

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

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Dear Reviewer,

Thank you for your time and effort put into reviewing the paper and for your helpful suggestions. Please find below our responses to your comments.

Major comments:

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

— STOPS is based on the CMAQ model and the structure and science processed  
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are the same as in CMAQ as mentioned in line 10-11 of the abstract and lines 7-10 on page 7624. Since CMAQ is well documented we did not see a need of repeating its description, instead we provided a reference to Byun and Schere 2006 in the manuscript (please see also the following link for additional CMAQ documentation <https://www.cmascenter.org/help/documentation.cfm> ). Therefore, in the manuscript we provided only information on modifications of CMAQ code related to STOPS structure and movement of its domain.

~When are which boundary conditions taken for STOPS. Is there only temporal or also some horizontal interpolation?

— In the original CMAQ there is temporal interpolation of boundary conditions; this is, hourly boundary values are interpolated to match smaller calculation time steps. In STOPS, in addition to this temporal interpolation, we also added spatial interpolation. It was needed for cases when the STOPS grids do not align with the grid cells of a CMAQ file used for boundary conditions.

~The transport is described in the text. If a column is taken. Is it one box or still divided into several cells?

— We keep the same vertical structure as in CMAQ, so the column(s) are divided into many vertical layers. Please also see a modified figure 1.

~What other processes are calculated? Chemistry? Convection? Deposition? Rain-out? Lightning? ..... How is this done in detail?

— For each grid cell in a domain the following processes are calculated: horizontal and vertical advection, horizontal and vertical diffusion, dry and wet deposition, chemical reactions in gas, aqueous and particle phase, as well as photochemical processes and chemistry in clouds. Please refer to Byun and Schere (2006) referenced in the manuscript as well as the following documentation of CMAQ <https://www.cmascenter.org/help/documentation.cfm>.

~Are the processes calculated in the column or flux changes taken from CMAQ?

— The processes are calculated for each grid cell inside STOPS domain. In and out-flow of pollutants between grid cells as well as at the STOPS domain boundaries is accounted for.

~Is there a difference between the output time and the calculation timestep? How is this organised?

— Usually outputs are saved as hourly values but a user has an option to change that. The calculation of science processes in CMAQ as well as in STOPS is based on so call synchronization time step, which is in a range of seconds to minutes and determined by the model to satisfy the Courant condition safe advection time step.

## 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.

— We will modify the manuscript as follow:

Page 7622 lines 23-25 was: "It can also be utilized to provide detailed process analysis information (mass budget and integrated chemical reaction rates) for a moving window domain to capture chemical evolution of plumes."

Will be: "It can also be utilized to provide detailed process analysis information (a contribution of physical and chemical process to a simulated mixing ratio) for a moving window domain to capture evolution of plumes."

Text from page 2624 line 16 to page 2425 line 4 will be replaced with the following and eq. 2 will be removed:

"The trajectory for STOPS movement is calculated based on the mean wind in the  
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middle column (thereafter mwind) that is averaged from surface layer up to the Planetary Boundary Layer (PBL) height and weighted by differences in pressure in each layer. The u and v components of wind (m/s) were calculated according to the following equations: (please see supplement for modified equation 1)

Where  $\sigma_F = 1 - \sigma$  and  $\sigma$  (unitless) is a scaled atmospheric pressure in a sigma coordinate system defined as follow: (eq 3).

## 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.

— Our goal was to evaluate STOPS performance for surface ozone mixing ratios (ppbV). The mean absolute error (MAE) would be the most rigorous metric for this purpose but the mean bias is useful too as it shows if model under or overpredicts values. We will remove equation 5 and 6 since we realized that the mean values are not shown in the manuscript and add units.

— The MAXD and MIND will be removed from the caption of tables 2, 3, and 4 as they are not shown in tables.

## 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.

— The following will be added before section 3.1: “We performed verification for three cases: (1) a case when the STOPS domain does not move, which was performed to test an effect of boundary condition on STOPS results; (2) cases with STOPS moving along different trajectories performed to test STOPS performance for different atmospheric conditions as well as an effect of different ways of trajectory calculation on STOPS results; (3) cases with different STOPS domain sizes to test an effect of domain size on the STOPS results.”

