Interactive comment on “Sensitivity of CHIMERE to changes in model resolution and chemistry over the northwestern Iberian Peninsula” by Swen Brands et al.

Anonymous Referee #2

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Quite a few different models are currently in use for chemistry transport modelling on the regional scale. Still many questions concerning the validity of the model results with respect to the necessary complexity of the chemistry mechanisms, the needed quality of underlying emissions or a sufficient grid resolution are not finally answered, yet. On the other hand these type of models are more and more applied for short term air quality forecasting. The present manuscript offers a sensitivity study conducted with the model CHIMERE, which was set up for the northwestern Iberian Peninsula, a region with complex topography and a long, structured coast line. Meteorological data from the WRF model was fed into CHIMERE, for the emissions the HTAP v2.2 inventory was used. Two different horizontal and two different vertical resolutions were tested...
as well as two chemistry mechanisms (SPARC-07 A and Melchior mechanism). Model derived nitrogen dioxide, PM10, PM2.5 and ozone concentrations are discussed and compared to observational data from a regional air quality network based on statistical measures. The comparisons were done for daily minimum and maximum values of those substances. The underlying investigation for the article is a straightforward sensitivity study with a pragmatic choice of varied parameters (∼12 km and ∼4 km horizontal grid resolution and 10 and 20 vertical layers to 500 hPA). The comparisons between the model set-ups is done (for daily extreme values only) by using the bias, Pearson correlation and standard deviation ratio for the chemicals under investigation in relation to respective observed values. In addition, a mean absolute error is chosen to compare the runs to a chosen reference case (the computationally cheapest). The results of this quite “technical” study may be interesting for those intending to set up CHIMERE for purposes, for which computing resources are a limiting factor. The result section is dominated by describing point for point in words, what the figures show anyway. No deeper investigation and discussion of possible reasons for the discrepancies among model runs for the different the set-ups are offered. E.g. for the strong statement in the conclusions section that “CHIMERE’s performance is very poor” it is in my opinion not sufficient to just speculate that the used emission inventory has deficiencies for the region: This definitely should be investigated (e.g. by consulting other inventories).

General comment: I doubt that the paper in its current form would be of great interest for the typical ACP readership. It fits not well into the journals scope. Neither the used procedures are sufficiently innovative nor the analysis of the results is deep enough to provide transferrable insights. The results, which might be interesting from a technical point of view, are addressing a specific region only, they could have wider implications for the modelling community in atmospheric sciences, if the analysis would look closer at the influence of the heterogeneous terrain and coastal flow effects on the findings. I leave a final consideration to the editor. In general, a more thorough discussion of reasons for the presented deviations between results from runs for the different model
set-ups and from the measurements is needed. Since the results have some value for air quality modelling, I would suggest to the authors considering a submission, though in a revised and extended form, to a journal, which is more devoted to technical analyses for modelling.

Some mayor points In addition to the remarks made above some further issues (shortcomings) of the manuscript need to be mentioned.

Emissions The backbone of air quality studies, especially when compared to observations, are suited emissions. The authors use HTAP v2.2 for the year 2010, while the study period are two summer months of 2018. A discussion of implications of this mismatch is missing. If the necessary observational data would be available, this technical study could have been performed for 2010 using appropriate meteorology. Or the 2010 emissions from HTAP could have been compared to more recent emission data and may be scaled (2010 compared to 2018). HTAP v2.2 emissions are provided on 0.1° x 0.1° grid, which does not directly fit the used resolution (0.15° x 0.15° and 0.05° x 0.04°). The regridding was done without downscaling. The authors do not explain what this mismatch means. But they should, since the resolution of the emissions may affect the results differently on the two grids, certainly a limitation of the study. HTAP v2.2 emissions are provided with a monthly time resolution. The authors do not inform the reader how they dealt with this coarse resolution when feeding the emissions into CHIMERE. Did they use time profiles on the emissions or did they feed in just the monthly means. A higher time resolution is needed, when comparing to daily maximum and minimum values of the observations (i.e. NO/NO2 and O3 relations are strongly dependent on the daily emission time profile). Any way, it is not adequate to state “CHIMERE’s performance for NO2 is very poor” and point at the same time to possible deficiencies in the emissions (in that case it is not CHIMERE’s performance). Page 17/Line 16 (1 on that page) To improve their manuscript, the authors need to devote an entire section to these emission issues.

Meteorology The study area is characterized by structured terrain and a complex coast
line. The question appears, whether the meteorological model in use (here WRF) is resolving the local flow features sufficiently well (terrain effects and summer sea breeze circulations)? The 12 km and 4 km runs might produce different results here, not unimportant, since quite a few of the observational stations are located near the coast or in hilly areas, where local flow fields might dominate the dispersion of emitted substances. Differences between modelled and observe concentration maxima/minima could partly be due to the quality of the meteorological simulations rather than entirely ascribed to CHIMERE. A discussion of the quality of the meteorological fields and reproduction of local features (best against observations) needs to be provided.

Data handling for results section The evaluation of the modelling results using observational data only considers maximum and minimum values. No information is provided how the values are taken from the respective series. There are several possibilities. Is the maximum taken from the observational time series and compared to the model result for the same time stamp? Or is the maximum taken from the observational time series and compared to the maximum of that day in the model series, which could occur at a different time (a considerable time shift might be possible). Or is the model output leading the selection? The same questions holds for the comparison of minimum values. It is interesting to learn whether maxima/minima are missed in general or whether there is a certain time shift. Although maximum values are important for air quality and health related studies, it would have been instructive to additionally analyse better time resolved concentrations to assess the models ability to reproduce daily cycles in different regions (i.e. O3) and the variability in the model and observational data. Both should be available with an hourly resolution. This could help also to discuss reasons for the deviations between the different set up. Show a few selected time series (for different quantities, different locations) of modelled versus measured concentrations (hourly resolution); may be more of that in the supplement. This would be very instructive. In an additional evaluation step the Mean Absolute Skill Score (using the reference run CS10) was provided separately for background, industry and traffic locations. In general no bad idea. It should be discussed, why for the background and
industry stations NO2 and O3 perform so differently for the different settings? Are they really that much decoupled? Are in case of the background stations O3 concentrations influenced predominantly by BVOCs from MEGAN? This needs a more thorough discussion. Quite a few of the stations used as bases for the statistical analysis are so called “traffic stations”. These stations are often hotspots for some of the considered substances (NO2, PM10), because local traffic emissions are dominating (not resolved by HTAP). The authors should inform the readers about these traffic stations. Are some of them located within street canyons, which channel the flow and dispersion near the ground? This very local data is compared to model results obtained with a relatively coarse resolution (4 km and more horizontally). This seems not to be appropriate. It would be recommended to nit consider traffic station in the statistical evaluation (or do it separately to see the effect). Also for the other measurement stations, it would be useful to know, how they are located within the modelling grid. A station, which is located close to the grid boundary or grid corner, might be better represented by the neighbouring grid cell(s), dependent on local terrain effects. A study of this localisation effects for the 12 km and 4 km grid resolution would be helpful. Point measurements are compared to grid box means. The issue of the spatial representativeness of the stations needs to be addressed. Which of the background stations are in forested regions (BVOC emissions)?

Minor points

Since computational costs ares one of the parameters of interest/motivation of this study, it would be helpful for the reader to get quantitative information on the model runtime for the different experiments.

On page 8, line 18, CS10 is flagged as the computational cheapest experiment. In table 3, in which the experiments are ordered according to their computational costs, CM10 is the first mentioned and here apparently the cheapest. Clarify.

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