Interactive comment on “Cloud system resolving model study of the roles of deep convection for photo-chemistry in the TOGA COARE/CEPEX region” by M. Salzmann et al.

M. Salzmann et al.

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We very much appreciate the careful review by this referee. We have tried to untangle the “clutter of other discussions in the paper and the supplement” by removing the dependence on the supplement by either extending or removing points, as appropriate for each case (see below for details). We chose to include a relatively large number of key points in a single manuscript since many of the issues are strongly inter-dependent (compare response to specific point 3 below).

Major points:

1) We think that the dimensionality issue related to the lightning NO\textsubscript{x} source should be kept in mind when implementing and applying any kind of “line” or “point” source in
a larger scale model using a super-parametrization for deep convection. However, in many of today’s global atmospheric models including chemistry, lightning NO is assumed to be instantaneously mixed over relatively large horizontal areas. While the discussion in our manuscript suggests that applying a source “inside” a super-parameterization would not automatically be a solution to this particular issue in large scale models, one could certainly speculate that this particular aspect of using a super-parameterization would at least not be inferior to the approach presently used in many large scale models. We recognize that more research would be necessary in order to address this question appropriately.

There is also another potentially interesting point related to deep convective chemistry transport in models using a super-parameterization, which goes back to Salzmann et al. (2004), and which we believe many of the super-parametrization users are already aware of. We briefly re-iterate it at the end of this reply.

2) A separation of results into 1) clear air only, 2) columns with clouds, and 3) columns with different cloud top heights is technically possible without a major effort, although such an exercise would indeed be somewhat limited by spatial and temporal (output every 30 min) resolution. In addition, one might, however, also have to distinguish between “background air” and convective outflow (beyond the (ice) anvils) in order to arrive at meaningful results. The latter is much more difficult than the separation suggested by the referee. In the present setup several mesoscale convective systems and isolated storms often co-exist within the domain, and systems downstream sometimes impact the outflow from systems upstream. Separating outflows would further be complicated by the use of specified lateral boundary conditions for tracers, implying that some air in the region has already been influenced by deep convection upstream. All in all such a separation would constitute a major additional effort. We did not attempt such a separation, mainly because our focus has been on longer term influences of several mesoscale convective systems and isolated clouds, on the budgets and certain properties of the profiles in the TOGA COARE/CEPEX region, rather than on the

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influence of a single system on a single profile. An example, where the three-modal structure of the cloud top heights could possibly play a role is found in the brief discussion of the cloud shading effect on ozone destruction in the end of Sect. S5.2. This is, however, also very difficult to separate from other effects (i.e. elevated mid-tropospheric ozone at the lateral boundaries) without further investigation.

3) We had originally intended to write two separate manuscripts from the material presented here, but finally decided against it, instead trying to retain some of the strong inter-dependence between the various key results (see also our reply to the next major point below). As a by-product of this decision, the number of focal points increased. We do not find a general problem with treating several points in one manuscript as long as there is a sufficiently good reason with respect to content, and we think that detailed supplements can be very useful for some readers. We do, nevertheless, understand the criticism by the referee. We have tried to almost completely remove the dependence on the supplement by either extending or removing points, as appropriate for each case (see below for details). Please note that we could find no stated guidelines for what is allowed in supplements, and based on the range of supplements in other papers (from collections of figures all the way to user’s manuals for models or components), we think the current supplement fits within this range. Nevertheless, a clear statement on the ACPD website as to what is acceptable as supplementary material would definitely be appreciated.

4) Our main motivation for this study has been to better understand the roles of (a) lightning produced NO and (b) ozone transport in the region, rather than only re-producing or explaining the very low upper tropospheric ozone mixing ratios observed during parts of the CEPEX cruise. Such extremely low ozone mixing ratios have also not been anticipated to be reproduced in the present simulations, as stated in the conclusions. Because the pioneering study by Wang and Prinn (2000) has raised some intriguing questions regarding the relative importance of lightning NO and transport for ozone, we found it important to discuss these issues together. We have further
stressed the connection between ozone profiles and locally produced lightning NO\textsubscript{x} in the introduction by mentioning lightning NO\textsubscript{x} explicitly in the second point of the listing starting on line 3, page 407. This point now reads as follows:

“ (2) Deep convective ozone transport (especially with regard to implications for its treatment in global chemistry-transport models), and, closely related to this, the role of regional scale ozone transport and lightning NO\textsubscript{x} in explaining ozone profiles in the TOGA COARE/CEPEX region.”

(Please note that the page and line numbers in this reply refer to the original ACPD manuscript, and that these will change in the revised manuscript.)

