

Interactive comment on “A new module for trace gas emissions in ICON-ART 2.0: A sensitivity study focusing on acetone emissions and concentrations” by Michael Weimer et al.

Anonymous Referee #1

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Review of M. Weimer et al.: A new module for trace gas emissions in ICON-ART 2.0: A sensitivity study focusing on acetone emissions and concentrations

The authors wrote an article presenting a new module for emissions of gas phase tracers in the framework of the ICON-ART model version 2.0. They describe a first application of their module in a sensitivity study of acetone concentrations near the upper-troposphere lower-stratosphere (UTLS) region. After a short general introduction to ICON, a detailed description of the algorithmic implementation and the procedure to apply gridded emission data sets to ICON-ART follows. Alternatively, they implemented the MEGAN model for biogenic volatile organic compounds. They briefly

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describe the basic properties of the MEGAN model. A first application of the new emission module is a sensitivity study of acetone in the UTLS region. All simulations are described and the emission data sets discussed. They use a simplified chemistry that is given in detail.

The subject of the paper is appropriate for Geosciences Model Development, however, I can not recommend it for publication without major revision. In fact, this paper merely describes how gas phase tracer emissions are applied inside ICON-ART, but it does not discuss the consequences of the various possibilities how emissions can be applied in such models nor do they reference other models using similar emission modules. Emissions in chemical transport models are widely used and nothing new. The reader is disappointed not to learn anything about these different methods although the title promises to present a sensitivity study on emissions. For a scientific evaluation of the emissions itself, the paper is too technical and “thin” with respect to the emissions themselves, but for a methodological paper, it’s not detailed enough in terms of the method. The short application to acetone is interesting but the emission module itself needs to be analysed in more detail.

General comment

Emissions of gas phase tracers, in particular surface emissions, can be brought into the model by at least three methods: (i) as a flux condition at the surface to vertical diffusion. In that case, a net flux on the surface is calculated by adding the dry deposition flux. The vertical diffusion distributes the tracer in the boundary layer. (ii) as a source term in the chemical kinetic equations in some appropriate model layers. (iii) as a tendency in some appropriate model layers near the surface. The authors chose method (iii) but should discuss the other methods also which are all associated with a certain operator splitting. What concerns me most is the fact that the criteria are unclear according to which the number of lowermost layers are chosen into which the

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emissions are brought as a tendency. The authors should discuss this choice, prepare an appropriate sensitivity study varying the number of levels and perform a simulation with emissions given as a flux condition to the vertical diffusion equation. In this latter simulation, the resulting tendencies in the lowermost model layers should be compared with the number of model layers used in method (iii). It would be particularly interesting to see the seasonal variation. Discuss other chemistry general circulation models and what methods they use.

Specific comments

p.2, l.26: The ICON model is not really “in development” anymore since the NWP physics is used for operational weather forecast.

p.3, Tab.1: The “official ICON grid number”: Give a citation here.

p.3, l.1: It should be clarified that Leuenberger et al. generalized the SLEVE coordinates

p.3, l.5 ff: The usual definition of volume mixing ratios is moles tracer per moles dry air. In ICON, tracers are defined per moist air for the horizontal transport. How do you treat these different definitions? How did you check mass conservation?

p.5, Fig.2: “reset simulation year from boundary year back to current year”: It’s not so clear what you mean here. You would like to say that the last year for which emissions are given is repeated for all years later than this year. By the way, this may even be error prone repeating the last year without warning.

p.6, l.10: Emissions are interpolated by a nearest neighbour interpolation. A flux conserving interpolation would sound more natural since you like to have the same amount of tracer going into the atmosphere irrespective of the used horizontal model resolution. Discuss this.

