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Geoscientific Model Development Discussions

Interactive comment on "Earth System Chemistry Integrated Modelling (ESCiMo) with the Modular Earth Submodel System (MESSy, version 2.51)" *by* P. Jöckel et al.

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We thank referee #2 for the very helpful and encouraging comments. Here are our replies:

- *The manuscript presents recent updates to the ECHAM/MESSy Atmospheric Chemistry (EMAC) model, describing the version that was used for a large set of simulations to be submitted to the Chemistry-Climate Model Initiative (CCMI) model intercomparison project. Selected results from a number of the simulations specified for CCMI are presented, including a comparison of different model con-*

figurations for many of these experiments. For example, results are compared between versions of the model with 47 and 90 vertical levels, including prognostic tropospheric aerosols versus specified aerosol fields and two different approaches to nudging the model dynamical fields to reanalysis for the Specified Dynamics simulations defined by CCMI. The effects of a number of problems with the CCMI simulations that were discovered after the simulations were quite advanced are also investigated by comparing these simulations with follow-on simulations with these errors corrected.

Reply: This provides a perfect summary, thank you very much.

- *The manuscript presents a great deal of information that will serve as an important resource for people analyzing the CCMI simulations and provides several interesting insights into how different choices in setting up the CCMI simulations affect the final results. The impact of the number of vertical model levels on stratospheric age of air and the effects of nudging wavenumber zero for temperature on lightning are good examples of findings that will be interesting to the modelling community.*

  Reply: Thank you very much for this positive and encouraging evaluation of our work.

- *My only significant concern with the manuscript in the current form is that I find the sheer volume of different simulations, including variations that test the effects of bugs, is overwhelming for the reader.*

  Reply: Yes, indeed. However, since the manuscript is intended to serve as a reference for further research with the data, rather than a study on a specific topic, the information density is naturally higher, since details might be important. Given the amount of data, close to 2 Peta-Byte, we think the extent of information is appropriate.

Obviously, the additional sensitivity simulations were not intended, but we think that the proper documentation of these is very important, in particular for further CCMI studies with the data, in order to avoid misinterpretations.

- *None of the analyses presented here show any significant differences between the RC1-aero-06 and -07 or the RC1-aecl-01 and -02 simulations that were run to test the effects of problems with the black carbon and organic carbon emissions. Yet the presentation of these four separate simulations complicates the interpretation of the results by the reader. It would seem possible to present the important caveat about the aero and aecl simulations while simplifying the presentation of the results by reducing the number of individual simulations discussed.*

  Reply: This point is well taken. However, the resulting small impact on the results (except for the fine mode aerosols!) derived from the overlapping time spans of RC1-aero-06/07 and RC1-aecl-01/02, respectively, was a priori not clear. Thus, we think it is an important result and we motivate this better in the revised section 3.12.3:

  "The fine mode aerosol distributions are, however, quite substantially impacted by the errors in OC/BC. Since the total budgets of many compounds are dominated by the larger size categories, they, except for OC/BC, are hardly affected. Furthermore, the impact on the aerosol optical properties of the small particles is also lower than for larger particles, such that the impact on radiation is also minor. For aerosol-cloud-interactions (*-aecl-*) the error is only in the very first phase of the simulation leading to an underestimation of cloud droplets. As the problem has been fixed before the dominant change in especially organic aerosol emissions, the effect of increased cloud droplets from the year 1970 onwards is included in the resulting time series of *RC1-aecl-02*. As a consequence, detailed analyses of OC/BC can safely be based on results from *RC1-aero-07* (from 1991 onwards) and *RC1-aecl-02* (from 1966 onwards), respectively."

  In this context, the additional section in the revised conclusions on "data usage

  recommendations", as suggested by referee #1 certainly helps as well. We added "Last, but not least, for further analyses on aerosol and aerosol-cloud effects, only *RC1-aero-07* (from 1991 onwards) and *RC1-aecl-02* (from 1966 onwards) should be used, respectively."

- *A similar argument could be made about the RC1-base-07a, 08a and 10a simulations.*

  Reply: Again, the results of the "unintended sensitivity simulations" have been a priori not clear and we need to prove the (small) impact of our "glitches". It is important to show that the base cases (i.e., the simulations without suffix "a") can be used, with only some limitations, for further analyses in the course of CCMI. Moreover, results from *RC1SD-base-10a* (so to say our best guess) are particularly suited for direct comparisons with observations. We hope, that the expanded conclusions on "data usage recommendations", as suggested by referee #1, clarifies this.

