Anonymous Referee #2

Received and published: 21 November 2017

This paper describes the BEATBOX framework, which enables users to perform and asses several data assimilation techniques using the BOXMOX model. The tool is open-source and should be of high interest to the atmospheric chemistry community. The online examples provide appropriate guidance to reproduce the results presented here.
I have only minor concerns with the manuscript concerning clarity. There are a few sections that are difficult to follow, and could be corrected by including more details, simplifying sentences, or fixing typos. I recommend publication after addressing the points below.

We thank the reviewer for his/her positive review and helpful comments. Please find our responses to the comments below.

Page 1, line 8: should be "allows users to conduct"
Fixed.

Is Figure 1 referenced anywhere?
It was not, thanks! Fixed, now referenced in the section just above it.

Page 5, line 17: Mention that BOXMOX is a standalone Linux executable (i.e. not written in python).
Sentence added: "[...] are possible input parameters. BOXMOX is a standalone C / Fortran program running on Linux or Mac OS X. In this work we have extended BOXMOX [...]"

Page 6, section 2.1.2: The last sentences of each paragraph in this section are essentially the same. Include it only once.
We have remove the first occurence.

Page 7: line 14: A single observation (p=1) means a single observation in space, but there can be multiple observations in time. Somehow clarify the time dimension here.
Here p=1 means a single observation in the assimilation window (1h), which means a single observation in space and time allotted within the window. We clarify the sentence as follow: "[...] In the BEATBOX framework a single observation in a given assimilation window (p = 1) and only the dimension along the chemical variables is considered [...]"

Page 8, line 2: should be "can be viewed"
Fixed.

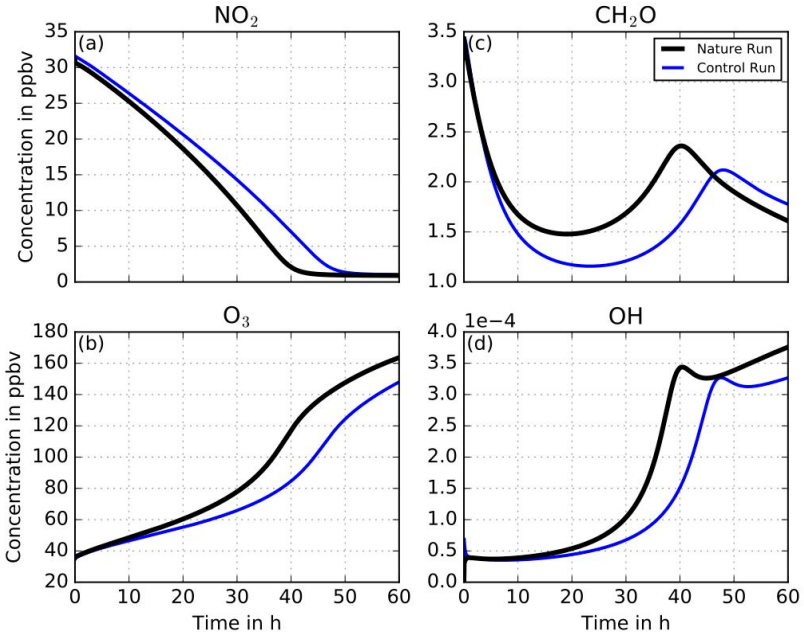
Page 11, line 1: Please provide more information on the setup. What meteorological parameters are varied with time? What is meant by VOC here? All measured VOCs and their oxidation products?
We have adapted sentence 2 which now reads: "[...] In the present simulations, all environmental parameters such as temperature and photolysis rates are kept constant. [...]" All

meteorological parameters are held constant. A sentence has been added at the end of the first paragraph to clarify what is initialized:
"[...] due to chemical reactions is allowed. Initial conditions for primary VOCs and inorganic compounds are provided using the FRAPPE observations. [...]"

Page 11 line 3: 'VOC-limited, NOX-limited, and transition region" . . . Indicate that these refer to ozone production. How was the placement of the vertical lines determined?
The paragraph has been amended to better explain why this was done: "[...] The vertical lines suggest the VOC-limited (VOC/NOx ratio <= 4), NOx-limited (VOC/NOx ratio > 15) and the transition region (4 < VOC/NOx ratio <= 15), to show that the simulation transitions through different O3 production regimes with possibly very different relevant chemical pathways. The measurements show an initially strongly VOC-limited air indicative of an urban air mass. The VOC/NOx-ratio of the aging air increases in time. During the first 15 h the simulation shows a strong VOC-limited regime. A transition regime spans from 15 h to approximately 30 h. After the transition period the chemical regime becomes NOx-limited, representative of more rural / background conditions. The toluene/benzene-ratio is used as qualitative measure of photochemical age. Toluene and benzene are considered to have the same sources but toluene is more quickly oxidized than benzene which leads to a decline in the ratio over time. [...]"

