Atmos. Chem. Phys. Discuss., 11, C3549–C3564, 2011
www.atmos-chem-phys-discuss.net/11/C3549/2011/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Development of a fast, urban chemistry metamodel for inclusion in global models" *by* J. B. Cohen and R. G. Prinn

J. B. Cohen and R. G. Prinn

jasonbc@smart.mit.edu

Received and published: 18 May 2011

We would like to thank the Referees for their time to review the manuscript and provide thoughtful comments. We hope that this exchange can continue until an improved manuscript is accepted into ACP. If there is any further feedback or clarification, please let us know. We have combined the Referees comments and will respond to them in a single document, since some overlap.

Referee#1: The use of assimilated meteorology rather than a grid-based prognostic meteorological model to drive CAMx does not reflect current best practices for regional- and urban scale photochemical modeling. It would be preferable to apply prognostic Eulerian mesoscale models such as MM5 or WRF to drive the CAMx simulations used to generate the urban metamodel.

Response: The most important thing about the meteorology fields used is that the dynamic variables are inherently consistent and mass conservative. A careful examination of the CAMx results shows that air and tracer mass is conserved. While many recent papers use a prognostic Eulerian mesoscale model to predict the meteorology at the urban scale, this method has both advantages and disadvantages over the method used. One advantage is that these models use very specific inputs (land-surface characteristics, boundary conditions, and radiation fields) to predict the dynamics over the corresponding regions precisely. A disadvantage is that these models cannot simulate more generalized areas, or areas under future conditions, as they rely on being fed a specific set of inputs. Presently, the majority of urban areas around the world does not resolve or publish the level of data required to create the necessary inputs required to drive these models. Future research could use such mesoscale models to generate meteorology under specific types of conditions that are quite different from those used in this approach (such as tropical urban areas or those with complex topography), and then use this meteorology to generate new metamodels. Comparisons between these approaches could be made and improvements could be found. Due to the demanding task of producing such set of meteorology, and the fact that they would not change the basic results, we believe this is best left to future research efforts.

Referee#1: The assumption that all anthropogenic emissions scale linearly with either CO or BC seems oversimplified. For typical CAMx applications, a more detailed emissions processing approach is employed to reflect the mix of source sectors and their temporal and spatial variability.

Response: The underlying emissions are based on the results of a detailed economic model that takes into consideration multiple economic and energy sectors, and computes the results for all nations or clusters of nations on a global scale. This modeling process includes many sources of uncertainty in terms of the emissions factors, economic conditions, policies, and competing energy sources. This data is then translated onto a global grid at the spatial scale of individual urban areas. When carefully forming the PDFs across these hundreds of different underlying emissions scenarios, it was found that there was a tendency for the results to scale with either BC or CO, with the most important component of this scaling related to the urban type. An initial attempt was made to perform this polynomial chaos expansion with each emitted species being represented independently. However, the end result was found to have inputs that were too strongly correlated. Therefore, for this work, it is assumed that the net emissions of each species scales linearly with either CO or BC, with different scaling ratios for each urban type: India, China, Developed Nations, and Developing Nations. If a given urban area has emissions ratios that fall somewhere in between two of these cases, both could be run and the value linearly interpolated. Secondly, the spatial and temporal distributions of the emissions within a given urban area are in fact highly variable. The distribution is controlled by two input parameters: "temporal weight" and "spatial weight", which respectively control the distribution of emissions as a function of time and geographic location. Given this method, a very large parameter space of different emissions distributions is reproducible. One of the key advantages of this method is that it is flexible. In even the world's most developed and best-studied urban areas, emissions inventories of critical species are still fraught with large uncertainties. In the majority of the world's urban areas, the ability to quantify emissions and their geographic and temporal pattern is poor at best. Furthermore, some of the most modern efforts for determining emissions are often based on a short snapshot or data that is quickly out of date. For example, the most recent census count of China, just released in 2011, shows that there are multiple large urban areas that just a few years prior, do not show up as polluted "urban areas" in the commonly cited emissions inventory of Zhang et al. (2009). This issue is not just restricted to China: throughout the developing world population and economic activity censuses are either not performed or not reported. Thirdly, the flexibility of this model allows for considerably higher or lower levels of the emissions and other input parameter space to be explored. This allows for policy scenarios, or future climate conditions, to be explored. When one restricts their emissions to such detail as appropriate for chemical weather prediction, they loose the

ability to adapt to the fact that urban areas change and evolve over time. Presently, urban areas are growing, evolving, and expanding rapidly around the globe, and they are expected to continue to do so into the foreseeable future.

