

Assessment of adjacency effect correction methods for Sentinel-2 MSI observations over mid-latitude lakes

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Abstract

Accurate retrieval of remote-sensing reflectance (R_{rs}) from lakes requires separating water-leaving radiance from atmospheric, surface and adjacency contributions. We assessed adjacency effect correction (AEC) methods for Sentinel-2 MultiSpectral Instrument (MSI) imagery using 329 satellite-in-situ matchups from four mid-latitude lakes: Greifensee, Lake Geneva, Lake Garda and Lake Trasim  no. The AEC methods TMART and RAdCor were combined with atmospheric correction (AC) methods ACOLITE, C2RCC and POLYMER, while GAAC was evaluated as an integrated AEC+AC approach. RAdCor+POLYMER produced the lowest median symmetric accuracy (MdSA) in three of the four lakes. The largest AEC benefit occurred in narrow Greifensee, where MdSA was 49.5 percentage points lower for RAdCor+POLYMER than for standalone POLYMER. Prior AEC reduced MdSA in 98 of 144 comparisons, with improvements most frequent at 705 and 740 nm. R_{rs} retrieval variation among AEC+AC combinations increased towards longer wavelengths: the median normalised interquartile range was 15.9% at 560 nm and 104.4% at 740 nm. Higher aerosol load was associated with larger AEC benefits in several combinations, whereas associations with sun zenith angle were generally small and varied among approaches and wavelengths. These results support routine inclusion of AEC in MSI lake R_{rs} processing, particularly for small or narrow lakes and products that use red and near-infrared bands. However, correction magnitude, sign and AEC benefit depended on water type, aerosol conditions, wavelength and downstream AC approach. Further method development and broader validation are required before AEC+AC combinations provide consistent benefit across inland waters.

Keywords: Remote-sensing reflectance; Atmospheric correction; Adjacency effect correction; Validation; MSI; Water quality; Lakes

1 Introduction

The blue-to-near-infrared spectral range of the Sentinel-2 MultiSpectral Instrument (MSI; 443–740 nm) is widely used to retrieve lake optical properties and water quality variables, including phytoplankton chlorophyll-*a*, suspended particulate matter, turbidity and water transparency (Toming et al., 2016; Bresciani et al., 2018; Werther et al., 2022b). These products depend on accurate retrieval of remote-sensing reflectance (R_{rs}). Atmospheric correction (AC) methods remove molecular scattering, aerosol scattering and surface reflection terms so that the remaining water signal can be expressed as R_{rs} . This step is difficult over inland waters because the radiance contribution from the water to the top-of-atmosphere (TOA) signal is typically small (1–10%), while atmospheric path radiance and surface-reflected radiance commonly dominate the signal measured by an optical satellite sensor over water (Gordon, 1978, 1985; IOCCG, 2010).

Several approaches are available for AC of MSI and Landsat OLI imagery over inland and coastal waters, including ACOLITE dark spectrum fitting (Vanhellemont and Ruddick, 2018; Vanhellemont, 2019), C2RCC neural network inversion (Brockmann et al., 2016), POLYMER spectral optimisation (Steinmetz et al., 2011), iCOR (De Keukelaere et al., 2018), and NASA SeaDAS l2gen (Gordon and Wang, 1994; Mobley et al., 2016). Intercomparisons over inland,

coastal and optically complex waters show that AC approach performance depends strongly on water type and wavelength, and that no single approach consistently outperforms all others across these environments (Warren et al., 2019; Pahlevan et al., 2021; Hu et al., 2025). For lakes and rivers, the AC problem is further complicated by sun glint, directional reflectance effects, wind-driven foam or whitecaps, and adjacency effects (Koepeke, 1984; Frouin et al., 1996; Steinmetz et al., 2011; Groetsch et al., 2017; Harmel et al., 2018; Wang et al., 2024; Pitarch et al., 2025; Paulino et al., 2025). The adjacency effect (AE) is particularly important for MSI and OLI observations over inland waters because these water bodies are often optically dark, spatially narrow and bordered by much brighter land surfaces. AE occurs when radiance reflected by neighbouring land, islands, shallow water margins, soil, vegetation, snow, urban surfaces or clouds is scattered by the atmosphere into the sensor field of view over water. This process produces an atmospheric point-spread contribution from the surrounding radiance field and can bias the apparent water signal, especially where land and water contrast is strong (Tanre et al., 1981; Tanré et al., 1987; Reinersman and Carder, 1995; Santer and Schmechtig, 2000; Bélanger et al., 2007). Radiative transfer studies show that the magnitude, spectral shape and spatial extent of AE depend on aerosol optical depth, wavelength, illumination and viewing geometry, land cover reflectance, water optical properties and shoreline morphology (Bulgarelli et al., 2014, 2017; Bulgarelli and Zibordi, 2018). For MSI lake applications, AE can extend beyond the first shoreline-adjacent water pixels wherever strong land-water contrast and atmospheric scattering affect the target radiance field (Bulgarelli and Zibordi, 2018; Lion et al., 2025).

AEC methods for aquatic applications follow several principles. Near-infrared (NIR) similarity methods assume that nearby water targets have similar NIR reflectance and use deviations from that similarity as an adjacency indicator (Sterckx et al., 2011). Environment-similarity methods compare the target with spectrally similar surrounding environments and are implemented, for example, in SIMEC and iCOR (Sterckx et al., 2015; De Keukelaere et al., 2018). Point-spread-function (PSF) approaches estimate the atmospheric scattering kernel that mixes neighbouring land and water radiance into the target pixel (Kiselev et al., 2015; Paulino et al., 2022). These studies show that AEC can improve nearshore water reflectance retrieval, while also pointing to important constraints: some methods rely on assumptions about NIR water similarity, others are tied to a specific AC approach, and many approaches have been validated for only one or a small number of algorithms, lakes or regions. More recent AEC methods include the Topography-adjusted Monte Carlo Adjacency-effect Radiative Transfer code (TMART), which uses Monte Carlo radiative transfer to estimate the atmospheric point-spread contribution from the surrounding land and water radiance field and subtracts this adjacency signal from TOA reflectance before AC (Wu et al., 2023, 2024); the Remote Sensing Adjacency Correction method (RAdCor), implemented in ACOLITE, which retrieves surface reflectance over heterogeneous scenes by accounting for contributions from surrounding surfaces with atmospheric PSFs and spatially resolved spherical albedo functions calculated for each wavelength and atmospheric state (Castagna and Vanhellemont, 2025); and the Genetic Algorithm for Atmospheric Correction (GAAC), which jointly retrieves aerosol optical depth, sun glint, adjacency terms, R_{rs} and inherent optical properties through a genetic optimisation framework (Pan and Bélanger, 2025). Recent, independent studies provide evidence that AEC can improve R_{rs} retrieval and downstream water constituent products, while also indicating that the benefit depends on approach choice, wavelength and scene context (Xu et al., 2025; Ansari et al., 2026; Giardino et al., 2025).

Despite this progress, two knowledge gaps remain. First, most AE studies evaluate one AEC implementation with one downstream AC approach. Cross-comparisons of the same prior AEC with several downstream AC approaches remain limited. Second, the conditions controlling AEC benefit over lakes remain insufficiently quantified. Lake environments often combine narrow basins, complex shorelines, islands, steep or heterogeneous surrounding terrain, strong seasonal illumination changes and large optical gradients between clear and productive waters. AEC may therefore be strongest where shoreline geometry, land-water contrast and aerosol scattering coincide. The sign and magnitude of the final R_{rs} change, however, may differ among approaches, wavelengths and optical water types (OWTs). OWT frameworks were developed to organise such spectral diversity for algorithm selection and interpretation (Moore et al., 2014; Spyraeos et al., 2018; Uudeberg et al., 2019; Bi and Hieronymi, 2024), but their use as indicators of AEC benefit remains limited.

The sparse availability of in-situ radiometry that has passed documented quality control limits the study of AEC implementations near lake shores (Peters et al., 2018; Braga et al., 2022; Avouris et al., 2025). Autonomous spectroradiometer systems such as the Water Insight SPectrometer station (WISPstation) can provide high-frequency above-water R_{rs} time series and have been used for validation. They are suitable for validation provided careful filtering is applied to account for illumination, cloud effects, glint, viewing geometry and spatial representativeness. These stations are often deployed close to shore or on fixed platforms, which makes them useful for assessing AEC under nearshore conditions. In this study, three fixed WISPstation datasets from Greifensee, the Lake Geneva LÉXPLORE platform and Lake Trasimeno provide repeated nearshore matchup observations, while a Lake Garda campaign dataset provides an additional long-term validation set with a broader range of station locations and

91 shoreline distances.

