Reply on RC2
Brandon McNabb and Philippe Tortell

Author comment on "Improved Prediction of Dimethyl Sulfide (DMS) Distributions in the NE Subarctic Pacific using Machine Learning Algorithms" by Brandon McNabb and Philippe Tortell, Biogeosciences Discuss., https://doi.org/10.5194/bg-2021-189-AC2, 2021

Lines 98-100 – Did the authors check for any additional data not included in the PMEL database?

*We did not, but we are unaware of any other databases for DMS.*

Paragraph starting on line 102 – Were any of these satellite derived parameters ground-truthed against in situ data during any of the cruises?

*We did not ground-truth the satellite predictors to in-situ data, per se, since there is a temporal mismatch between the monthly resolution satellite predictors used here and in-situ data from individual cruises (prior to binning). However, several studies have previously assessed the accuracy of these predictors, and we now note in L127-128 that each likely has uncertainties associated with it.*

Lines 150-152 – The Nightingale et al. (2000) parameterization of k is not really appropriate for DMS. It is becoming more and more clear that the k wind speed-based parameterization for DMS should be linear (Blomquist et al., 2017; Bell et al., 2013; Zavarsky et al., 2018).

*Thank you for this suggestion. We have revised our calculations throughout using the Goddijn-Murphy et al. (2012) parameterization, which is both linear and validated against satellite data. Relevant changes can be found in L154-161 and L284-292, Figures 1, 4, and 5 and Table 2. This new parameterization has only a small effect on the magnitude of the sea-air flux estimates and doesn’t change the dominant spatial patterns reconstructed by the ML methods.*

Line 224 – typo, should be ANN not AAN

*Thank you, this is now corrected.*

Section 3.4 – It seems highly likely (and I believe the authors allude to this too in the discussion starting on line 388 paragraph) that the correlations found (especially with SSH) are indirect. The real driver of DMS distributions is likely nutrients and type of microbes present. If the SSH represents eddies carrying the relevant nutrients, SSH is not really a universal parameter that can be used to describe DMS distributions everywhere. It
would be good to see how that works in other regions without much eddy activity. Were phosphate and bacteria looked into? It seems that bacterial counts and types are important, but difficult to account with things like satellite data. Is it possible to compile that info from the in-situ measurements – or is that too low resolution for the techniques?

We agree that the usefulness of SSHA as a predictor requires further analysis, and current follow-up work is focusing on applying these techniques to the Southern Ocean (another DMS hotspot) where numerous studies have noted the importance of eddies to nutrient supply and productivity.

Bacteria are likely very important to DMS distributions, but in-situ data are currently too sparse (both spatially and temporally) to incorporate into these models. To our knowledge, there are also no reliable algorithms for estimating bacterial counts from satellite data. However, it may be interesting in future work to apply these machine learning techniques to bacterial counts, from which the resulting product could then be used to aid in modelling DMS.

We did initially assess phosphate as a potential predictor, but preliminary analyses found its inclusion yielded no substantial improvement in predictive accuracy.

Discussion (and Intro) – Why was this region chosen instead of one with more data coverage? Or why not try two different regions and compare findings? The area and number of data points (compared to the region that is mapped) seems small (i.e., Figure 4).

The NESAP was of interest as it is a well-known hotspot for DMS with particularly high turnover between DMS and its related compounds (see, for example, Asher et al., 2017, Herr et al. 2019, and the distributions from the Lana et al. (2011) climatology). As mentioned in L73-74, this region has benefitted from increased sampling frequency over the years with the development of novel instruments, and although the region is small, the relative proportion of data coverage to the area mapped is not unreasonable when compared to global studies using these ML techniques (ex. Roshan & DeVries, 2017). Part of the motivation for this work was also to demonstrate these models are not just limited to global scales but can be successfully applied to smaller regions and still yield good results. As mentioned above, the encouraging results found here have motivated us to apply similar analyses to the Southern Ocean.

Section 4.1 (and methods section starting on line 187) – Why don’t the two iron limitation proxies resemble each other at all? Also, the use of SSN is not really a unique identifier (e.g., effect of nutrients and photochemistry, as stated in the paragraph starting on line 388). How can this be practically handled when using SSN as a predictor? And if the relationships cannot be understood, why is it used?

The more complicated NPQ-corrected fluorescence yield ($\varphi_f$) was an early attempt to remove fluorescence associated exclusively with photoinhibition effects (i.e. excess light energy dissipated through NPQ pathways), with the assumption that the remaining fraction of the total variable fluorescence better captures the response to iron limitation from space. However, more recent work (see Westberry et al. 2019) has suggested that that the simple ratio between total variable fluorescence (including NPQ pathways) and chlorophyll can be sufficient to detect a signal physiological response from space using past iron fertilization experiments as evidence.

There are a few reasons we feel the inclusion of SSN is warranted. First, and most simply, model performance is degraded when SSN is excluded, indicating it does have an important, albeit partly obscure, role in the DMS dynamics within this region. Additionally, since these regression models use non-linear solving equations, predictors are also more
“dynamically weighted” in space/time when compared to linear regression for example, which produces a fixed coefficient for all cases. In a practical sense, this means that these models will still benefit from the inclusion of predictors such as SSN, despite our limited mechanistic understanding of the underlying relationships.