Referee#1: Given that both the preparation of input meteorology and emissions for CAMx appear simplified compared to typical regional- and urban scale CAMx applications, output from the CAMx simulations performed in this study should be compared to observations before being used to develop a metamodel for use within a global model. While the metamodel output is compared to observations in Section 8, similar analysis should be performed for the underlying CAMx runs. In particular, the authors state that some of the discrepancies between the metamodel output and observations arise from the incompatibility between ground-level measurements vs. column-integrated metamodel outputs. By directly comparing CAMx output for the first model layer against observations these incompatibility could be reduced and the credibility of the CAMx setup used in this study could be established. If similar discrepancies exist even between the actual CAMx output and observations (i.e. large overestimation of ozone, underestimation of CO), it is hard to justify the use of these CAMx outputs for developing the metamodel.

Response: A set of comparisons between the metamodel and CAMx for the lowest 100m average concentrations over the domain have been made. These figures were removed from an earlier draft to help shorten the length of the manuscript. They match each other quite well, as explained in the text. A comparison between the bottom 100m average concentrations of the 50,000 sensitivity runs can be made with observations, if it helps to improve the reviewer's confidence in this methodology. If this is what is suggested, either of these can be done and added as an additional figure or table respectively. However, to overcome the issues of incompatibility between "ground-level measurements vs. column-integrated metamodel outputs", especially since the emissions are not tuned or distributed for chemical weather forecasting, then measurements of a similar type will need to be compared with the metamodel. It is not known to us where there are publically available urban measurements made to represent similar spatial and temporal scales to what the metamodel is predicting: coverage over a roughly 100km by 100km single urban area, for 24 hours a day. However, we will gladly use any such data to compare with the sensitivity runs if it is available. The point of making comparisons with measurements is to show that the metamodel can reasonably simulate realistic conditions and that it behaves as it is expected to, based on how the underlying chemical and physical routines integrated within the parent model. It is over and beyond the scope of this effort to evaluate CAMx, which is itself open and available in the public domain.

Referee#1: The introduction section should be shortened. The order of figures some figures and tables is out of sequence, e.g. Table 5 is referenced before Table 3, and Figure 8 is referenced before Figure 7. The CAMx setup should be fully described in Section 3, yet most details of the setup are only described in Sections 5 and 6. Sections 2 and 6 both deal with prior work and should be combined, i.e. Section 6 should be folded into Section 2.

Response: The introduction has been shortened, with parts completely removed and other parts edited for both space and clarity. Figures 6, 8, 10, and 12 have been eliminated, with the relevant information from these figures folded into the existing Table #6. This includes the means and statistics of the concentrations as predicted by the metamodel as well as the mean and maximum concentrations provided by the respective measurements. The following Tables have been re-labeled so that they now are in correct order: Tables #5,3,4 and Tables #7,8,6. The portion of the CAMx setup described in section 5 (the final paragraph) has been integrated into section 3. The first three paragraphs of Section 6 have been folded into Section 2. The remaining paragraphs of Section 6 relate to the overall conclusions and have, at the recommendation of Referee #2 been integrated into the conclusion section. Section 6 now no longer exists.

Referee#1: Pages 4633 – 4636: There should be some references to modeling systems that pursue global-to-urban nesting approaches (e.g. GATOR

http://www.stanford.edu/group/efmh/jacobson/PDF%20files/GATORGCMOM1008.pdf; GU-WRF, http://www.cmascenter.org/conference/2010/slides/karamchandani_development_grid_2010.ppt) rather than sub-grid scale parameterizations to characterize urban scale phenomena in global modeling studies. Please provide some brief discussion on the advantages and disadvantages of each approach.

