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Atmospheric Chemistry and Physics Discussions

Interactive comment on "The impact of resolution on ship plume simulations with NO_x chemistry" *by* C. L. Charlton-Perez et al.

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We would like to thank the reviewer for his remarks and helpful suggestions. In particular, thanks for bringing our attention to the Franke, et al. (2008) study which we now include references to in this paper. We appreciate the many comments which strengthen and clarify the text.

1. In several instances, the introduction and abstract present a relatively inaccurate overview of the previous literature and current state of modelling, to the extent that I am familiar with it. In particular:

    - Most importantly among the historical perspective issues, the authors have

overlooked a recent study which makes similar steps towards developing a parametrization of ship plume emissions, though using the approach of employing a Gaussian dispersion model: Franke et. al.. The results are in some ways similar, such as the strong overestimate of ozone by dilution to global model scales. The results of the present study should be placed in the perspective of the Franke et. al. study.

We now include a discussion of the Franke et. al. study in the introduction section. We have also referred to the Franke et. al. study in the conclusions section.

- The abstract mentions the 'reduction in model skill' without indicating which reduction it is referring to (see below).

  We have changed the text to explain this (see response to the comment below).

- The terms 'first time' and 'explicit' in the abstract are not really accurate, since other studies have already examined this issue in principle (eg. using nested box models) and since the finding will only really be explicit when it is done with a large-scale 3D model including something like a plume in grid or similar parametrization which can be directly compared with observations.

  We use "first time" to refer to a non-box model study without any parametrization of the plume at all. We are confused as to why a plume-in-grid parametrization would be considered explicit and a better comparison to observations than a high resolution simulation where no parametrization of plume behavior is used? Surely the ultimate experiment would be something like a model with a domain of size 1x1 degree with model resolution down to 10s of meters with interactive chemistry and meteorology?

  We have changed the text to "For the first time, by explicitly reducing the model spatial resolution we show that there is a significant reduction in model skill in accurately simulating the aforementioned quantities due to the

ACPD

9, C3356–C3370, 2009

coarse resolution of these CTMs and the non-linear nature of atmospheric chemistry."

- In the introduction, which studies are the authors referring to which indicate that there is generally a substantial reduction in model skill for the MBL when ship emissions are included? A few early studies such as Kasibhatla et. al. (2000) and Davis et. al. (2001) did indicate this to be the case. However, in contrast to this assertion, the recent study of Eyring et. al. (2007), an intercomparison of ten models, inclusing a comparison with the limited observations that er presently available, concluded that 'in the lower troposphere.. the models are capable to reproduce ozone and nitrogen oxides reasonably well.'

  We have re-written the introduction to address this concern. In the next to last paragraph of the introduction, the work by Eyring et. al. (2007) has been added. "However, in a later study, Eyring, et al (2007) used a multi-model approach to compare both the ensemble mean as well as individual model results to observational data and found better agreement than in these previous studies of ship emissions."

- 'ship emissions are not typically included in global 3D CTMs' ; although several authors have noted the uncertainties and problems with current emissions inventories, most models that I am familiar with nevertheless do include some representation of ship emissions. This statement needs to be either modified or justified with citation of several models which currently neglect ship emissions.

  We have modified this paragraph in light of this comment and in response to Reviewer 2's similar comment.

- 'this overestimate is usually attributed to ... resolution'; this should be 'partially attributed', since many studies have indicated this cannot explain all discrepancies.

ACPD

9, C3356–C3370, 2009

Yes, 'partially' is more precise and we have editted the text.

- The studies of Song et. al. and von Glasgow et. al. should be mentioned in the introduction to better put this study into proper context (at least P 8591 L 5 if not earlier).

  We have now added references to these two studies in the introduction.

- It would be easier to read if the discussion of Lawrence and Crutzen (1999), Kasibhatla et al (2000) and Davis et al (2001) were put in chronological order, also mentioning that is Lawrence and Crutzen, some observations such as those from the OCTA campaign compared to the model output did support the computed effect of ship NOx emissions, while the mode extensive data available to Kasibhatla et and and Davis et al indicated the model simulations tended to overestimate the observations. The comparison with observations in Eyring et al (2007) could also be added to this perspective.

  We have rewritten this paragraph to improve the clarity and impact as suggested.

- Rather than 'have been attributed by some authors to model resolution effects' more accurate would be 'proposed' or ' hypothesized to be due to..'

