Comments on *The MESSy chamber DWARF: a box model for simulating chamber experiments (based on MESSy v2.55.2)*

The authors present an extension to the MESSY DWARF box model called chamber DWARF. In broad terms it seems to consist of preprocessing code for the DWARF box model, along with postprocessing for analysis, facilitating evaluation and planning of further simulations. According to authors the novelty lies in that it enables direct comparison between a chamber simulation and a chemical and aerosol scheme of a three-dimensional regional or global model, such as are used in ESM or CTM.

In the introduction, the problem that the paper is addressing is presented in a rather high-level and ambiguous fashion. The intro leaves the reader somewhat confused about what specifically the practical problem that they set out to solve is, what other solutions (or possibly failed attempts) there exist already and how (in broad terms) they will address the problem. I suppose this is unintentional because the authors know their particular problem and methods so well, but a reader with some knowledge and expertise in chemical modelling should be able to grasp the motivation to the work by the end of the introduction. The paper would benefit from more clear description of what new applications or features their model brings in the pool of so many existing aerosol and chemistry box models – of which only a fraction were referenced in the introduction.

The paper evaluates the model by simulating chamber experiments in three different chambers and setups. The two first examples are rather simple experiments, which show that the model is able to apply a kinetic chemistry system, whereas the third experiment couples the chemistry with aerosol dynamics and multiphase chemistry, again demonstrating that the model can apply chemistry, and the uptake of inorganic and organic compounds to aerosols, including the wall losses for gases and particles. Even if some of the simulated results did not agree with observations, this is most likely because of the underlying MESSy modules, or parameters regarding the volatility. However, the paper does not discuss, whether the user can do anything about these – how married is the chamber DWARF to the current chemistry systems, and if it is not, how flexible is it? For example, could the full MCM be used, even if it is not applicable in a three dimensional model environment, but at least to evaluate the lumped chemistry. This, I imagine, would be one of the main use of such a model – improve the lumped chemistry schemes to eventually improve large scale models?

I suggest that the text be edited so that the titles of the numbered sections better described the contents of that section. Also, there needs to be more emphasis on the description of the model processes and how the model is used in practice. Is a user manual available? A model description paper should be written in a way that the reader has at least a general idea of the necessary and optional input data and parameters needed to run the model (without relying solely on the supplementary material). Instead the text contains a lot of self-evident statements, such as " *all data required to constrain the simulation must be read by the model*" or rather strange statements in the context of numerical modelling such as "*The SCALC submodel enables the execution of mathematical operations on data for each simulation time step*".

All this said, I think the style of the writing is still quite pleasant to read, does not fall into jargon, even if the text could do with a more concise and specific expressions. Some of my comments likely stem from unclear or high-level description of the matter; please consider it as a sign that improvement is necessary. With further editing and addressing the specific comments, this paper could be considered to be published in GMD.

Specific comments:

Section 2, "Model description"

This section is not a model description. It describes a standard way to setup and control a Fortran program with namelist files, and mentions in generic way of preprocessing scripts that aid the user in writing the namelists and collecting input data to a format for the DWARF model. The text is so generic that it feels more like an introduction to a user manual. I suggest the authors expand this section by combining and rearranging with section 3.

Line 35: Introduction lists a few box models which are written in other languages than Fortran, and from this seems to imply that (usable or practical) Fortran models would not exist, and that these would not be included in three dimensional models. I suggest the authors find and discuss models which are written in Fortran, as there are plenty; most notably the Kinetic PreProcessor (KPP, gas phase chemistry) – which is used in regional three

dimensional models (such as WRF), but others exist, some even with similar functionality that is presented in this paper.

Lines 44-45: It is unclear, what processes are meant here. A box model is zero-dimensional by design, and when applied in a three (or other) dimensional model the mixing, transport, losses etc. are handled by other, external modules. I suggest authors clarify, why in practice a box model would not be applicable as a chemistry (or aerosol) solver in a gridded environment. These details might become more clear later in the paper, but at this point the reader would benefit from clarity in describing the problem and the novelty the proposed model offers.

Line 47: Consider adding a sentence or two briefly describing what MESSy framework is, to carry the reader deeper into the topic (or possibly rearranging some text in this paragraph).

Line 52: The text mentions “numerous studies and publications” bur offers no references; the references are model description papers.

Lines 58-59: I hope there will be an explanation how the MESSy DWARF transfers a detailed chemistry to lumped, or is this just applying a lumped chemistry in the chamber?

Line 61: Minor detail, “Table“ should not be abbreviated (see GMD guidelines). This form appears also later in the text.

Line 73: Consider rearranging the sentence to make it more fluent.

Line 98: Text mentions the possibility of modelling experiments that “manifest nucleation”, but the nucleation mechanism of the model is not described at all.

Line 119-120: Please specify clearly what is meant by “They are kept constant at the observed value during the integration” – is ‘integration’ the ‘time step’ mentioned earlier (Line 114) or the total simulation? For example temperature can (and it should be able to) vary during a simulation, so it does not have to be *constant*.

Line 130-131: Similar comment to previous: please, be very specific what you mean by ‘constant values’.