92 This study makes three specific contributions. First, we implement RAdCor as a modular MSI preprocessing
93 step that produces a Level-1C-equivalent product for independent downstream AC approaches. Second, we validate
94 TMART+AC and RAdCor+AC combinations against standalone AC products for the same matchups. Third,
95 we link AEC benefit to OWT, aerosol load, observation geometry and lake spatial context to analyse AEC as a
96 differentiated implementation effect whose magnitude and sign may vary among scenes, wavelengths and approaches.

97 The analysis is guided by two hypotheses. First, we hypothesise that explicit AEC improves MSI lake R_{rs} accuracy
98 relative to standalone AC. We expect the largest gains in the red, red-edge and near-infrared bands, where weak
99 water-leaving radiance and atmospheric estimates influenced by nearby soil, vegetation, built surfaces, shallow
100 margins or islands can strongly affect R_{rs} retrieval. Under this hypothesis, prior AEC methods such as TMART and
101 RAdCor, and the integrated AEC+AC GAAC approach, should reduce matchup errors across many lake, approach
102 and wavelength combinations, although the gain may differ strongly among downstream AC approaches.

103 Second, we hypothesise that the validation benefit of current AEC implementations is context-dependent. We
104 expect the magnitude and sign of the R_{rs} correction to depend on OWT, aerosol loading, acquisition geometry,
105 shoreline configuration and downstream AC approach. We expect AEC to produce band, scene and approach
106 dependent R_{rs} changes, with both increases and decreases possible after correction.

107 To evaluate these hypotheses, we compare three standalone AC approaches, ACOLITE, C2RCC and POLYMER,
108 with AEC+AC approaches based on GAAC, TMART and RAdCor. We combine exact paired AEC+AC versus
109 standalone AC comparisons with OWT stratification, conditional analyses of aerosol load and observation geometry,
110 and spatial case studies to identify where AEC improves MSI lake R_{rs} retrieval, where its validation benefit is weak
111 or adverse, and which factors are associated with the magnitude and sign of the retrieved correction.

112 2 Datasets

113 The assessment dataset consists of two sample types: first, observations from fixed WISPstations installed on
114 Greifensee (2022, 2023, 2025), Lake Geneva (2022, 2023, 2025) and Lake Trasimeno (2018–2025), and second, a
115 spatially distributed field campaign dataset (2015–2024) from Lake Garda (Fig. 1). The three WISPstation sites
116 provide autonomous above-water R_{rs} observations. Greifensee is a eutrophic, 2.3 km² lake in the Swiss Midlands,
117 with the WISPstation mounted on a platform close to shore (≤ 300 m). Lake Geneva is a large peri-alpine lake; the
118 LÉXPLORE platform is located about 500 m offshore and provides a fixed station in the western basin of the lake
119 (Wüest et al., 2021). The western basin provides a geometrically complex shoreline setting for spatial analyses. Lake
120 Trasimeno is a shallow, productive and often turbid Italian lake; the WISPstation is located on a platform about
121 400 m north of Isola Polvese, a small island. These three fixed station records provide the in-situ component needed
122 to generate matchups with MSI imagery under consistent local sampling geometry and distance from shore.

123 The Lake Garda dataset provides a complementary validation case. Unlike the WISPstation sites, Lake Garda
124 was sampled through targeted MSI field campaigns at multiple stations and distances to shore from the launch
125 of Sentinel-2A until 2024. This long-term campaign record extends the validation beyond nearshore or platform
126 locations and allows AEC performance to be assessed over a broader spatial gradient within a large, deep peri-alpine
127 lake bordered by steep terrain and characterised by generally clear waters. Together, the four lakes span contrasting
128 lake sizes, optical regimes, shoreline morphologies and surrounding topography, all of which are relevant for assessing
129 AEC methods.

130 2.1 In-situ WISPstation remote-sensing reflectance

131 WISPstations installed at Greifensee, Lake Geneva and Lake Trasimeno provided autonomous fixed-position above-
132 water hyperspectral radiometry. The instruments measured downwelling irradiance, $E_d(\lambda)$, downwelling sky radiance,
133 $L_s(\lambda)$, and upwelling water-leaving radiance, $L_u(\lambda)$, from 350 to 900 nm at 15 min intervals. The Greifensee
134 and Lake Geneva stations were mounted on floating platforms, and the Lake Trasimeno station was installed on
135 a pole-mounted platform approximately 3 m above the water surface and about 400 m north of Isola Polvese.
136 Measurements were transmitted to WaterInsight WISPcloud and, for the Swiss stations, are available in near-real
137 time through Datalakes (see Code availability section).

138 Level-1 radiometric components were processed to R_{rs} with the three-component above-water reflectance model,
139 hereafter referred to as 3C. The 3C approach derives R_{rs} from measured $E_d(\lambda)$, $L_s(\lambda)$ and $L_u(\lambda)$, while estimating
140 residual surface reflection from direct sun glint and diffuse sky glint. The spectral glint formulation underlying this
141 processing follows the work of Gege and Grötsch (2016) and the subsequent validation of the 3C model by Groetsch
142 et al. (2017), with further assessment by Pitarch et al. (2020). A recent update by Pitarch (2026), published while

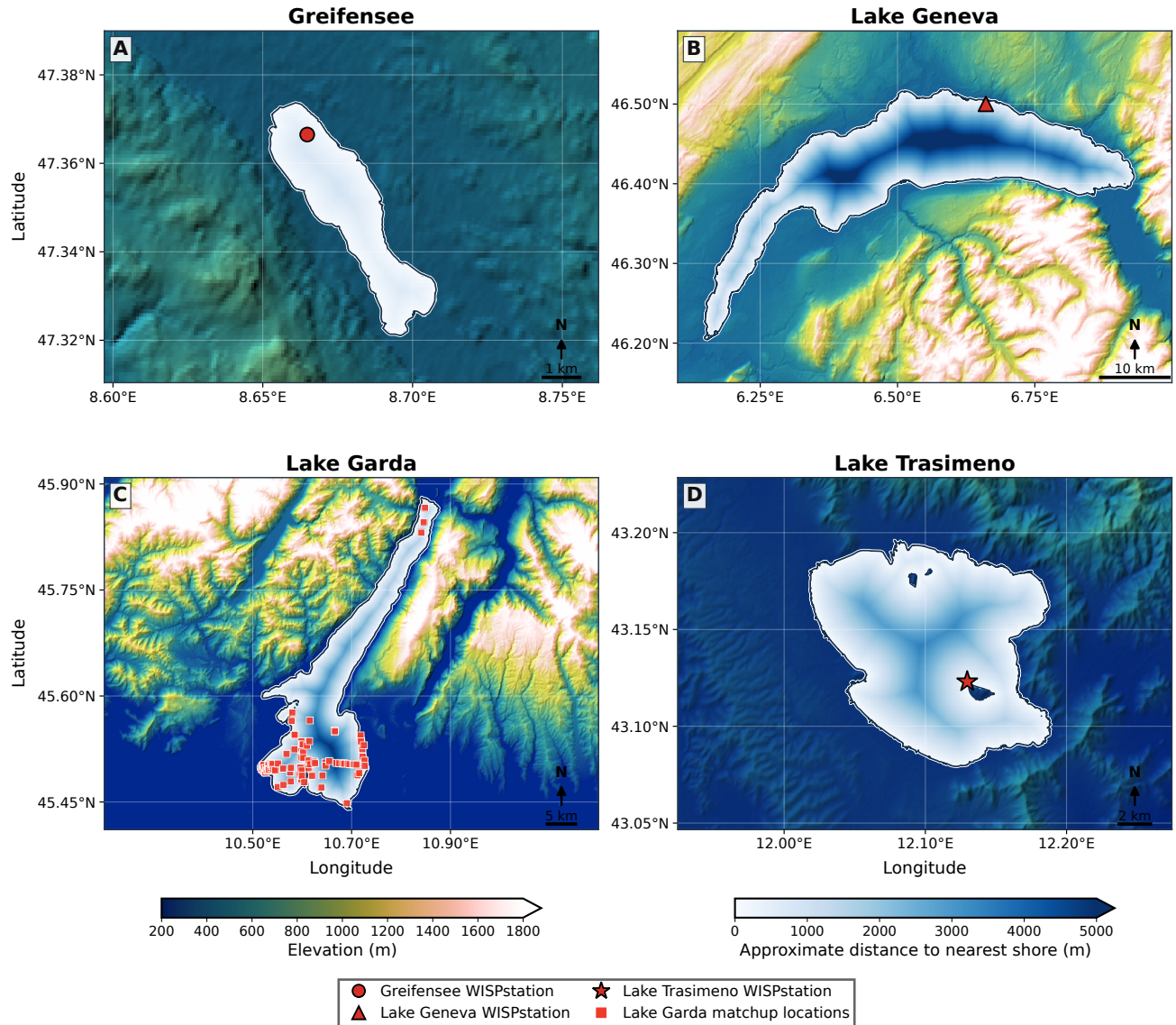


Figure 1: Locations retained for the assessment in Greifensee (A; CH), Lake Geneva (B; CH/FR), Lake Garda (C; IT) and Lake Trasimeno (D; IT). Land colours show elevation; colours within each lake show approximate distance to the nearest shoreline.

this manuscript was being finalised, introduced the 3C-O25 formulation. Processing of the matchup dataset had already been completed with the existing 3C formulation when 3C-O25 became available.

For this study, we implemented the 3C equations in a differentiable JAX workflow to accelerate batch processing of the WISPstation time series and to make the optimisation step reproducible within our processing pipeline. The spectral model structure was retained, and ancillary atmospheric and geometric inputs were updated dynamically for each individual measurement. Relative humidity and air pressure were estimated from COSMO meteorological fields (Baldauf et al., 2011), solar zenith angle (SZA) was computed with `pvlib` (Holmgren et al., 2018), and viewing geometry was read from the WISPstation metadata. These changes improved processing consistency across stations and acquisition times. The in-situ-satellite matchup residuals played no role in selecting the ancillary inputs or geometry. The Greifensee WISPstation record and related quality control checks have been independently described and used for hyperspectral phytoplankton taxonomic analysis and validation against imaging microscopy (Maire et al., 2025).

2.2 In-situ Lake Garda field campaign measurements

Lake Garda in-situ R_{rs} spectra were obtained from targeted MSI matchup field campaigns beginning after the launch of the mission in 2015. This dataset has been steadily extended over the years and used in several studies related to AC and bio-optics (Giardino et al., 2014; Cazzaniga et al., 2016; Bresciani et al., 2018; De Keukelaere et al., 2018). The measurements were acquired with different radiometers: the handheld WISP-3 radiometer covering 400–800 nm and full-range ASD FieldSpec-FR and Spectral Evolution radiometers operating from 350–2500 nm. The above-water acquisitions recorded $E_d(\lambda)$, $L_s(\lambda)$ and $L_u(\lambda)$. WISP-3 acquired the radiometric components simultaneously, with water and sky views approximately 40° from nadir. ASD and Spectral Evolution acquisitions were sequential: downwelling irradiance was measured with a cosine receptor, and water and sky radiance were measured with a 5° fore-optic at approximately 40° from nadir and 135° relative azimuth from the Sun, following the SeaWiFS above-water protocol (Bresciani et al., 2018; De Keukelaere et al., 2018).

2.3 Matchup generation

Matchups between in-situ and satellite-derived R_{rs} were generated in three steps. First, hyperspectral observations from the WISPstations and Lake Garda campaigns were converted to glint-corrected hyperspectral R_{rs} , because the 3C correction requires hyperspectral input. The corrected spectra were then convolved with the spectral response functions of the corresponding S2A, S2B and S2C MSI instruments, using the ESA Sentinel-2 spectral response function release (European Space Agency, 2024), to obtain MSI band-equivalent in-situ R_{rs} . Second, Sentinel-2 scenes were retrieved from the archive for observations that passed the field radiometry quality criteria in Section 2.3.1. Third, satellite pixels were masked using the IdePix water, cloud, cloud shadow, snow/ice and invalid pixel flags, then assessed for local homogeneity. Paired analyses were restricted to records for which both the standalone AC product and the corresponding AEC+AC product were available.

2.3.1 In-situ R_{rs} quality control

For the WISPstation sites, WISPstation observations around candidate Sentinel-2 overpass times were evaluated with a Level-1 radiometric $E_d(560)$ illumination indicator. This illumination stability check follows the WISPstation quality control logic described by Maire et al. (2025); here it was applied only to the overpass window used for satellite matchup selection. For each site and candidate overpass, measured $E_d(560)$ in a ± 15 min overpass window was compared with a modelled clear-sky daily irradiance curve (Fig. 2). The curve was a sine-shaped clear-sky proxy scaled with the 90th percentile of noon $E_d(560)$ observations within a ± 15 day window. Candidate overpasses were retained when the mean absolute percentage error (MAPE) between measured and modelled $E_d(560)$ in the overpass window was $\leq 20\%$. This filter was introduced because a spectrum can pass shape-based spectral criteria while still being acquired under transient cloud, shadow or rapidly changing illumination near the satellite overpass; $E_d(560)$ provides an independent high-frequency indication of whether the in-situ and satellite observations sampled a comparable illumination state. The $\leq 20\%$ threshold was chosen as a conservative compromise that removes unstable overpass windows without rejecting normal clear-sky variability in the station irradiance record. For the retained matchups, the median overpass window $E_d(560)$ errors were 3.2% for Greifensee, 7.4% for Lake Geneva and 5.5% for Lake Trasimeno; for the 172 Trasimeno matchups, the 95th percentile was 16.1%, below the 20% threshold. The closest WISPstation R_{rs} measurement within the overpass window was then selected for the in-situ side of the matchup. Lake Garda field campaign spectra were processed from the matched hyperspectral records and convolved to MSI band-equivalent R_{rs} .

All retained in-situ spectra were additionally evaluated using the Quality Water Index Polynomial (QWIP) and retained when $|QWIP| \leq 0.2$ (Dierssen et al., 2022). The maximum absolute QWIP values were 0.190 for Greifensee, 0.179 for Lake Geneva, 0.200 for Lake Trasimeno and 0.1377 for Lake Garda.

2.3.2 MSI scene selection

S2A, S2B and S2C MSI Level-1C products were retrieved for dates and locations that passed the in-situ quality control. Level-1C products are TOA reflectance products that are radiometrically calibrated, geometrically corrected and distributed in UTM projection (Drusch et al., 2012). AC outputs and matchup validation spectra were evaluated on a common 20 m grid. Earlier inland water validation studies commonly used small resolution neighbourhoods around the station; for example, Bresciani et al. (2018) used centred 3×3 pixel windows, whereas De Keukelaere et al. (2018) used 5×5 , 3×3 and single pixel supports for the 10, 20 and 60 m Sentinel-2 bands, respectively. All analyses were performed on a common 20 m grid because adjacency effects were assessed using the complete validation band set, including the native 20 m bands at 705 and 740 nm. This choice preserves the native spatial