  We have changed the text to reflect this comment.

2. The simulations do not include NMVOCs. Although this will be appropriate for some regions, much of the worldwide ship traffic is near the coasts along the route between the North Sea, the Mediterranean, Suez Canal and across the Indian Ocean thought southeastern Asia where NMVOCs are likely to have a substantial impact on the results. Also, ships emit NMVOCs themselves, ther is still a considerable uncertainty in this. The importance of this should be discussed.

   After the paragraph starting "Table 1 summarizes the chemical reactions we use to model" we have now included the following sentences: "VOC chemistry is not

ACPD

9, C3356–C3370, 2009

included in the model. The primary reason is numerical efficiency, as the addition of VOC chemistry adds a significant computational burden to the model. A second reason is to simplify the experimental design, allowing the present experiments to focus solely on NO_x photochemistry, rather than attempting to map the more uncertain NO_x-VOC parameter space. Thirdly, in the conditions explored here the background VOC levels are low due to the remote nature of the atmosphere being simulated. At the low concentrations typical of the remote ocean the impact of VOCs on OH and O_3 production is small (Sommariva, et. al. 2006)."

3. The simulations are done for tropical conditions; likely differences for extratropical conditions should be discussed, especially in the perspective of comparing to some of the other previous studies.

   In the Conclusions section we now state in paragraph 2 that "This model-resolution dependence may be somewhat sensitive to the tropical meteorological conditions adopted here; consequently, an obvious extension of this work is to determine the robustness of our results over a wide range of different MBL locations and conditions." and we also suggest in paragraph 4 some potential differences for other meteorological scenarios with more active BL dynamics possible in the extratropics.

4. It should be made clear in the setup description that it is assumed that the ship smokestack stays fixed at the right edge of the domain and the relative wind streams past this.

   We have taken this suggestion. Please see response to the following reviewer comment.

5. A wind speed of 1 ms^{-1} is used in the simulation since this is assumed to be the relative wind speed in the reference frame of a fixed smokestack. However, won't the surface drag and the turbulent energy spectrum be different for a simulation with a 1m/s wind relative to the ground compared to one with a 10 m/s wind? At

ACPD
9, C3356–C3370, 2009

least this would be expected in reality even if the model does not capture this. Please discuss the implications for this study.

The reviewer is correct in that although a 4 ms^{-1} wind with a ship travelling at 5 ms^{-1} in the same direction gives the same ship-relative wind as a 11 ms^{-1} wind with the ship travelling at 12 ms^{-1}, the two cases give different surface drag and so different boundary-layer turbulence. It is beyond the scope of this study to explore the large parameter space of various possible boundary layers, with different depths, stabilities, mean winds etc, so this approach was used as a first order estimate, but this limitation should have been noted in the text. We now state,

"The ground-relative mean wind speed in our simulations is taken to be 1 ms in the negative x-direction and the ship source is held stationary relative to the ground. Typical translation speeds of merchant and military ships used in previous studies range from 7.7-12.6 ms^{-1} (Liu et al., 2000) and 5-12 ms^{-1} (Hobbs et al., 2000). Therefore, if the variations in boundary-layer structure with the ground-relative wind are neglected, the prescribed wind field of 1m/s relative to the ship can be interpreted as representing a ground-relative wind of 4-11.6 ms^{-1}, with the ship moving in the same direction as this steady breeze. Explicitly simulating these stronger ground-relative winds (with a moving ship) would be expected to increase the shear-driven mixing in the turbulent boundary-layer, but since investigating the role of a variety of boundary-layer structures was beyond the scope of this study this effect was neglected. Other ship-relative wind relationships are also of interest (e.g. Song et al., 2003), but due to the difficulty of resolving the plume over a much larger domain, which would require substantially greater computational resources, we choose to concentrate on the aforementioned scenario."

6. P 8596 L 24 What is meant by the winds being interpolated back to the starting conditions every six hours; are they not simply reset to the initial values? If not, please explain. Also please comment on whether the temporal discontinuity will

ACPD

9, C3356–C3370, 2009

have any implications for the simulation.

