Interactive comment on "The chemistry CATT–BRAMS model (CCATT–BRAMS 4.5): a regional atmospheric model system for integrated air quality and weather forecasting and research" *by K. M. Longo et al.*

Author's response to interactive comment from Anonymous Referee #2

We thank the referee for his (er) thoughtful comments and suggestions, which are addressed below.

Referee #2 General questions and comments

1) What about aerosols? It does not really become clear whether you treat aerosols at all (as prognostic variables, that is), or not. Sometimes you mention it, but then there is no mentioning of e.g. nitrate, and how it is connected to the gas-phase, or sulfate from the gas-phase, or organic material. This needs to mentioned - either how it is done, or stated explicitly that this is missing.

Authors:

In this model version the aerosols are treated as prognostic variable, which means they are emitted, transported (as mass mixing ratio), and removed by dry and wet deposition process. However, aerosols are treated as generic PM2.5 particles for urban and biomass burning sources, without considering the evolution of its composition and size distribution.

We are currently implementing/evaluating a full aerosol microphysics model in CCATT-BRAMS based on the Multiconfiguration Aerosol Tracker of mIXing

state model (MATRIX, Bauer et al., 2008). This should be available in the next model version.

The following phrase was included in the manuscript.

"… the aerosols are treated as generic particles (with diameter smaller than 2.5 µm) from urban and biomass burning sources, without considering the evolution of its composition and size distribution, not accounting for interaction between aerosol and gas-phase chemistry."

Bauer S. E., D. L. Wright, D. Koch, E. R. Lewis, R. McGraw, L.-S. Chang, S. E. Schwartz, and R. Ruedy, MATRIX (Multiconfiguration Aerosol Tracker of mIXing state): an aerosol microphysical module for global atmospheric models. *Atmos. Chem. Phys.*, 8, 6003-6035, 2008.

2) While you mention direct (radiative) effects it does not become clear how much (if any) climate feedbacks are included. Do you have them? Or is there just the provision to include them in future work? (Also relates to the previous question - no aerosols, no climate feedback, probably).

Authors: Presently the climate feedback is associated to direct effect only and it has a significant impact on areas dominated by high level of biomass burning aerosol during the dry season on South America.

In the manuscript, there is a statement about that:

"…this model version already takes into account the interaction of aerosols with solar and long wave radiation and the feedback to the atmospheric model in terms of heating rates (Longo et al., 2006)."

In fact, Moreira et al. (2013) have shown the impact of inclusion of this process on 2-meters temperature with an improvement of model's skill prediction on weather scale.

3) Please ensure that the manuscript goes through the English copy-editing process to polish grammar, structure and wording.

Authors: We appreciated the recommendation. The paper went through a careful English revision in order to improve its reading and the specific points addressed were corrected.

Referee #1 Specific comments

Page 1175, line 13: *remove "atmospheric" from "atmospheric weather"*

Authors: Done

Page 1175, line 14: *"user defined chemical mechanism(s)" plural. Remove text in brackets.*

Authors: Done

Page 1175, line 15: *"trace gases emissions" -> "trace gas emissions"*
Authors: Done
Also, corrected in the legend of Figure 1.

Page 1175, line 16: *"atmospheric fields" sounds strange. Use something like "interpolation of initial and boundary conditions for meteorology and chemistry" instead.*
Authors: Done

Page 1175, line 26: *"research" singular.*

Authors: Done

Page 1176, line 3: *rephrase "the dynamics is forced" to sth. like "transport is calculated based on"*

Authors: Done

Page 1176, line 9: *"the past ten years"*

Authors: Done

Page 1176, line 12: *"cloud resolving models" would need to be on the microscale (<1km) and at least be LES type models. Do you really mean that? Or rather "convection-permitting" models?*

Authors: You are right, thanks for the correction. It is more appropriate to say convection-permitting models. This correction was incorporated to the manuscript.

whole paragraph: what about aerosols? They need considerable computation time as well, if not even more than gas-phase chemistry? Mention them.

Authors: In general, an aerosol microphysics model can be very costful. However, since the current model version has a very simple aerosol module, the associated computation time is not significant compared to other processes.

In this introductory section we included "for both aerosol and gas phase" in the following phrase:

"Simulation using fine resolutions, large domains and detailed chemistry, for both aerosol and gas phase, over long duration is computationally still too demanding."

