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Interactive comment on "Development cycle 2 of the Modular Earth Submodel System (MESSy2)" *by* P. Jöckel et al.

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We thank referee #1 for the very helpful and encouraging comments. Here are our replies:

- *My major comment concerns the overall presentation and length of the manuscript. The paper is a mixture of technical description of new and modified submodels, user manual and a rather short model evaluation that consists mainly of a large number of not commented figures in the supplement.*

  Indeed, the focus of this manuscript is the technical description of the new developments, whereas the evaluation has been deliberately kept short, as the pre-

  vious version of the model has been extensively evaluated before (Jöckel et al., 2006; Pozzer et al., 2007). The intention was not to repeat earlier findings but rather to provide only the main improvements and changes. We agree, however, that we overshot this mark by showing no figure in the main text. We will expand the evaluation section in the revised manuscript.

- *I recommend to shorten the paper by moving the 'user manual'-like parts to a separate submodel documentation as it is already done for the submodels TIMER and CHANNEL.*

  We have chosen supplementary material for TIMER and CHANNEL, because these infrastructure submodels require a rather extensive documentation for the users in addition to the main ideas presented in the text. For the other submodels, we have chosen the main text for documentation, because a much shorter description is sufficient to be able to apply these. Moving parts of it to yet another supplement will further increase the amount of text a user has to read. Many things need to be doubled in this case, because we feel that the main ideas and illustrating examples should remain in the main text and cannot be easily (i.e., without creating additional overhead) detached from the description of the underlying techniques and namelist control. For this reason, we are very hesitant to basically move / double all submodel descriptions, but we would be interested to hear the opinion of the editor.

- *Furthermore, I suggest a revision of the evaluation section. In the current state this section is neither fish nor fowl. The authors might either extend the discussion or decide to publish a detailed model evaluation as a companion paper.*

  As stated above, the material is not sufficient to justify another model evaluation

paper in addition to Jöckel et al. (2006) and Pozzer et al. (2007). But indeed, the new results need to be highlighted more. Therefore, we will revise the evaluation section.

Specific Comments:

- *Fig 1, 3, 5, 7, etc: I suggest to omit the example namelists of the new submodels and to provide a detailed submodel documentation including the example namelists as an additional supplement.*

  For most of the new submodels, the presented details are sufficient for their application and do not justify a separate supplement. A separation of methodology, the methodologies' reflectance in the namelists and the illustrating examples would make understanding even harder and create a lot of additional overhead.

- *CHANNEL: For ECHAM5 users the CHANNEL submodel sounds like the stream elements used in ECHAM5. Maybe the authors can give some more information about differences and the changes necessary to make the data storage and management more generally applicable.*

  Indeed, stream elements and channel objects share some basic ideas, such as the application of concatenated pointers, Fortran95 structures etc. In the EMAC (ECHAM/MESSy Atmospheric Chemistry) model based on MESSy cycle 1, we apply the ECHAM5 stream approach as memory management and I/O interface. However, it turned out that the ECHAM5 stream management is too tightly connected to ECHAM5 (too specific) and not sufficiently flexible for intended further extensions. Therefore we implemented CHANNEL "from scratch" having a complete legacy model independence in view. The main differences between the two approaches are therefore: (1) the stream concept is very tightly connected to the ECHAM5 model, whereas CHANNEL is completely independent of any

legacy model (and of all the rest of the MESSy infrastructure); (2) the concept of the (object oriented) hierarchy of attributes, dimensions, dimension variables, and in particular representations is unique in CHANNEL and does not exist for the streams; (3) the I/O in CHANNEL is completely namelist controlled (for the ECHAM5 streams code changes are required, if a variable shall be output or not); CHANNEL also includes the option for additional (or alternative) output of statistics w.r.t time (whereas the ECHAM5 stream implementation does not contain the (namelist controlled) possibility to output such statistics, such as for instance the "maximum over the output time interval").

- *Has MESSy2 already been used with another GCM except ECHAM5? It would be very interesting to see how much effort is required to couple MESSy to another GCM.*

  We are currently coupling MESSy2 to the COSMO-CLM model and to CMAT2. The documentation on these activities can hopefully be submitted soon.

- *Sect. 5.2, SCOUT.: Is it possible to select an individual output interval for the submodel SCOUT or is the output interval identical to the GCM output?*

  Since for each location a separate channel is created, the output is completely controlled via the channel namelists. This implies that the output interval can be chosen (via a standard namelist) independent of all other output intervals, even individually for each SCOUT location. This is stated (discussion paper) on page 1436 in lines 23-26: "Operating with channel objects enables automatically all namelist controllable output features for sampled data (see Sect. 2), such as for instance time averaging, output redirection, etc. With SCOUT, high frequency output of model data for comparison with stationary observations can be provided, examples are shown in Fig. 6." We will add "output frequency" to this list

and rephrase “the hourly output” into “hourly output” in the caption of Fig. 6.

- *Sect. 7.1.1: In my opinion this section is dispensable and could be removed or at least substantially shortened.*

  We cannot agree with this statement. This section describes an essential progress we made for KPP based chemistry modeling in higher dimensional models. The application of KP4 as “post processor” to the automatically generated KPP Fortran90 code increases the run-time performance by a significant factor. This section documents this and it might be of interest for other chemistry modelers, who apply KPP.

