Atmospheric Chemistry and Physics Discussions

Interactive comment on "Assessment of high to low frequency variations of isoprene emission rates using a neural network approach" *by* C. Boissard et al.

Anonymous Referee #1

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General comments

The emission of biogenic volatile organic compounds, hereafter referred to as BVOC, is well accepted as a dominant factor in atmospheric chemistry and physics. Despite this wide acceptance we still face significant gaps in our knowledge of emission budgets and emission regulation. We need more data on emission qualities and quantities which can only be gained by experimental work providing support to develop better modelling to describe the complex regulation and dependencies. Simple models relying on light and temperature sometimes describe astonishing well emission processes without taking into account any further environmental, ecophysiological or biochemical

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factors. However, it is well documented that complex interactions with these factors increase the uncertainties of all modelling and upscaling exercises. The authors developed a neural network approach in order to assess the low frequency, i.e. long-term, regulation of isoprene and monoterpene emissions by plants.

This work is important and contributes to a better understanding of the relations between the environment and the biological emission source. It also provides a nice overview on field studies indicating and partly demonstrating the potential role of long-term acting factors on BVOC emission. Therefore, the study principally deserves publication in ACP. However, there are some gaps and misinterpretations of the general background and of cited papers as well as. Some major corrections may improve the quality of the paper.

Specific comments

1) Chapter 2: There are a few things to be rewritten. This is not a review but it should contain some more references. Especially seasonality of monoterpene emissions might be stressed a little bit better. There are recent papers which contribute quite significantly to this topic. Seasonal development of light driven emissions from European beech has been reported by Holzke et al. (2006). Seasonal behaviour of Quercus ilex emissions is excellently reported by Ciccioli et al (2001; Ciccioli, P., Brancaleoni, E., Frattoni, M., Brachetti, A., Marta, S., Loreto, F., Seufert, G., Vitello, M., Tirone, G., Manca, G. and Valentini, R. (2001). "Daily and seasonal variations of monoterpene emissions from an evergreen oak (Quercus ilex L.) forest of southern Europe." Eighth European Symposium on the Physico-Chemical Behaviour of Atmospheric Pollutants" was "A Changing Atmosphere". Torino, Italy, from 17th to 20th September, 2001; http://ies.jrc.cec.eu.int/Units/cc/events/torino2001/torinocd/Documents/Terrestrial/TO4.htm. The seasonality of monoterpene emissions from the evergreen species Quercus ilex L. was investigated through laboratory and field experiments. A strong seasonality in the basal emission was observed. The original version of the G93 algorithm was modified to account for seasonality effects. A modified version of the CANOAK model

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was developed for predicting the seasonality of monoterpene emissions and that of the reduced carbon losses in relation to gross carbon assimilation (GPP). The results seems to indicate that present estimates on the fraction of the GPP allocated to isoprenoid emission must be revised since they are one order of magnitude higher than what was measured before.

2) On page 12421, lines 13-16, the authors mention seasonality in tropical and sub-tropical regions to vary with a much lower magnitude than in temperate regions. That is true, if we regard the forest as a whole. However, there are significant dynamic changes in emissions and emission quality if we go to the tree species level. Some trees even shed their leaves completely and develop new ones when first rain falls. Others obviously increase their emission rates. See Kuhn et al. (2004). We should not make it too easy for us in dealing with the complete forest and ignoring processes within the forest which may cancel out each other. Is it reasonable to describe seasonal adaptation of trees by leaf shedding during the dry season (best guess: 30% of tropical trees) using low frequency environmental data? Changes in emissions are secondary effects in this case. This should at least be discussed.

3) A few lines later, line 22-23, the authors discuss limonene and trans-ß-ocimene emissions from a pine tree in dominating in winter and summer, respectively. It might be a help for the reader to know whether that this is the effect of two different features. The Ocimene was exclusively emitted during sunlit hours in the main vegetation period, whereas limonene (and others) was emitted day and night and throughout the seasons. The results demonstrate that different terpene emission sources in P. pinea foliage exist.

4) The effects of drought are shortly discussed at the end of the introduction. We have to take into account that there are short term and long term effects. The long term drought may lead to a decrease of isoprene emission as nicely reported by Staudt et al 2002.