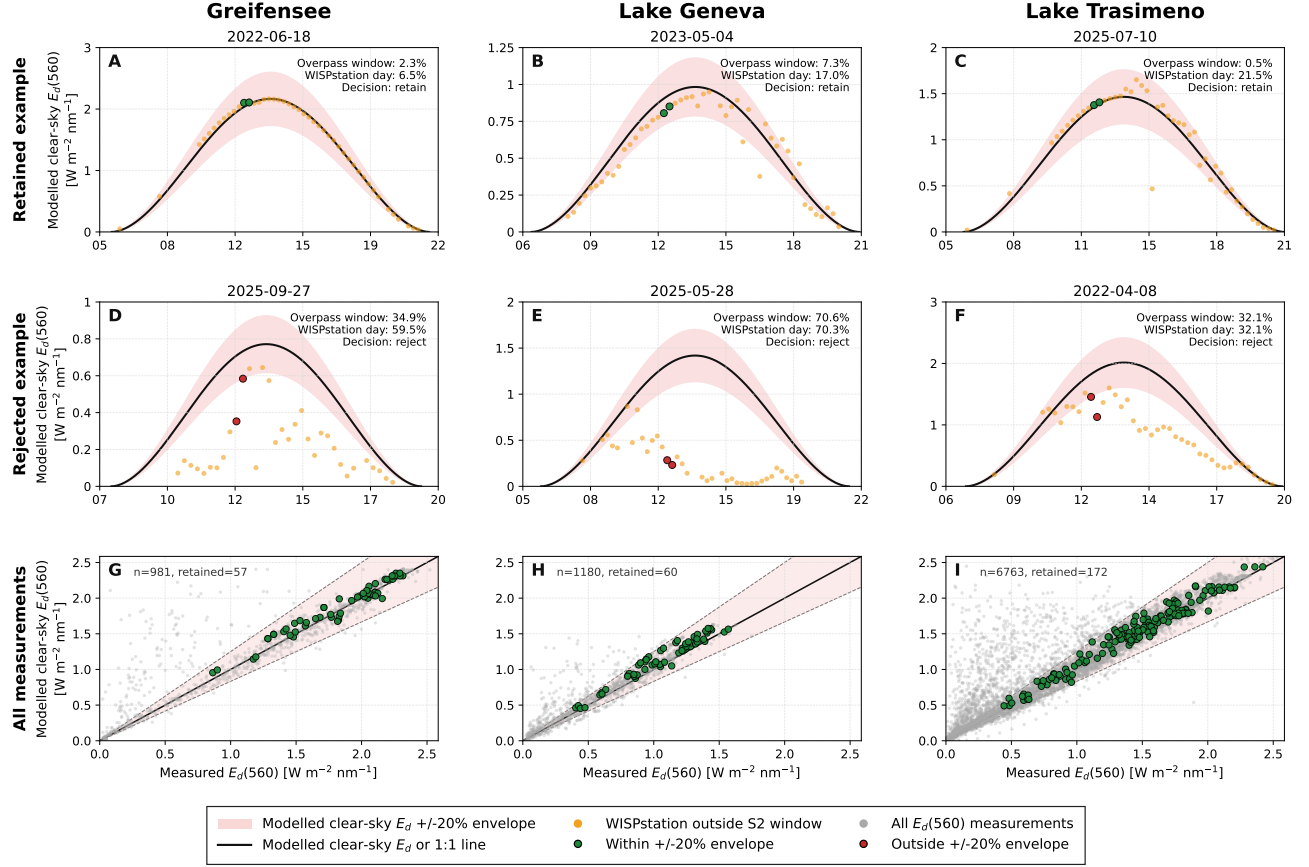


Figure 2: Downwelling irradiance quality control for WISPstation measurements at Greifensee, Lake Geneva and Lake Trasimeno. Panels A–C show retained MSI matchup days; panels D–F show rejected examples. Panels G–I compare measured $E_d(560)$ with the modelled clear-sky proxy for all available measurement days. The black curve in panels A–F is the clear-sky proxy, the light red band is the $\pm 20\%$ acceptance envelope, orange points fall outside the ± 15 min satellite overpass window, and green and red points within that window fall inside and outside the envelope, respectively.

support of the analysis while avoiding resampling to the coarser 60 m resolution. Platform-specific adjacency effects at Greifensee and Lake Geneva remain part of the 20 m observations and were not removed by this choice of spatial resolution. The 443 nm band therefore remains constrained by its native 60 m information content but is evaluated at the common 20 m approach output to maintain a consistent spatial grid across validation bands and approaches.

Satellite imagery was masked with IdePix, a multi-sensor pixel classification tool. For MSI, only pixels classified as water and free of cloud, cloud shadow, snow or ice, and other invalid conditions were retained (Skakun et al., 2022; Wevers et al., 2025). Following established ocean colour matchup protocols, local spatial homogeneity was assessed using the spatial coefficient of variation of native 10 m Level-1C B03 TOA reflectance at 560 nm, hereafter CV_{560} (Zibordi et al., 2009; Concha et al., 2021). A centred 3×3 window was extracted at each in-situ coordinate, and CV_{560} was calculated as the population standard deviation divided by the mean of the finite positive pixels. Matchups with a finite $CV_{560} > 0.25$ were excluded. Median CV_{560} values were 0.0056 for Greifensee, 0.1037 for Lake Geneva, 0.0043 for Lake Trasimeno and 0.0054 for Lake Garda.

Candidate in-situ matchup measurements differed between the continuous WISPstation records and the discrete Lake Garda campaign observations and are therefore described separately. For Greifensee and Lake Geneva, the stable illumination control described in Section 2.3.1 retained 57 and 60 candidate Sentinel-2 MSI overpass dates, respectively. Application of the $|QWIP| \leq 0.2$ criterion retained 29 matchups for Greifensee and 31 for Lake Geneva.

Of the 338 candidate Lake Trasimeno matchups, 190 met the IdePix valid water criterion, Level-1C CV_{560} and

QWIP criteria. The resulting dataset comprised the 172 matchups that also met the stable illumination criterion described in Section 2.3.1. For 230 original Lake Garda records, same-day MSI matching and IdePix valid water pixel identification yielded 97 matchups. All 97 satisfied the QWIP and Level-1C CV₅₆₀ criteria. All WISPstation matchups were acquired within 15 minutes of the Sentinel-2 overpass, whereas the Lake Garda matchups were date-matched, with a mean absolute time difference of 1.84 h and a median of 2.01 h.