Response: These two approaches are different from each other. The approach used here is to parameterize urban processing, so that the physical and chemical alterations can be approximated under widely divergent sets of conditions. The point is to make it so that the effects of this processing can be applied throughout the World, under present-day, future, and past conditions, and under different types of geographic and policy constraints. The method should be applicable to urban areas characterized based on different densities, transportation styles, and major emissions sources. Finally, it should be applicable for areas not well characterized or for sensitivity studies. This approach is rapidly scalable and computationally quick enough that it can be applied to a GCM that needs to run for many decades or centuries. It can be run in such a way that new urban areas can suddenly come online or be turned off. Finally, the model is designed to interact in a 2-way fully coupled manner. We are not overly familiar with the two models used as examples above, but based on the information provided, believe that they use a different approach. These methods seem to work in one direction only: it is our understanding that a full 2-way coupling of dynamics from regional to global scales has only been published one time in the peer-reviewed literature, Lorenz and Jacob (2005), and that there has been no follow-up on that work. We have thus not been able to find a 2-way coupling of chemistry, physics, and dynamics, of aerosols and gas species, since this would involve requiring a two-way dynamical coupling. Additionally, it seems that these methods are based upon and fine-tuned to operate under current day conditions. Since the grids are not dynamically updateable, changes in the locations of, size of, and distribution of urban areas seems like it is not possible. While this method could potentially be used to explore chemical weather over a short time period, we do not see how it could be expected to make such computations under conditions where urban areas or the climate itself evolve in the future. Perhaps, for future work, there is a way to use these global to urban approaches, under thousands of different emissions, climate, and urban conditions to improve the ability of the modeling system? A combination of these approaches could potentially yield more information on the urban scale. If it is deemed important for the validity of this study, such a detailed inter-comparison can be included in a revised manuscript.

Referee#1: Page 4634, line 29: replace "areas" with "area's"

Response: Done.

Referee#1: Page 4639, line 28 – page 4640, line 2: please provide more details on the procedure used to assimilate the meteorological data. Which two days were simulated? The OTAG episode lasted for about a week. Why wasn't a prognostic model used, possibly in data assimilation mode? How many sites were developed to generate the assimilated meteorological fields for the 4km CAMx domain described in Section 5?

Response: The two days were chosen to correspond to the two-daily average maximum in rainfall, minimum in rainfall, maximum in integrated wind speed, and minimum in integrated wind speed, over a contiguous urban area. The two days simulated were not the same for each set of meteorology chosen for the four different meteorological conditions. The rationale was to choose data that was as extreme as possible, and yet still contained within the weeklong episode. The above paragraph has been folded into the manuscript. The use of a prognostic model, as mentioned in response to another question, would provide an excellent additional piece of information, and would be most useful for studying an area that has a completely different meteorological pattern. We do believe that this can be done as future work.

Referee#1: Page 4640, line 15-16: please provide more details or a reference for the "newer and more detailed representation"

Response: An appropriate reference has been added.

Referee#1: Page 4641, line 8: what are some of the other mathematical techniques? What are the advantages and disadvantages of the method chosen for this study?

Response: This line has been altered and expanded upon to describe advantages and disadvantages of this method.

Referee#1: Section 3 (pages 4642 – 4647), CAMx model: please provide more details on the setup of CAMx: height of vertical layers, model top, size of horizontal modeling domain, number of grid cells, grid cell spacing, lateral boundary conditions etc. Some of this information is later provided in Sections 5 and 6 and Table 4 but should be provided upfront.

Response: Based upon the other changes made and described in this response document, we do believe that all of this information is now up-front and clear.

Referee#1: Page 4644, line 2. The assumption that all emissions are proportional to either CO or BC does not generally hold true, at least not when considering complex urban areas at a fine spatial scale. Please provide a justification for making this simplifying assumption and discuss how it may affect the accuracy of the model outputs when compared to observations.

Response: This has been answered in full or in part by other responses.

Referee#1: Page 4644, lines 15: please provide a reference that found the chosen approach to be "superior" to that of Mayer et al. (2000).