The interpolation prevents discontinuity, insofar as the model is discrete by nature. We did not reset the values to the initial values because this might introduce a big jump in the wind values which we wanted to avoid, as the reviewer suggests. We interpolate the end of the time series values back to the initial values. We performed tests on the wind interpolation in time. At the time resolution required to satisfy the CFL condition, the winds vary smoothly enough to prevent any numerical problems and are physically reasonable as well. We have explained our method in the text on P 8596 L 19-25.

7. The domains of the LES which provide the winds are tiled together along the plume axis; please indicate whether this is done for the LES that produce the winds, or only for the CTM simulations that use the winds (in that case from the smaller parent model domain) and if the latter, whether that introduces discontinuities in the winds along the boundaries where the tiling is done and any implications this would have.

   The LEM domain is periodic in the horizontal and divergence-free. This means that we can tile the domain in either x or y directions without losing the divergence-free property and without any discontinuity in space. The LES is performed with a single tile and the winds are used in the CTM in a tiled format. P 8596 L3 and L 6 have been changed to clarify this point.

   "To increase our domain size with the minimum off-line computational expense, we "tile" the output of the LEM (not the LEM domain itself) along the zonal direction to form an extended domain for the plume to occupy. The periodic boundary condition used for the initial LEM simulation is ideally suited for this. We use 12 tiles for the chemistry-advection model, and thus we go from a 9.6 km $\times$ 9.6 km $\times$ 1.92 km LEM simulation to a 115.2 km $\times$ 9.6 km $\times$ 1.92 km simulation with the chemistry transport model."

ACPD

9, C3356–C3370, 2009

8. P 8592 L 19 Indicate the background of the values of ship speeds from the previous studies (e.g. are these based on Lloyds of IMO statistics or similar?)

   They are actual ship speeds measured and confirmed during field campaigns. We have added the sentence: “In both of the previous studies ship speeds were measured in field campaigns; Hobbs (2000) used data gathered from ships in the Monterey Area Ship Track (MAST) study.”

9. Are there any mean transverse winds, or is the tendency of the plume to move off to one side of the domain the result of asymmetries in the turbulent eddies and if so where do these originate?

   The domain is periodic in the across-plume direction and it is the LEM winds which transport the plume in this direction. There are no mean transverse winds, but the asymmetries in the plume appearance are due to the eddies which are of the size appropriate to the eddy-resolving scales of the LEM.

10. P 8598 L 27 The plume width does increase with distance, but the plume height actually does not; it increases for the first 4 km, but the decreases up to 8 km and stays about the same up at 20 km; if possible please analyze the 3D fields more closely to explain this apparently unusual behavior (perhaps it is a function of the chosen contour intervals).

    The contour intervals are the same in all 4 panels of Figure 2. Indeed the highest NOx concentration contour does not appear to increase with height at each of the points downstream, but from 1 to 4 km only. Dilution effects downstream in the presence of cleaner ambient air and the effect of the wind could both be responsible for the decrease in height of the highest contour value. Defining a plume edge is a tricky thing, and in this case, we were speaking qualitatively of the plume edge as the contour value 316, which does expand in y and z as one looks downstream. If one were to define the plume edge as the location of the highest contour value, then the plume edge would have descended downstream

ACPD

9, C3356–C3370, 2009

from the source. We have rewritten the text to clarify the description of figure 2 because the interpretation of the plume is subjective in the description.

"Defining the plume boundary is subjective, but the [NO_x] = 316 pptv isosurface can be taken as a reasonable definition, and is also contoured in Figure 1. Then the plume height and across-plume width generally increase with distance downstream from the source. The height does not appear to increase from 8 to 20 km downstream and we note that much of the plume remains generally trapped in the vertical below the level of imposed subsidence in the LEM model (approximately 1.5 km)."

11. P 8600 L 19 The speculation that the asymptotic behavior between C1 and C2 depends on the similarity in the meteorology seems inconsistent with the basic idea of the study that the main effect on O3 and the related species is due to the dilution (i.e. the dependency of O3 and OH on NOx levels and the feedback this has on NOx lifetime), which one might expect to apply regardless of the similarity in meteorology. Is it possible that there is a limit to the dilution effect at very small scales such as C1 and C2? It would be very enlightening if some deeper analysis or further sensitivity studies could be done to elucidate this interesting aspect.

    We cannot think of a limit to the dilution effect at very small scales and the similarity between C1 and C2 is consistent with most of the fluxes in C1 being on scales that are captured by C2. This asymptote at small-scales is not important for our conclusions about the coarser scales, and the explanation is clearly described as speculation in the text, so we have left this text unchanged.

12. P 8601 L 2 The study of von Glasgow et. al. (2003) used a box model, not a global chemistry model, to examine the effect of dilution of ship plumes (this is mentioned in the first sentence of the abstract of that study, which needs to be read through more carefully by the authors so that the present study can be put in a more proper perspective with respect to the previous literature).

ACPD

9, C3356–C3370, 2009

Yes, in the abstract in the von Glasgow paper, the authors state that they use a box model. However, in the paper they also state: "To study the global effects of ship emissions we used a simple upscaling approach which suggested that the parametrization of ship emissions in global chemistry models as a constant source at the sea surface leads to an overestimation of the effects of ship emissions on O_3 of about 50% and on OH of roughly a factor of 2." Even though the authors use a box model, with the upscaling approach that they apply, they make a meaningful comparison with global chemistry models.

To clarify this point we have re-written the sentence as:

"In a study by (von Glasgow et al., 2003), using a box model which is modified via a "simple upscaling approach" to compare with global chemistry models and where ship emissions were taken to be a constant source at the sea surface, they found that OH can be overestimated by a factor of 2."

13. It would be elucidating to compare the rate of plume expansion (horizontal and vertical) in this study with the assumed or computed rates in the earlier studies like von Glasgow et. al and Song et. al. (a brief note of this is already made in the text, but would be helpful to be more detailed on this point of comparison).

    Indeed, this would be an interesting topic to pursue. However, it would entail defining the plume edge precisely before being able to compute the rate of expansion of the plume and this is not a simple exercise, but would take some careful thought and planning of more objective measures or criteria than we have used so far. We, unfortunately, are not currently in a position to continue this line of investigation and will have to leave this as a suggestion for future work.

14. P 8601 L 13-15 It would be good to mention explicitly that the approximation of equating NOx loss to HNO3 production is exact in these simulations, since the reaction of HNO3 with OH and its photolysis are neglected.

    Yes, we have changed the text to incorporate this comment.

ACPD

9, C3356–C3370, 2009

15. P 8601 L 23 (also P 9603 L 22) 'as suggested by Chen et. al.'; was this suggestion based on observation? If so, please describe, that will help make the conclusion stronger (and perhaps indicate what other competing candidates for NOx loss would come into question).

    This study used a box model forced by data obtained from observations of 8 transects of ship plumes in the ITCT ship experiments. NO and O_3 were among the inputs, while OH and HNO_3 were some of the outputs. Chen et. al. (2005) state that "The variation of the lifetime is anticorrelated with OH levels. This strong anticorrelation reflects that OH + NO2 is the main NOx loss process, contributing 85 to 90% for west A through D and 65 to 75% for the rest of later transects. The other significant ship plume NOx sink involves formation of PAN." In our study we consider PAN decomposition, but not the formation of PAN.

    We have added to the text to answer the questions raised in this comment.

16. P 8602 L 13-15 The 'OH halo' result is very interesting; would this be influenced much by the inclusion of complex NMVOC chemistry (eg. near coasts)?

    Yes, there probably would be an influence, but we would need further studies to simulate this. We have added a line to the text to say: "The magnitude of the change in NO_x lifetime may be influenced by VOCs, but the general feature should be robust."

17. P 8603 L 1+ for the simulations with halved emissions are the OH and NOx slopes also approximately half as large as with the full emissions? Can the authors offer any explanation for the contrasting behavior of the OPE?

    The OH slope is not halved with the halved emissions, but is about one third of the value of the full emissions case. The NO_x lifetime slope is not halved but is about a sixth of the of the value of the full emissions case. We cannot offer any explanation for the OPE behavior and have removed this result from the text along with the other halved emission results.

ACPD
9, C3356–C3370, 2009

It is not surprising that resolution effects fall away rapidly with decreasing source strength, as they depend critically on nonlinearity in the chemistry. There would be no resolution effect at all for a very weak (i.e. linear) source.

Please see our response to a similar comment from reviewer 2.

18. P 8603 L 21 (and elsewhere where appropriate in the conclusions): make clear that this result is specific to these conditions and may vary under other conditions.

    We have modified the text to reflect this comment.

19. Somewhere in the manuscript it would be worth briefly discussing what the resolution does to the mean NOx mixing ratio, not just the NOx lifetime, since it is the mixing ratio which is measured and compared to in previous studies like Lawrence and Crutzen (1999) and Kasibhatla et. al. (2000).