- *A related concern, if the article is to serve as a reference for the set of EMAC CCMI simulations, is that it is not clear how the different simulations described in the manuscript correspond to simulations that will be available for analysis within CCMI. For example, the RC1-aecl-01 simulation stops at 1972 and the RC1-aecl-02 simulation covers 1965 – 2011. Will the EMAC REF-C1 simulation with the model setup of aecl be constructed by combining these two simulations?*

  Reply: Thank you very much for pointing this out. This information is indeed missing. We do not intend to construct combined time series, however *RC1-aero-07* can be used from 1991 onwards, and *RC1-aecl-02* from 1966 onwards (e.g. from the CERA database at DKRZ). Only those simulations covering consistently the requested time periods will be uploaded to BADC for CCMI.

  In the revised manuscript, we state this more precisely in the conclusions and "data availability" sections, respectively.

- *Aside from difficulties dealing with the number of simulations, I have no significant concerns with the manuscript. A few minor suggestions are given below.*

  Reply: Thank you very much.

- *Page 8640, Lines 15-21. It is mentioned here that the chemistry and reaction rates have been updated. From the wording, it is not clear if the reaction mechanism has been modified or if the updates were just to update the reaction rates. If there have been some modifications to the chemistry, it would be helpful to have them briefly described. The issue of the chemistry is discussed in more detail in section 3.5.1, but what updates have been made, if any, are not mentioned.*

  Reply: The differences between the mechanisms are small. Apart from updated rate coefficients, the product distributions were also updated for a few reactions (e.g. C_2H_4 + O_3). In addition, previously neglected, chemically inert or ubiquitous products like CO_2, H_2O and O_2, have now been added in order to fix the mass balance of some reactions. Since Hg chemistry is not considered in this study, all Hg reactions were switched off.

  We add this additional information to section 3.5.1 of the revised manuscript.

- *Page 8643, Lines 3-5. It is not clear to an outside reader what SCALC is designed to do. The use of the term 'channel objects' is also a mystery – to me, at least.*

  Reply: Yes, indeed. As it reads, it is only understood by MESSy insiders. Therefore, we add some clarification: "The term *channel object* was introduced as part of the MESSy terminology by Jöckel et al. (2010). In brief, it describes a specific Fortran95 structure comprising the data and corresponding meta-data of prognostic and diagnostic variables according to an object-oriented approach. The individual model components (i.e., what we call *submodels*) operate on these *channel objects*. SCALC, in particular, is used to provide, defined by namelist, new *channel objects* (e.g., the total loss rate of a reactive compound), consisting

  of the sum of (optionally scaled) individual objects (e.g., the process specific loss rates of that compound)."

- *Page 8646, Lines 21-27. It is mentioned that the changes to the clouds produce a 3.4 W/m2 increase in the shortwave balance, that is designed to offset the -3.3 W/m2 net balance using the original set of parameters. Is there any impact on the longwave balance from the revised parameter values and what is the overall radiative balance with the revised parameters?*

  Reply: Both altered parameters mainly affect the shortwave radiation (4.3 $W\,m^{-2}$), and the effect on the longwave radiation is only small (0.9 $W\,m^{-2}$). The value of 3.4 $W\,m^{-2}$, given in the manuscript, is the combined change of the OLR and the TOA net shortwave radiation, unlike stated in the original manuscript. The text in the revised version is changed accordingly.

- *Page 8648, Line 7. I believe 'divers' should be 'diverse', but both are valid English words with subtly different meanings.*

  Reply: Funny, indeed! Something that the spell-checker cannot find. It is corrected in the revised manuscript.

- *Page 8659, Lines 14-17. Here it is stated that the isoprene emissions are reduced by a factor of 0.6 to give realistic isoprene mixing ratios in the boundary layer. Is there a physical reasoning behind the reduction, perhaps to account for reactions within the canopy, or is it a purely pragmatic choice?*

  Reply: As shown by Arneth et al. (2008)[1] (and references therein) the global emission of isoprene in literature is estimated to be approx. 500 Tg(C)/year. And indeed, our emission algorithm calculates values close to this. However,

[1] Arneth, A., Monson, R. K., Schurgers, G., Niinemets, Ü., and Palmer, P. I.: Why are estimates of global terrestrial isoprene emissions so similar (and why is this not so for monoterpenes)?, Atmos. Chem. Phys., 8, 4605-4620, doi:10.5194/acp-8-4605-2008, 2008.

those result in unrealistically high isoprene mixing ratios in the boundary layer. The reason for this discrepancy could be missing processes below the canopy or shortcomings in our simplified isoprene degradation scheme (MIM1). This is under investigation but beyond the scope of the present study.

Thus, in conclusion the selection of the scaling factor 0.6 is a purely pragmatic choice, as also stated by Jöckel et al. (2006)[2]: "The additional scaling factors adapt the parameterisations in order to achieve realistic mixing ratios of isoprene in the boundary layer". A more detailed discussion on the isoprene scaling factor is provided by Pozzer et al.(2007)[3], who also compare with global emission values used in other models.

We add this information to the revised text.

- *Page 8667, Line 18 – Page 8668, Line 3. The error with extinction is discussed here, section 3.12.1. Since most of these runs use prescribed SSTs, the impact of the volcanic eruptions will already be present in the tropospheric temperatures. Does the error also impact the infrared interaction of the aerosols, in which case the stratospheric temperature response will be significantly effected?*

  Reply: Both, solar and infrared radiative transfer, are affected. The underestimation of the solar effect leads to an overestimated radiative transmission into the troposphere and hence a too strong warming. This is partly compensated near the surface by the prescribed SSTs. In the infrared the volcanic aerosol is,

[2]Jöckel, P., Tost, H., Pozzer, A., Brühl, C., Buchholz, J., Ganzeveld, L., Hoor, P., Kerkweg, A., Lawrence, M. G., Sander, R., Steil, B., Stiller, G., Tanarhte, M., Taraborrelli, D., van Aardenne, J., & Lelieveld, J.: The atmospheric chemistry general circulation model ECHAM5/MESSy1: consistent simulation of ozone from the surface to the mesosphere, Atmospheric Chemistry and Physics, 6, 5067-5104, doi: 10.5194/acp-6-5067-2006, URL http://www.atmos-chem-phys.net/6/5067/2006/ (2006)

[3]Pozzer, A., Jöckel, P., Tost, H., Sander, R., Ganzeveld, L., Kerkweg, A., & Lelieveld, J.: Simulating organic species with the global atmospheric chemistry general circulation model ECHAM5/MESSy1: a comparison of model results with observations, Atmospheric Chemistry and Physics, 7, 2527-2550, doi: 10.5194/acp-7-2527-2007, URL http://www.atmos-chem-phys.net/7/2527/2007/ (2007)

however, of minor importance, especially due to its low water content. Consequently, even though the stratospheric temperature response is underestimated, the effect is weak and not statistically significant in most regions (see attached Figure).

In the revised manuscript, we modify/add: “But very important: the dynamical effects of large volcanic eruptions (e.g., Mt. Pinatubo 1991; El Chichón 1982) are essentially not represented in the simulations, **except for the contribution to the tropospheric temperature signal induced by the prescribed SSTs. The effect of stratospheric volcanic aerosol on infrared radiative heating is weak, as shown by mostly insignificant differences between *RC-base-07a* and *RC-base-07*, and *RC-base-08a* and *RC-base-08*, respectively (not shown).**”

- *Page 8673, Lines 17-26. Figures 16 and 17 show values of the deposition flux from sedimentation, yet many of these simulations use specified aerosol fields. There is, apparently, a calculation of sedimentation for model runs using specified aerosols. In Section 3.5.4 there should be a mention that sedimentation is calculated for simulations with specified aerosols and, perhaps, a brief description of any important features of how this calculation is performed.*

  Reply: We add to the revised section 3.5.4 the missing information: “In the simulations without prognostic aerosol chemical and microphysical properties (i.e., all except for *-aero-* and *-aecl-*), sedimentation fluxes are calculated by SEDI for the residual aerosols originating from evaporation of clouds and precipitation leading to particles. In these cases, particle size distribution (mean radius = 5×10^{-07} m, $\sigma = 2.0$) and particle density ($\rho = 1841.0$ kg/m^3) are prescribed.”

- *Page 8676, Lines 5-11. This section of text places the EMAC methane lifetime alongside the methane lifetime from other models. I have no objection to this discussion, but the text should also discuss the observationally based estimates*

of methane lifetime of closer to 11.2 +/-1.3 years from methyl chloroform (Prather et al., 2012).

Reply: Thank you very much for pointing this out. We add the reference.

- *Page 8678, Lines 6 – 9. The text discusses how ozone in the summer decreases more rapidly in the model than in the observations, leading to an underestimate in the model above the tropopause that peaks during June-July-August. Figure 21 shows an overestimate of CH4, notable because the model underestimates CH4 in much of the upper troposphere. Could the underestimate of ozone and overestimate of CH4 be related to problems with cross-tropopause transport?*

  Reply: This could indeed be the cause for the two differences between the model and measurements. But an investigation in this direction is beyond the scope of the present study, as it only presents first results in the sense of a baseline study.