- *Sect. 7.1.2: Is there any reference for equation 6?*

  We will add the reference “(see Jacobson, 2005, Eq. 11.150)” to the revised manuscript.

- *Sect. 7.2: The submodel PSC and HETCHEM are obsolete, but remain available for compatibility with MESSy1. At the same the authors argument that maintaining different modules with the code is error-prone and not desirable. Does that mean that there will be no bug-fixes or updates for HETCHEM and PSC anymore?*

  Currently, we schedule an update/bug-fix release of MESSy (and EMAC) every half a year. The development cycle 2 is new and most of the users apply EMAC based on MESSy1 for their ongoing projects. Thus, both development cycles (1 and 2) will be maintained and released in parallel for some time. To simplify the incorporation of bug-fixes and improvements found/implemented by cycle-1 users into the new submodels, PSC and HETCHEM will, for the time being, also

be kept in cycle 2. If cycle 1 will not longer be supported, the decision has to be made, which submodels should be kept in cycle-2.

- *Sect. 7.3., LNOX: In the new version of LNOX the calculation of the flash frequency is based on a fractional instead of an integer land-sea-mask. Has this change any effect on the total amount or the distribution of NOx emissions from lightning? The decrease in flash frequency over Indonesia and Middle America is an improvement compared to MESSy1. How about the increase in flash frequency over South America and Africa? Is this also an improvement? Are the changes statistically significant?*

  There is no absolute increase of the flash frequency over South America and Africa. In Fig. 21 the supposed increase appears, because both results have been normalised to the same global integral flash frequency. (cf. page 1460, lines 11-14: “Since the normalised flash frequency is shown and both simulation results have been normalised with their respective average (in time) integrated (in space) flash frequency, Fig. 21 (lower panel) indicates a relative redistribution of flashes into the continental, lightning-active regions.”) This implies that in grid-boxes over land and over sea no change in the lightning-NOx production occurs, whereas in coastal (i.e., mixed land-sea) grid boxes the lightning production is either increased or decreased, depending on the integer land-sea mask used before. This is a systematic, algorithmic change and therefore statistically significant. The impact on climate (through coupling the chemical state of the atmosphere via the radiation calculation on dynamics) is far beyond the scope of this manuscript.

- *Sect. 9: The description of the model configuration and set-up (9.1) is as long as the presentation of the model results (9.2). If the authors want to keep this section (see general comment), I suggest to extend the re-evaluation of the new*

model version. A few comments are given below.

As mentioned above, we will extend the evaluation section.

- *Sect. 9: EMAC based on MESSy2 could be referred to as EMAC2.*

  We will use this where appropriate.

- *Sect. 9.1.: How do the total biomass burning emissions differ between the current model simulation and the simulation S2 from Jöckel et al. (2006)?*

  In S2 of Jöckel et al. (2006) biomass burning emissions from the GFED database version 1 incorporated into the EDGAR3.2FT2000 database have been used (monthly averages of the year 2000 repeated every simulation year). In the present study, we applied the Global Fire Emission Database (GFED version 2.1, 5 Randerson et al., 2007; Van der Werf et al., 2006) for the years 1998 to 2006 (monthly averages); for the years 2007 and 2008 we applied climatological monthly averages of the previous years.

  We will add a table with biomass emission totals to the revised supplementary material and indicate this in the revised manuscript.

- *Sect. 9.1.: Please give some information about the role of mercury in atmospheric chemistry.*

  For the benefit of readers who are not familiar with atmospheric mercury chemistry, we will add the following paragraph to the revised manuscript: "Mercury is a highly toxic element that has both natural and anthropogenic sources. Gaseous elemental mercury (GEM, Hg0) is quite inert and can be transported in the atmo-

sphere over long distances. Once oxidised to reactive gaseous mercury (RGM), it is deposited to aerosols and to the surface quickly."

- *Sect. 9.2.: I recommend to present the figures discussed in this section in the paper, not only in the supplement.*

  We will move the respective figures to the main text.

- *Sect. 9.2.: The discussion of the model results concerning mercury is rather sparse. Getting the best results by switching off certain oxidation reactions does not inspire much confidence. Please provide more details.*

  Indeed, it is a strange result that switching off oxidation by OH and O3 leads to better results even though it is normally assumed that they are the main sinks for most atmospheric pollutants. However, it is very difficult to measure Hg + OH and Hg + O3 in the laboratory. Therefore, the uncertainties of the rate coefficients are very large and testing with a model if these reactions are needed at all is a viable approach. Our results are in line with the study of Holmes et al. (2010).

  We will add this information and reference to the revised manuscript.

- *Fig. 11, right panel: This figure is not clear to me. The orbit position corresponding to the time of the model output is already shown in the left panel.*

  The left panels show global model snapshots for 16:00 UTC on January 15, 2006. In the middle panels (SORBIT output for January 15, 2006) the UTC time depends on latitude and longitude, but due to the geometry of sun-synchronous orbits, the local time is only latitude dependent (see Eq. 3), which is shown in the right (narrow) panels. The red triangles in the left and middle panels show

real ENVISAT orbit positions, which directly correspond to the underlying model output w.r.t. time. We will clarify this by rewriting the figure caption.

- *Supplement, evaluation of MESSy2, Fig 1-3: For a better comparison I suggest to add the respective figures from Jöckel et al. (2006).*

  We will add the desired figures to the supplement.

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