**Uncertainty document for PACE chlorophyll Fluorescence Line Height (FLH) and Net Primary Production (NPP)**

**Toby K. Westberry, Michael J. Behrenfeld, Jason R. Graff**

Our team is responsible for delivering algorithms to estimate 1) chlorophyll fluorescence via a line-height approach (nFLH, units of mW cm-2 m-1 sr-1) and 2) the rate of daily, water-column integrated net primary production (NPP, units of mg C m-2 d-1). Approaches for the two products differ due to the differences in complexity of the algorithms and are described below.

Uncertainty for PACE nFLH will follow from heritage approaches. For MODIS, Bands 13-15 (central wavelengths of 667, 678, and 748 nm) were used to calculate nFLH:

Uncertainty for this approach (nFLH) can be calculated directly using standard laws of error propagation and knowledge of the uncertainties associated with individual reflectance bands, such as those collected as part of AERONET-OC and other observations in the SeaBASS archive. This approach has been described in detail as part of the PACE Technical Report Series (Volume 6, see Appendix 5.7, McKinna and Cetinic, 2018). McKinna and Cetinic (2018) used two representative reflectance datasets (taken from Chase et al., 2017) and assumed a fixed 5% uncertainty to show that the median uncertainty on resultant nFLH was ~42%. The PACE nFLH algorithm is not yet finalized, but will still use the line-height approach, albeit with different, possibly dynamically adjusting bands:

Thus, the same approach can be used to derive pixel level uncertainties, so long as the uncertainty in discrete wavebands is characterized. The latter is required to be provided by the PACE mission. Thus, following McKinna and Cetinic (2018):

where the *Rrs* terms are uncertainties in individual reflectance bands, and the partial derivatives can be derived analytically from the definition of nFLH above.

Generating uncertainties for NPP rates is more difficult than for nFLH and cannot be easily accomplished using standard laws of error propagation. We have proposed to use multiple different approaches to best estimate NPP uncertainty. Direct, one-to-one matchups between *in situ* measured NPP and NPP estimated using the PACE algorithm will be carried out, despite a limited validation dataset (N<50). The requirement(s) for hyperspectral optical properties curtails this effort and renders most existing NPP matchup datasets (e.g., the Primary Productivity Algorithm Round Robin dataset, Saba et al., 2011) of little use because ocean color inputs are not sufficient to initiate the PACE NPP algorithm. Nevertheless, this direct approach allows calculation of typical uncertainty metrics (e.g., Bias, RMSE, MAPE, etc.) such as reported for other ocean color properties (e.g., Seegers et al., 2018). However, these are usually ‘aggregate’ uncertainty metrics and not necessarily applicable to pixel-level NPP. It may be possible that we can estimate a median relative error within finely discretized bins across the observed NPP gradient which can then be assigned to pixel‐level NPP estimates that fall within each bin. If the data allow, the median relative error may further be empirically modeled as a function of NPP, which would provide a continuous error function for the full range of NPP rates encountered in the ocean.

We note that since the validation dataset is so small, the resultant uncertainties may be subject to significant change as more validation data becomes available. Further, the uncertainties may only be applicable over a more limited dynamic range (defined by the dataset) than exists in the global ocean. Conveyance of this fact will be achieved with data quality ‘flagging’, as discussed in the PACE SAT.

Additionally, we will conduct sensitivity analyses for the majority of empirical expressions and input parameters in the PACE NPP model, similar to what we have done with the CAFE NPP model (Table 2 in Silsbe et al., 2016). The bounds of these sensitivity studies will be guided by expected or documented uncertainties in input products (e.g., spectral phytoplankton absorption, particulate backscattering, chlorophyll concentration, etc.), which are better characterized than for NPP itself. This approach is similar to work conducted with the Vertically Generalized Production Model NPP (VGPM, Behrenfeld and Falkowski, 1997) to determine the range in model variance that can be attributed to known or assumed uncertainty in individual ocean color input products (Milutinovic & Bertino, 2011). This amounts to a Monte Carlo‐like estimate of the upper bound for NPP error, in lieu of formal error propagation. Model parameters (or inputs) can be varied iteratively or in combination with one another. A similar ‘brute force’ approach has also been successfully used in the past for assigning uncertainties to inverted ocean color products (Boss and Roesler, 2006; Wang et al., 2005).

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