Empirical Orthogonal Functions to Diagnose and Correct OCO-2/3 Calibration Errors Robert

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The Orbiting Carbon Observatory (OCO) -2 and -3 instruments have provided precise estimates of the column-average dry air mole fraction of carbon dioxide since 2014 and 2019, respectively. High-resolution spectra are acquired in three infrared channels centered at 766, 1608, and 2064 nm. Each spectrometer channel has its own slit, grating, and focal plane array, while the three share common entrance optics. In the spatial dimension, the active region of each focal plane array is divided into eight along-slit footprints. OCO-2/3 Level 2 full physics retrievals are performed using the Atmospheric Carbon Observations from Space (ACOS) algorithm. The modeled and measured spectra are often slightly mismatched for a number of reasons. These include imperfectly specified surface albedo, aerosol scattering, absorption coefficient (ABSCO) tables, and instrument line shapes. A number of radiometric calibration errors with spectral structure also appear, including uncorrected bad pixels, stray light, and biases in the prelaunch gain and inflight gain degradation coefficients. To improve goodness of fit and accuracy, the final operational retrievals include channel-dependent scalar multipliers based on empirical orthogonal functions (EOFs) in the state vector.

EOFs are generated by processing a large volume of data without EOFs, ideally spanning as much of the record as possible in space and time. For operations, only ocean data filtered to remove all but the clearest scenes has been used, though land data has also been evaluated as a diagnostic. The principal components of the spectral residuals are saved separately as a function of spectral column for each spatial footprint of each channel. They are ranked by the fraction of variance explained, with the top three or four used in the final retrievals, depending on channel. Importantly, the scalar multiplier, or "loading", of each EOF is unique for each sounding, but the spectrally-dependent shape is fixed. Visualizing the shapes of the EOFs and trends of their loadings with time are important indicators of data quality and yield key insights into which aspects of the dataset need to be improved in future versions. While the forward model, and therefore its error, is the same for all soundings over a given surface type, radiometric calibration is spatially varying and updated once or twice each week to describe instrument response changes with time, temperature, and contamination level. As a result, EOFs that change shape with footprint and loadings that change with time are the most sensitive metrics available to assess calibration data quality. However, there are limits to relying on EOFs to eliminate biases from calibration, especially when features change shape over time as in OCO-3 Version 10.3.

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