Response: To our understanding, this paper is the first one that makes the comparison. Mayer et al. (2000) simulated ozone to a larger uncertainty than these results and was not capable of simulating many of the more chemically complex species (eg: aerosols). Mayer et al. (2000) use a similar mathematical approach, at a lower order of magnitude fit, and thus is expected to be mathematically less robust. The results in terms of the quantification of the goodness of fit, and the ability to simulate more physically relevant outputs (such as aerosols and urban concentrations) further validate that this approach is superior. It is hoped that subsequent work can be done to further refine and expand upon this question. Furthermore, one co-author on this paper was also a co-author on Mayer et al. (2000) and this person approved the use of "superior" that is quoted by the referee.

Referee#1: Page 4645, line 1: what is the top of the urban modeling domain? This information is provided in subsequent sections but should be presented upfront.

Response: This has been moved forward.

Referee#1: Page 4648, lines 26-28: While 72 hours may be sufficient to dampen the effect of initial conditions, boundary conditions are expected to be very important for a modeling domain covering only 108 km x 108 km. How were boundary conditions specified, and how sensitive are the CAMx results to these boundary conditions?

Response: Boundary concentrations user defined input variables. The boundary conditions are the mole fractions and concentrations of the appropriate species at all five of the boundaries of the domain. This value, once chosen, is held constant for the length of the model run. This works perfectly for use within a global modeling framework, where this information is at coarse resolution. The results of the 50,000 sensitivity runs include this aspect of the sensitivity. If it is deemed important for the study, another set of sensitivity runs can be performed which only contain variations in the boundary conditions. However, this alone is likely not sufficient, since the response of the boundaries under different levels of emissions is likely to not vary in a linear manner. This seems like it would be better handled as future work.

Referee#1: Page 4652, line 1: The CAMx studies listed in Section 3 were for a more sophisticated setup of CAMx, including prognostic meteorology. As stated in my major comments, the authors do need to show that the more simplified CAMx setup used in this study is accurate with respect to observations.

Response: The point of this CAMx setup is to quantify the effects of processing of high

levels of emissions from urban areas. Specifically, we are interested in how the urban scale processing of chemical, physical, and dynamical mechanisms lead to changes on urban-scale concentrations and net export fluxes. We believe that the comparisons made and presented here are sufficient for this task. If there are specific further comparisons that can improve this manuscript, we would be happy to look into them and to include them in any revised manuscript. Based on our understanding, many regional scale models use emissions that are or were previously constrained based on measurements. This type of forecasting can be made at high precision for a specific urban area at a specific time, assuming that the physics, chemistry, and sub-grid scale approximations are valid. This level of precision is not generally translatable to other urban areas, especially if the other areas are poorly or differently characterized, or if environmental conditions or the climate have changed. Given that the model chemistry, physics, and sub-grid parameterizations are being run in a standard mode, that the meteorological inputs fulfill the consistency issues, and that the emissions are prepared to the correct units and magnitude, there should be no reason to assume that the CAMx will behave incorrectly. Looking at diagnostics from the CAMx results we have determined that the mass and number fluxes, concentrations, chemical and physical production and destruction and deposition rates all match. If there is something that has been missed, please let us know and we will carefully examine if there is indeed an issue to further explore.

Referee#1: Page 4656, line 22 – Page 4658, line 27: Figures 6,8,10,12: The panels in these figures are too small. The dots representing the median values of the metamodel runs are barely visible. It is unclear which range of observations is represented by the lines: Page 4656, line 27 states that the minima, medians, means, and maxima for the measurements are shown on these plots, but only a single line is shown for each site. Furthermore, what were the sampling periods and number of sites for each of the observed ranges? For example, what is represented by the line labeled "Delhi BC"? A single site or multiple sites? The range between minimum and maximum observed values? Over which time period? Why is only a single observational site used for ozone for all four metamodels? “Guadalajara” is misspelled in the figure legend. The figure captions do not state that the plots also contain observational results. Why are no observational results shown for BC and OC even though they are discussed in the text? I am also confused about the results presented in Table 6: assuming the ranges reflect the results from the 50,000 metamodel runs, how are the median and maximum values defined? As the median/maximum values over all grid cells over the entire simulation period for each metamodel run?