— Section 3.1 will be renamed to: “Effect of boundary conditions”. Section 3.2: “Uncertainties related to movement of STOPS”. Section 3.2.1 will be changed to 3.3: “Effect of domain size”. 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.

— We will replace the sentences on page 2623 lines 24 through page 7624 line 5 with the following description: “CMAQ domain is divided into grid cells with certain number of rows and columns in a horizontal direction and layers in a vertical direction. STOPS can be considered as a sub-domain of CMAQ, which is also divided into a grid cells in horizontal and vertical direction and moves with the mean (Figure 1). At its starting position STOPS grid is aligned with CMAQ grid, but as STOPS moves with wind its grid may not necessarily align with CMAQ grids. STOPS uses initial condition and the dynamic boundary conditions from saved original CMAQ simulation results. Because of that STOPS movement is limited to CMAQ domain boundaries.”

~ Title: "Development" -> "Description"? (also section name)

— The whole manuscript is a description of STOPS and its evaluation, in the title we wanted to underline that we both developed and evaluated this model.

~ The authors sometimes use ppb and ppbV. Is there a difference? Is it mass versus volume mixing ratio? Please use it uniformly.

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— We will modify the text to uniformly use unit “ppbV” which indicates volume mixing ratio.

~ Similar with CST and UTC. The use is correct, but it makes it harder to read. Please use one time only.

— We will modify the manuscript to consistently use UTC.

More detailed comments:

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

— We will replace “columns” to “parcels” in the description of Lagrangian approach in the Introduction.

l19 : “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.

— What we meant is that there is only parcel movement with wind but there is no advection in and out of the column, a process that is considered in Eulerian models. We will modify it as follow:

“The air parcels move along with the prevailing winds (being advected), there is no mass exchange between parcels and surroundings except emissions of pollutants that are accounted for when the air parcels pass over source regions.

l23-28: Please rephrase, since there are Lagrangian chemistry models!

— We will rephrase as follow: “Often they do not account for chemical transformations as the chemistry is modeled as first order decay of pollutants; in such cases they are unable to adequately predict the atmospheric concentrations of species with short lifetimes, such as fast reacting ozone-forming VOCs and air toxics, an example of which is 1,3-butadiene.”

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p7622 l8 "... 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 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?

— While tagging could be used in source-receptor applications it increases number of model species and therefore computation time. It also does not give information about response to emission changes. Our goal was to get a fast tool that simulates effects of perturbation in emissions and STOPS is just one approach that we thought might be useful for that purpose.

p7623 l 6 Delete "A"

— we will delete it.

p7624 l 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?

— You could think of STOPS as being CMAQ with a much smaller domain that moves with wind. As STOPS is based on CMAQ's code, the same subroutines are used and the same process included. We modified only several subroutines to account for movement of a domain and added a new module as described in the manuscript.

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

— It will be corrected.

l 20ff add units to the variables. Every sentence is a paragraph that is irritating. Clarify pl (midlevel pressure?). Explain why the mean wind has units m/s/kg. (sigma is a number;

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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 uin 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?

— The idea was to calculate average wind based on wind values in each layer and weight it by mass of air in each layer. We approximated mass by calculating differences in pressure which in sigma coordinate system could be calculated from differences in sigma layers. We will remove eq. 2, modify equations 1 and 2 as well as rephrase the text as follow: The trajectory for STOPS movement is calculated based on the mean wind in the middle column (thereafter mwind) that is averaged from surface layer up to the Planetary Boundary Layer (PBL) height and weighted by differences in pressure in each layer. The u and v components of wind (m/s) were calculated according to the following equations: (please see supplement for modified eq.1)

Where  $\sigma_F = 1 - \sigma$  and  $\sigma$  (unitless) is a scaled atmospheric pressure in a sigma coordinate system defined as folloq: (eq 3).

Section 3:

Please clarify the Si - Hi matching: It is unclear to me how the matching of Hi and Si 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.

— Explanation will be added on page 7627 just before section 3.1: "Since STOPS grids do not necessarily align with CMAQ grids the CMAQ values from grid cell corresponding to a STOPS cell are interpolated by means of weighted averaging of CMAQ values."

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## 2. Please clarify units of Si Hi

— We will add the following at the end of section 3 on page 7627: “where Hi and Si corresponds to instantaneous mixing ratios (ppbV) obtained with CMAQ and STOPS, respectively.”

