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High-frequency multi-solute calibration using an in situ UV – visible sensor

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Abstract

Monitoring the temporal variation of solute concentrations in streams at high temporal frequency can play an important role in understanding the hydrological and biogeochemical behaviour of catchments. UV – visible spectrometry is a relatively inexpensive and easily used tool to infer those concentrations in streams at high temporal resolution. However, it is not yet clear which solutes can be modelled with such an in-situ sensor . Here, we installed a UV – visible spectrometer probe

(200–750 nm) in a high-altitude tropical Páramo stream to record the wavelength absorbance at a 5-min temporal resolution. For calibration , we simultaneously sampled stream water at a 4-h frequency from February 2018 to March 2019 for subsequent laboratory analysis. Absorbance spectra and laboratory-determined solute concentrations were used to identify the best calibration method and to determine which solute concentrations can be effectively inferred using in situ spectrometry through the evaluation of six calibration methods of different mathematical complexity. Based on the Nash–Sutcliffe efficiency (NSE) and Akaike information criterion metrics, our results suggest that multivariate methods always outperformed simpler strategies to infer solute concentrations. Eleven out of 21 studied solutes (Al, DOC, Ca, Cu, K, Mg, N, Na, Rb, Si and Sr) were successfully calibrated (NSE >0.50) and could be inferred using UV – visible spectrometry even with a reduced daily sampling frequency . It is worth noting that most calibrated solutes were correlated with wavelengths (WLs) in the low range of the spectra (i.e., UV range) and showed relatively good correlation with DOC. The latter suggests that estimation of metal concentrations could be possible in other streams with a high organic load (e.g., peat dominated catchments). In situ operation of spectrometers to monitor water quality parameters at high temporal frequency (sub-hourly) can enhance the protection of human water supplies and aquatic ecosystems as well as providing information for assessing catchment hydrological functioning. © 2021 John Wiley & Sons Ltd.

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