* In light of the aforementioned lower stratospheric humidity bias in coarse resolution models, we are especially interested to identify possible causes of such biases.

This paper is structured as follows. The next section provides a brief description of the GEM model and the configuration of the simulation experiment, as well as the observation data for comparison and a trajectory model used to link the simulated and observed samples. This is followed by the analysis of the GEM simulation results, with a focus on the lower stratospheric water vapor budget. We then conclude with a summary of the findings and perspectives for further studies.

2. Method

2.1 NWP model simulation

The NWP model used in this study is the GEM model of Environment and Climate Change Canada (hereafter ECCC, Côté et al., 1998; Girard et al., 2014). The dynamics of GEM are formulated in terms of the non-hydrostatic primitive equations with a terrain-following hybrid vertical grid. It can be run as a global model or a limited-area model and is capable of one-way self-nesting. Milbrandt et al. (2016) described the self-nesting configuration with horizontal grid-spacing $\Delta x \geq 2.5$ km; Leroyer et al. (2014) and Bélair et al. (2017) did the same for $\Delta x = 0.25$ km. For the experiments reported here, four self-nested domains are used with areas of 5000x3600, 3000x2000, 1500x1000 and 375x375 km²

which corresponds to horizontal grid-spacings of 10, 2.5, 1 and 0.25 km, respectively. The four nested domains are shown in Fig. 1. All simulations use 77 vertical levels, with vertical grid-spacing $\Delta z \approx 250$ m in the UTLS region.

5 For the three high-resolution simulations with 2.5, 1 and 0.25 km horizontal grid-spacings, the double-moment version of the bulk cloud microphysics scheme of Milbrandt and Yau (2005a, b; hereinafter referred to as MY2) is used. This scheme predicts mass and number mixing ratio for each of six hydrometeors including non-precipitating liquid droplets, ice crystals, rain, snow, graupel and hail. Condensation (ice nucleation) is formed only upon reaching grid-scale supersaturation with respect to liquid (ice). For the simulation with 10 km horizontal grid-spacing, the Kain-Fritsch deep convection scheme (Kain and Fritsch, 1990, 1993; hereinafter referred to as KFC) is incurred. The liquid and solid cloud water content from KFC scheme are later passed to the MY2 scheme as hydrometeors of non-precipitating liquid droplet and ice crystal category, respectively.

15 In addition to the MY2 and KFC schemes, the planetary boundary-layer scheme can also produce implicit clouds, particularly cumulus and stratocumulus (Bélaïr et al., 2005). It predicts mean liquid and ice water contents as well as cloud fraction. The shallow convection scheme (Bélaïr et al., 2005) is the third means by which GEM can produce clouds. It predicts mean liquid and ice water contents and cloud fraction for cells that contain shallow cumulus clouds.

20 The simulation at 10 km grid-spacing is initialized with conditions from the ECCC global atmospheric analysis at 00:00 UTC 24 Aug 2013. It runs for 96 hours until 00:00 UTC 28 Aug 2013. The second nested simulation at 2.5 km grid-spacing runs for the same period of time. The simulations at 1 and 0.25 km grid-spacing are initialized at 12:00 UTC 25 Aug 2013 and run for 24 hours during which the convective event that we focus on in this study developed. Model outputs are saved every 1 minute for the 2.5, 1 and 0.25 km simulations and every 5 minutes for the 10 km simulation.

2.2 In situ observation

25 We use the water vapor measurements from a NASA field campaign, the Studies of Emissions and Atmospheric Composition, Clouds and Climate Coupling by Regional Surveys (SEAC⁴RS, Toon et al., 2016). During this campaign, an ER-2 aircraft provided *in situ* high altitude observations in the UTLS region. These data are used here to verify the model simulated water vapor content at the lower stratosphere. The ER-2 flight on the day of 27 Aug 2013 began from Huston at 16:46 UTC. It performed four descending-ascending movements between ~20 km and ~13 km height crossing the tropopause between 18:00 and 21:00 UTC in an area to the south of the Great Lakes (cyan lines in Fig. 1). The locations where the descending trajectories ended and corresponding times are shown in Fig. 1. The humidity data used here are from the Harvard Lyman- α photo-fragment fluorescence instrument (hereafter named LYA, Hintsa et al., 1999; Weinstock et al., 2009) and are shown in Fig. 2. The corresponding altitude and temperature are also shown in this figure. The measurements with air pressure lower than 115 hPa and water vapor concentration are also shown in this figure. The measurements with air pressure lower than 115 hPa and water vapor concentration higher than 8 ppmv are marked in all the three panels. These measurements indicate water vapor contents much higher than the standard values (~5 ppmv) in the lower stratosphere. [Some areas with ice water content between the altitude](#)

of 14 and 15.5 km are also observed by the Fast Cloud Droplet Probe (SPEC Inc.) onboard the ER-2 aircraft which suggests the possibility of long distance transport or the formation of ice in these areas.

2.3 Back trajectory simulation

5 In order to include all the different convective events potentially responsible for the moistening of the lower stratosphere captured by the aircraft measurements on 27 Aug 2013, we start the GEM simulations with the largest, low resolution domain (see Fig. 1) and several days earlier. Several mesoscale convective events developed on different days near the Great Lakes within this domain. To identify the source of water vapor for the aircraft-measured samples, the back trajectories of the air parcels are simulated using the trajectory model, LAGRANTO (Sprenger and Wernli, 2015) and GEM-generated wind fields. *Using this technique, we find that the large water vapor anomalies*
10 *observed by the aircraft in Domain B on 27 Aug 2013 originated from two deep convection events. The first one began at the end of 25 Aug and ended at the beginning of 26 Aug in Domain A (100° W to 87.5° W, 46° N to 50° N, ~860x445 km²) as illustrated in Fig. 1 (see more discussions below). This convection has major contribution to the water vapor content in the lower stratosphere of domain B. The second source is the convection began at the end of 26 Aug and ended at the beginning of 27 Aug in Domain A. This second convection increases the water vapor content in the*
15 *northern part of domain A. This agrees with the results of Smith et al. (2017) in which the humid air parcels observed by the aircraft near 19:40 UTC (Fig. 1, northeast of domain B) are traced back to the convection began at the end of 26 Aug.*

3. Model results and analysis

3.1 Convective system

20 We first examine how well GEM simulates the general features of the deep convection events of central interest (within Domain A). Figure 3 shows the brightness temperature for the middle-infrared atmospheric window, which indicates the cloud top height, synthesized from the GEM simulations at different horizontal resolutions and observed by GOES-13 geostationary satellite (the 11.2 μm channel, Knapp et al., 2018). The synthetic radiances are calculated for the 10.2-12.2 μm spectral interval using the Rapid Radiative Transfer Model for GCMs (RRTMG, Mlawer et al,
25 1997; Iacono et al., 2000, 2008) with GEM-simulated atmospheric and surface properties as inputs. The target convective event simulated by the high-resolution models (2.5, 1 and 0.25 km) begins at around 18:00 UTC 25 Aug. The convection is initiated a bit later in the 10 km grid-spacing simulation, at around 21:30 UTC. To account for this difference, the synthetic images from model simulations are all taken at 5 hours after the initiation of the convection. The 0.25 km simulation is limited to a small domain due to the limits of computational resources. Its domain is centered
30 where the convection is initiated (95.5 W, 48.5 N). With an eastward movement, parts of the storm system quickly move outside of the simulation domain. We therefore do not include the 0.25 km simulation for the comparison in Fig. 3.

From Fig. 3, we can identify the location and extent of the convective system from the white-colored areas that signify low cloud top temperatures (high cloud tops). GEM succeeds to predict a strong convective system in the area near the Great Lakes. The locations of the convection are slightly different from one simulation to another. The 10 km simulation places the convective system west of Lake Superior. The two higher resolution simulations put the same convective system slightly north-west of Lake Superior. The satellite imager shows the storm system over Lake Superior. Another difference is the horizontal extent of the anvil clouds. The two higher resolution simulations generate anvil clouds of very similar forms to the observation. The 10 km simulation however generates clouds that extends in the northeast-southwest direction and covers a noticeably larger area than what is observed by the satellite. We notice that the 10 km simulation has a larger area with the brightness temperature lower than 210 K (magenta line highlighted areas) than those in the high-resolution simulations as well as that in the GOES-13 images. These highlighted zones with cold cloud tops represent the intensive convective areas. For all three simulations with different horizontal grid-spacings, the convective areas are all located within Domain A during the 5-hours period after the initiation of convection.

In order to inter-compare the simulations at different resolutions, we perform the evaluation for Domain A which encompasses the convective event of interest in the three simulations at 10, 2.5 and 1 km grid-spacing. The time window for the evaluation is the initial 5 hours of the convection development. During this time, the convection system of interest initiated, developed multiple overshooting tops and moved from the west to the east end of Domain A. At the end of the evaluation time window, the heights of overshooting tops are observed to generally decrease (not shown), which evidences that the chosen window captures the primary cross-tropopause transport of water by the convective system. Due to its limited domain area, the results of the 0.25 km simulation are not included for Domain A-based inter-comparisons. Instead, the first hour of the convection event in this simulation (before the system begin to move out of the simulation domain illustrated by the green box in Figure 1) is analyzed for comparing some aspects of the convection (see below).

3.2 Overshooting tops and gravity wave breaking

We examine the overshooting tops in the GEM simulation and especially the gravity wave breaking process that was found to primarily account for the water transport into the lower stratosphere in overshooting events. In our simulations, we find both the 1 and 0.25 km simulations generate similar structure of “jumping *cirrus*” to the previous studies (e.g., Wang et al. 2009, 2011). To illustrate the results, we show in Fig. 4 vertical cross-section in Domain A at 19:46 UTC on 25 Aug from the 1 km simulation. In addition, two movies made from this simulation are included in the Supplementary Materials (Qu, 2019).