Response: Figures 6, 8, 10, and 12 have been removed and are replaced by an extended Table 6 (now renamed to Table 8). This table contains the mean, statistics, and maximum values that the papers report. These values are also reported and described more fully in the text, and the underlying meta-properties found in the papers have been made clearer. An additional site has been included for Ozone measurements. BC concentrations are mentioned in the text and the modified table. The median value is the value at which 50% of the runs are less than and 50% of the runs are greater than. The maximum value is defined as the largest of the set of 50,000 runs. In each case, there is a range, since there are 16 different metamodels. The values being shown are the concentration as predicted by the metamodel: the daily average concentration over the urban area.

Referee#2: General comments: It seems to me that the paper is missing a section where the results of the method would be used to demonstrate both the necessity and the significance of the method described.

Response: We believe that this result is significant in that it allows for a way to quantify the chemical and physical processing occurring in present, future, and simulated urban areas. We further believe that the result is important because it is flexible enough to be implemented within the framework of a GCM or to be used to perform various sensitivity analyses of emissions scenarios, background concentration influences, urban-scale policy formulations, or many other applications. Furthermore, this is the first work to offer a significant advance based on the widely cited paper of Mayer et al. (2000).

Finally, the result shows that on an urban average level, that concentrations and export fluxes can be successfully simulated over many urban types of conditions.

Referee#2: pg 4656, line 6: What happens at the extremes? It seems that this could potentially be significant, especially if the metamodel is extrapolated from very few sites / episodes to general conditions.

Response: At the extremes, the mathematical approximation made to form the metamodel breaks down. However, the inputs were chosen to prevent this from causing a problem when extrapolated to general conditions. It has been shown that running the metamodel approximation of the largest 215 World Cities from the period 2002 through 2006 leads to none of the metamodel inputs being within 15% of either extreme [see Cohen et al. (2011)]. This example was chosen using present day conditions and only including large urban areas (those with more than 3 million people). Under future emissions scenarios, for example, with a rapidly changing emissions profile, it is possible for the emissions or background concentrations to approach the extreme values. An additional source of this occurring is if large urban areas continue to aggregate, pushing up the emissions towards the upper extreme. In the cases of the inputs becoming too low, these urban areas should behave similarly to the “dilution” assumption, and are best no longer treated as urban areas. In the opposite case, break up the urban areas into multiple urban areas, and run the metamodel sequentially from upwind to downwind. The important thing is to set flags and carefully monitor the values of the inputs, so as to make sure that they do not drift towards the extreme ends of the input PDFs. Further metamodels can also be made, if necessary.

Referee#2: pg 4658, ln 2-27: Comparison with air quality data. Maybe a table would make this data clearer. Also, what was the selection criteria? I appreciate that doing a comparison is a potentially endless task, but it seems that some extra justification / citations are needed here, including reference to meta-analyses. The comparisons in fig 6-12 are inadequate (and the figures are very hard to read, even as electronic versions). For example, why are China results compared with Guadalajara (not Guadalara, by the way)? Maybe the number of comparisons could be narrowed down, but be made more thorough. Fewer cases, but comparisons could include histograms of actual data? At any case, Fig 6-13 felt like a core dump that was hard to sift through.

Response: A Table has been created. The selection criteria is to test how well the metamodels are at reproducing urban concentrations over regions which have the largest number of urban areas. Presently, the majority of these are in China, India, and the Developing world (respectively). It is also preferred to use data from regions that are generally less well studied, since these are more likely to provide a challenging test for the metamodel. Your advice to include more citations and references to meta-analyses has been incorporated into the updated table and throughout the text, where appropriate. Figures 6, 8, 10, and 12 have been removed. Figures 7, 9, 11, and 13 have been made slightly larger and easier to view. While there were no histograms of data provided by any of these papers, statistics of the measurements, where available, are provided in the updated table and in the text.

Referee#2: Introduction: There is only one citation. Surely there is a larger literature on the regional impact of urban plume processing that would be relevant here? This could include urban field campaigns as well as meta reviews of experimental work.

Response: More citations regarding the regional to global scale impact of urban scale plume processing have been added.

Referee#2: Section 2: This covers only 3 papers. Aren't there any others that would be relevant, has anybody else used the papers cited?

Response: There have only been these papers so far on this topic, a reason why this result is relevant and timely. We have thus added in some of the more critical papers that have cited these 3 papers.