Page 11 line 15: replace "slighter" with "smaller".
Done.

Figure 4, legends are needed.
Added:



Page 13 line 22: remove period before “either”
Done.

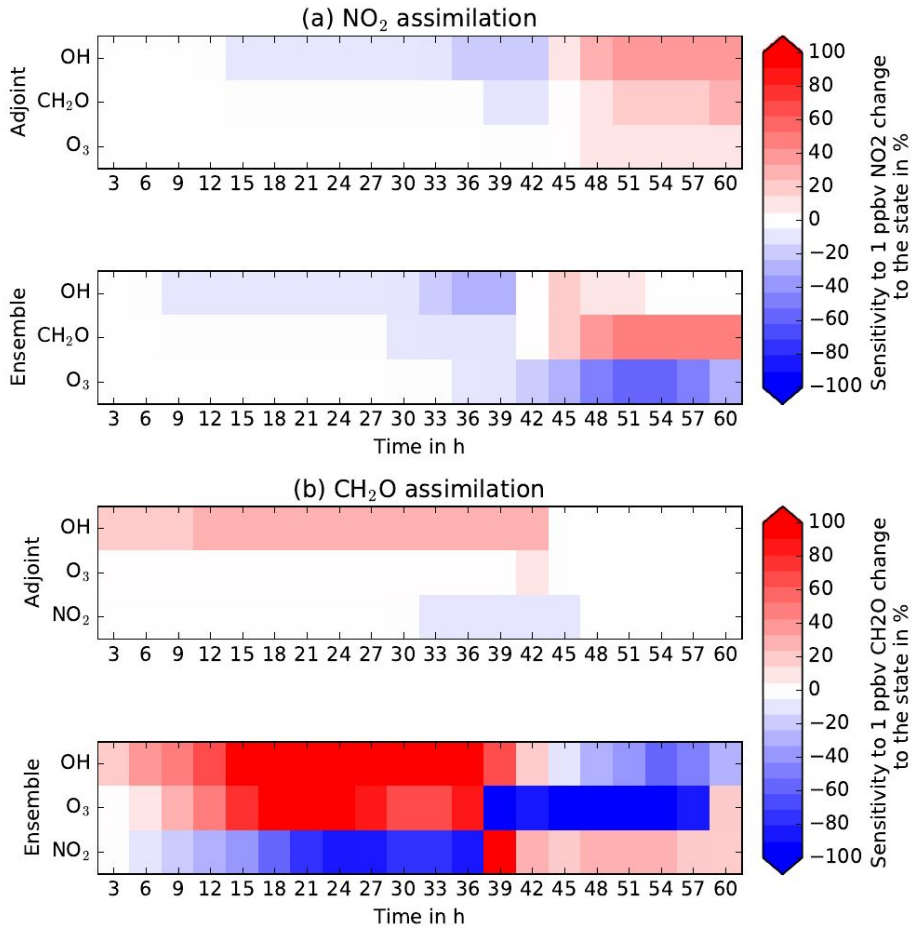
Page 13 line 24: what is “secondary” production?
This sentence was unclear and has been rephrased: “[...] After 40 hours, NO_2 concentrations drop to very low values, NO_2 assimilation increments are very small, hence almost no inference on the other state variables is observed. [...]”

Page 13 line 26: remove one instance of “that case”
Done.

Page 15 line 5: replace “is willing to come back to” with “returns”
Changed, see reviewer 1.

Page 15 line 6: replace “as” with “a”
Fixed.

Figure 7, bottom panel: are the colorbars saturated more often than not? If so, adjust the colorbar scaling.
We have extended the color bar range, but had to find a balance with visibility of changes in the top panel, as we wanted to keep the color bar range identical for all plots to aid comparability.



Page 15 line 17: "form" should be "from"
Thanks for spotting this one!

Page 17 line 22: Simplify sentence starting with "We recall that". . . to read "Most state-of-the-art EnKF methods use this approximation"
Done.

Page 17 line 31: Fix "The adjoint inference do not strongly changes"
Changed.

Page 17 line 33: Change the model "wants to go back to" to "returns"
Changed, see reviewer 1.

Page 20 line 9: Replace "more at a loss" with "negative".
Updated.

Page 20 line 10, Simplify the sentence starting with "If we now...", to read "The CR rates are significantly faster than the AR ensemble rates, and the slopes of the rates (i.e. the second derivative of the concentration evolution) also differ".
Done.

Figure 9: These are difficult to compare with the different y axis. Consider an additional plot that contains net production and net loss for each run, and including these all on the same axis (without individual reactions).
We have added an additional plot that only contains the net fluxes for each run: