

Geosci. Model Dev. Discuss., referee comment RC1
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Comment on gmd-2022-180

Anonymous Referee #1

Referee comment on "Halogen chemistry in volcanic plumes: a 1D framework based on MOCAGE 1D (version R1.18.1) preparing 3D global chemistry modelling" by Virginie Marécal et al., Geosci. Model Dev. Discuss., <https://doi.org/10.5194/gmd-2022-180-RC1>, 2022

Rev of gmd-2022-180

Marecal et al., MOCAGE-1D (version R1.18.1) preparing 3D global chemistry modelling

First, my abject apologies for letting my review slide past the deadline. The authors deserved a more timely review than I provided. I began several weeks ago, reading from the beginning, and making typical, small-correction notes for the authors to improve the manuscript's readability. Then at L326, I "hit the wall" in terms of what the model was doing. I did not know how to continue with the review when I was unsure as to the physical representation of this new model.

The intervention by the Editor Ham regarding the paper's suitability pushed me to quickly finish this review so that it may still be useful. I would like to see this work published, but it does need some more clarity for the science, and documentation of the model as noted by the Editor.

First, this appears to be a 0-D box-in-box model since there is no interaction in the vertical? Is there not interaction between the overhead plume and the photolysis rates? There appears to be no other 1D connection.

Second, from the three bullets (L344-349) it is not clear that any chemistry is calculated within the P box. I presume it is – Yes it is so stated in Figure 1.

Third, is the plume constantly injected over multiple time steps? That would seem odd as the upper layers are moving across the volcano, not hovering. From Figure 1, the P-box stays exactly over the emission plume for the whole time of the eruption. That makes no sense given normal atmospheric winds.

at time T1 you have a volcanic plume (size = P-box) going into the M-box, OK

at time T2, you have done chemistry on both boxes and then mixed at some rate

in your step 3 (not T3) you state that you mix unidirectionally from P-box to M-box, does not the P-box shrink? but then in step 4, you mix M-box air back into P-box. OK

but at step 5 you add more fresh volcanic emissions to the P-box does that not include new air mass?

does the P-to-M mixing rate control the rate of new emission flux into P-box?

This model implies that the outflow of chemically processed P-box air keeps going into the same M-box air. Possible, but sounds difficult. If so, then the original P-box should become more dilute.

Fourth, the mixing between P box and M-P box should be based on a mixing frequency defined by the inverse time to mix the P box (e.g., 4 /hour for 15min). Presumably you conserve air mass and mix equal parts air mass of the M-P and P boxes and then put it back into both boxes? I cannot tell if that was done. YES, after reading the Fig 1 caption, it is clear stated. You need to be more precise in the sentences describing this in the text and not rely on the Figure caption.

Fifth, you should really show that your results converge as you reduce the time step. That shows you are reasonably modeling a continuous process. That is why mixing rates need to be in per hour.

Basically the model looks sort like a smokestack model, but even there the exhaust is constantly encountering new background (M-box) air. Putting emissions of trace gases into the P-box is maybe convenient, but in reality these emissions come with an air mass that must be incorporated into the P-box. Is this the way you would model a standard smokestack plume?

So, overall, I am not sure what kind of plume you are modeling. The physics of injection and mixing seem not to be realistic for volcanic plumes. I am readily willing to be convinced otherwise if the authors can make a clear case.

Comments below may be helpful for language use when revising this paper.

Title: awkward, try maybe: Halogen chemistry in volcanic plumes: a 1D framework based

on MOCAGE-1D (version R1.18.1) preparing 3D global chemistry modelling

L20 – maybe "a 1-D **single-column** configuration...."

L28 – how about also to the background atmospheric conditions?

Abstract – Overall, it is too long, can you shorten?

L42 – Iodine clearly eats O₃, does CL do much in the troposphere? (not sure)

L104 – 'no possibility' is too strong, how about 'no direct way to '

L122 – I am confused, a 1D single-column model really has not horizontal resolution, yet here you talk about it grid size and a sub-grid parameterization.

L123 – 'also' not needed.

L135 – Make its shorter and easier to see the 3 things:

There are three reasons behind the choice of this volcanic eruption: (1) Mount Etna is one of the largest known emission sources of halogens (Aiuppa et al., 2005); (2) the Etna volcano is also continuously and extensively monitored by INGV (Istituto Nazionale di Geofisica e Vulcanologia) including gas composition needed for the model; and (3) satellite observations above the Mediterranean region are available.

L146 – 'passive' = 'non-eruptive'

L150 – "The composition of Mount Etna plumes has extensively been characterised before this case study by both in situ (e.g.,....

L152 – drop the "as"

L153- 'location' instead of 'space' ??

L155 – ' ... more distal, safe locations, are...'

L158 – 'such' instead of 'similar'

L161 – eruptions are available, and none for 10 May

L169 – I would drop the clause: 'being representative of Etna emissions'

L176 - 'al., 2021). MOCAGE is developed"

L177 – drop ' Due to the low computational cost', just say simply that: "This 1-D configuration of MOCAGE allows us to make a large set of sensitivity tests on the..."

L179 – very confusing ("It does not..."), do you mean: "MOCAGE 1D does not focus on the very early stages.... " then stop and delete "but to" this is already said or implied.

L182 – "corresponds here to the vertical column" I do not agree with this. You need to make it clear that the 1-D column model does not connect across vertical layer with transport or photolysis (? does it). It starts as a 1-D column, but the layers shear out as separate as they would in 3D. Right? OK OK, I see this in L187, so maybe combine this information.

L190 – the problem is the entrainment mixing on the way up. You should consider doing LES models or other models to find the entrainment factor as a function of altitude

L195 – do not keep mentioning 'future' – "The 1-D configuration of MOCAGE is designed so that the chemistry model developed for volcanic emissions can be seamlessly inserted into MOCAGE-3D.

L201 – " MOCAGE-1D start with those in MOCAGE-3D,

L233 – I am looking forward to a plot of chemistry vs time showing this Br explosion

L245-256 – All this makes sense and seems logical.

L255 – 'of volcanically derived sulphate' The volcano emits sulphate or SO₂? if both (below) then make this clear

L262 – "The RELATIVE TRACE GAS composition in the plume is ...Table 1.

[What is unclear here is the absolute concentration in the plume at each level?]

L266 – the high temperature (magma?) chemistry should be already taken into account in Table 1.

L276 – 'given in Table 2' – this really needs to be combined with Table 1.

L302 "THAT PARTICULAR eruption..."

L307 – the aerosol mass, diam and surface area should be in Table 1+2. Do not scatter critical input parameters.

L321 – (resp. 'D.BGD)' (spelling)