Page 1177, line 3: *if possible list those "specific developments for the tropics/subtropics" briefly*

Authors: There is a detailed description of the specific developments for the tropics/subtropics within BRAMS model in Freitas et al. (2009), which was already referred in the manuscript. We understand that it is not necessary to repeat this description here.

Page 1177, line 5: *"run at horizontal"*
Authors: Done

Page 1177, line 6: *I don't believe your model is "fully optimized", as this is not possible unless you write machine code directly. You optimized it, not more, not less. Rephrase.*
Authors: Done. "Fully optimized" was replaced by "optimized".

Page 1177, line 10: *"code optimization specifities" -> "details on code optimizations"*

Authors: Done. "…code optimization specificities…" was replaced by "…details on code optimization…"

Page 1180, line 4-5: *it is "loss term", not "lost term".*

Authors: Done

Page 1181, line 7-10: *does this mean you speciate VOCs in PREP-CHEM-SRC? If so, where do you get speciation information from? If not, mention that only simple conversions are possible and VOC speciation is done somewhere else.*

Authors: Yes, the VOCs are speciated in PREP-CHEM-SRC. When only total VOCs emissions per source are reported, the disaggregation follows the OxComp (tropospheric Oxidant model Comparison - Wild and Prather, 2000; Derwent et al., 2001) specification for the hydrocarbon mixture, as reported in

the Third Assessment Report of IPCC (Prather et al., 2001). Subsequently, the resulting disaggregated VOCs are reassembled into lumped species via compatibility files specific for the chosen chemical mechanism. This information is now in the manuscript.

Derwent, R.G., Collins, W.J., Johnson, C.E., and Stevenson, D.S.: Transient behaviour of tropospheric ozone precursors in a global 3-D CTM and their indirect greenhouse effects. Clim Change, 49:4, pp 463-487, 2001.

Prather, M., Ehhalt, D., Dentener, F., Derwent, R. G., Dlugokencky, E., Holland, E., Isaksen, I. S. A., Katima, J., Kirchhoff, V., Matson, P., Midgley, P. M., and Wang, M.: Chapter 4. Atmospheric Chemistry and Greenhouse Gases, in Climate Change 2001: The Scientific Basis, J.T. Houghton et al., eds., Cambridge U. Press, pp. 239-287. 2001.

Wild, O. and Prather, M.J.: Excitation of the primary tropospheric chemical mode in a global CTM. J. Geophys. Res., 105, 24647- 24660, 2000.

Page 1181:

** please briefly mention whether your anthropogenic emissions are emitted only in the lowest layer, or whether you include point sources (e.g. stacks) aloft.*

Authors: Currently, all urban emissions are released in the lowest model layer. However, if emissions from point sources (e.g. stacks) are available, the information of stacks height can be easily included.

We have included a phrase in Section 2.2 (Emissions) explaining that users have flexibility to incorporate new emission datasets in PREP-CHEM-SRC, including point and line sources.

** also, is your plume rise calculated online, that is with the correct meteorology?*

Authors: Exactly. The plume rise is treated as a sub-grid transport mechanism simulated by embedding a 1-D cloud model with appropriate lower boundary conditions in each column of the transport model and fire information from PREP-CHEM-SRC. A detailed description can be found in

Freitas et al. (2006, 2007, 2010). These references are all in the paper and we rephrased the text to clarify this information:

" The biomass burning emission estimate is divided into two contributions: smoldering, which releases material in the lowest model layer, and flaming, which makes use of an embedded online 1-D cloud model in each column of the 3-D transport model to determine the vertical injection layer. In this case, the cloud model is integrated using current environmental condition (temperature, water vapor mixing ratio and horizontal wind) provided by the host model. (Freitas et al., 2006, 2007, 2010)."

Freitas, S. R., Longo, K. M., and Andreae, M. O.: Impact of including the plume rise of vegetation fires in numerical simulations of associated atmospheric pollutants, Geophys. Res. Lett., 33, L17808, doi:10.1029/2006GL026608, 2006.

Freitas, S. R., Longo, K. M., Chatfield, R., Latham, D., Silva Dias, M. A. F., Andreae, M. O., Prins, E., Santos, J. C., Gielow R., and Carvalho Jr., J. A.: Including the sub-grid scale plume rise of vegetation fires in low resolution atmospheric transport models, Atmos. Chem. Phys., 7, 3385–3398, 2007, http://www.atmos-chem-phys.net/7/3385/2007/.