Figure 4 shows a few key variables that highlight the impacts of overshooting tops and induced gravity wave breaking. Two overshooting tops are well identified between the longitudes of 95.94° W and 95.57° W by the upward extruding isentropic lines in Fig. 4a. The temperature within the overshooting tops are noticeably colder. To the right of the overshooting tops near 95.60° W, the region with overturned isentropic lines and convective instability ($d\theta/dz <$

0) is marked by a red circle. As found in the previous studies (e.g., Wang 2003; Wang et al. 2009, 2011), this instability develops in association with the breaking of gravity waves near the overshooting tops. The wave breaking leads to sudden jump of air flow and transports both ice particles and water vapor upward into higher altitudes in the stratosphere, which is visible from the IWC and water vapor distributions in Fig. 4b and 4c. At the time shown in Fig. 4, the wave breaking region mentioned above is forming a “jumping *cirrus*” patch that is marked by the red arrows. Two other jumping *cirrus*, formed earlier, can be found near -96.10° W and -95.75° W, as marked by the two magenta arrows. In our simulations, we find that the jumping *cirrus* can extend to 2 to 3 km above the tropopause (~14.5 km, according to the WMO definition, i.e., the altitude with lapse rates Γ decreased to 2 °C km⁻¹ or less). The lower stratospheric regions around the jumping *cirrus* are also characterized by high water vapor concentrations (up to 20 ppmv, see Fig. 4c). The water vapor plumes generated are typically 10 x 10 km² or less in size. However, in some cases, continuously occurring overshooting produces aggregated plumes, which have a size as large as 30 x 30 km². The continuous development of the overshooting tops, breaking gravity waves and jumping *cirrus* are shown by the movie in the Supplementary Materials (Qu, 2019). Ice plumes are also formed near the areas where the gravity wave breaking happens. Two sources are found: the direction transport of ice and the formation of ice under supersaturation condition within humid plumes. Their sizes are generally smaller than those of the water vapor plumes, because ice will be completely sublimated/sediment within a short period of time, generally within one hour.

The cloud ice properties are different in the overshooting tops and in the thin ice plumes. At the altitude of ~15.5 km (~ 1 km above the tropopause) within domain A at 19:42 UTC 25 Aug, the ice water content in the overshooting tops is relatively high with values from ~0.5 g m⁻³ up to ~2.8 g m⁻³. In the thin ice plumes the ice water content is generally lower than 0.1 g m⁻³. We calculated the effective radius for each solid category, e.g. ice crystals, rain, snow, graupel and hail. We find that in the cloud overshooting tops, the mass weighted effective radius for ice increases with the ice water content from ~300 to ~700 μm. On the other hand, the mass weighted effective radius for thin ice plume is usually lower than 30 μm. The area of cloud overshooting top occupies only 2.3% of the cloudy area but contains 68% of the total ice mass at this altitude.

We find in our simulations that the breaking of gravity waves occurs in many ways similar to the breaking of lee waves, which are formed when air flows through a mountain range. On the leeward side of the mountain, when the wave amplitude reaches a critical level, a convectively unstable region develops and consequently leads to wave breaking (Wurtele et al, 1993; Dörnbrack, 1998, Strauss et al, 2005). In the regime of gravity wave breaking, we can identify a sudden jump of the stratiform flow (Houghton and Kasahara, 1968). In its vicinity, wave energy is dissipated through turbulence which causes a strong mixing. It was found that such wave breaking occurs when the horizontal wind speed perturbation opposes the mean flow and causes stagnation, meeting a prognostic condition (Baines, 1995; Sachsperger et al., 2016):

$$|u'/U| \gtrsim 1 \quad (1)$$

where U is the mean flow speed and u' is the horizontal wind speed perturbation, which can be derived from the vertical wind speed perturbation w' using a 2-dimensional incompressible mass continuity constraint:

$$|\partial u' / \partial x| = |\partial w' / \partial z| \quad (2)$$

5 where x is the horizontal distance and z is the vertical height. Larger obstacles will generate larger w' which in turn derives larger u' . When u' is large enough to satisfy the condition in eq. 1, wave breaking occurs.

10 Analogies can be drawn to the gravity wave breaking near the overshooting tops. The overshooting tops carry air mass of different horizontal velocity into the lower stratosphere and act to block the pre-existing horizontal flow there (westerlies, speeds ranging from 5 to 25 m/s at different altitudes). The obstructed stratified flow in the lower stratosphere is forced to pass around the overshooting tops, creating a similar situation to air flow passing a mountain range and inducing gravity waves.

15 Fig. 5 shows several key variables for the same cross-section shown in Fig. 4 but 4 minutes earlier (19:42 UTC) when the condition of gravity wave breaking (eq. 1) is satisfied. At this moment before the formation of “jumping *cirrus*”, the cloud overshooting top near -95.6° W is falling after reaching its maximal altitude with a speed of $\sim 10 \text{ m s}^{-1}$ (Fig. 5c, dark blue area between the altitude of 15 and 16 km). This downward movement will eventually bring the majority of overshoot ice and vapor back to the equilibrium level below the tropopause. The falling of the overshooting top generates a strong vertical wind speed gradient (right hand side of eq. 2) just above the overshooting top near the altitude of 16 km. Using eq. 2, we calculated the corresponding horizontal wind speed perturbation (u') shown in Fig. 20 5d. An area with strong u' with maximal value of $\sim 6 \text{ m s}^{-1}$ can be found above the falling cloud overshooting top as pointed by the black arrow. This value is of the same range as the background horizontal wind speed in the west-east direction at the altitude of 16 km ($\sim 5 \text{ m s}^{-1}$ on Fig. 5e). The condition in eq. 1 is then satisfied which leads to the stagnation of air flow and the breaking of gravity wave. The breaking of gravity wave further formed the jumping *cirrus* shown in Fig. 4 (red arrow). In this process, a significant amount of ice and water vapor is transported 25 irreversibly into the lower stratosphere instead of falling back to the equilibrium level.

We emphasize the “irreversibility” of the vertical upward transport during the gravity wave breaking event. In case of a non-breaking gravity wave, the ascending air will later descend after reaching the wave ridge. In this case, the upward transport is “reversible”. In addition, there is weaker turbulent mixing to bring up the moister air below 30 because the wave energy is less transferred to turbulence but is propagated away. In the case of gravity wave breaking, a sudden jump of air flow occurs. The wave energy is dissipated through turbulence in the vicinity of the jump which enhances the mixing and the transport of water vapor and ice from upper troposphere to lower stratosphere.

The occurrence of gravity wave breaking depends on the intensity of the overshooting strength. As shown in eq. 2, the magnitude of the horizontal speed perturbation is linked to the vertical wind speed perturbation, which in this case

is related to the overshooting strength. This is in agreement with the finding of Dauhut et al. (2018) that stronger overshooting tops favor wave breaking and thus facilitate more vertical water transport.

5 We find in our simulations that the overshooting tops and wave breaking are frequently observed in the 0.25 km and 1 km simulations, with the breaking waves and jumping *cirrus* of typical horizontal sizes of 2 to 3 km. These phenomena are visible in the 2.5 km simulation, although with less frequency and intensity, and are not found in the 10 km simulation because the grid size cannot resolve the process.

3.3 Humidity and ice field

10 *We further examine the water vapor fields simulated by GEM at different horizontal grid-spacings. Fig. 6a and 6b show the mean vertical profiles of water vapor volume mixing ratio and temperature within the afore-defined Domain A and 5-hour time window. All the simulations show irregular moisture profiles near 16 km, where the vertical trend of the humidity profiles bends and produces ‘bumps’ (elevated water vapor contents) above the tropopause (indicated by the circles in Fig. 6, hereinafter the tropopause is defined by the altitude where the mean lapse rate Γ within Domain A and 5-hour time window decreased to 2°C km^{-1} or less).* Surprisingly, the low resolution (10 km) simulation predicts the highest water vapor content in large part of the UTLS. This is interesting because, as described above, the overshooting tops and the gravity wave breaking processes are only resolved in the higher resolution simulations, which causes vertical water transport and explains the moistened lower stratosphere in these simulations. The moister lower stratosphere in the 10 km simulation (compared to the 1 and 2.5 km simulations) warrants further investigation. In this subsection, we first use satellite remote sensing and aircraft *in situ* observations to validate the vertical humidity profiles, to find out which simulation better approximates the reality, and then, in the following subsection, we diagnose the causes of the identified model biases.

It is challenging to observe the humidity at the levels near tropopause. Nadir-view satellite remote sensing instruments, such as the Atmospheric Infrared Sounder (AIRS) onboard NASA Aqua satellite, usually cannot accurately measure the low water vapor concentrations in the lower stratosphere (e.g., Divakarla et al., 2006), although attempts have been made to improve the retrieval under special circumstance (e.g., Feng and Huang 2018). Limb-view sounders such as the Microwave Limb Sounder (MLS) on board Aura satellite have higher sensitivity and provide measurements of water vapor content in the UTLS, although biases have also been noted in these datasets. **These biases might be caused, among many others, by the averaging kernels of limb sounders which smear out the strong vertical gradient in water vapor at the tropopause (Hegglin et al., 2013).** For instance, an underestimation of water vapor with mean bias up to -25% and biases for individual case up to -85% between 100 and 300 hPa were reported for the MLS retrieval (Read et al., 2007; Vömel et al., 2007, Livesey et al., 2018). It is important to bear in mind the uncertainty in the satellite data when comparing the simulations with the observations.

35 **Figure 6c, 6d show the comparisons between the GEM simulations after applying averaging kernels of MLS and MLS retrievals (v4.2). Because of the scarcity of the collocated satellite data and also the afore-mentioned mismatch in time**

and location of the simulated convective system, we conduct the comparison with respect to area-averages rather than individual samples. The MLS measurements used here include five MLS footprints located between [38°N, 45°N] and [95°W 93°W], taken on 26 Aug 2013 around 19:00 UTC, about 15 hours after the dissipation of the convection system (Fig. 7, red diamonds). We applied the averaging kernel of MLS on the mean profiles of GEM simulated humidity and temperature within the 100x100 km regions centered on the MLS footprints. The comparison here suggests that both model simulations give higher estimations of water vapor content in the UTLS comparing to MLS retrievals, although the higher-resolution simulation better approximates the satellite observations. It is also found that GEM slightly overestimated the temperature comparing to MLS retrievals. This suggests that warmer temperatures in comparison to MLS could lead to slower ice crystal growth and thus less dehydration and thus higher gas-phase water. The spatial-temporal errors of the model simulation, e.g. shifted convection location or time, might also contribute to the discrepancies between the GEM and MLS profiles. Furthermore, the lower value of water vapor content from MLS near the level of 160 hPa may be subject to the aforementioned negative bias in the MLS data.