Specific points:

1. We re-arranged the short summary of the results in the abstract in the following order, almost completely retaining the original scope:

   - O\textsubscript{3} transport (2-D vs. 3-D runs)
   - small impact of lightning on O\textsubscript{3} in all runs
   - lightning unlikely to explain near zero ozone
   - NO\textsubscript{x} loss (2-D vs. 3-D runs)
   - downward transport of ozone (compare specific point 12)
   - role of the ISO for ozone profiles

We acknowledge that the perceived relevance of each of the points to a certain extent depends on the personal interest of the individual reader.

2. We replaced the sentence "Anvils are identified as described in Sect. S1.4." by: "For each system, the anvil is identified as follows: First all grid points in the entire domain with a cloud top height $z_{ct}$ between $z_{ctw}$-1400 m and $z_{ctw}$+1400 m are flagged. Then, one grid point wide connections between flagged regions ("bridges") and single points ("bumps") on the edges of the flagged regions are removed. Finally, all the
flagged points are identified which lie inside the region in which the column with the maximum updraft velocity is located, and which are less than 80 km away from this column (see Sect. S1.4 for details). This fairly simple method allows us to assign anvils to the convective systems which have previously been identified by fitting rectangles as described above.

3. Location of the upper mode

The location of the upper mode is chosen to depend on the development of the cloud. Fixing the location at -45°C could lead to unrealistic flash altitudes computed during the early growth stages, when clouds produce almost exclusively IC flashes. We have extended the sentence starting on page 410, line 20 as follows: “In the present study, the upper mode of the IC distribution is assumed to be centered at \( z = z_{(-15)} + 0.8 \cdot (z_{ctw} - z_{(-15)}) \), where \( z_{(-15)} \) is the altitude of the -15°C isotherm, thus allowing the altitude of the upper mode to vary depending on the growth stage of the cloud.”

Placement of CGs in the vertical column where \( w_{\text{max}} \) is located

In order to better justify this choice, we have indicated (page 410, line 23) that placing CG in the vertical grid column at the location of the maximum updraft velocity is consistent with Ray et al. (1987), who based on dual Doppler radar and VHF lightning observations found that in a multi-cell storm, lightning tended to coincide with the reflectivity and updraft core. Note that in general CG flashes tend to be co-located with the most intensive cores close to the leading edge of mesoscale convective systems. In the response to Referee #2, we argue that the assumption of CG flashes being placed at the location of \( w_{\text{max}} \) is also not inconsistent with more recent observations by Dye et al. (2000). Note also, that in the LTN3D (base) run, only \( \approx 9\% \) of all flashes are placed at the location of \( w_{\text{max}} \), accounting for less than 18% of the total NO production. Furthermore, the assumption of placing CGs in the column where \( w_{\text{max}} \) is located is consistent with Wang and Prinn.
Flash rate calculation each 56 s

The 56 s are chosen mainly for computational efficiency. However, given that the flash rates are often relatively low, this choice to some extent mimics the discreteness of flashes. At times of maximum flash rates this choice could lead to a slight over-estimate of the computed maximum NO\textsubscript{x} mixing ratios. However, since the strongest updrafts tend to have timescales longer than one minute, one would expect this potential over-estimate to be rather small, and we expect that the latter effect might be less important than the first effect. Furthermore, the simulated grid box average NO maxima due to lightning might still be below local maxima in reality, because the lightning NO is assumed to be instantaneously mixed over the size of a grid box (base area: 2 x 2 km\textsuperscript{2}). Therefore, the last sentence of Sect. 2.1 has been changed to: “For numerical efficiency, lightning NO production is calculated every 56 s in the 3-D run and every 60 s in the 2-D runs. This choice to some extent mimics the discreteness of flashes at times when flash rates are low.”

4. The lack of measurements has been indicated at the end of the 2\textsuperscript{nd} to last paragraph of the introduction: "Unfortunately, chemistry and flash rate observations are not available for the episode (19–26 December 1992) simulated in this model sensitivity study. In order to constrain the simulated flash rates and for the discussion of our chemistry results, we instead rely on observations from nearby regions and/or at other times." (Compare response to Anonymous Referee#2.) Please note that here we simulate a 7-day episode while most chemistry observations have concentrated on outflow from a single isolated storm or MCS. Please note also, that we are currently setting up another version of the same model for studying a recent field campaign for which direct observations of chemistry and meteorology will be available.