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p.9, l.14: “for each time step” may sound like model time step here, but you mean times for which emissions are provided. Please, rephrase.

p.7, Fig. 3: Lines are cut and not completely displayed.

p.7, l.5: Fig. 3 shows \LaTeX not \TeX code.

p.7, l.6: “the number of emission”: is it emission sectors, emission types? Be more specific.

p.7, l.7: “...account only the number...” an “if” is missing. “...is then used globally”: Explain better that “the number” is then a globally applied emission mass flux.

p.8, l.2: “emission date” may be misinterpreted as the date when emissions are applied (actually, they are applied in every time step), but “emission date” refers to the date for which emission fluxes are provided. Please, rephrase.

p.8, l.9: Just a remark: Is it necessary to have such a fixed time limit of 11–years? Volcanic emissions could be very irregular, farther away than 11–years and should not be interpolated?

p.8, l.13: “After interpolation the emission is converted to VMR ($C_{emi,i}$)”: Rephrase “emission” to “emission flux”; furthermore, you mean a VMR tendency here, the symbol c is normally used for molarity, so $dX_{emi,i}/dt$ would be the correct symbol. Divide eq. (2) by time.

p.8, eq.(2): In mathematics, sums \sum are not counting backwards, write $\sum_{l=k_{lev}-k_{emi}+1}^{k_{lev}}$. If $k_{emi} = 1$, I guess that all emissions should go into the lowest level k_{lev} , consequently, the sum has to go from k_{lev} to k_{lev} . The lower limit needs a +1 therefore. Explain the symbols.

p.9, l.1: Explain the choice of k_{emi} in more detail.

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- p.9, l.5:** Websites are not a good reference in general. If necessary, add in a footnote the date when you accessed the sites the last time. Similarly: p. 9, l. 15, p. 11, l. 25, p. 16 the footnote, p. 22, l. 3/5
- p.11, l.17:** Avoid to start a sentence with a mathematical symbol, in particular when it repeats the symbol of the last sentence.
- p.11, l.28:** “derived” instead of “defined”.
- p.12, l.6:** “sunlit leaves” instead of “sun leaves”
- p.13, fig.6:** Explain better how you calculate the means. First, the word “global” is irritating, since you are calculating means over “S–America”? In fact, you calculated means over a rectangle in longitude and latitude with sea points contributing to the surface but not to the emissions.
- p.15, l.7:** “...due to Reactions (R5) and (R6)” you probably like to say that (R5) is the rate–determining step.
- p.17, l.20:** ICON contains several time steps, which one do you mean?
- p.17, l.20:** Output interval of 23 hours, meaning output at 0h, 23h (of next day), 22h (of next day), 21h (of next day), and so on?
- p.18, l.1:** Temporal variability of OH at which time scale?
- p.19, l.15/20/Fig. 8:** OH–chem(off): Better choose OH–chem(megan–off) or similar acronyms to make clear that it is not the OH–chemistry being switched off. Fig. 8: Show the free troposphere in an additional panel such that the interannual variability becomes visible.

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- p.19, l.12 ff:** Your reasons for the underestimation are pure hypotheses and more confusing than explaining your results. The reader is lost what refers to your simulations and what is speculation. Make it clear where your considerations are general and what concerns your situation.
- p.20, fig.9:** Remove unnecessary axis and titles of the plots. Create one color bar for all panels instead. Instead of a pressure range, give the geometric altitude of the tropopause.
- p.20, l.3ff:** Describe your result first, then interpret/explain
- p.20, l.13:** Acetone life time of 1.5 years versus 28 days? This is worth an explanation.
- p.21, l.5 ff:** The conclusions should contain information about the choice of k_{emi} and the sensitivity studies versus a flux condition in vertical diffusion.
- p.22, l.1–5:** Code availability: give a contact person only since there seems to be no icon license available at the site given (address not found!). The ART license is referring to a person anyhow.
- Appendix A:** “Concentration” should be either “molarity” or “number concentration” since concentration can be anything, mole fraction, volume mixing ratios, molality, molonity and the like. It’s confusing to have a species index and a time step index on c in the same section. Put $c_{i,t}(x)$ where x refers to the location, i to the species and t is time. Write the equations for an arbitrary integration step from t to $t + \Delta t$. From (A2) on you can, if you like, omit the index i . Mark the various solutions with superscripts ^(e) for explicit Euler and ^(pc) for the predictor–corrector method.
- p.23, l.9:** Better: “If Δt becomes larger than...”. What do you mean with “unstable”?
- p.27, l.8:** Give the page in Pandis/Seinfeld.

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Technical corrections

p.1, l.12: “dominated concentrations”: missing space

p.2, l.28: delete one of the “to”

p.13, l.11: “The tracer loss rate” or “the loss rate of the tracers”

p.19, l.8: “Maximum” instead of “Maximal”