- *Page 8679, Lines 24-26. Could the authors clarify what they mean by 'The seasonal cycle is, however, reproduced when taking more model data into account (not shown).' Is this referring to more data in the same region of the atmosphere, or sampled over different geographic locations?*

  Reply: The latter. To clarify this, we reformulate: "The seasonal cycle is, however, reproduced when taking more model data from the UTLS into account, including data from longitudes different to those where CARIBIC flies (not shown)."

- *Page 8685, Lines 6 – 9. Total column ozone from the model is compared with the Bodeker Scientific dataset (BSTCO) for the years 1980-2011. Averaging over the 1980-2011 period mixes years from the early 1980s, when ozone depletion was more modest, with years in which it was more fully developed from the mid-1990s onward. Wouldn't a comparison of, say, 1995-2011 be a more straightforward averaging period? Do the trends over 1̂980-1995 contribute to the variance used in the test for statistical significance*

  Reply: To test the effect of the chosen period we repeated the analysis for the shorter period (1995-2011) as suggested (see Figure below). We find only small differences between the results for the two periods and the main conclusions that we draw from this plot are not changed. However, the regions of significant differences between the simulations are slightly larger for the shorter period. This may result from the fact that the trend is not removed and indeed contributes to the variance.

- *Page 8738, Caption for Figure 19. There should be mention in the figure caption, as there is in the text, that the data used is restricted to the latitudes 35 – 60N.*

  Reply: We add this information to the caption: "Comparison of O_3 climatologies **(35^o N – 60^o N)** based on data from the years 2005–2013."

- *Page 8691, Line 6. The term 'sulphite' is used here, as it is in a few other places through the manuscript. Should that be 'sulphate'? I'm not sure myself, but I am more used to seeing sulphate.*

  Reply: SO_2 scavenged by clouds and precipitation is not completely converted to sulphate (depending on the pH). Therefore, the term sulphite corresponds to all species with sulphur in oxidation state +4 (S(IV)). On the other hand the oxidised sulphate corresponds to all compounds which could be summed as S(VI).

  We add the definition to the first occurrence of "sulphite" in the text.

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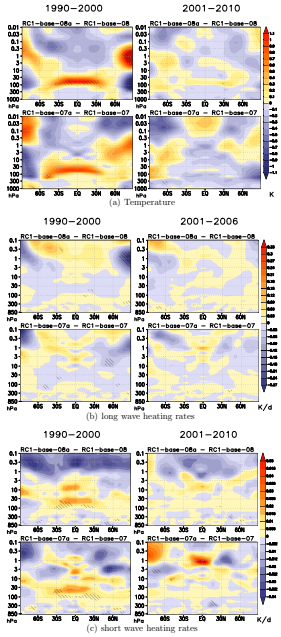

Figure 1: Differences of the long-term, annual mean for (a) temperature, (b) long wave heating rate, and (c) short wave heating rate. In hatched regions the differences are significant at the 95% level.

1

Fig. 1.

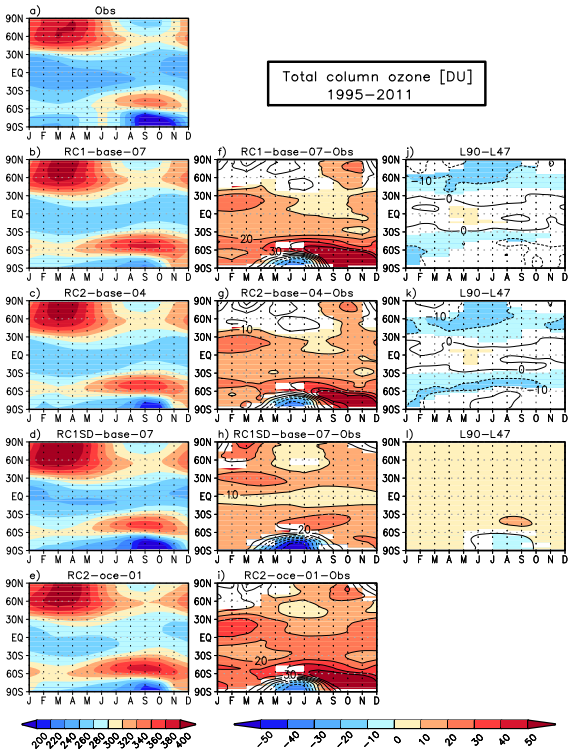

Fig. 2. Same as Figure 27 of the GMDD manuscript, however, for the period 1995 – 2011.