High accuracy hygrometers onboard high-altitude aircrafts provide benchmark water vapor measurements, although the temporal and spatial coverage of the aircraft data are limited. On 27 Aug 2013, the ER-2 aircraft deployed in the SEAC⁴RS field campaign obtained UTLS water vapor measurements located to the southwest of the Great Lakes as shown in Fig. 1. Using back-trajectory calculations we find that the measured air samples in Domain B are in the downwind direction of our studied convective system in Domain A. For the back-trajectory calculations we use the wind field simulated by GEM at 2.5 km grid-spacing. It is used to trace air parcels at 56 locations on 8 vertical levels between 14 and 17.5 km and 500 m intervals. Figure 7 shows the back trajectories of 16 selected air parcels starting at the altitude of 15.5 km and at the time of 19:40 UTC, 27 Aug around which time the aircraft measurements were taken. Through the back trajectories, we find that most of the air parcels in Domain B previously passed through Domain A where the convective system analyzed above developed. The high moisture content samples located in the southwest corner of Domain B are especially found to be moistened by the overshooting convection. Figure 8 illustrates the evolution of a few properties of one of these convectively moistened air parcels located in the southwest corner of Domain B at the tropopause altitude of 15.5 km. Similar results are found for the other altitudes above (not shown). The results here establish a connection between Domain A and Domain B for the lower stratosphere. It is particularly evidenced that the ER-2 aircraft measured UTLS air samples characterize the moistening effects of the overshooting convection that occurred earlier (and analyzed above) in Domain A.

One particular note for Fig. 8 is the formation of ice shortly after 19:40 UTC 27 Aug when the humid air parcel slowly ascends with decreasing temperature and increasing relative humidity with regard to ice. At these altitudes, the ice water content is relatively low ($\sim 1 \times 10^{-5}$ g m⁻³). The ice particles will gradually fall to a lower altitude and eventually be sublimated again. This process will partly dehydrate the upper layer of the atmosphere where the ice is forming, and later hydrate the lower atmospheric layer through ice sublimation. However, this dehydration has minor impact for the air parcels above the tropopause. We observe that the water vapor mixing ratio of the air parcel at the 15.5 km altitude (i.e., the upper layer) increased slightly after 19:40 UTC (Fig. 8a). This might be the results of the mixing

with the adjacent air in the northeast side of the parcel which is more humid (pointed by the black arrow in Fig. 7). As ice formation in Domain B is found to have limited impact on the humidity field above the tropopause, our interpretation of the stratospheric water vapor injected in domain A by linking it to the water vapor simulated/observed in domain B is therefore not affected in a significant way.

5
For the atmospheric layer under the tropopause between the altitude of 13.5 and 14.5, the horizontal wind speed increases significantly. The back-tracking results show that the humidity and ice field in the northern part of Domain B are linked to the convection initiated at the beginning of 27 Aug in domain A. The locations of ice water content in domain B from the simulation partly agree with what are observed by the aircraft in Fig. 2b. Based on the back tracing
10 results, we noticed that the ice in Domain B is not originally formed during the convection, but later during the slow ascent of the humid air parcel. This is similar to the dehydration process discussed above but at a lower altitude below the tropopause. The ice formed at this lower altitude is more abundant (in the order of $1 \times 10^{-3} \text{ g m}^{-3}$). The impact of dehydration (via ice formation and falling) at this level is more significant which can be seen in Fig. SI.3 near 15:40 UTC with an amplitude of about 20 ppmv. The readers are referred to the supplementary materials for more
15 discussions on this topic (Fig. SI.2 and Fig. SI.3, Qu 2019)

Given the variability of water vapor in Domain B as shown in Fig. 7 and possible errors in the location and time of GEM-simulated water vapor features, it would not be meaningful to compare the aircraft measurements with GEM simulations at the exactly matched locations and times. Instead, we compare the mean vertical profiles averaged for
20 Domain B between the aircraft observations and GEM simulations in Fig. 6e, 6f. We note that only the 10 and 2.5 km simulations cover Domain B where aircraft data are available (see Fig. 1). We observe a slight temperature bias from both model simulations of $\sim 2 \text{ K}$ above the tropopause level at 15.5 km (Fig. 6f). For water vapor content, Fig. 6e shows that the 2.5 km model well predicts the aircraft measurements, which indicates noticeable moistening around the altitude of 16.5 km. Although it also captures this moistening feature, the 10 km simulation generally overestimates
25 the water vapor contents in the UTLS region. This is consistent with the comparison made in Domain A against satellite measurements (see Fig. 6c and discussions above). This noticeable moist bias in the 10 km simulation warrants an investigation of its cause. As the convective parameterization is turned on at this resolution, both resolved vertical air motions and parameterized vertical transport (via the KFC scheme) potentially account for the convective moistening in GEM. This is similar to the simulations of GCMs, which also generally overestimate the UTLS
30 humidity. In the next subsection, we diagnose how an overly moist UTLS occurred in the coarse resolution simulation.

3.4 Budget analysis

We diagnose the water vapor transported across the tropopause into the lower stratosphere in the GEM simulations. The water budget is calculated for the rectangular box surrounded by a given lower boundary (e.g. tropopause) and model top ($\sim 30 \text{ km}$) as well as the four lateral facets of Domain A. Using the wind, water vapor and tendency fields
35 generated by GEM, we calculate the contributions to the change in total water vapor in the stratospheric box due to vertical advection of water vapor, as well as the sublimation of ice.

First, we use the Reynolds decomposition (eq. 3-5) to diagnose the **direct** vertical transport (**vertical advection**) of water vapor for the two high resolution simulations (1 and 2.5 km grid-spacings). For the 10 km grid-spacing simulation, the vertical advection is composed of two parts: the grid-scale advection which is solved explicitly and the parameterized sub-grid scale transport (tendency on water vapor due to KFC) which makes this case not suitable for Reynolds decomposition.

$$w(x, y, t) = \overline{w(x, y)} + w(x, y, t)' \quad (3)$$

$$q(x, y, t) = \overline{q(x, y)} + q(x, y, t)' \quad (4)$$

$$\begin{aligned} & \sum_{nt=1}^{nt=Nns=M} \sum_{ns=1} \delta t \delta S w(x, y, t) q(x, y, t) = \\ N \delta t & \sum_{ns=1}^{ns=M} \overline{\delta S w(x, y) q(x, y)} + \sum_{n=1}^{n=N} \sum_{ns=1}^{ns=M} \delta t \delta S w(x, y, t)' q(x, y, t)' + \\ & \sum_{n=1}^{n=N} \sum_{ns=1}^{ns=M} \delta t \delta S \overline{w(x, y) q(x, y, t)'} + \sum_{n=1}^{n=N} \sum_{ns=1}^{ns=M} \delta t \delta S \overline{w(x, y, t)' q(x, y)} \end{aligned} \quad (5)$$

We decompose the vertical wind speed w and humidity q into the time averaged terms and fluctuation terms as shown in Eq. (3) and (4), where x and y represent the coordinates of longitude and latitude and t represents the time. The integrated product of w and q for the evaluation domain and time is shown in the Eq. (5), where N is the total number of time steps of the simulation during the evaluation window, M is the total number of horizontal grid boxes in the Domain A, δt is the length of each time step, δS is the horizontal surface of a given model grid box.

Applying Eq. (5) at the tropopause level in Domain A (mean $\Gamma < 2^\circ\text{C km}^{-1}$), we obtain a first-order approximation of the vertical transport of water vapor through the tropopause. Among the four terms on the right side of the Eq. (5), the last two terms are negligible. The first term on the right side of the equation measures the transport of water vapor through tropopause by the mean updraft (or downdraft). The second term on the right side of the equation includes transport by “eddies” generated by wave breaking. Through the decomposition for the 1 km simulation, we find that the first term represents 39% of the total vertical transport and the second term represents 59%, which highlights the important role of wave breaking. With the decrease of model’s horizontal resolution, the weight of the eddy term decreases to 29% for the 2.5 km simulation. This suggests that the importance of wave breaking in direct vertical transport of water vapor decrease with the model resolution.

Secondly, we calculate the total transport of water vapor and the contributions from direct transport and ice sublimation for each simulation. The comparison between the high-resolution simulations and the 10 km simulation is less straightforward because their tropopause heights are different (Fig. 6a and 6b). We therefore calculated the water vapor change due to the vertical advection and ice sublimation/**vapor deposition** with different altitude levels as the lower boundary from 14 km to 16 km. These results are shown in Fig. 9.

The vertical advection simulated by the high-resolution models is relatively constant from 14.5 km to 16 km altitude with positive values (upward transport, Fig. 9a). This upward advection is linked to the gravity wave breaking (see discussion in Subsection 3.2) which makes the stratospheric air flow ‘jump’ by about 2 km upward and transports humidity into the stratosphere. The vertical advection in the 1 km simulation is generally stronger than that of 2.5 km simulation due to the more important role of wave breaking. This is in agreement with the results from Reynolds decomposition.

It is not a surprise that the higher resolution NWP models tend to produce stronger direct vertical transports across the tropopause because, as shown in Subsection 3.1, the transport is closely related to the strength of overshooting and the breaking of the gravity waves. Similar to what was found by Weisman et al. (1997), we find in our GEM simulations that the simulated maximal vertical wind speed is inversely proportional to the horizontal grid-spacing of the NWP model. The stronger vertical wind speed in the convection updraft leads to higher cloud overshooting top. In our cases with high resolution simulation, the maximum cloud top altitude is 16.64 and 16.96 km for 2.5 and 1.0 km simulation respectively. We find that the stronger overshooting wind speed in the higher resolution simulations leads to favorable conditions for gravity wave breaking (see the discussions in Subsection 3.1) and thus more direct vertical transport. This agrees with Dauhut et al. (2018). In total, the direct vertical transport of water vapor contributes to 40% of the total transport at the tropopause level for the 2.5 km simulation and makes up to 89% for the 1.0 km simulation.

The total vertical advection from 10 km simulation is different from those of the two high resolution simulations. It can be decomposed into two parts: the grid scale explicit advection (blue dashed line in Fig. 9a) and the sub-grid scale advection by KFC (blue dotted line in Fig. 9a). The grid scale vertical advection of 10 km simulation is positive below the altitude of 14.3 km. It turns to negative values from 14.4 km. One of the reasons for these negative values may be the lack of representation of gravity wave breaking. Another reason is possibly the large-scale circulation induced by the convection. In the convective area, the air transported to the level above 14 km is relatively dry and cold, whereas the descending areas surrounding the convective zone are moister due to the sublimation of the ice. The sub-grid scale advection is strongly negative in lower altitude. In KFC, this downward transport comes from the effect of compensating subsidence outside of the convective updrafts. This strong downward transport gradually reduces to zero near the tropopause.

We find large discrepancies in the contribution of ice sublimation throughout the UTLS region between the high-resolution simulations (1 and 2.5 km) and the 10 km simulations. Ice sublimation (hydration) and vapor deposition on ice (dehydration) are two opposing microphysical processes competing for a dynamical balance. We use hereinafter ‘sublimation’ to denote the combined effect of these two processes. The positive value signifies that the ice sublimation is faster than the vapor deposition, and the negative value signifies the other way around. In this study, the value of sublimation includes all the ice-phase categories. For the two high resolution simulations, the contribution of ice sublimation reaches their maximal positive values near the altitude of 14.5 km. Toward higher altitude, the

contribution of ice sublimation decreases gradually to a small value. *To focus on the tropopause level, ice sublimation has a non-negligible contribution to the total transport of water vapor for the 1 km simulation (11%) and a larger contribution for the 2.5 km simulation (60%). For the 10 km simulation, the mean ice sublimation rate is large and always positive. Ice sublimation is therefore the primary source of moistening of the UTLS region above the altitude of 14 km. Vertical advection does not contribute to the moistening of the UTLS region but transports a significant part of water vapor back to lower altitudes. Overall, the contribution from both processes generate a strong moistening of the UTLS region for the 10 km simulation (Fig. 9c).*

An additional comparison including the 0.25 km simulation for a smaller domain (see Fig. 1) and shorter period (1 hour) corroborates the above finding that simulation tends to have a larger contribution from advection and less contribution from sublimation as the resolution increases (see Supplementary Fig. SI.1, Qu, 2019).

It is, however, interesting that compared to the high-resolution simulations, the sublimation induced lower stratospheric moistening is stronger in the lower resolution simulations (10 km grid-spacing), as shown by Fig. 9b. We find that this higher sublimation rate may be contributed for the following reasons: First, more abundant ice particles in the lower stratosphere in the 10 km simulation, as shown by Figure 10. The cause of this higher mean ice water content may be due to the lack of the parameterization of downward transport to bring the ice within the cloud overshooting tops back into the upper troposphere in the KFC deep convection scheme. In this scheme, the ice transported into the lower stratosphere by the parameterized updrafts will be distributed uniformly into the $10 \times 10 \text{ km}^2$ model grid box. The ice will then be passed into the MY2 microphysical scheme in the hydrometeor “ice” category. Part of these ‘ice’ particles will eventually be transformed through aggregation or diffusional growth into other larger hydrometeors such as “snow”. But all these solid hydrometeors can only fall back into the upper troposphere through gravitational sedimentation. In the reality, and as evident from the high-resolution simulations here, the majority of ice transported into lower stratosphere within the cloud overshooting tops will be brought back to troposphere when the overshooting tops fall back to the equilibrium level. This suggests that the simple entrainment-detrainment model in KFC might not well represent the complexity of the different mechanisms near the tropopause level.

A separate test run with 10 km model grid-spacing without the KFC scheme has been performed and shows that the ice water content at the UTLS region above the altitude of 14 km is very close to the 2.5 km simulation (Fig. 10a, purple line). These results suggest that the over-estimation of ice is partly due to the use of the deep convection parameterization. With the reduction of ice in the test run, we find that the mean ice sublimation tendency is largely reduced (blue line and purple line in Fig. 10b). However, with similar amount of ice in the UTLS, the 10 km simulation without KFC still shows a higher ice sublimation rate above the altitude of 14.5 km compared with the two high resolution simulations.

This second reason leading to stronger moistening of the lower stratosphere in the coarse (10 km) resolution simulation is due to the sublimation efficiency of ice. We find that the ice transported into lower stratosphere is largely sublimated

into water vapor in the 10 km simulation and much less for the higher resolution simulations. The amount of ice transported across the tropopause at the 1 and 2.5 km simulations are similar: 2.3 and 2.6×10^9 kg respectively out of which only 2% and 6% are sublimated. In contrast, in the 10 km simulation, the vertically transported ice across the similar altitude (~ 14.5 km) is 3.9×10^9 kg and 21% is sublimated. If evaluated at the tropopause determined from the 10 km simulation (~ 15.5 km, higher than the tropopause in the higher resolution simulations), 75% of the 4.8×10^8 kg ice is sublimated in the 10 km simulation. In summary, the coarse resolution simulation strongly over-estimates the fraction of ice that is sublimated in the lower stratosphere comparing with higher resolution experiments.

What leads to the drastically different ice sublimation processes in the coarse-resolution simulation? We find that one important factor influencing ice sublimation efficiency in the lower stratosphere is the spatial distribution of ice. Fig. 11 shows the ice sublimation rates, IWC distributions and a few related fields, from the GEM simulations at different resolutions, at the level of ~ 15.36 km in Domain A at 23:25 UTC 25 Aug 2013. From the panel Fig. 11a, we can identify that the 10 km simulation is populated with many pixels with high sublimation tendency (in yellow) corresponding to the edges of convective cloud areas. These areas are in-between the supersaturated air (relative humidity over ice ~ 1.08) within the convection clouds and the surrounding dry mid-latitude lower stratospheric air (Fig. 11d, g). The ice sublimation rates in the higher resolution simulations are very different. In these higher resolution cases, the areas loaded with ice are much smaller than that in the 10 km simulation and are of much higher spatial heterogeneity. The majority of the ice is concentrated in the very limited areas (Fig. 11e, f) with low temperature (Fig. 11k, l) and high relative humidity (Fig. 11h, i), corresponding to the locations of the overshooting tops. That is, the majority of ice is “trapped” in the overshooting tops. As shown by Fig. 12, this trapping effect is also evidenced by the distributions of ice with respect to temperature (panel a) and relative humidity (panel b), respectively, calculated by summing up the mass of ice in the grid boxes whose temperature or relative humidity values fall within each specific interval and then dividing it by the total mass of ice in the whole domain. We find that the majority of ice of the two high resolution simulations are trapped in cold temperatures between 195 and 201 K and high relative humidity inside the overshooting tops. The horizontal extent of the areas with high ice water content is thus small. The trapped ice therefore has less contact surface with the surrounding dryer stratospheric air. This factor significantly limits the ice sublimation rate in the higher resolution simulations. In contrast, in the 10 km simulation, the ice is not trapped in the cold overshooting tops but distributed over larger areas with the warmer temperatures (> 201 K). This leads to significant larger contact area with dry air and higher sublimation.

4. Conclusions and discussions

In this study we use the GEM model of ECCC to reproduce a mid-latitude lower stratospheric moistening event over North America near the Great Lakes during 25-26 Aug 2013. Simulations are conducted with a set of nested domains at increasing resolutions from 10 km to 0.25 km grid-spacing. Satellite remote sensing data from MLS as well as aircraft *in situ* observations from the SEAC⁴RS campaign are used to evaluate model simulations, complemented with trajectory simulations to associate those observations with model forecasts over specific regions. Comparisons conducted here suggest that while the higher resolution simulations well approximate the observed water vapor fields

in the UTLS region after the deep convective events, the coarse resolution simulation simulates a substantially moister UTLS.

5 Intercomparison of simulations using different horizontal resolutions, we find that the high-resolution simulations
(with grid-spacing $dx \leq 1$ km) can properly resolve the key dynamical features of the overshooting convection,
including the overshooting tops, the gravity wave breaking process and the visible jumping *cirrus* phenomenon. The
overshooting convection may significantly elevate the water contents (both vapor and ice) up to 1-2 km above the
tropopause. The size of the high-concentration water vapor plumes is typically less than 10 km although they can
aggregate to sizes greater than 30 km. Coarse resolution simulations ($dx \geq 10$ km) cannot resolve these features,
10 although a moister UTLS region results from the parameterized deep convection and associated water transport.

A lower stratospheric water budget has been performed to quantify the contributions by different processes. It shows
that vertical advection of water vapor is one main contributor to the lower stratospheric moistening in the overshooting
events. In the high-resolution simulations (0.25 and 1 km) where the gravity wave breaking process is well simulated,
15 eddies resulting from wave breaking are found to mainly account for the direct vertical transport of water vapor into
the lower stratosphere. This transport mechanism is largely dependent on the strength of overshooting (updraft speed),
with higher resolution simulations generating stronger updrafts which enhance overall the transport of water vapor
into the stratosphere.

20 Another important source of water vapor in the lower stratosphere is ice sublimation. The comparisons conducted in
this study show that the 10 km simulation has considerably higher ice sublimation rate. One of the possible reasons is
that the KFC convective scheme that is turned on in this simulation bring more ice into the UTLS region which
enhances the production of water vapor through the ice sublimation process. The cause of this overproduction of ice
is likely associated with the lack of downward transport of ice that is observed after the cloud overshooting tops reach
25 their maximal height in the lower stratosphere. The simple entrainment-detrainment model used in KFC scheme may
not well represent the complex processes near and above tropopause during the convective event. One solution is to
add an element in the KFC scheme to take into account this downward transport above the tropopause. Another
solution is to increase the ice particle size in the UTLS so that the ice can sediment faster and hence reduce the ice
water content at these levels. Another possible reason why the 10 km model has higher sublimation rate is the high
30 ice sublimation efficiency. This high efficiency is due to the different distribution of ice water contents comparing to
the those of high-resolution models. This results from the inability to resolve overshooting tops by the coarse grid
boxes (10×10 km²) and the failure to represent the trapping of ice by the cold air within the overshooting tops. One
possible solution to address this problem is to add a parameterization to reduce the ice sublimation rate in the lower
stratosphere or to condition it on the sub-grid scale temperature or relative humidity variability. The moist bias
35 identified in the coarse resolution simulation of GEM here is reminiscent of the moist bias in many GCMs. The ideas
for remedying this issue stimulated by the diagnoses here warrant further investigations.