Freitas, S. R., Longo, K., Trentmann, J., Latham, D.: Technical Note: Sensitivity of 1D smoke plume rise models to the inclusion of environmental wind drag, Atmos. Chem. Phys., 10, 585-594, 2010.

** Is MEGAN coupled so that it uses model temperature etc. variables?*

Authors: In the current model version, MEGAN emissions are included in PREP_CHEM_SRC only as a function of the zenithal angle. We are currently implementing MEGAN online with CCATT-BRAMS explicitly using the model variables state needed to calculate the emission of biogenic species. This capability should be available in the next CCAT-BRAMS model version.

Page 1183:

Is rain evaporation possible? Do you release species back to the atmosphere? How do you do that for aerosols? Do you cloud-process them (i.e. do they grow in size)?

Authors: No, this is all ongoing work.

Page 1185-1186

** isn't setting up the numerical integrator part of M-SPACK? If so, you did not develop this method in this work, but it has been described somewhere else, probably in Djouad et al. 2002, no? If so, this section is nice but unnecessary, please remove. If you modified it, state the differences.*

Authors: The SPACK version we based on for M-SPACK only had the very simple quasi-steady-state approximation (QSSA). We implemented the ROS2 and RODAS3 Rosenbrock solvers and the different settings of the operator splitting for time integration. As well, we included in M-SPACK the LU factorization method to take advantage of the sparseness of the Jacobian matrix.

Therefore, we will keep this description in this manuscript.

Page 1187, line 1: *do all these options have any impact on the result? Or is it only speed? Which one is preferred? Why?*

Authors: The numerical solutions using different choices of splitting are slightly different. For example, for highly reactive species (like ozone) these differences are less than a few percents. It is recognized that the sequential splitting is more accurate than the parallel one. So, this splitting should be preferred. However, we also implement the sequential symmetric splitting, where the integration of chemistry is done between 2 or more integration of the dynamics, using time step 2 times or more higher. In Figure 1, we show the difference for the ozone (%) resulting from the sequential integration for time steps of chemistry from 2 to 6 times larger than the one used for the dynamics relative to the symmetric integration. These differences are of only a few percents at megacities areas.

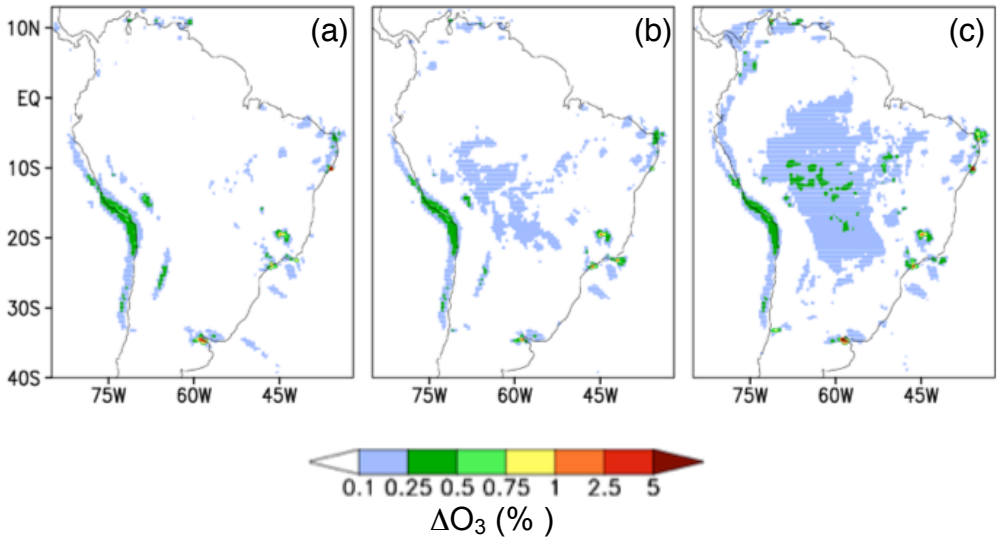

Figure 1: Difference of ozone (%) using sequential integration for time steps of chemistry (a) 2, (b) 4 and (c) 6 times larger than the one used for the dynamics relative to symmetric integration. These are test results performed for 07 August 2008 at 21UTC.

Figure 2 shows the elapsed time of several model runs using different solvers and operator splitting. The best compromise between accuracy and computing time was achieved using RODAS3 and symmetric splitting with a chemistry time-step four times larger the time step of the dynamics. This setting is used operationally at CPTEC.

