Anonymous Referee #2

1 General comments

The paper describes a new open-source box model designed primarily for runs using the Master Chemical Mechanism (MCM), although other mechanisms can also be modelled provided they are entered in the correct format. The model comes in two forms, one (the original) available online via a web-interface, and a downloadable one (AtChem2) suitable for more advanced studies including batch runs that can be executed on the user's machine. The box model is presented as being free and easy to use, and having functionality that makes it particularly suitable for comparison against observational data, due to the way it handles constrained variables with different time frequencies. It is applied in two case studies to chamber and field data respectively to illustrate that it can handle these scenarios and allow us to reach some conclusions about which parts of the mechanism need to be reviewed. I believe this paper will be suitable for publication subject to revision.

We thank the referee for their comments and suggestions. Please find below our replies and the related modifications to the manuscript. The line numbers refer to the version of the manuscript published on GMDD.

2 Specific comments

The text in the paper is generally well-written and easy to follow. The figures are less clear, however. In particular, Figure 2 is too small to make much sense of even when zoomed in on (due to the scale); the outlier marker is larger than some of the box-and-whiskers. Figure 3 is missing some arrowheads, and the ones that are there are too small to be clearly seen. In Figure 6, the ozone and nitrogen oxides lines/markers are not labelled as to which is which; I would also recommend using different marker shapes when presenting multiple datasets in one graph in addition to using different colours.

The sizes of Figure 2 and 6 have been increased.
The arrows in Figure 3 have been fixed.
Markers have been added to Figure 6 and the legend has been corrected.

I think the paper could highlight in detail what makes AtChem stand out over specific other box models. The two forms (online/offline) appear to have different unique benefits, and perhaps need to be discussed separately. It appears that the online model can at present only be run with login details (is it only for use by the EUROCHAMP community?), which might restrict takeup (especially for teaching purposes), but I hope this is something the authors are planning to address. I also note that the online form does not seem to readily support the newest MCM version; perhaps this can be updated?

The referee is correct that the two versions of AtChem presented in this paper have different objectives, as well as different benefits and limitations (please note that the login details are available to anybody upon request, as indicated on the AtChem-online website, at https://atchem.leeds.ac.uk/webapp/). The history and the purpose of the two versions of AtChem are explained in the Introduction and in Section 2.1; we have also added more information about other open-source models in the Introduction (see the reply to a comment by referee #1).

Both versions of AtChem can be used with any version of the MCM, or with any general set of chemical reactions, as long as they are in the prescribed format. In fact, the examples in Section 3 were run with two different versions of the MCM (see below).

Given the commonality of the codebase we don't think it makes sense to divide the paper into two parts, each discussing a version of AtChem, as this would result in much repetition. We feel that the features and the characteristics that distinguish the two versions of the model are clearly identified as such in the manuscript.

Parts of the paper are using different versions of the MCM and perhaps also different versions of AtChem(2). In particular, on page 12 the section on lines 358-360 describes that the previously published results were off by a small amount due to a bug in a previous version of AtChem; however, at no point does the paper make reference to which version(s) of AtChem(2) were used in the runs. I would suggest carrying out all the model runs with the latest version of AtChem2 and annotating them as such. If the latest MCM version was not used for modelling the field study data for consistency with the previous paper analysing this data, I would comment on this, but also perhaps rerun the simulation with the newest MCM version for comparison.

All the model results discussed in Section 3 have been run with the same version of AtChem (version 1). The sentence on page 12, lines 358-360 refers to the model results published in Sommariva et al. (2011), not to those presented in this manuscript. The following changes have been made to the manuscript to clarify these points:

Lines 71-72: changed to "This paper presents version 1 of AtChem, and is divided into two parts"

Line 78: added "(version 1.5, rev. 146)"

Line 92: added " Version 1.0 of AtChem2 (doi:10.5281/zenodo.3404021) is presented here, and has been used for the model simulations shown in Sect. 3."

Line 358: changed to "The results obtained with version 1 of AtChem2 and with the beta version of AtChem used by Sommariva et al. (2011a) differ by ~3%"

It is true that different versions of the MCM are used in the paper. Specifically version 3.3.1 was used in Section 3.1 (chamber study example) and version 3.1 was used in Section 3.2 (field campaign example); the reason for this is that we wanted the model used in this paper to be directly comparable with the model used by Sommariva et al. (2011), in which the full model/measurement time series is presented.

For the objectives of this paper, the comparison between different versions of AtChem is more relevant than the comparison between different versions of the MCM, which is extensively covered in the updates to the original MCM protocol (e.g., see Saunders et al., 2003; Jenkin et al., 2015). If the same version of the MCM is used with the same configuration/constraints, then any difference between the two models can only be due to changes in the AtChem code (which was the case, see lines 358-360). To make this point clearer, Figure 7 was modified by adding the model results from Sommariva et al. (2011) and the text was modified as follows:

Lines 350-351: "The chemical mechanism used here was extracted from the MCM v3.1 (as in Sommariva et al. (2011a)): it included the inorganic chemistry scheme, the oxidation mechanism of 65 VOC, the dimethyl sulfide (DMS) oxidation mechanism from Sommariva et al. (2009), plus dry deposition terms and heterogeneous reactions for the appropriate gas-phase species."

Lines 354-356: moved to line 349.

3 Technical corrections

p7, line 204: change “studies" to “study"

Corrected.

p7, line 214: change “results" to “result" and correct spelling of “stiffness"

Corrected.

p8, line 224: Eq. 3 appears to use two different forms of the multiplication sign

Corrected.

p12, line 351: IUPAC spelling is “sulfide"

Corrected.

p22, label on Figure 4: the local time is GMT–7 in the winter, but GMT–6 in the summer due to daylight saving time

The plot is showing the correct times in GMT. The caption of Figure 4 has been corrected as suggested.

p27, in Table 1: “SO2" should have 2 as a subscript.

Corrected.

There is inconsistent use of American and British spellings (s/z) in the manuscript, and though it is a very minor issue, this can perhaps be standardised. I also feel that a few more hyphens would aid easy parsing of the text in places (e.g. p7, line 205 as well as Figure 2 label: “9-days"; p9, line 250 as well as p8, line 226: “two-stream").

The spelling has been corrected to British English. The hyphens have been added, as suggested.