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5) I like the discussion around soil quality and activity on the emission of VOCs (page 12433/12434). Taking such influences into account would help to make a step forward.

6) How do the results and conclusion hold, if the more reactive species are included? The authors conclude that their neural network does not work as good for monoterpenes as for isoprene. How can they explain this difference? Isoprene and monoterpenes are both synthesized within the plant chloroplast and underlie the same regulation. I was surprised to see this result. However, Simon et al. (2005) demonstrated a convincing modelling by a neural network for isoprene as well as for monoterpenes. The closer the modelling was related to plant physiological parameters, the better was the correlation of modelled with measured emission. I guess Boissard and co-workers know that paper though they did not cite it. The model application to monoterpenes is described quite shortly and the whole procedure remains unclear (network architecture, parameter selection, training). Furthermore the model performs poorly which has to be addressed in more detail since the overall approach should work in principle also with other BVOCs. Therefore, alternatively, I recommend to take the monoterpene part completely out of the paper and to focus on isoprene including a more detailed description of the emission database

7) I agree with the authors that the processes underlying sesquiterpene emission are much more complex compared to the emissions of isoprene and monoterpenes because these compounds are synthesized via different pathways and located in different subcellular components. Furthermore, they have clearly dedicated functions as signalling compounds for example. However, I do not tend to agree with the authors that the monoterpene pathway in plants is more complex compared to the isoprene pathway (Page 12436, line13-17). Some monoterpenes are also produced for such a function but most of them underlie the same regulation steps as those for isoprene.

8) The terms „low" and „high frequency" variations are a bit misleading i.e. to physical in my opinion since the biogenic VOC emissions are primarily regulated by biological processes that respond to short and long term acting

environmental factors (as described at P12419 L14-16)

9) In my opinion, the paragraph on biochemical regulation at the end of section 2 points to the clue of a better understanding of the short and long term variability of BVOC emission and should therefore be moved to the beginning of the introduction.

10) The isoprene emission database provides a nice and, although it is far from being complete, comprehensive overview on isoprene emissions by plants which deserves to be published. I suggest to provide additional information in table 2 (species, emitter type etc and especially the standard emission factor according to G93) and to simultaneously remove redundant information from table one. Just as an idea, it would be nice to have the complete dataset including the micrometeorological driving data available on a web site for extension and future model applications also by alternative approaches.

11) I suggest modifying the outline of the study. The literature review should be moved to the introduction section. The result section is very short compared to the first part and Section 4.2 (the section title “Development of ISO_DB ..” is probably wrong) belongs to the methods section. However, since the isoprene database represents a useful result and outcome of the paper (see above), it should be moved to the beginning of the result section. In my opinion, there is no need for an appendix. Appendix A can be represented as a figure with caption, and Appendix B and C can be easily represented as tables within the text.

12) I do not agree with the interpretation of some of the results of the sensitivity analysis. It must be clarified that the observed sensitivities to input parameters do not necessarily reflect direct relationships (see e.g. P18 discussion on STL1u). In the presented approach, this is a general problem of multi-linear regression methods because most of the input parameters (see Appendix B) are not linearly independent which violates the mathematically assumptions. However the neural technique may serve as a good tool to address the “proportion of the emission intensity that is not yet

parameterised” (see 2nd paragraph in section 3.1) as a black box model. Beside that, as a further result, it would be nice to have a further visualization of the trained network parameterization e.g. by showing the inferred relationship between the predicted relative emission in relation to the full observed range of each single input parameter, while all other parameters are held constant at the mean observed value.

13) The procedure of data processing is not completely clear (section 3.4). If the authors really use different units for the same parameter, it would make much more sense, in my opinion, to first convert the input data from different data sets into the same units before normalization. Furthermore, concerning the output parameter (i.e. the BVOC emission), I miss (at least) a discussion of using mass based emission rates but not using emissions rates based on leaf area. The results might differ substantially.

14) The notation of mathematical symbols is often unclear. The use of matrices, vectors and scalars must be clarified.

