

Interactive comment on “Global Simulation of Semivolatile Organic Compounds – Development and Evaluation of the MESSy Submodel SVOC (v1.0)” by Mega Octaviani et al.

Anonymous Referee #1

Received and published: 8 April 2019

General Comments:

This paper addresses the modeling of atmospheric PAH transport and chemistry/physics, which is certainly within the scope of GMD. It addresses some important processes for PAHs which have been, to the best of my knowledge, previously unresolved in models of its kind. This model built into the MESSy framework is a substantial contribution to the modeling of PAHs in the atmosphere. The methods are clearly outlined, and important assumptions are explicitly tested and discussed, leading to a reproducible work. The authors have given due emphasis to the existing literature, and their own contribution is clearly documented. The overall presentation of the paper

C1

is good, including language, adherence to title and abstract requirements, and formulae. The supporting information is very strong, but the code corresponding to the work appears to be not immediately accessible.

Specific comments:

L194: Soil density is a parameter of the capacity for PAH uptake. Is this density spatially specified? What is the origin of the value used (spatial database, land model or otherwise)?

L201: Similarly to above, is the fraction of organic carbon in soil spatially varying? What is its origin?

L215-220: Some clarifying statements on the application of volatilization from vegetation are warranted. Particularly, it is not clear to me how this CV is applied. Is the CV at 7 days after application used to calculate a timescale for complete revolatilization? i.e. to fit an exponential return to the atmosphere for deposited PAHs. Or is the fraction not volatilized after 7 days assumed to be permanently deposited? Also, is a single CV applied to all plant types?

L255: The ocean is treated with comparatively little detail. Some discussion of how this could impact the strong bias of the model compared to measurements over the oceans would be informative. (Currently it is simply listed as a possible contributor to the bias)

L289-291: With a second-order representation, a higher value of kOH only suggests OH as the dominant loss pathway if concentrations of all three oxidants are equal. The concentration of OH would be expected to be much lower than the concentration of ozone, however.

L314-316: The assumption of the rate doubling every 10 degrees is presented without reference. An explanation of the rationale behind this number should be included here.

L332: Why are gaseous reactions switched off for BaP?

C2

L434-436: This output was selected as the single output for analysis, but other quantities could be analyzed using the same model experiments. Were any others investigated, and if so do they show similar behavior? I.e. are the factors affecting total PAH concentration representative of the factors affecting other outputs?

L626-630: The CoV is compared between observations and model output. But the observations may not be representative of the same time-variations as the model. From the screening flowchart (Figure S3), it seems likely that many stations' "monthly" observations represent less than a full month's integration. This should make their monthly values more sensitive to synoptic-scale variations than their model counterparts, and much more sensitive to local-scale phenomena (e.g. convective precipitation and subsequent wet removal).

L775-776: Does the underestimate follow the same pattern as SOA concentration? The omission of SOA in the model should be mentioned in the methods section.

Technical corrections:

L417: I believe this should read: "Two options for this factor were tested:"

L435: The word "selected" is repeated.

L453-454: I believe that point (2) should be reworded. "... physically interpret." would be better than "... physically justify." if I understand correctly.

L462: "are higher" should read "being higher" at the start of this line.

L597: "On the contrary," should read "In contrast,"

L618: "occur in the gas..." should be "occurring in the gas..."

L645: "in a qualitative agreement" -> "in qualitative agreement"

L714: "ocean shipping and do" -> "ocean shipping and does"

L715: "potential origins" -> "potential point of origin"

C3

Interactive comment on Geosci. Model Dev. Discuss., <https://doi.org/10.5194/gmd-2019-19>, 2019.

C4