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 specied 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.

— Our goal was to evaluate STOPS performance for surface ozone, so the statistics is calculated for ozone mixing ratios in ppbV. The mean bias is the most widely used in atmospheric model evaluations therefore it is useful for comparing our results with other studies, also it provides information on model under or over predicts values. MAE and RMSE are the more rigorous metrics that we thought would be useful to show.

Explain what stationary mode means. What is stationary? windfield? chemistry? zero wind?

— When we use “stationary” we refer to a domain that is not moving. To clarify this we will modify the first sentence in that paragraph (p. 7627 lines 14-16) as follow: “First, the correctness of the STOPS code implementation was verified by performing STOPS simulations in the stationary mode, this is when it is not moving. In this configuration STOPS domain is like a CMAQ sub-domain in which the grid cells are aligned with CMAQ grid cells; thus, STOPS calculated values can be directly compared with CMAQ values from corresponding grid cells.”

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 inter-

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vall?

— The calculation time step is in order of minutes. The output time step is usually 1 hour. We will rephrase the paragraph on page 7628 (lines 7 – 18) to provide clarification on that.

6. Throughout the text “interpolation” is used. I first thought a horizontal interpolation is meant to match locations. Please clarify.

— Temporal interpolation of hourly input values is performed for most of the input data, including boundary conditions, in CMAQ as well as STOPS. In addition, for the case when STOPS domain travels; thus, may not necessarily align with the grid cell of input data, we also perform spatial interpolation.

p 7627 l 16/17 “of either initial or boundary values”, but what is with the Hi values?

— The following will be added at the end of section 3 on page 7627: “where Hi and Si corresponds to instantaneous mixing ratios (ppbV) obtained with CMAQ and STOPS, respectively.”

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

— Here STOPS was just like a sub-domain of CMAQ, so its grid is located inside CMAQ grid and aligns with CMAQ grid cell. We were comparing values from STOPS grids cells with the corresponding grid cells in CMAQ. We will rephrase this sentence to make it clear. Please refer to a modified figure 1.

## 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/ ...)

— As mentioned above we will provide some additional information at the end of section 3, before section 3.1.

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

— We will rephrase it as follow: "or CMAQ values from several cells have to be interpolated to the corresponding STOPS cell by calculating weighted average from the CMAQ values."

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?

—You are right, that was a mistake and we will rephrase it as follow: "CMAQ concentrations were spatially interpolated to be compared with STOPS mixing ratios." Number of STOPS values depends on the size of its domain; since we compared only surface values there were N values as specified in equation 4, where NCOL and NROW is number of columns and rows in STOPS domain, and NTSTEP number of output time steps. As STOPS moves it calculates mixing ratios for different locations.

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

— We will replace the graphs with color ones.

"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?

— yes, we looked at surface ozone (ppbv). We will add this information into a manuscript.

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.

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— Since STOPS is based on CMAQ model so in this context we believe it is right to evaluate STOPS against CMAQ.

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

— We prefer to show all the statistics currently listed in those tables and therefore would like to keep the tables.

Section 4:

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

— We will add the following explanation in line 19 p. 7632: "The additional emission was added between 11 and 12 UTC in the location of the middle cell of STOPS domain at its starting position."

Why did you change between UTC and CST?

— We will modify to UTC to be consistent with other parts of the manuscript.

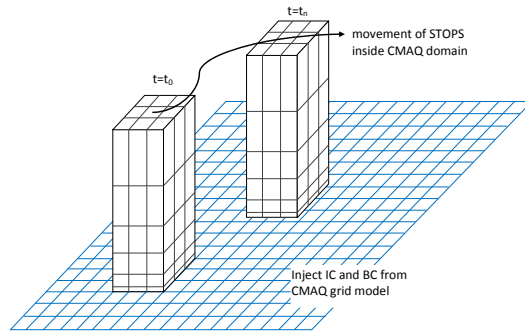
Please also note the supplement to this comment:

<http://www.geosci-model-dev-discuss.net/7/C3502/2015/gmdd-7-C3502-2015-supplement.pdf>

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Interactive comment on Geosci. Model Dev. Discuss., 7, 7619, 2014.

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**Fig. 1.**

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