15) Abbreviations are used too excessively. I recommend removing all abbreviations from the abstract

16) Abstract: Suggestion: remove paragraph on Ulex e. (confusing)

17) P12418 L22: Suggestion: remove abbreviation CTMs (single use)

18) P12418 L26: Suggestion: remove abbreviation for VOC (single use)

19) P12419 L12-16: Suggestion: Change to “These parameterisations are base on photosynthetic active radiation and leaf temperature and account for relatively short term (minutes to hours) physiological adaptations.”

20) P12419 L27 The presented approach is not new. Simon et al. (2005), Plant, Cell and Environment 28, 287-301, presented a back propagation neural network approach applied to tropical species (data from Kuhn et al. 2002,2004),

21) P12420 L11-14 Suggestion to remove “This section [..] observed variabil-

ity.”

22) P12420 L19 – P12421 L1 the paragraph “Both studies …conditions” is unclear and confusing

23) P12421 L13 Suggestion: replace “between springtime and summertime” by “early summertime”

24) P12422 L17-18 Suggestion: remove “suggesting some complex unexplained regulation processes”

25) P12422 L19 Suggestion: remove “Some rather simple environmental indicators such as”

26) P12423 L2 Definition of ETS unclear (˜ 400 days $>$ 5degree ?)

27) P12424 L12-16 Suggestion: remove beginning of Section 3.1

28) P12426 L2-6 Suggestion: remove first paragraph “The neural network …. Further “; I also suggest rewriting the following paragraph introducing the notations. What is the bias?

29) Eq. (3) “For this study, E was” This is a general equation representing the first order derivative of Eq (2). Minimization in the training phase gives network improvement

30) Section 3.3 Enumerations are too long.

31) P12428 L2-3 “No canopy flux data … phenomenon” This is not an argument for excluding these parameters. It just confuses the reader because the overtraining effect has not been explained before. I suggest removing this remark

32) P12428 L8-9 Suggestion: remove “…, much larger than .. methods.”

33) P12428 L15-16 Suggestion: remove “, although these .. 25 min-

utes:”. Parameter integration time should be provided in overview table (see above). What is the integration time of the emission data?

34) P12428 L23-26 Suggestion: remove “Some of them… variations …(see review section).” (Repetition)

35) P12429 L1-3: What about soil humidity reflecting potential effects of drought stress?

36) P12429 L12-16: There is meteorological data available from a nearby tower (see Andreae et al. 2002, Biogeochemical cycling of carbon, water, energy, trace gases and aerosols in Amazonia: The LBA-EUSTACH experiments, JGR 107 (D20), 33.1-25).

37) P12429 L20-22: How has the position in the canopy been derived? This information should be available in the overview table (see above)

38) Section 4.1. Here I miss a comparison of the network approach using temperature and light as input with the Guenther et al. 93 standard algorithm

39) P12432 L4-6 “.. with MSE_validation” values higher than MSE_training ..” Isn’t that the normal case? Usually, the network performs better on the training set because it has been trained on it. However, when the network has been trained too much (i.e. too many iterations) the MSE_validation increases while the MSE_training still decreases. What is the stop criterion of the algorithm?

40) P12434 L6 Replace “the isoprene emission rate” by “the predicted isoprene emission rate”

41) P12434 L15-16 Replace “weight on isoprene emission regulation” by “weight on predicted isoprene emission”

42) P12435 L4-11 Suggestion: remove “Using … rates.” (Repetition of the abstract). Conclusions?

43) P12435 L9-14: Suggestion: replace by "A maximum of 60% of the observed isoprene emission variability could be explained by air temperature and light".

44) P12439 L7 "soil water contents in fraction (0-1)" I guess fraction of volume?

45) Acknowledgements: Check spelling of J. "Kesselmeieir"

46) Appendix C / Figure2: It would be useful to change the notation of the weights by indicating the connection type for example x_i, n_j, and y_k are connected by the two weights $w_{(i,j)}$ and $w_{(j,k)}$

47) Table 3: Could be removed since the relevant information is already described in the text

48) Figure 4 could be larger. These are the most important and impressing results of the study

49) Page 12423, line 18: It should read Fischbach not Fishbach.

50) Page 12429, line3: It should read "Except" instead of "Expect".

Interactive comment on Atmos. Chem. Phys. Discuss., 7, 12417, 2007.

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