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Interactive comment on “Development and evaluation of the Screening Trajectory Ozone Prediction System (STOPS, version 1.0)” by B. H. Czader et al.

Anonymous Referee #2

Received and published: 2 January 2015

The authors present a Lagrangian-Eulerian Diagnostics (STOPS), which allows for a more detailed analysis of emitter-receptor relations. They chose 3 meteorological situations to analyse the performance of STOPS and provided an application, which are well chosen. The content fits well the scope of GMD and should be published, however only after substantial modifications. The presentation of the model and the verification is hard to understand and to interpret since a lot of information is missing or partly given at a later stage.

Major comments:

1. More detailed description of STOPS

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I recommend a more detailed description of the STOPS model. A work flow could be helpful. This description should include:

- When are which boundary conditions taken for STEPS. Is there only temporal or also some horizontal interpolation?
- The transport is described in the text. If a column is taken. Is it one box or still divided into several cells?
- What other processes are calculated? Chemistry? Convection? Deposition? Rainout? Lightning? How is this done in detail?
- Are the processes calculated in the column or flux changes taken from CMAQ?
- Is there a difference between the output time and the calculation timestep? How is this organised?

2. Units and equations

Please add units to all variables. It makes it easier to understand. If the word "mass" is used I would expect something like a unit "kg". But here it seems not to have a unit at all. Some variables, like delta sigma are not explained properly and some equations have little errors.

3. Chosen performance metrics

I know that these metrics are often used. It would be helpful to first clarify for what purpose they can be used. What is the scientific question? And which metric is answering this question best? E.g. total ozone for maintaining the mass budget. Or difference in ozone mixing ratios for ... ? There are some issues if the mass or volume in the individual CMAQ cells are differing, e.g. in the vertical. That should be clarified in more detail. MAX and MIN is used in the text but is missing in the description.

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4. Concept of verification.

The chosen stepwise verification seems to be valid, but hard to judge, since I couldn't follow in detail. Please include a subsection explaining the procedure, motivation, and interpretation of the experimental set-up in more detail. (see also questions below). The fact that there is only one subsection in 3.2 might indicate that there are some more thoughts on the structure necessary.

Some more general comments:

- Please explain rows and columns in CMAQ. And make a difference between the CMAQ column and STOPS vertical column. This is confusing.
- Title: "Development" -> "Description"? (also section name)
- The authors sometimes use ppb and ppbV. Is there a difference? Is it mass versus volume mixing ratio? Please use it uniformly.
- Similar with CST and UTC. The use is correct, but it makes it harder to read. Please use one time only.

More detailed comments:

I 17: Why "columns of air.", I rather would say air parcels. Most are only points in the atmosphere, but some actually have an extension.

I19 : "so there are no advection terms in the set of governing equations.". Please rephrase. It sounds like there is no advection. Of course the air parcels are advected.

I23-28: Please rephrase, since there are Lagrangian chemistry models!

p7622 I8 "... tool to study a source-receptor relationship". Still there are diffusion processes, turbulence etc, which is normally not resolved, but which leads to a inter

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parcel exchange. This normally limits the efficiency of source-receptor relationships. This might come later, but should somehow be mentioned here. On top, there are other methods to resolve source receptor relationships, such as tagging. That should be mentioned somehow. Lagrangian methods are not the only one. Probably a combination would be most favourable?

p7623 | 6 Delete "A"

p7624 | 8 "physical and chemical processes in STOPS are the same as in the full domain CMAQ model" Please clarify: Are the same subroutines used, i.e. there is a call of the e.g. chemistry package from STOPS or are chemical changes from the CMAQ simulation extracted and applied to the column in STOPS?

I 19 Correct "I=PBL" -> "PBL" (in all equations!)

I 20ff add units to the variables. Every sentence is a paragraph that is irritating. Clarify p_l (midlevel pressure?). Explain why the mean wind has units m/s/kg. (sigma is a number; w in m/s?; and M in kg?) In eq. (2) M is defined as a unitless number, namely the ratio of the PBL-mass to the total model atmosphere mass in the respective column. Please revise either the equations or the naming. A mass should have kg as a unit. Explain delta sigma. Difference of what?

Section 3:

1. Please clarify the $S_i - H_i$ matching: It is unclear to me how the matching of H_i and S_i is done, e.g. to calculate the mean bias in eq. (7). Background: The column in STOPS is moving. Hence after a couple of timesteps the column is covering in the horizontal fractions of different CMAQ grid cells. Which of these grid cells is taken? Or is a weighted mean calculated? See e.g. also Grewe et al., 2014 (Meteorologische Zeitschrift) for problems in Eulerian-Lagrangian cell matching.
2. Please clarify units of S_i H_i

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3. Please motivate more the use of the performance metrics. Clarify why the difference of (i guess) ppbvs is taken in eq. (7)? For example, if the mass or volume of the individual cells in the column is differs largely, then one cell might dominate the total mass in the column. The mass of a species simulated with STOPS and CMAQ might be basically equal, but the performance metrics might show a large discrepancy because it is dominated by cells with low mass.
4. Explain what stationary mode means. What is stationary? windfield? chemistry? zero wind?
5. The naming "output time step" is confusing. Is this the time step of STOPS? or is STOPS run with shorter time steps and just the output of STOPS is at a different interval?
6. Throughout the text "interpolation" is used. I first thought a horizontal interpolation is meant to match locations. Please clarify.

p 7627 l 16/17 "of either initial or boundary values", but what is with the H_i values?

p 7628 l12 Please define what is meant by "from the corresponding grid cells".

Section 3.2

Here a couple of things are now explained, which partly clarify some of the questions above. Please give this information earlier. (stationary/alignment of cells/ ...)

p 7629 l8-9. How is the interpolation done?

p 7630 l 21 "STOPS concentrations were spatially ..." I would have thought that the CMAQ values have to be interpolated (or redistributed?). How many STOPS values are available? Where are they located?

Figure 5: triangles and crosses can not be identified. Please plot differently, e.g. in color.

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"Very good performance was found on 28 August with the averaged mean absolute error of 1.3 and 1.5 for the urban and industrial domains, subsequently" What is looked at? Surface ozone? 1.3 and 1.5 ppbv? kg?

p 7631 "STOPS system were validated against CMAQ calculated concentration". This assumes that CMAQ is the reference. But what is if the lagrangian transport is just more accurate, with less diffusion. Then a difference would be an enhancement of the model. But the statistics would show the opposite effect. Please explain.

Table 5 and 6 could be converted into a figure to better show the convergence?

Section 4:

At what time is the release? 6:00? And where exactly?

Why did you change between UTC and CST?

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