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Comment on bg-2021-189

Anonymous Referee #1

Referee comment on "Improved prediction of dimethyl sulfide (DMS) distributions in the northeast subarctic Pacific using machine-learning algorithms" by Brandon J. McNabb and Philippe D. Tortell, Biogeosciences Discuss., <https://doi.org/10.5194/bg-2021-189-RC1>, 2021

Review of "Improved Prediction of Dimethyl Sulfide (DMS) Distributions in the NE Subarctic Pacific using Machine Learning Algorithms" by Brandon J. McNabb and Philippe D. Tortell

General comments

This study applied two different machine learning techniques to estimate the distribution patterns of the climate-active gas DMS in the Northeast subarctic Pacific (NESAP) during the summer, and their relationship with several environmental variables. Given the current large uncertainty in the estimation of DMS emission at large scales, application of these novel statistical techniques to improve their accuracy is very welcome. Although these algorithms do not provide mechanistic understanding per se, their application can help identify previously unrecognized patterns.

I was particularly glad to find that the authors evaluated the optimal spatial scale for the ML predictions. However, and this is my first criticism, they did not perform a similar evaluation for the temporal resolution of the data, and used only monthly-binned DMS datasets. My questions: How compatible is binning to monthly resolution with the claim that your ML methods can resolve DMS concentration at the mesoscale? I.e., is this temporal resolution sufficient? Changes in DMS cycling regimes often match the timescales of meteorological forcing, i.e. days to weeks (Royer et al., 2016), and several meteorological re-analysis products are readily available as inputs for the analysis of the optimal temporal scales of the ML models.

My second general criticism concerns the comparison between the ML models and previous DMS algorithms based on simpler traditional statistics. Such comparison would be useful to readers if conducted differently, but in its present form it is too shallow, and

its sole purpose seems to be highlighting the better performance of the ML models (which one can take for granted, as shown by abundant recent literature on the subject). In my view, each approach has its pros and cons, and both of them should be included in a fair evaluation. First, in my view the predictive power of the different approaches should be compared at the same spatiotemporal scale. Second, the regional tuning of the global algorithms shown in Fig. 2 should be described more in depth somewhere, not just referring to Table 5 of Herr et al. (2019). Tuning each of the previous algorithms for a particular region is a complicate task in itself. Table 5 shown in Herr et al. 2019 made evident that the tuning they applied was not always effectively improving the algorithms: it improved some skill metrics (e.g., correlation) at the expense of other (e.g., RMSE degraded notoriously in many cases). Third, it would also be interesting to learn why regionally tuned algorithms that explained nearly 10% (VS07) or 7% of the DMS variance in the NESAP now appear to explain less than 1%. I do not think that the datasets used by Herr et al. (2019) and this paper are that different... is the difference only due to the finer resolution used in the present study?

My third general criticism concerns the way regionally aggregated emissions are reported (Table 2; line 20 in the abstract; lines 258–263 in the Results). First, it is incorrect to call “annual sulfur emissions” what actually are summertime emissions. Second, the total regional summertime emissions cannot be the mean of the three individual months (0.3 Tg S) but their addition. Only in this way the range reported in the abstract, 0.5–2 Tg S (pear year? Per summer?) can be compatible with the monthly emissions reported in Table 2. Finally, the authors must explain how they obtained the uncertainty range of 0.5–2 Tg S pear year (but, do they refer to summer only or the whole year?) given in the abstract and in line 158.

Finally, I prompt the authors to improve the Discussion. I provided some ideas in the specific comments in the hope that they will be useful.

Specific comments

Introduction

L25-26: a more up-to-date reference would be good here.

L29: DMS does not seem to be an essential substrate for most pelagic prokaryotes, but for rather specialized methylotrophic taxa, as suggested by Vila-Costa et al. 2006. Most taxa do not seem to use it as a carbon source, and the enzymes that degrade it might be quite unspecific. Please rephrase with additional supporting references. Suggestions:

- Schäfer, Hendrik, Natalia Myronova, and Rich Boden. "Microbial degradation of dimethylsulphide and related C1-sulphur compounds: organisms and pathways controlling fluxes of sulphur in the biosphere." *Journal of experimental botany* 61.2 (2010): 315-334.
- Green, David H., et al. "Coupling of dimethylsulfide oxidation to biomass production by a marine flavobacterium." *Applied and environmental microbiology* 77.9 (2011): 3137-3140.
- Hatton, Angela D., et al. "Metabolism of DMSP, DMS and DMSO by the cultivable bacterial community associated with the DMSP-producing dinoflagellate *Scrippsiella trochoidea*." *Biogeochemistry* 110.1 (2012): 131-146.
- Lidbury, Ian, et al. "A mechanism for bacterial transformation of dimethylsulfide to dimethylsulfoxide: a missing link in the marine organic sulfur cycle." *Environmental microbiology* 18.8 (2016): 2754-2766.

L75-78: I missed here references to 2 important studies in the NESAP:

- Royer, Sarah-Jeanne, et al. "Microbial dimethylsulfoniopropionate (DMSP) dynamics along a natural iron gradient in the northeast subarctic Pacific." *Limnology and oceanography* 55.4 (2010): 1614-1626.
 - Steiner, Nadja S., et al. "Evaluating DMS measurements and model results in the Northeast subarctic Pacific from 1996–2010." *Biogeochemistry* 110.1 (2012): 269-285.
- These studies suggested an important role for phytoplankton community species composition (prymnesiophytes, dinoflagellates) and higher bacterial DMS yields from dissolved DMSP in Fe-poor offshore NESAP waters.