5. We estimated the flash rate per day per km\textsuperscript{2} from the Petersen et al. (1996) 24-h CG flash number to be 800/600\textsuperscript{2} = 0.0022. Since Petersen et al. applied a three point smoother to the data in their Fig. 10, this number constitutes a lower bound for the observed maximum daily flash number. Tuning the model to a 50% smaller
flash number would, however, not alter our conclusion that lightning NO production in the domain has a small influence on domain averaged ozone. Note that in general, mesoscale convective systems in the TOGA COARE/CEPEX region tend to produce much smaller flash rates compared to more intense continental thunderstorms.

6. Most of the lightning NO\(_x\) produced by CG flashes is indeed transported upwards (Fig. 8b, Fig. 6). This result is consistent with Pickering et al. (1998) who simulated a single TOGA COARE squall line. (The maximum NO\(_x\) concentration in the domain nevertheless depends on the vertical flash distribution, since higher maxima in the DeCaria et al. parameterization compared to a constant vertical distribution are also advected upwards.) We do not see a clear multi-modal structure of the vertical NO\(_x\) distribution, neither in the LTN3D run, nor in the LTN2D run, in which the lightning NO\(_x\) signal is stronger (Fig. S9), presumably because most lightning NO\(_x\) comes from MCS with high cloud tops. A further study of the vertical distribution of lightning NO\(_x\) in the LTN3D run is currently under way in a related project.

7. The justification for \(\alpha\) is given in line 26, page 409 to line 3, page 410: "\(\alpha\) is an empirical scaling factor which is adjusted to improve the agreement with available flash rate observations. For a mid-latitude supercell storm Fehr et al. (2004) applied a scaling factor of 0.26." Regarding the smallness of \(\alpha\), we changed page 413, line 25ff to: "The scaling factor \(\alpha\) in Table 1 is smaller for the 3-D run than for the 2-D run because of generally higher vertical velocities in 3-D simulations compared to 2-D simulations (Redelsperger et al., 2000; Phillips and Donner, 2006). In spite of the smaller \(\alpha\) in the LTN3D run, the number of flashes and the number of NO molecules produced are greater in the LTN3D run than in the LTN1 run."

8. p. 415, lines 21–23: We removed the references to specific tables in the supplement and added the sentence "More details on the NO\(_x\), PAN, and HNO\(_3\) budgets can be found in the supplementary material" as suggested by the referee. We also removed several other non-essential references to the supplementary material.
9. We added in Sect. 2. that the NOLTN as well as the LTN1, LTN2, LTNWP, and LTNHWP run are 2-D runs.

10. There is a pronounced influence of cloud scattering on local photolysis rates inside deep convective clouds as indicated by Wang and Prinn, 2000. However, Fig. 11 indicates that strong ozone depletion due to the reaction with NO takes place only in the LTNHWP, and to a lesser extent also during the LTNWP run, predominantly during nighttime. Fig. S15 indicates that during day-time, cloud shading can lead to a slower ozone depletion in the marine boundary layer. Salzmann (2005, Sect. 9.5), conducted a sensitivity run in which cloud formation was suppressed by turning off the microphysics and the not using the large scale advection terms. This run yielded a similar domain average column integrated chemical net loss rate of ozone as a 2-D run including lightning (which was similar to the LTN1 run in this study).

11. In Fig. 11 we are dealing with fairly localized minima and maxima. The maximum difference between the minimum surface layer ozone mixing ratio and the 10\textsuperscript{th} percentile surface layer ozone mixing ratio in the 248 × 248 km\textsuperscript{2} run, for example, is 3.48 nmol mol\textsuperscript{-1}, the mean difference over the whole time series is 0.76 nmol mol\textsuperscript{-1} (and the standard deviation of the difference is 0.73 nmol mol\textsuperscript{-1}), reflecting the relatively high spatial variability of the surface minimum, which is mainly due to the high temporal variability of the mixing ratios at the inflow boundary. (For comparison: the corresponding differences between the surface ozone minimum and 50\textsuperscript{th} percentile surface ozone mixing ratio are: 6.04 nmol mol\textsuperscript{-1} (maximum difference), 1.92 nmol mol\textsuperscript{-1} (mean difference), 1.44 nmol mol\textsuperscript{-1} (standard deviation). Especially the ozone minima in the very high NO\textsubscript{x} 2-D simulations tend to occur rather localized. The comparison of local extrema is meant to inform us about whether small scale processes, such as undiluted transport or ozone titration in the vicinity of the flashes are taking place. In order to better quantify the role of these processes for the average trace gas mixing ratios in the domain, we have used budget calculations.