Line 137: Please specify how the actual light spectrum in the SAPHIR-chamber compares with MCM-clear sky, or is spectral actinic flux data (and corresponding parameters, perhaps from MCM) used to calculate the J-values. Based on Eq. 1, the function is not wavelength-dependent, and therefore would assume a fixed spectrum.

Line 157: The text says SMPS (or similar) measurements are used to constrain (or intialize?) the model, and continues “ the standard deviation of the log-normal distribution (σ), and the mean diameter determined from the number size distribution are prescribed”. Please specify how you arrive to the parameters of the log-normal distribution, is the fitting done in the pre-processing step, or during simulation? Also, is a single mode assumed in the fitting? At this point, the reader who is not familiar with DWARF, does not know what kind of aerosol model it has – sectional or modal, which makes this part of the text both confusing and irrelevant.

Line 161: SMPS measures dry diameter, however the LWC depends on the particle composition. It would be good to mention the assumptions made (or perhaps additional information) to derive the wet particle volumes from SMPS.

Fig 3. X-axis says hours, but apparently shows month-day-hrs. I suggest for ease of use, changing to hours (starting from zero).

Lines 223→ Section “Multi-phase kinetic… “ briefly describes the gas phase chemistry scheme. Is the model restricted to these reactions, and how easy it is to add new reactions. Maybe this would not make sense if the aim is to have exactly the same chemical description as in a large scale 3-D model, but in that case, what is the point of this model except for simulating the simplest systems? For example, is the chemistry scheme able to simulate autoxidation reactions of VOCs, which can account for more than half of aerosol yields?

Line 241: Is the wall loss of soluble components based on water content of the wall?

Line 267: Minor detail – reader would perhaps like to know if other methods (or user input) for estimating Henry’s constant can be used.

Line 278: Consider adding that Eq. 7 (and later 11) is based on Hatch-Choate conversion equations.

Line 278-281: This partly answers my earlier comment regarding line 157; consider rearranging this information so that this part becomes clear when it is first discussed.

Line 282, Eq. (7) (and later Eq. 11). Very minor detail: Although in this particular equation it is of no consequence, I would always like to see either $\log_{10}$ or ln in equations to make them unambiguous. Here, with ln(), the equation would simplify further.

Lines 337-339: Eqs. 15 and 16 and following text, for reproducibility of science, please explain $C_{org[i]}$, C_{OA} and i. Also, in "..ratios are averages weighted by the concentrations of each organic species.." for clarity, specify mass or molar concentrations.

Line 355: Why does the user have to select the precursor class – can't the model automatically select the correct class? If the question is silly, clarify the text.

Line 365: Can the $k_{f,wall}$ and $k_{b,wall}$ be measured? Previously many factors affecting the loss rate was mentioned, such as turbilence, bag material, A/V ratio of the chamber – how are these in practice taken into account in the model; or if it is up to user to account for them, how?

Line 381–387: Minor detail: This part of the text – which was properly referenced – is nearly verbatim that of Novelli et al. 2018. Please consider making it more clear in the text if larger parts are "adapted [nearly as such] from A.B. et al. xxxx for the benefit of the reader", or something of similar effect. Alternatively, use direct quotation and […] for omitted parts, if necessary. Ultimately the form of the citation should follow the practices of GMD.

Line 383: Consider expressing the H_2O concentration also in (approximate) RH.

Line 400: Interestingly, the slope of OH increases are also higher in the measurements – could this be linked to HO2 discrepancy? Could the MOM-scheme slightly under-estimate the production of OH and HO2 from the down-the-line reactions of MBO oxidation products?

Line 414: Despite the scatter in measured NO, consider adding it along with modelled concentrations.

Line 421-431: In addition to the discussed error sources, discuss the impact of omitted wall losses/emissions in the model. Isn't it safe to assume *some* NO_X emission from the Teflon walls, which would further reduce the necessary initial H_2O_2 in the model and/or photolysis rates? How plausible is an error of this scale in the estimated initial [H2O2], vs. a tired UV lamp.
What exactly is meant by: "*... the calculation of the introduced H2O2 may not be fully transferable between different studies and chambers*". Surely the reported concentrations in a given study are the best estimations (if not perfect) for that study only, what kind of transferability would there be? Please clarify.

Line 470: "The slightly higher prediction…" remove "slightly" (replace with a percentage if you want to quantify how slight).

Line 471-474: "*...attributed to the production of more highly soluble species under lower NOx*" needs editing. Is the model overestimating the solubility, or concentrations of soluble compounds? Can LWC on the walls explain the discrepancy between model and measurement (this goes back to my earlier comment on Line 241).

Line 485: "*...larger Henry's law coefficients (smaller volatility)...*" The model estimates the gas-particle partitioning with parameters that combine solubility and volatility (on average), but I would not equate the two in this way.

Figure 9 and the discussion of it: As GMD is primarily focused on model description, the reader might be interested how reactivity analysis such as this is done in the proposed model – if the model offers some tools for it in addition to the concentrations, rates and stoichiometry?

Line 543: "*The model matched the observed organic aerosol mass concentrations...*" except in low NOx conditions. Note, I am not saying the DWARF model is to blame, it is most likely the MOM chemistry or the simplified partitioning scheme – what goes in, eventually comes out.