Author contribution

Y. H., P. A. V., J. N. S. C., M-K. Y. and K. A. W. conceptualized the research goals and aims. Z. Q. and Y. H. designed the experiments and Z. Q. carried them out. Z. Q. developed the model code, performed the simulations and prepared the manuscript with contributions from all co-authors.

5 Competing interests

The authors declare that they have no conflict of interest.

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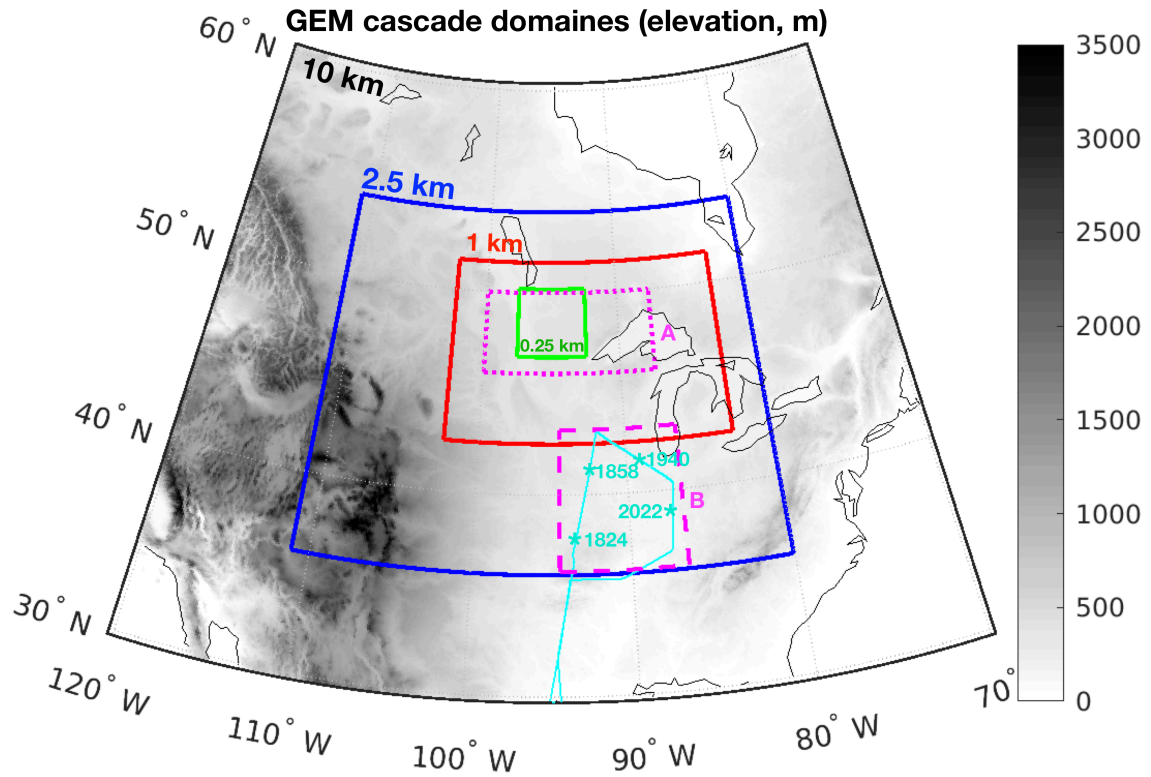


Figure 1: GEM cascade domains. Thick solid lines in black, blue, red, and green represent simulation domains at 10, 2.5, 1 and 0.25 km horizontal grid-spacings, respectively. Thin cyan line represents the ER-2 aircraft flight path on the day of 27 Aug 2013. Magenta dotted line represents evaluation Domain A which covers the major convective events of this study. Magenta dashed line represents Domain B for comparison between aircraft observations and model simulations. The four cyan stars show the locations and times (UTC) of the lowest location of the descending-ascending trajectories of the aircraft.

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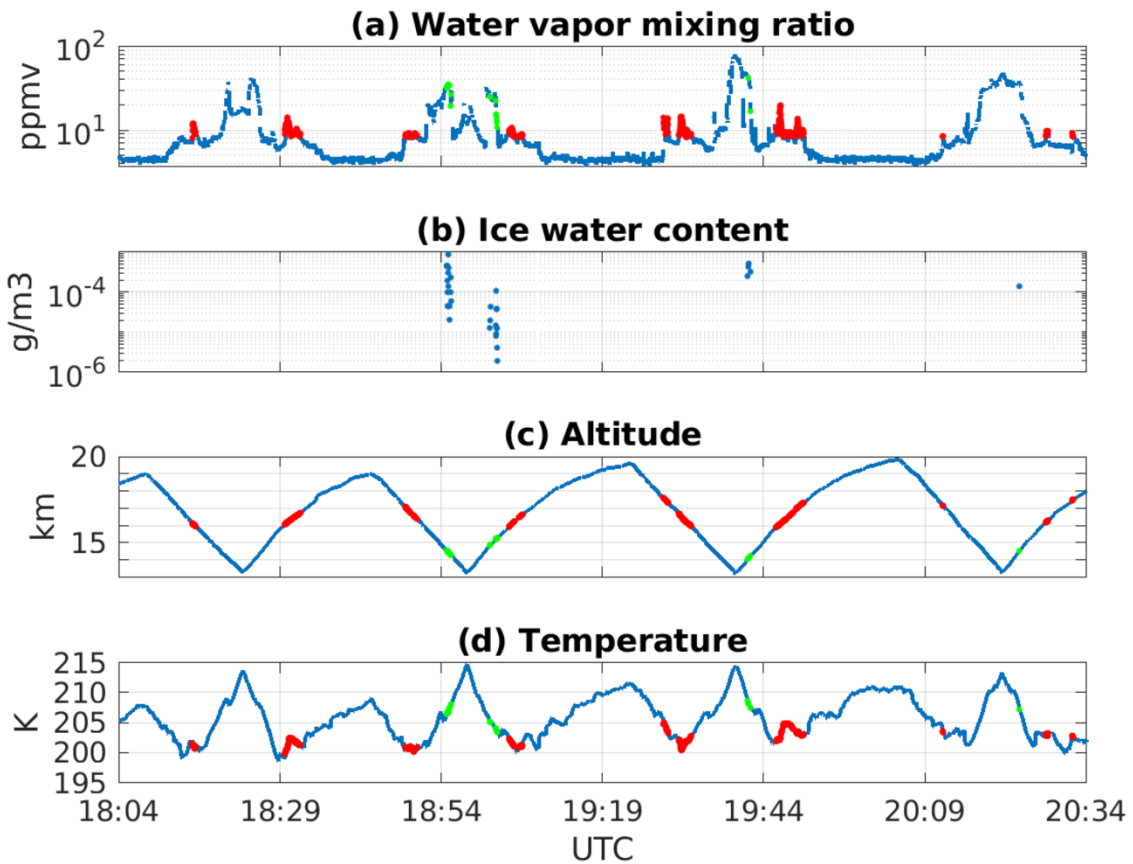


Figure 2: ER-2 aircraft observation of a) water vapor mixing ratio in ppmv in logarithmic scale, b) ice water content in g m⁻³, c) altitude in km and d) air temperature in K, on 27 Aug 2013. The red dots highlighted the measurements with pressure lower than 115 hPa (tropopause) and water vapor volume mixing ratio greater than 8 ppmv. The green dots highlighted the measurements with the presence of ice.

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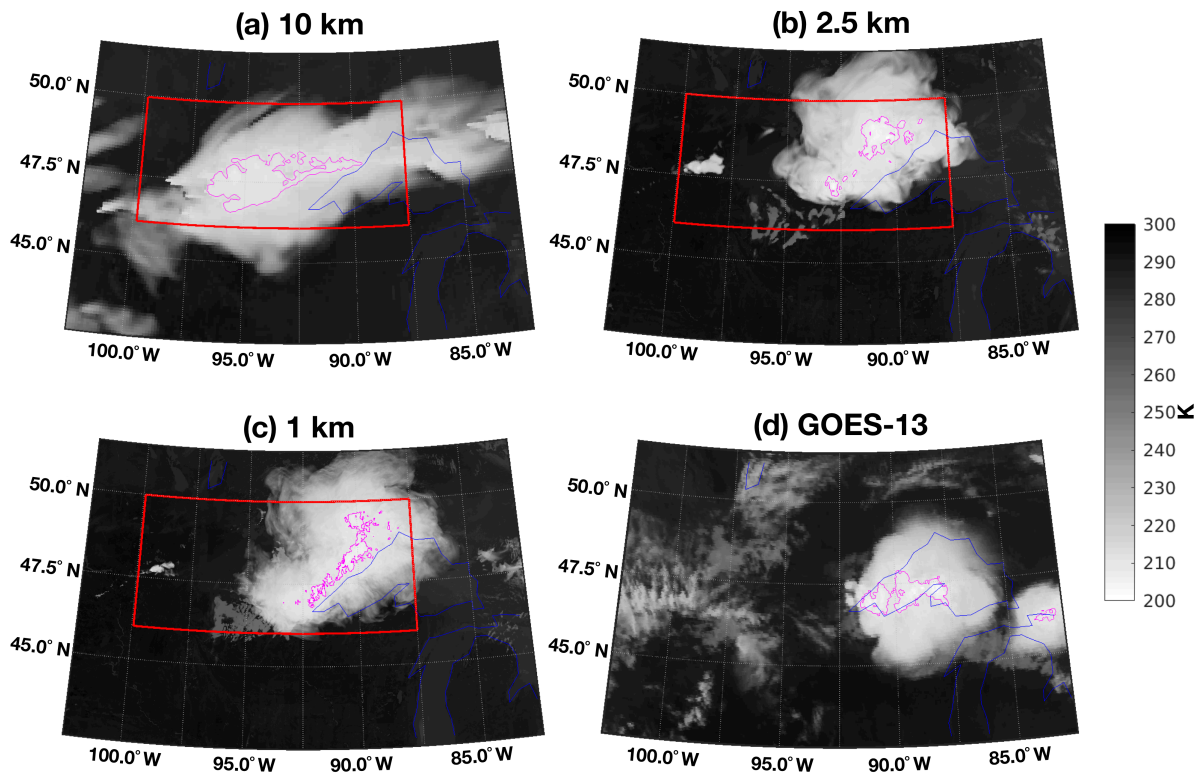


Figure 3: GEM-simulated deep convective clouds compared to satellite observation. Brightness temperatures are simulated using the RRTMG radiative transfer model, from GEM simulations at three resolutions with 10 km (02:30 UTC 26 Aug), 2.5 km (23:00 UTC 25 Aug) and 1 km (23:00 UTC 25 Aug) grid-spacing, and compared to the brightness temperature of 11.2 μm channel of GOES-13 satellite (06:00 UTC 26 Aug). The red rectangles mark the Domain A. The magenta lines highlight the area with brightness temperature lower than 210 K.

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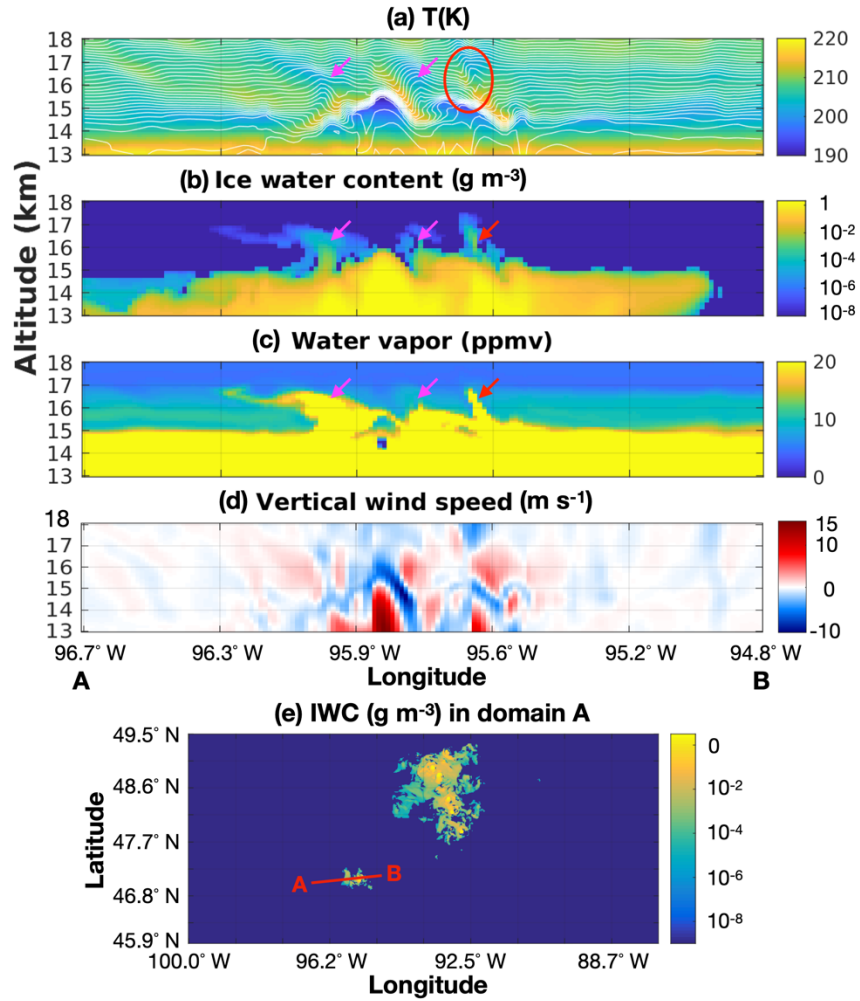


Figure 4: GEM-simulated overshooting convection. The results illustrated here are taken from the 1 km simulation at 19:46 UTC 25 Aug 2013: a) temperature (colour) and potential temperature (thin white lines); b) ice water content, in logarithmic scale; c) water vapor mixing ratio in ppmv; d) vertical wind speed (m s^{-1}); e) ice water content in domain A at the level of 15.24 km at 19:46 UTC on 25-08 from the 1.0 km simulation. The red line shows the location of the cross-section A-B.

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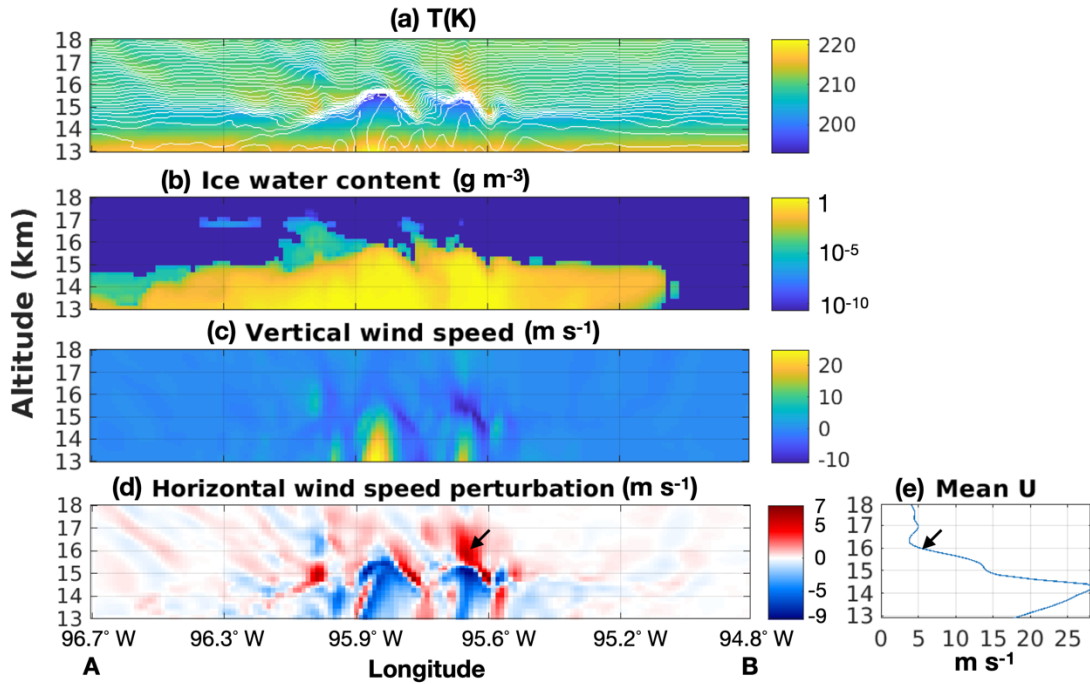


Figure 5: cross-section as shown in Fig. 4 but for 19:42 UTC 25 Aug 2013: a) temperature (color) and potential temperature (thin white lines); b) ice water content, in logarithmic scale; c) vertical wind speed (m s^{-1}); d) horizontal wind speed perturbation based on eq. 2 (m s^{-1}); e) the mean horizontal wind speed on west-east direction.

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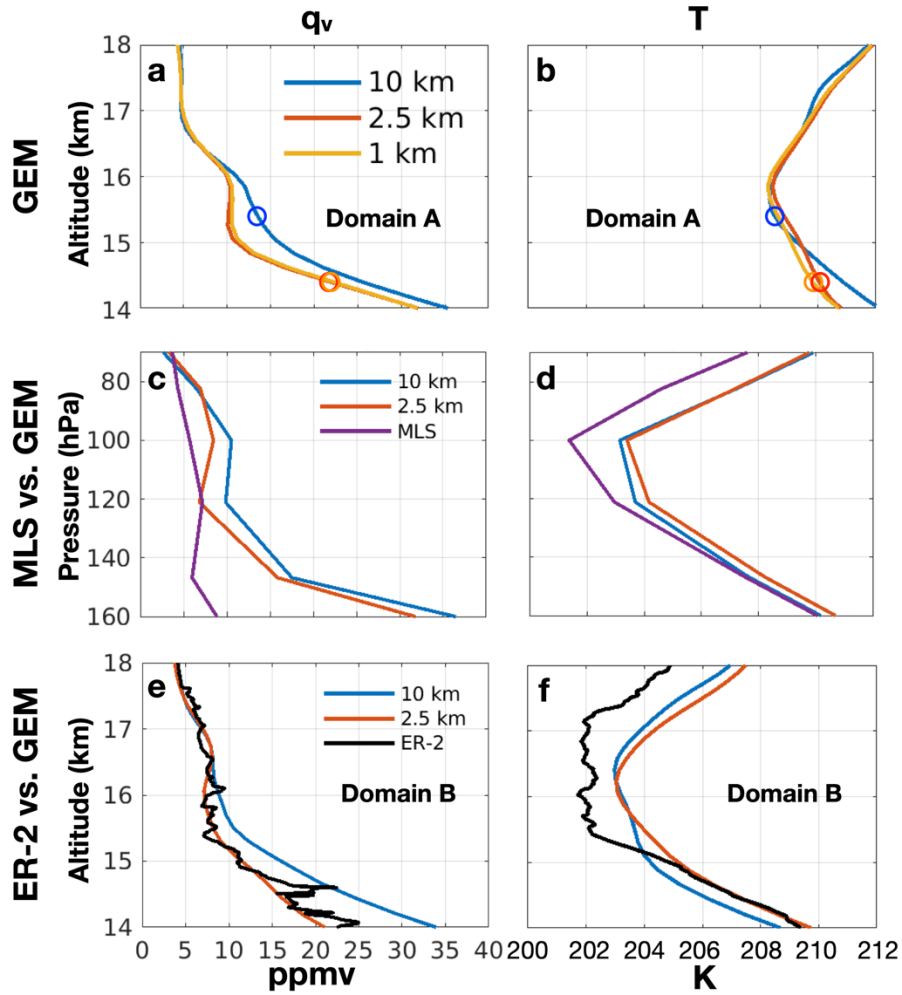
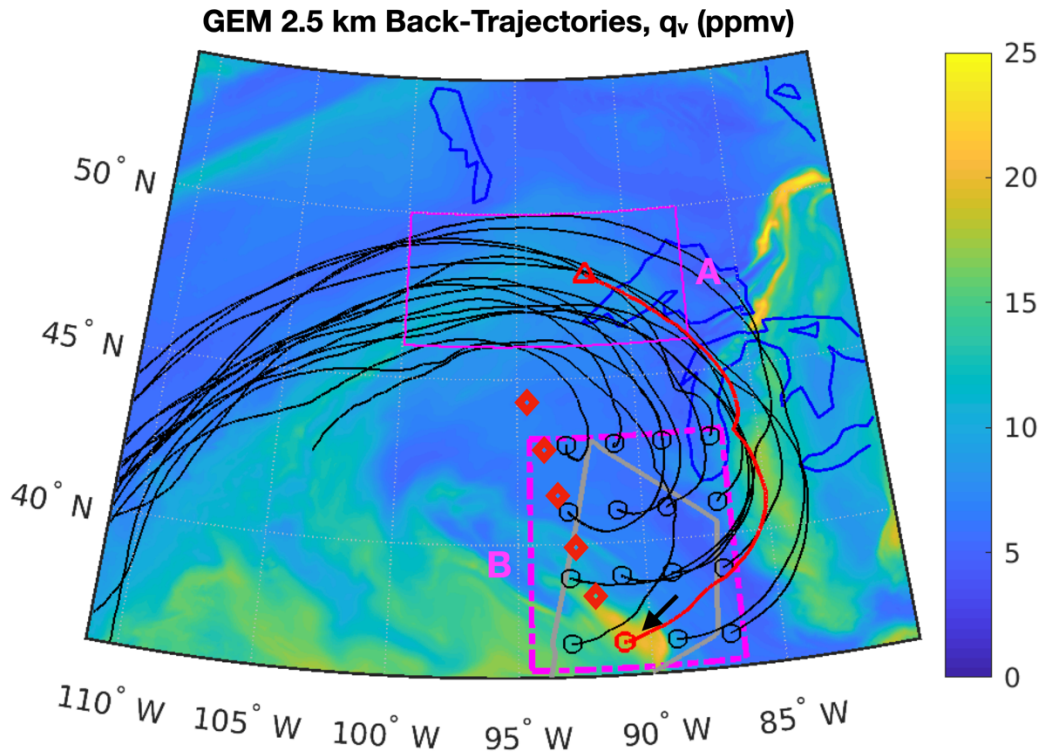