Methods

L103: Please specify NASA reprocessing (e.g., R2018).

L103: the resolution looks wrong. I am not aware of any NASA product with 0.036 degrees resolution. The 1/24th degree resolution probably used here corresponds to ~0.042 degrees.

L137-138: A short discussion of this finding might be useful for future studies.

Figure 1: please use the same left and right y-axes in both panels.

Results

L208-209: R2 reported twice, the range given in L208 suffices.

L226: I understood from the Methods that the ML models were used to estimate sea-surface DMS concentration, not sea-air fluxes directly. This would make more sense because sea-air fluxes are derived from a known parameterization. Therefore, is the sentence "the models showed lower predictive power for sea-air DMS fluxes at coarser resolution (Fig. 1)" accurate?

Figure 3: if DMS is arcsinh-transformed, the nM units no longer make sense. Either modify the axes to show actual DMS concentrations, or remove the nM units. In the latter case, it would be useful for the readers to know the range of DMS shown in the scatterplots.

L258-263: see general comment about the regional emissions.

L261: How was this range obtained? It seems that the actual range resulting from the combination of regional and global uncertainty ranges should be larger, assuming their errors are uncorrelated. For example, 0.5/28 gives a minimum of ca. 2%, 2/15 gives a maximum of 13%...

L303: why the central Alaska gyre, and not other subregions within the NESAP?

L318-322: correlations between DMS and other variables that can be directly observed (SST, SSHA) are not comparable to those between DMS and variables output by empirical or prognostic models, such as NPP (VGPM) or NCP. This should be mentioned, as the skill of that latter models is quite limited in some regions.

L327: Royer et al. 2010 L&O, too.

Discussion

L352-355: The sulfur overflow hypothesis may describe sulfur metabolism in species with high intracellular DMSP concentration and where DMSP is the main sulfur osmolyte. This hypothesis may not be relevant for species with low intracellular DMSP that produce other sulfur metabolites in similar or higher quantities, e.g. DHPS (Durham et al., 2015). Might this be the case for the northern part of the Alaska gyre?

- Durham, Bryndan P., et al. "Cryptic carbon and sulfur cycling between surface ocean plankton." *Proceedings of the National Academy of Sciences* 112.2 (2015): 453-457.

Moreover, total phyto biomass is, per se, a strong predictor of DMS outside the subtropical and intertropical areas, and is strongly negatively correlated to nitrate I guess... this would give a more straightforward explanation of the negative DMS-nitrate correlation found here.

L380-383: The authors mention only physiological aspects of the effects of (UV) irradiance on DMS cycling. Please consider giving a wider view that considers community-level effects, for which ample evidence exists, for example:

- Lizotte, Martine, et al. "Macroscale patterns of the biological cycling of dimethylsulfoniopropionate (DMSP) and dimethylsulfide (DMS) in the Northwest Atlantic." *Biogeochemistry* 110.1 (2012): 183-200.
- Galí, Martí, et al. "Diel patterns of oceanic dimethylsulfide (DMS) cycling: Microbial and physical drivers." *Global Biogeochemical Cycles* 27.3 (2013): 620-636.
- Vance, Tessa R., et al. "Rapid DMSP production by an Antarctic phytoplankton community exposed to natural surface irradiances in late spring." *Aquatic microbial ecology* 71.2 (2013): 117-129.

L386-387: Correlation analysis between DMS and potential predictor variables should perhaps consider the different spatiotemporal scales of variation each variable is capturing. For example, in the case of PAR, the negative correlation might arise solely from the fact that DMS peaks in August-September (as does Chl), whereas the highest PAR is in June (summer solstice). The kind of information we obtain from the DMS-PAR correlation is very different from that provided by SSHA, which informs mostly about mesoscale variability, or SSN, which reflects circulation patterns. Therefore, what the authors wrote in L377-379 possibly applies to irradiance effects as well.

L398: Please examine your argumentation more in depth and rephrase accordingly, because it is currently at odds with the reference chosen to support it. Sunda et al. 2002 found that Fe-induced oxidative stress upregulated DMSP synthesis and its cleavage to DMSP intracellularly. Note that DMSP cleavage can be catalyzed by lyases, or proceed through OH radical attack on DMSP intracellularly (i.e. in species lacking DMSP lyase; Spiese et al., 2015), followed by quick DMS release through cell membranes (Lavoie et al., 2018). In general, the work of Sunda et al. is used to explain enhanced DMS leakage out of algal cells upon oxidative stress, not enhanced DMS consumption.

- Spiese, Christopher E., et al. "Dimethylsulfide membrane permeability, cellular concentrations and implications for physiological functions in marine algae." *Journal of Plankton Research* 38.1 (2016): 41-54.
- Lavoie, Michel, et al. "Modelling dimethylsulfide diffusion in the algal external boundary layer: implications for mutualistic and signalling roles." *Environmental microbiology* 20.11 (2018): 4157-4169.

L410: cyclonic eddies in particular, with upwards doming isopycnals at their core?

L426: note that satellite PIC reflects detached coccoliths from senescent coccolithophore blooms, and may therefore be a poor predictor of DMS production during bloom initiation and eventual plateauing.

Minor corrections

L172: Spearman.