**NASA PACE Science and Applications Team**

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**Uncertainties estimation for OCI water remote sensing reflectances (***Rrs***), UV irradiances (*ES*), and Machine Learning (ML) retrievals**

**1. OCI hyperspectral *Rrs* algorithm.** We developed a novel hyperspectral OCI atmospheric correction (AC) algorithm which is based on RTM (VLIDORT) calculation of the TOA reflectance, *Lt,calc* and adjusting water leaving radiance, *Lw*, to match OCI-measured reflectance, *Lt,meas*.We demonstrated the algorithm using proxy *Lt,meas* data from OMI to retrieve remote sensing reflectance, *Rrs= Lw(adjusted)/Es* every 5 nm from 315nm to 500nm. We validated OMI retrievals using MOBY hyperspectral *Rrs* measurements in UV without using vicarious calibration.

We use OMI measurement noise, δ*Lt,meas*~1%( and RTM calculated Jacobians: to estimate random *Rrs* uncertainty δ*Rrs* ~10% ( at blue wavelengths increasing to ~15% at 350nm, and ~20% at 320nm. We estimate larger systematic uncertainties in *Rrs* due to variable aerosol backscatter. Scaling MERRA-2 spectral AOD to match OMI retrieved AOD388 in UV and removing highly absorbing black carbon (BC) component greatly improved OMI *Rrs* comparisons with MOBY. After PACE launch, we plan to use OCI retrieved aerosol AOD and SSA as inputs to our *Rrs* algorithm. Our hope is that aerosol measurements obtained from OCI and SPEXone combined with new GMAO reanalysis will satisfy the important need for accurate UV aerosol optical properties in this challenging spectral range.

Going forward we plan to apply our *Rrs* retrievals to more complex coastal (Case II) waters and for harmful algae blooms, where the benefits of UV ocean color measurements hold a great deal of promise [Kahru and Mitchell 1998]. To evaluate these results, it would be useful to use *Rrs* spectra collected on research cruises or from the next generation of autonomous in-situ hyperspectral measurement systems that are well calibrated in the UV down to ~320nm.

**2. Hyperspectral surface and underwater UV irradiance algorithm.** PACE OCI retrievals of hyperspectral surface UV irradiance, *ES*(, are required to estimate remote sensing reflectance and as a boundary condition for calculating underwater downwelling irradiance, *Ed*( We extended OMI operational *ES* algorithm [Krotkov *et al.,* 1998; 2001; 2002] hyperspectrally from 290 to 399nm (every 1nm) over land and oceans to accommodate variable biological action spectra required for different PACE applications. The *ES* uncertainties are estimated by propagating uncertainties in input parameters: column ozone, surface pressure, and cloud and aerosol UV reflectivity. For cloud- and aerosol-free conditions random *ES* uncertainties *δEs* ~10%( in UVB and *δEs* ~7%( in UVA (see Table 5.5 in [Krotkov et al., 2002]). These estimates were confirmed with MOBY *ES* comparisons: on cloud-free days. UV-absorbing aerosols (smoke and dust) attenuate *ES* much stronger than clouds and non-absorbing aerosols [Krotkov et al., 1998] thus, require additional *ES* correction using OCI retrieved aerosol absorption optical depth AAOD in UV [Arola et al., 2021].

To calculate underwater scalar, *E0*((actinic flux) and planar, *Ed*(, irradiances we use LUTs computed with the Hydrolight RTM [Mobley and Sundman 2008]. We calculate hyperspectral diffuse attenuation coefficients for planar, *Kd*, and scalar, *Ko*, irradiances, as well as 10% penetration depths for action spectrum weighted irradiances. Major uncertainties of the underwater irradiance are introduced by our IOP model (Case 1) which is comprised of several empirical relationships between the scattering and absorption coefficients and Chl [Vasilkov *et al*., 2005]. Uncertainties of those empirical relationships are poorly known. An additional difficulty of modelling the IOPs in UV is related to the presence of strongly absorbing mycosporine amino acids (MAA) which may not be correlated with photosynthetic pigments. One more source of the IOP uncertainties is pure water absorption in UV. Unlike Vis, there are no consensus values for the pure water absorption in the UV. All those considerations lead to a conclusion that it is extremely hard to estimate the underwater irradiance uncertainties through the propagation of the uncertainties of separate components of the entire chain of computations. That is why we decided to estimate the underwater irradiance uncertainties using a comparison of computed *Kd* values with those derived from in situ measurements of underwater irradiance. In situ data used in the comparisons are from two cruises: the Aerosol Characterization Experiment (ACE) where measurements of *Ed* were carried out at 313, 320, 340, and 380nm [Vasilkov et al., 2005] in the Northern Pacific Ocean and the BIOSOPE cruise where measurements were carried out at 305, 325, 340, and 380nm [Tedetti et al., 2007] in the Southern Pacific Ocean. The comparisons showed that the relative RMS error for all the cruise stations did not exceed 20%. We accept this number as a maximum uncertainty of out underwater irradiance product at all wavelengths in the UV spectral range of 300 to 400 nm. We plan to compare with the new PACE vicarious calibration systems data when available.

**3. Machine Learning (ML) algorithm for atmospheric correction.** Our team has been exploring ways to use ML to enhance retrieval coverage under less-than-ideal conditions such as cloud, sun glint, and aerosols [Fasnacht et al., 2022]. In this technique, the coefficients of the principal components derived from OCI measured spectra are used as inputs to a neural network trained to predict ocean color properties derived from collocated physically-based retrievals. Assuming that our training is comprehensive (i.e., we cover all possible retrieval situations), there are two major sources of uncertainties: (1) uncertainties of the inputs and (2) how these translate into predicted outputs. These can be quantified by running sensitivity tests adjusting the inputs by their uncertainties and determining the impact on the predicted quantities, such as Chl and *Rrs*. The other source of uncertainty, which is more difficult to quantify, is the uncertainty of the random errors in the neural network itself. To estimate such uncertainties, we plan to develop an ensemble of neural networks, essentially retrain the same NN model many times, and analyze the variability of the model ensembles.

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