**Atmospheric
Chemistry
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Discussions**

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Interactive comment on "Technical Note: Coupling of chemical processes with the Modular Earth Submodel System (MESSy) submodel TRACER" *by* P. Jöckel et al.

P. Jöckel et al.

We thank the anonymous referee for her/his awareness of our attempt to improve the accepted standard of model documentation and the valuable and constructive comments.

Here is our reply:

- Abstract and PTRAC:

  – "tagging techniques": Tagging is a widely used concept in atmospheric chemistry modelling (e.g., Lamarque et al. [1996], Horowitz and Jacob [1999], Grewe [2004, 2007], Meijer et al. [2000], Ma et al. [2002], Gong

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et al. [2006], Heald et al. [2004], Builtjes et al. [2003]) and it is applied to derive additional information from the model which cannot be derived from measurements. The most prominent application is the "source region" tagging, where one (or more) chemical species is (are) artificially split into parts and each part is labelled with its source region. Nevertheless, we will reformulate the respective sentence in the revised abstract.

– "limited precision": This simply means that the numerical calculations are not exact. Since this is also stated in the term "rounding errors", we will remove it.

– PTRAC: Indeed, the only purpose of PTRAC is to be able to define prognostic tracers **alternatively** via a Fortran95 namelist without recompilation. However, we neither stated that this is the only way to define prognostic tracers, nor did we distinguish between "prognostic" and "diagnostic" tracers. In fact, the standard method to define tracers is in the code, more precisely in the SMIL of a given submodel, using the interface routines described in detail in the supplement. Changes in the code, however, require recompilation and this is not always desirable. Furthermore, all tracers are "prognostic" in the sense that they constitute "prognostic variables" of the system (i.e., are subject to change by the various processes like advection, convection, etc.), no matter if they generate feedback or not.
In addition to this simple method of defining tracers via namelist, we describe the special features that are required if these tracers should be treated as aerosol. However, we did not state that aerosol tracers are more suited for a definition via PTRAC than gas-phase species.
In the revised version we will clarify these misunderstandings.

• TRACER_PDEF: As the referee emphasises, TRACER_PDEF is **not** designed to correct conceptual errors of arbitrary advection algorithms. An important prerequisite for the functionality of TRACER_PDEF is that every tracer related

process implementation in itself is positive definite. TRACER_PDEF is only designed to correct for technical problems, such as rounding errors. We will clarify this in the revised version of the manuscript.

In the paragraph on page 17084 (starting at line 21) we clearly state that we are aware of the risk of masking potential severe errors and of the issue of mass conservation violation. This, in our opinion, implies that - as is true for any other numerical technique - TRACER_PDEF must not be "naively" applied. The application is yet simplified by the ability to set thresholds.

– Since we are very well aware of the (typically very small) mass conservation violation, TRACER_PDEF does not only (optionally !) correct negative overshoots, but in addition tracks and diagnoses the resulting mass conservation violation to provide a quality control measure for the result. We have taken this most simple approach, because any attempt to redistribute the "negative" mass globally likely introduces other problems such as unphysical instantaneous long range transport, violation of the monotonicity etc. A brief discussion will be added to the revised manuscript.

– Small numerical positive overshoots are very dependent on the specific numerical algorithm and can hardly be detected and fixed a posteriori. This is not the purpose of TRACER_PDEF and we did not claim that.

– We completely agree with the referee that the global mass based analysis is not the only possible method. Certainly alternative criteria are possible and we welcome very much any extension to the module.

– A guideline of what is "sufficiently small" cannot be given in this context, since the allowed error must be related to the scientific question for which the model system is applied. Since TRACER_PDEF is designed solely to

correct for numerical errors, the error in terms of mass conservation violation in most cases is probably by several orders of magnitude lower than the total mass (as shown in the two typical examples in Figure 2).

We will take into account the detailed comments for the revised manuscript, however, the very last becomes obsolete by the clarification above.

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