**Association of Uncertainties to PACE surface radiation products**

The PACE surface radiation products include global maps of spectral and wavelength-integrated (UV and PAR spectral ranges), instantaneous and daily downwelling planar solar irradiance just above and just below the surface, scalar solar irradiance just below the surface, and average cosine for total light just below the surface. The quantities below the surface are essentially derived from the planar fluxes just above the surface following Frouin et al., 2018a). Associating uncertainties (algorithmic and other) to these products on a pixel-by-pixel basis is needed to assess product utility and ensure that variability and trends revealed in product analyses are significant (larger than uncertainty). This requires modeling the measurement, identifying all possible error sources (e.g., noise in the input variables, imperfect or incomplete mathematical model), and determining the combined uncertainty. Algorithmic uncertainties are those due to model approximations and parameter errors (e.g., decoupling effects of clouds and clear atmosphere, using reanalysis data for aerosol properties, absorbing gas contents, and diurnal variability of clouds) assuming that the input variables (top-of-atmosphere reflectance) are known perfectly. Other uncertainties originate from imperfect knowledge of the satellite measurement, which may be due to radiometric noise, calibration errors, and processing to Level 1b.

The statistical procedure adopted to estimate and provide, for each pixel of the above-surface planar flux product, the algorithmic component of the total uncertainty budget, which is expected to dominate, is described in Frouin et al. (2018a,b; see also Frouin et al., 2022). The uncertainty probability distribution function (PDF) is obtained by simulating as a function of clear sky flux and cloud factor (characterizes the effect of clouds on surface flux and varies from 0 to 1) the satellite measurements (TOA reflectance) and the corresponding surface flux values and comparing the latter with the satellite estimates. From this PDF, and knowledge of the clear sky flux and cloud factor of a given flux estimate, the bias and standard deviation uncertainties are obtained and assigned to the flux estimate. This is accomplished in practice using pre-calculated look-up tables (LUTs). In the final product, however, the flux estimate is corrected for the bias uncertainty, and the corrected value is provided with only the standard deviation uncertainty.

The uncertainties on below-surface quantities are obtained by propagating the uncertainty on the above-surface flux through the model equations used to estimate those quantities (see Frouin al., 2018a). The Monte Carlo approach to uncertainty estimation (JCGM101, 2008) is used. The model equations depend on the cloud factor and coefficients varying with wind speed, latitude, and day of the year. A large number of numerical simulations of the model equations are generated from the uncertainty PDFs for cloud factor and coefficients, from which the PDF of a given below-surface variable is computed. It is assumed, in these simulations, that the uncertainty PDFs of the various input parameters are not correlated. The mean and standard deviation of the output PDF yield the variable estimate, therefore its bias, and its uncertainty. LUTs are created to compute bias and standard deviation uncertainty as a function of cloud factor, wind speed, latitude, and day of year. The estimates are finally corrected for the bias uncertainty, as done for the above-surface planar flux.

Evaluation of the uncertainty estimation for above-surface planar flux will be performed using in-situ measurements at offshore stations equipped with downwelling solar irradiance cosine sensors. From these measurements and estimates of the clear sky flux from radiative transfer calculations and ancillary data (e.g., from reanalysis), the cloud factor will be derived. The bias and standard deviation uncertainties will then be obtained by comparing the estimated and measured fluxes, and they will be examined as a function of cloud factor. These uncertainties will be related to those generated theoretically, as described above. If the two types of uncertainties (measured and predicted) differ significantly, especially if the predicted uncertainty is too small, we will consider including uncertainties in the TOA reflectance. This will require knowing the covariance matrix of the noise in the L1b OCI imagery, which can be estimated using structure functions. The procedure described above for algorithmic uncertainties will be used, but with noisy TOA measurements. Figure 1, obtained for daily mean PAR derived from MERIS data (2005-2012), shows that experimental uncertainties at the COVE site resemble algorithm uncertainties generated from simulations without noise, suggesting that the procedure to associate uncertainties is adequate (Frouin et al., 2018b).



***Figure 1****: Uncertainties (bias, standard deviation) on MERIS daily mean PAR estimates at the COVE site (Chesapeake Bay). Red curves: using MERRA-2 data (simulation, see text); Blue curves: comparing satellite PAR estimates with in-situ measurements. MERIS and COVE PAR data acquired during 2005-2012 were used.*

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