    We have now included this information in the results section.

20. P 8604 L 3 running the LEM at even higher resolution to explore the convergence (also see the note about its interpretation above) is an excellent idea for this study: if at all possible (within computational limitations) it would be very much worth doing so in a revised version.

    We acknowledge the reviewer's comments about running the LEM at higher resolution and have had the same thoughts ourselves. We could in the future (with greater computational resources than we currently have) run a variety of LEM simulations at extremely high resolutions to try to understand this interesting subtlety and have left this thought in the conclusions as a suggestion for future work. However, for the scope of this paper we do not believe that this would add any major insights into the conclusions which do not rest upon these details.

ACPD

9, C3356–C3370, 2009

0.1 Technical comments

1. For the Forster et al (2007) reference, the IPCC should be mentioned.
   We have changed the reference to refer to the IPCC.

2. P 8589 L 28 'around 10% of the total radiative forcing' - is this 10% of the increase since preindustrial times or of the absolute total.

   From reading Endersen et. al. (2003) Table 17 and section 6.8, I believe that we are looking at the absolute total. We have rewritten this paragraph to be more precise.

3. P 8591 L 21 Since there are many other errors such as mixing processes, chemistry and emissions of other tracers, as well as an incomplete observation set for model evaluation in the ship-affected regions, it will unfortunately not be possible to 'fully account for the erroneous representation...' this should be rephrased.

   We have rephrased to 'partially account for.'

4. P 8592 L 17+ The description of the winds need to be written more clearly.

   We have re-written the description including some clarification on the typical ship speeds gathered from previous studies.

5. P 8600 L 16 'linearly dependent on resolution' should be 'linearly dependent on the logarithm of the grid box volumes.'

   We have changed the text here.

6. P 8601 L 16 'NOx loss' should be 'NOx concentration'

   Yes, we have changed this.

7. P 8602 L 1 'emission' should be 'plume'

   Yes, we have changed this.

ACPD
9, C3356–C3370, 2009

8. P 8602 L 5+ indicate whether the simulations discussed here were done at high resolution

   The simulations were done for C2-C48 resolutions, but not at the highest resolution because the zero emission runs were not significantly different at all other resolutions. We thought it was not necessary to run at the highest resolution since the C1 runs are so expensive. We have made a note in the text that C2-C48 are the resolutions we are referring to. See the response to the next comment.

9. P 8603 L 6+ are the no-ship simulations done are at all the resolutions? If so, are there notable differences between the various no-ships runs themselves due to the resolution, or are they all relatively homogeneous? Please indicate briefly in the text.

   We have changed the text in response to this comment and the one before: "We calculated the mean NO_x lifetime in the entire domain (not shown) for a model run with a ship plume and without at different resolutions (C2-C48). There were no notable differences in the zero emission runs between different resolutions."

10. P 8604 L 13 'starting point' is not really valid since in principle a couple other studies have already looked at the resolution/dilution issue for ship plumes (albeit with simpler approaches than used here); 'important step forward' would be more fitting.

    We have changed the text.

11. P 8604 L 16 the link to power plant plumes is in principle appropriate but that research has a long history of its own and is affected by very different chemistry so that it is more likely that the ship research community will learn from them than the other way around.

    Indeed, the power plant plume research community has a long history of its own. Our reference to power plant plumes was as another application for our model.

ACPD

9, C3356–C3370, 2009

Yes, our model chemistry would need to be modified and perhaps different meteorology would be needed to drive the model. However, in principle, our model and approach could easily be applied to study power plant plumes. We have changed the text to reflect the intent of our remark more clearly.

"Our model may also be modified to study other plumes, such as those from power stations, at high resolution and without parametrization of the plume."

12. Make figure 8 into Figure A1 to avoid confusion.

    We have changed the figure numbering.

13. P 8606 L 19 'dimishes' should be 'diminishes'

    Yes it should. We have corrected this typo.

14. From figure 5,6,7 move the text on the no-ships run into the main text.

    We have a line at the end of the results section with the same values for the no-ship emissions or clean case. However, we think that it helps the reader to have the statements handy in the captions as well for when they are studying the figures.

Interactive comment on Atmos. Chem. Phys. Discuss., 9, 8587, 2009.