12. The discussion of the downward transport is important in the light of the results by
Wang and Prinn (2000), who found that deep convection "induces downward transport and actually leads to increases of O₃ mole fractions in the upper troposphere, despite the local reduction in convective areas caused by high NOₓ in the lightning runs" while their "simulations have shown that the upward transport of O₃-poor air from the boundary layer does not significantly decrease O₃ concentrations in the upper troposphere". We find that the transport of O₃ poor air to the upper troposphere does decrease upper tropospheric mixing ratios and that, while we also simulate downward transport, on the whole this does not offset the upward transport of O₃ poor air (Sect. 4.3). In Sect. 4.3, we attribute the difference between our result and the result of Wang and Prinn (2000) to the use of different initial profiles. Downward transport of O₃ has also been found in other 2-D model studies and has also been observed (as noted at the beginning of Sect. 4.3). We nevertheless agree with the referee on the need for further studies using 3D setups with high vertical resolution in order to better quantify this transport, as indicated in our conclusions, though in a full chemistry setup, this would of course require extensive computational resources. Note that the vertical resolution in the 2-D runs has been 350 m, which is better than the 500 m in the 3-D run.

13. Sect. 5 explains why we do not see an increase of the NOₓ lifetime with increasing NO production as did Wang and Prinn (2000), who found an almost complete depletion of OH instead of an increase due to the NO+HO₂ reaction in their lighting sensitivity runs (compare discussion at the end of Sect. 3.3). Furthermore, average OH and HO₂ profiles can yield some valuable insights regarding the photochemistry simulated in the domain. While we find increasing average OH concentrations and decreasing HO₂ concentrations with increasing lightning NO production in our runs, there are several other possibilities (compare Fig. 3, Logan et al., 1981): at extremely high NOₓ in the direct vicinity of the flashes, OH and HO₂ can both decrease. On the other hand, the effect of upper tropospheric O₃ and OH increasing away from the lightning NO source can be expected to overcompensate the effect of such a potential initial HO₂ depletion, so that OH and HO₂ would both increase. (This is because the photolysis of one O₃ molecule in the presence of water vapor can yield two OH radicals, potentially
amplifying OH production). Therefore, we did not expect to necessarily find increasing OH and slightly decreasing average HO$_2$ with increasing lightning NO production. One could speculate that this might also be different in the close vicinity of mid-latitude storms which produce far more lightning.

14. Advection by non-stationary windfields is a complicated subject, and one could think of a number of scenarios in which either $u$ lags O$_3$ (e.g. upstream flow temporarily meandering over a NO$_x$ source region) or O$_3$ lags $u$. For the much simpler theoretical case of a stationary windfield (and a constant precursor source), one would neither expect $u$ to lag O$_3$ nor O$_3$ to lag $u$. In our case, including a lag does not improve the correlation significantly, indicating that the lag could be rather coincidental. The cross equatorial flow tends to occur east of the study region over the Indonesian Archipelago, so that one might expect a weaker correlation between O$_3$ and $v$ than between O$_3$ and $u$.

15. Since the main wind direction during the westerly phase of the ISO is indicated by the thick arrows in the schematic in Fig. 20, the reference to Fig. S3 is not essential, and we removed this reference from the manuscript.

16. CEPEX started during a WP (Fig. 17 of Kley et al., 1997). At about 170°E, the lower tropospheric winds shifted to easterly. Wang and Prinn simulated a squall line for 8 March 1993, when the CEPEX research vessel *Vickers* was located southeast of the TOGA COARE IFA, and the area was still under the influence of the WP. Note that neither Kley et al. (1997) nor Wang and Prinn interpreted their results in relation to the ISO. Kley et al. (1997) indicate, however, that in the low upper tropospheric ozone observed on 15 March “upper tropospheric outflow from other convective areas elsewhere must be involved” since “convection had been absent from the area for three days”. This is in line with our suggestions regarding the influence of the ISO. Most of the time our domain has also been influenced by a WP. We added the sentence: “The seven-day episode from 19–26 December 1992 is characterized by the onset of a strong WP” to Sect. 6 (p. 422, line 12). During WP’s, ozone rich air is advected into the
TOGA COARE area in the lower troposphere, so that local deep convection is unlikely to cause extremely low upper tropospheric ozone mixing ratios due to transport. Since in the upper troposphere, the wind tends to be easterly, bringing in air from the remote Pacific, horizontal transport in association with deep convection upstream is likely to play a role with regard to low ozone mixing ratios in the upper troposphere.