Referee#2: Section 3: Again, more care should be shown in citing relevant work.

Response: As per your recommendation, a few more references, specifically citing the

various different assumptions used in the CAMx run, have been added.

Referee#2: Pg 4639, ln 8-10 is somewhat sloppy. Could you be a bit more specific? There should be a more detailed discussion of the strengths and weaknesses of CAMx.

Response: An additional couple of sentences have been added describing some strengths and weaknesses of using CAMx.

Referee#2: Pg 4639, ln 22-30: There is a strange switch from general comments (which could be reduced to the actual point of importance for this study) and specific information about the method. This should be better organized. I would like to see some more information about the specific sites and about the selection criteria used.

Response: In reference to a question asked by Referee#1, this part has been made more detailed and expanded. If this section still does not provide sufficient organization and information, kindly let us know how to improve it.

Referee#2: Pg 4640, ln 16: The aerosol modeling is treated as if it were a totally standard component of the model. As I understand it, there are numerous options and versions available. The paper should be clearer about which models are used and outline some of the expected strengths and weaknesses.

Response: One sentence has been removed and an additional three sentences have been added to explain which aerosol options were used, and to explain their strengths and weaknesses. The gist is that the CMU scheme, over 10 equally spaced size bins (in log space) from 10nm up to 5000nm. The technique provides the most reasonable approximation size evolution of the aerosols allowable by CAMx. However, it is not a full two-moment scheme and hence does not perfectly conserve both mass and number at the same time.

Referee#2: Pg 4640, ln 27-28: This is an example of a careless statement that could be rephrased more scientifically.

Response: These sentences have been re-written to be more precise as follows. The computational expense of running a detailed urban model, such as CAMx, is too large to individually simulate the largest hundreds or thousands of urban areas, over the multiple decadal to century time scales required for climate modeling.

Referee#2: Section 6: It would help to clarify that you are comparing with Calbo / Mayer. Maybe the first 3 paragraphs could be integrated more smoothly in the method section (sec.4). The last 2 paragraphs (pg 4650) seem like they belong in the discussion.

Response: We clarified in the first sentence of section 6 (now section 2) that this is in reference to Calbo / Mayer. Given a suggestion from referee #1, these first three paragraphs have been folded into section 2, related to prior reduced form urban models. Furthermore, the final two paragraphs have been moved to the conclusions section. The fifth paragraph has been broken into parts and incorporated into existing paragraphs, while the fourth paragraph has been moved intact.

Referee#2: Equation 8: Would it help to be clearer about "Flux", possibly by including "Flux In" and "Flux Out", or specifying "Net Flux". This is alluded to briefly in line 15. To what extent is transport of pollutant across urban areas significant? (eg. Biomass burning plumes, industrial plumes?)

Response: The term "Net Flux" has been introduced in place of "Flux. The presence of external plumes is modeled through the boundary concentration terms. Urban areas that are located upwind from other urban areas (or regions of biomass burning) will have elevated mass (and for aerosols, number) concentrations at their boundaries. This term has a significant impact on the results in cases where the plume has different chemical or physical processing under the conditions within the urban area, as compared to the diluted background.

Referee#2: pg 4653, ln 19 to pg 4654, line 13: the discussion is not as easy to follow as it could be. "Sulfur is not predicted as accurately... Sulfur is predicted reasonably well..."

Response: This paragraph has been shortened and re-written for clarity.

Referee#2: Table 1: Presumably these are real cases for real cities. It would help to have this information, and to give each one a name based on the dominant feature. This would facilitate the discussion.

Response: Table 1 has had a column added to give a name based on the dominant feature of each meteorology type. The dominant feature for each type has also been clearly added in the text.

Referee#2: pg 4633, ln 18-22 is a run-on sentence

Response: This has been shortened so as not to run on.

Referee#2: pg 4645, ln 13: to improve this upon this

Response: The first word "this" has been removed.

Referee#2: pg 4652 ln 18 "the the"

Response: One "the" has been removed.

Referee#2: "EFs" should be defined in fig 7 etc.

Response: In each figure, a link from the term EF has been made back to the corresponding definition given in the text (Equation 8).

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 4631, 2011.