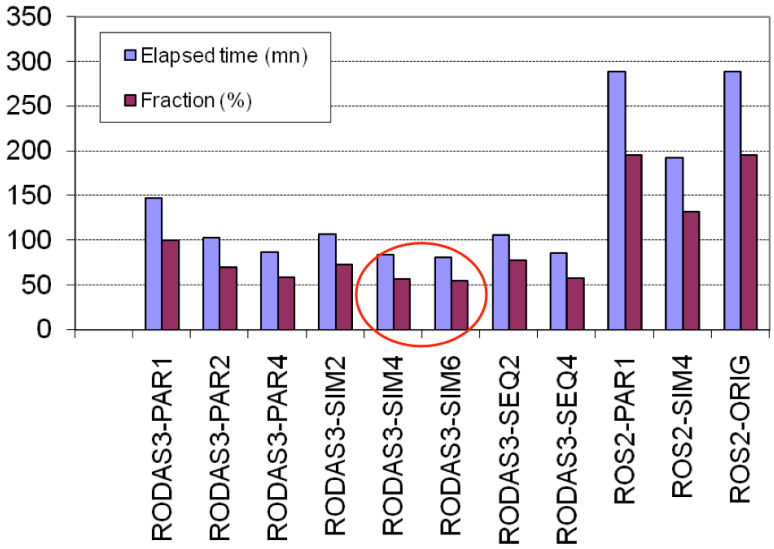

Figure 2: Elapsed time (mn) and fraction (%) of several model runs using different combinations of solvers and operator splitting. ROS 2 (2nd order, 2 stages) and RODAS 3 (3rd order, 4 stages) Rosenbrock's. Model test are performed for a grid domain covering South America with 60 km horizontal resolution, CB07 chemical mechanism, 4DDA using MOCAGE/CPTEC analysis, 88 amd/opteron processors with 2.8GHz, atoll=10^{+7}, rtol=10^{-3}.

Page 1187, line 10: *this is a rule you deliberately set, but it is not enforced by Fortran, i.e. these fields are not "read-only" for other modules. Programmers should be aware about that.*

Authors: Ok, you are right. "As a general rule…" was replaced by "As a general BRAMS design and coding rule…"

Page 1187, line 12: *is this the case on every architecture with every compiler? I doubt that. Either cite work that proves it or remove. (Also for several mentionings further along in the text.)*

Authors: You are right, since the argument does not apply for current GPGPU architectures and cache misses may depend on the actions of the compiler run-time on mainstream x86-based architectures. Our experiments on this issue were restricted to a single compiler on a single implementation of the x86 architecture. Following your suggestion, we removed the sentence and two other sentences further along the text that originally mentioned the cache issue.

Page 1187, line 28: *I do not understand what sc_p should be, please make a realistic example. Is sc_p a certain species like e.g. no2? Why do you need another index nspecie? Or is it an ancillary field you need to calculate some rate (temperature, pressure)? Or do you only do "chem(nspecie, ngrid)%sc_p(z,x,y)" because you want to avoid sth. like "chem(ngrid)%sc_p(nspecie,z,x,y)"?*

Authors:

In the manuscript, the paragraph:

"CCATT–BRAMS data structure extends the original BRAMS data structure in a natural way. Derived data type *chem* contains history-carrying variables introduced by the chemistry. Multiple grids are represented by an array of type *chem*. But since each species requires its set of history carrying variables at

each grid, the array has to be indexed by species number and grid number. Consequently, *chem g(nspecie,ngrid)%sc_p(z,x,y)* stores field *sc_p* at grid point *(z,x,y)* of species *nspecie* at grid *ngrid*. This organization keeps at nearby memory addresses all fields of one species of one grid."

was replaced by:

"CCATT–BRAMS data structure extends the original BRAMS data structure in a natural way. Derived data type *chem* contains variables related to one chemical species such as current mass concentration, its tendency, its decrease due to dry and wet deposition, etc. Let *sc_p* be one of these fields. Multiple grids are represented by an array of type *chem*. But since each species requires its set of variables at each grid, the array *chem* has to be indexed by species number and grid number. Consequently, *chem g(nspecie,ngrid)%sc p(z,x,y)* stores field *sc_p* at grid point *(z,x,y)* of species *nspecie* at grid *ngrid*. This organization keeps at nearby memory addresses all fields of one species of one grid."