17. We find our results regarding downward transport important in the light of the results by Wang and Prinn (2000), who also based their findings on 2-D simulations. We find downward transport to be qualitatively much less important for the upper tropospheric ozone budget than Wang and Prinn and attribute this difference to the difference in initial profiles between the two studies. We agree, however, that further research on this issue is necessary as indicated in Sect. 4.3 (line 10, page 420) and in the conclusions (line 24–26, page 424). Furthermore, in the conclusion, we argue that “Because multi-day 3-D runs are still computationally expensive (to our knowledge this is the first multi-day cloud system resolving study including chemistry), 2-D sensitivity runs can nevertheless be useful, especially for comparing with 2-D sensitivity runs from a previous study.”

18. We appreciate the suggestion by the referee to write the section with more tact and adopted large parts of the referee’s formulation. The revised paragraph now reads:

“The causes of extremely low $O_3$ mixing ratios in the upper troposphere were examined through a series of sensitivity studies. We found that low $O_3$ mixing ratios can be a result of lightning-produced NO when high NO production rates and flash rates are used in a 2-D run, similar to Wang and Prinn (2000). However, a recent review of NO production by lightning (Schumann and Huntrieser, 2007) indicates that the NO production rate used in this sensitivity simulation is 10–100 times greater than most values reported in the literature. We therefore think this source is unrealistic. We find vertical transport of ozone poor air to play a larger role in causing low upper tropospheric mixing ratios than Wang and Prinn (2000), who specified an initial $O_3$ profile with a relatively small vertical gradient between the boundary layer and the upper troposphere. A repro-
duction of the extremely low \( O_3 \) concentrations observed during CEPEX (which started in the TOGA COARE region) was not to be anticipated in the present study since during the westerly phase of the intra-seasonal oscillation (ISO), relatively \( O_3 \)-rich air is transported to the region by low level westerlies. Correlations between zonal wind and ozone volume mixing ratios from MATCH-MPIC for 31 October 1992 to 31 March 1993 suggest that vertical ozone profiles in the TOGA COARE/CEPEX region are strongly influenced by the ISO. This influence can help to explain the lack of coincidence between upper and lower tropospheric \( O_3 \) minima observed during CEPEX."

**Technical details:**

1. we corrected \( Z=0.27 \) on page 411, line 16 to \( Z=2.76 \) as suggested by Anonymous Referee #1.

2. We moved the paragraph “Using a pressure scaled but otherwise constant vertical distribution ... “ to the end of the section.

3. The sentence containing "On the other hand ...” has been re-written. Please see reply to point 3 of the specific points.

4. a. We assume that the referee is mainly referring to Fig. 16? The aim of this figure is to show the general structure of the squall line and in particular the location of the downdrafts containing high ozone mixing ratios. Unfortunately, the format of Fig. 16 is not very well suited for ACP(D) and can not easily be changed without losing some of the information in the figure.

b. Figs. 6, 7, and 14 are indeed mostly intended to show the general structure.

**Additional remarks regarding convective chemistry transport in models using a super parameterization (compare point #1)**

Traditionally, models with a super parameterization apply horizontally homogeneous large scale tendencies to the fine grids, which can in certain ways be viewed as an analogue to the so-called "large scale forcings" used for water vapor and potential
temperature in numerous cloud system resolving studies, including the present study. This appears appropriate for temperature/water vapor having relatively small horizontal gradients due to rapid condensation/adjustment by gravity waves on the scale of a few tens to a few hundred kilometers. It is, however, certainly not as appropriate for an insoluble chemical tracer with a source in the planetary boundary layer which is transported inside some narrow convective updraft, since one would expect such a tracer to be horizontally smeared out over the entire 2-D sub-domain by applying horizontally homogeneous tracer large scale forcings (compare discussion in Salzmann et al., 2004). Since in global 3-D models large scale advection has to be calculated in two horizontal directions and since the cloud system resolving models in the super-parameterization use only one horizontal dimension, it might not be trivial to entirely avoid such a smearing out of tracer concentrations. In an approach which e.g. uses a super-parameterization to calculate so-called transient matrices, and then uses these matrices to calculate the "instantaneous" transport of tracers or some alternative approach of this sort (which is currently also being pursued by some researchers) this would, however, not necessarily be a problem. The very same issue regarding horizontally homogeneous large scale forcings for tracers could also limit attempts to apply observation derived large scale forcings for tracers in cloud system resolving models, as can be directly inferred from the discussion in Salzmann et al. (2004). (We decided to mention the latter in the last sentence of the conclusion: "Furthermore, as discussed in Salzmann et al. (2004) the application of observation derived large scale forcings for trace gases would, unlike for water vapor and potential temperature, be problematic.") We are now concentrating on nested studies in association with a recent field campaign.

**References not in the ACPD manuscript**


Interactive comment on Atmos. Chem. Phys. Discuss., 8, 403, 2008.