

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

Anonymous Referee #2

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This technical note describes the submodel TRACER of the MESSy system. This note belongs to a series of papers describing the various modules of MESSy. The authors should be commended for their ambition to describe in detail in the peer reviewed literature, an ambition that goes far beyond the standard for the documentation of comparable models. I very much recommend that, eventually, the paper should be published by ACP. However, I believe that work is required before the paper is ready for publication.

I have several reservations about the paper as it stands at the moment. Overall, I recommend that the paper is revised to make it better understandable to the ACP

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readership. The authors have invested great effort to make their code accessible to a wider group of scientists than those who originally wrote the code and this paper is part of this effort, but the paper can serve its purpose only if it is lucidly written and easily accessible to the potential readership.

The problem is already evident in the abstract. I do not understand the sentence describing ‘tagging techniques’ at all. And I do not believe that the term ‘tagging techniques’ is an established term in the field. And what is meant by ‘limited precision’ in line 20 of the abstract? Is it the precision in the sense of ‘double precision’ in ancient Fortran or is it the issue of over and undershoots caused by some numerical advection schemes (and related numerical problems)? Further, the only real information given in the abstract (and indeed in the paper) about the PTRAC module is the technical point that ‘prognostic tracers’ are defined via a Fortran95 namelist. So one is tempted to conclude that ‘diagnostic tracers’ are those that are not defined via a namelist – but this is surely not the point here. Some of these concepts can be better understood when reading the paper but an abstract must stand on its own.

Particularly confusing is the discussion about the PTRAC module. The only real information given in the in the paper is the technical point that ‘prognostic tracers’ are defined via a Fortran95 namelist. But clearly other chemical species are ‘prognostic’ quantities in the sense that their chemical and advective (etc.) tendencies are calculated. The example that is given in the paper, namely that a simple aerosol model would be a good candidate for being dealt with by PTRAC does not help. Why should the properties of aerosol particles be more suited to be defined via a Fortran95 namelist than say ozone or methane?

The most serious problem I have with the present paper regards module TRACER_PDEF. This module is designed to “correct negative overshoots” in quantities such as mixing ratios that are positive definite. The suggested procedure is setting negative concentrations/mixing ratios to zero. Clearly this will work. But a disadvantage of the suggested technique is that it systematically violates mass conservation.

Of course, this problem could be avoided by redistributing the accumulated ‘negative’ mass globally and enforce mass conservation. This would perhaps be a better solution than the one put forward in the paper. But still one that employs a global fix for a local problem (namely negative undershoots). Further, overshoots, caused by the same numerical problem as undershoots and equally unphysical, are not addressed at all in the current TRACER_PDEF formulation. Alternatives have been suggested to *locally* fix such problems in many papers e.g. those on positive definite advection schemes cited in the paper. There is a long history discussing such problems in the literature that is largely ignored in the paper as it stands [for example, Mon. Wea. Rev., 120, 1407-1415, (1992); Mon. Wea. Rev., 126, 1541-1580 (1998); Mon. Wea. Rev., 130(8), 2088-2097 (2002), and references therein].

The paper as it stands could be *misunderstood* recommending the use of more or less arbitrary advection schemes and parametrisation and to let TRACER_PDEF ‘do the job’ of fixing negative tracer values. Such a misunderstanding should definitely be avoided. All parametrisations, advection schemes etc. in a model should be designed to be positive definite. The role of the module TRACER_PDEF should be limited to remove any *technical* problems remaining such as rounding errors. If the authors agree, they should state this very clearly in the paper.

I am convinced that a naive application of the module TRACER_PDEF as it is described at the moment could lead to substantial model errors in simulations that are not easily detected. For example, I would predict that the advection of methane in the atmosphere by a very simple centred-space, leap-frog scheme should lead to substantial *local* errors in the stratosphere (for example in the vicinity of the sub-tropical or the polar night jet) that are then ‘fixed’ by the TRACER_PDEF module. And I would be surprised when such problems would be detected using the mass-based ‘quality-control scheme’ because most of the atmospheric mass of methane resides in the troposphere. Why are not alternative schemes discussed (at least as a potential extension of the module) that are based on a different measure than global mass? And

the paper currently fails to give a guideline what a “sufficiently small” negative mass is or even what strategy should be followed to select an appropriate threshold.

A few detailed Comments:

p. 17071, l. 11: I suggest to add ‘mixing’ to atmospheric transport processes.

p. 17078, l. 8: Unclear what ‘for this’ refers to.

p. 17083, l. 18-20: It is not correct what is stated here, numerical advection schemes as those cited here (and many others) are designed to avoid negative values. Moreover, I would expect (but I am not sure) that even negative values produced by parametrisations such as linearised sinks would be removed by the schemes cited in l. 17. in any event, this could be easily tested.

Interactive comment on Atmos. Chem. Phys. Discuss., 7, 17069, 2007.

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