Figure 6: a), b) the mean profiles of water vapor volume mixing ratio (q_v) and temperature (T) for Domain A during the 5-hour period. The circles indicate the positions of the tropopause (mean $\Gamma < 2^\circ\text{C km}^{-1}$); c), d) mean profiles (q_v and T) after applying averaging kernels of MLS on GEM 2.5 km, 10 km simulation (100x100 km areas centred on 5 MLS footprints) and MLS profiles; e), f) the vertical profiles (q_v and T) within Domain B for GEM 10, 2.5 km simulations and for ER-2 aircraft *in situ* observations.

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5 Figure 7: Back trajectories of air parcels. All the trajectories, in black lines, are initialized in Domain B at 15.5 km altitude and 19:40 UTC 27 Aug. The circles indicate the initial locations of each back trajectory. The gray line here illustrates the ER-2 aircraft flight path (in clockwise direction). The background image shows the water vapor content in ppmv at this level from the 2.5 km simulation. The red line highlights the back trajectory of one air parcel from its initial location in Domain B to its location in Domain A at around 23:00 UTC 25 Aug 2013 when the overshooting convection occurred. The evolution of the properties of this air parcel are shown in Fig. 8. The red diamonds indicate the center of 5 MLS footprints on 26 Aug.

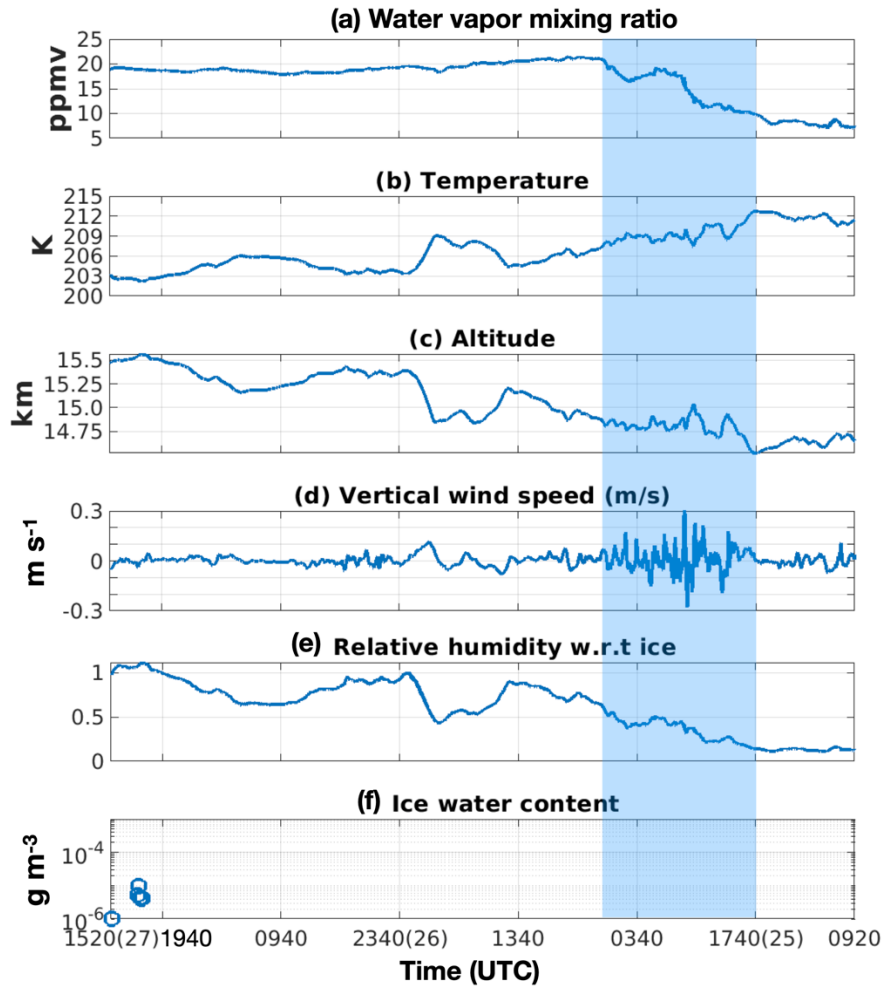


Figure 8: The changes of the properties of a tracked air parcel (red circle highlighted in Fig. 7) along its back and forward trajectory. The beginning time of the back/forward tracing is 19:40 UTC 27 Aug. Highlighted in the rectangular shaded area is the encountering of the air parcel with the overshooting convections in Domain A at around 22:40 UTC 25 Aug which is evidenced by fast rising water vapor concentration, decrease in temperature, rise in altitude and sudden changes in vertical wind speeds.

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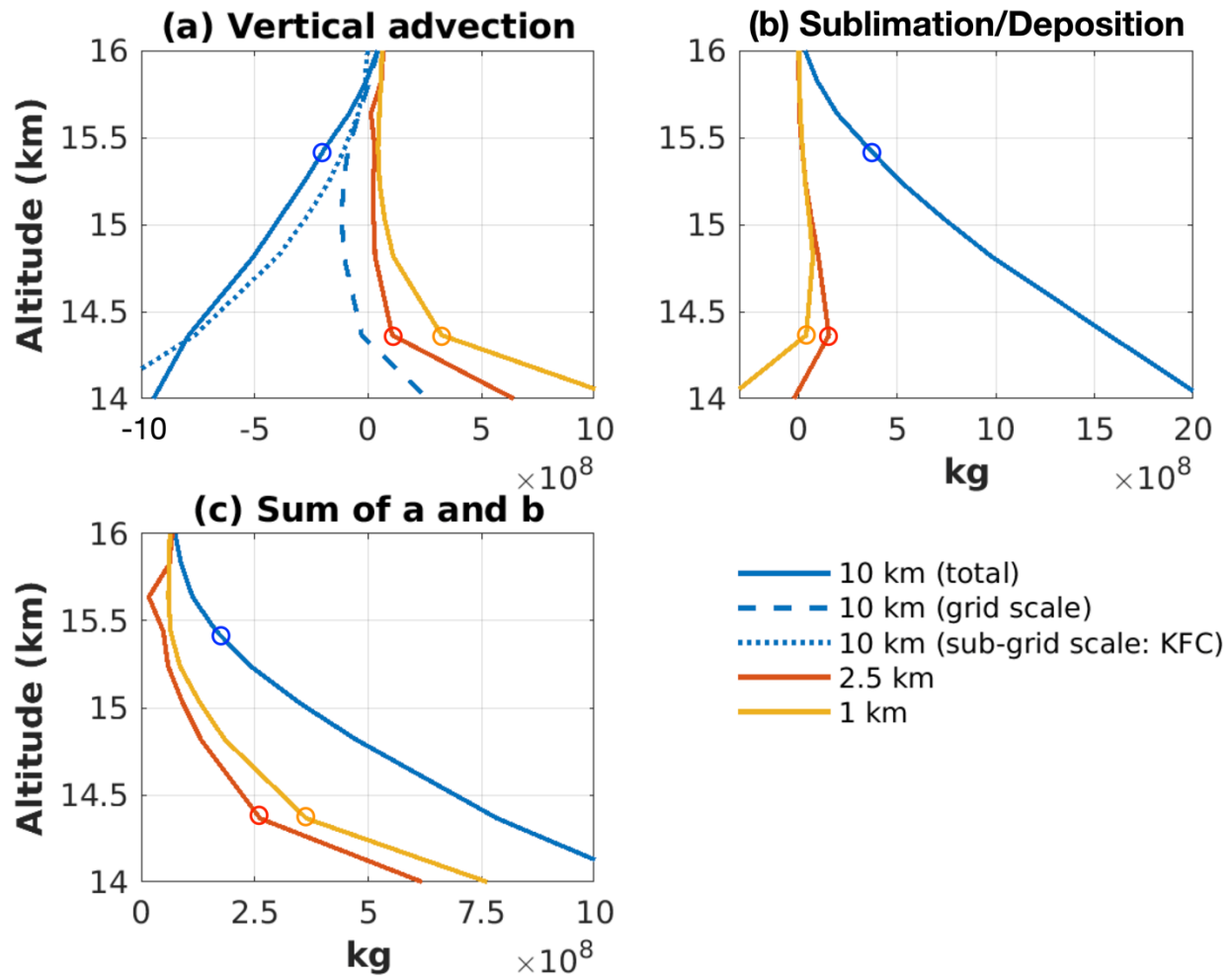


Figure 9: Change of water vapor in Domain A during the 5-hour evaluation period with different altitude levels as the lower boundary. The circles represent the height of tropopause (mean $\Gamma < 2^\circ\text{C km}^{-1}$).

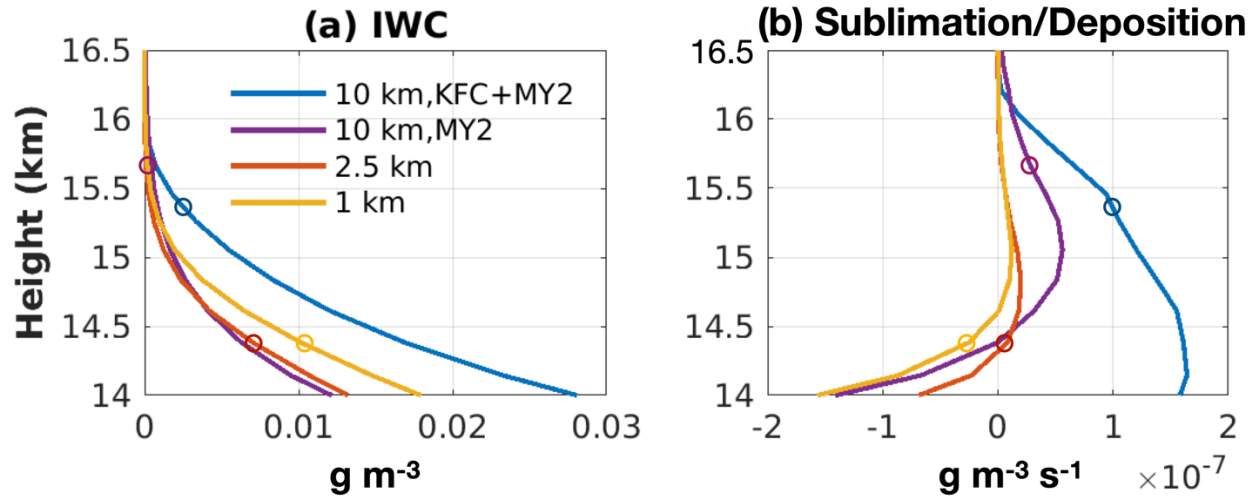


Figure 10: mean profiles between 14 km and 16.5 km within Domain A and evaluation time window (5 hours): a) ice water content; b) ice sublimation/vapor deposition tendency. The circles indicate the position of tropopause (mean $\Gamma < 2^\circ \text{C km}^{-1}$).

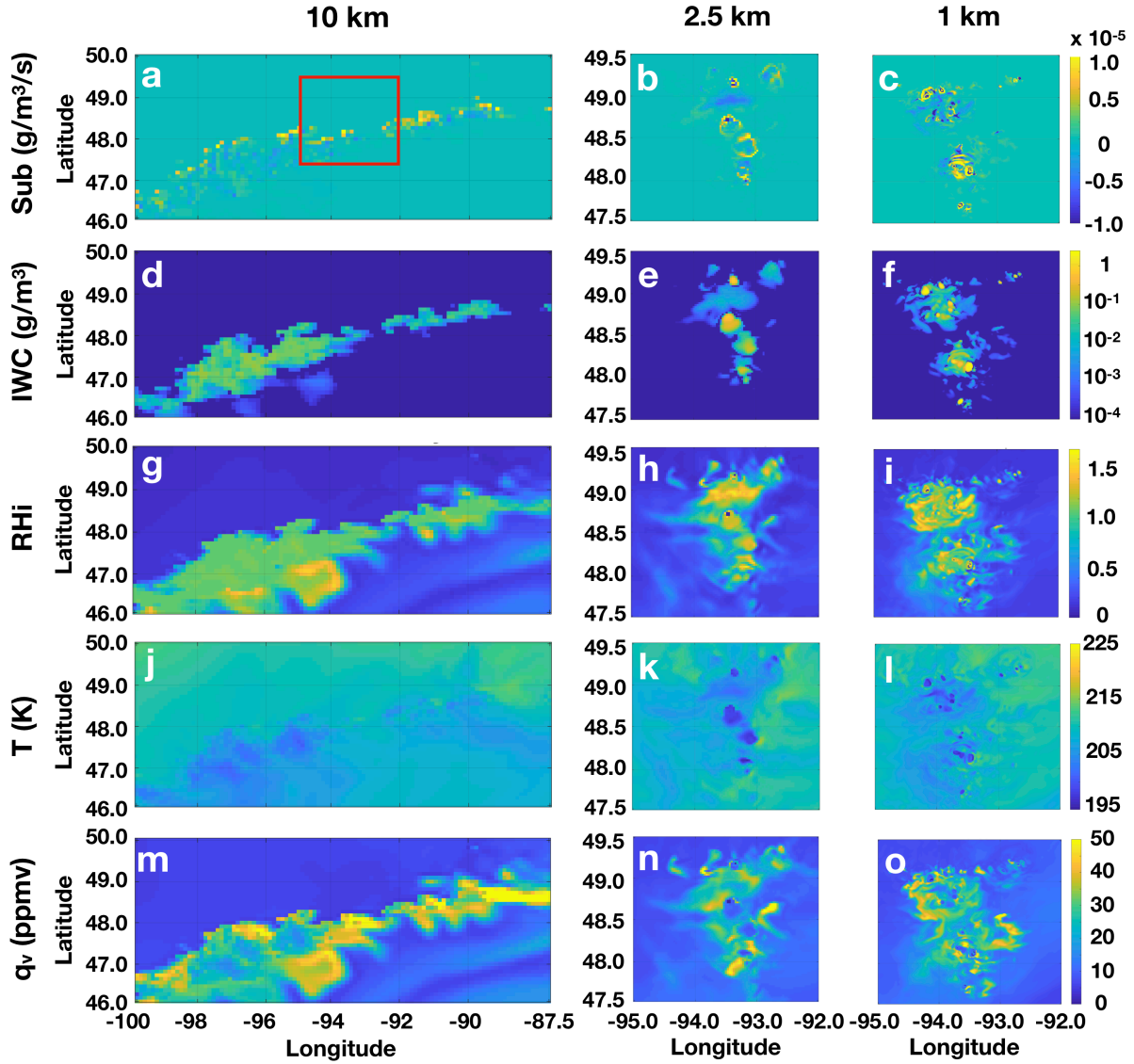
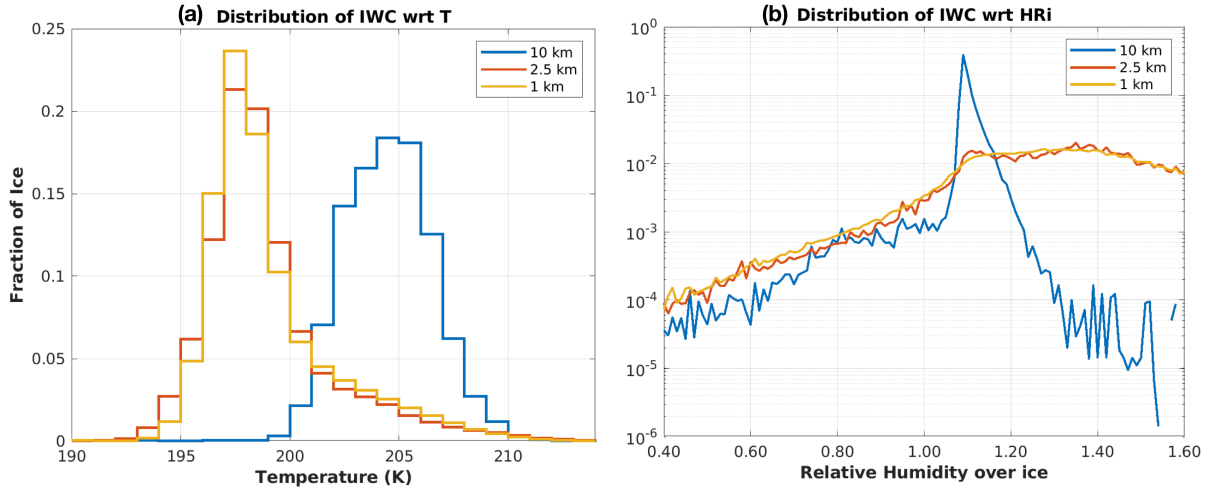


Figure 11: Distribution of a few variables in Domain A during overshooting. The results are taken from one instance: 23:25 UTC, 25 Aug. 2013. and one vertical level of ~15.36 km (above the tropopause). Shown in the three columns are the simulations at 10 km, 2.5 km and 1 km horizontal grid-spacing, respectively. The area shown for the 2.5 and 1 km simulations corresponds to the red rectangle in the first image. Short names for each row are used for notation, Sub: sublimation; IWC: ice water content, RH: relative humidity with regard to ice, T: temperature; q_v: water vapor volume mixing ratio.

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5 **Figure 12: Distribution of ice with respect to a) temperature and b) relative humidity. The results are based on the variables in Domain A at as shown in Figure 11. The temperature and relative humidity intervals are 1 K and 1%, respectively. The mass fraction value at each temperature or relative humidity interval is calculated by summing up the mass of ice in the grid boxes whose temperature or relative humidity values fall within the specific interval and then divide by the total mass of ice in the whole domain.**