2.4 Regional aerosol reanalysis data

Regional aerosol conditions were characterised with two global reanalyses of atmospheric composition. The primary dataset was the Modern-Era Retrospective analysis for Research and Applications, Version 2 (MERRA-2), produced by the National Aeronautics and Space Administration (NASA) (Gelaro et al., 2017; Randles et al., 2017). We used the hourly M2T1NXAER aerosol collection on its native 0.5° latitude $\times$ 0.625° longitude grid. The extracted variables were total aerosol extinction optical thickness (AOT) at 550 nm, $\tau_{\text{ext}}^{\text{aer}}(550 \text{ nm})$ (TOTEXTTAU), and total aerosol scattering AOT at 550 nm, $\tau_{\text{sca}}^{\text{aer}}(550 \text{ nm})$ (TOTSCATAU). These variables were almost perfectly correlated in the matchup dataset. We therefore retained $\tau_{\text{sca}}^{\text{aer}}(550 \text{ nm})$ as the primary MERRA-2 aerosol descriptor because atmospheric scattering directly contributes to adjacency radiance.

The comparison dataset was the European Centre for Medium-Range Weather Forecasts (ECMWF) Atmospheric Composition Reanalysis 4 (EAC4), distributed by the Copernicus Atmosphere Monitoring Service (CAMS) (Inness et al., 2019). CAMS EAC4 provides global atmospheric composition fields at 3-hourly intervals on a $0.75^\circ \times 0.75^\circ$ grid. We retained total aerosol optical depth at 550 nm, hereafter AOD₅₅₀, as the CAMS aerosol descriptor. Throughout the manuscript, AOT refers to the MERRA-2 optical thickness variables, whereas AOD₅₅₀ refers to the CAMS total aerosol optical depth at 550 nm.

Both products were extracted over $42.0\text{--}48.5^\circ\text{N}$ and $5.0\text{--}13.5^\circ\text{E}$. MERRA-2 fields were interpolated to the matchup coordinates and Sentinel-2 sensing time, while CAMS EAC4 fields were matched to the available 3-hourly analysis times. MERRA-2 $\tau_{\text{sca}}^{\text{aer}}(550 \text{ nm})$ was available for 328 of 329 matchups. CAMS AOD₅₅₀ was available for 323 of 329 matchups across all four lakes.

3 Methods

We evaluated ten AC and AEC+AC approaches (Fig. 3): standalone ACOLITE/DSF, C2RCC and POLYMER; TMART followed by each of these three AC approaches; modular RAdCor preprocessing followed by C2RCC or POLYMER; the original ACOLITE/TSDSF approach using RAdCor internally; and GAAC as an integrated AEC+AC approach. The AEC and AC approaches are described in Sections 3.1 and 3.2, respectively.

The assessment first compared satellite-derived and in-situ R_{rs} for each standalone AC or AEC+AC approach and then quantified the change in retrieval error produced by adding AEC before the same downstream AC. This paired AEC benefit was used as the response in the conditional analyses of solar geometry, optical water type and aerosol load. These variables were analysed jointly because their distributions differed among lakes and acquisition conditions. We used Huber M regression to estimate the conditional associations while limiting the influence of extreme response residuals. Sentinel-2 scene identifiers defined the clustering unit because multiple matchup events could originate from the same satellite acquisition. Section 3.4 defines this common estimation and scene-clustered inference approach. The validation statistics and paired AEC benefit response are defined in Section 3.3. Section 3.4 describes the sensitivity analyses, including the OWT and shoreline analyses and the conditional solar geometry and aerosol models.

3.1 Adjacency effect correction

3.1.1 Topography-adjusted Monte Carlo Adjacency effect Radiative Transfer (TMART)

TMART simulates millions of photon paths in a 3-D land–atmosphere–water system and derives a scene-specific PSF for every wavelength. The PSF is then deconvolved from the original Level-1 radiance product to produce an AE-corrected Level-1B product that can be forwarded to any AC (Wu et al., 2024). In this study, the public `tmart` v2.5.1 code was run with its default Monte Carlo configuration (10^6 photons, 1 km cut-off radius) and the same 20 m grid as the AC approaches.

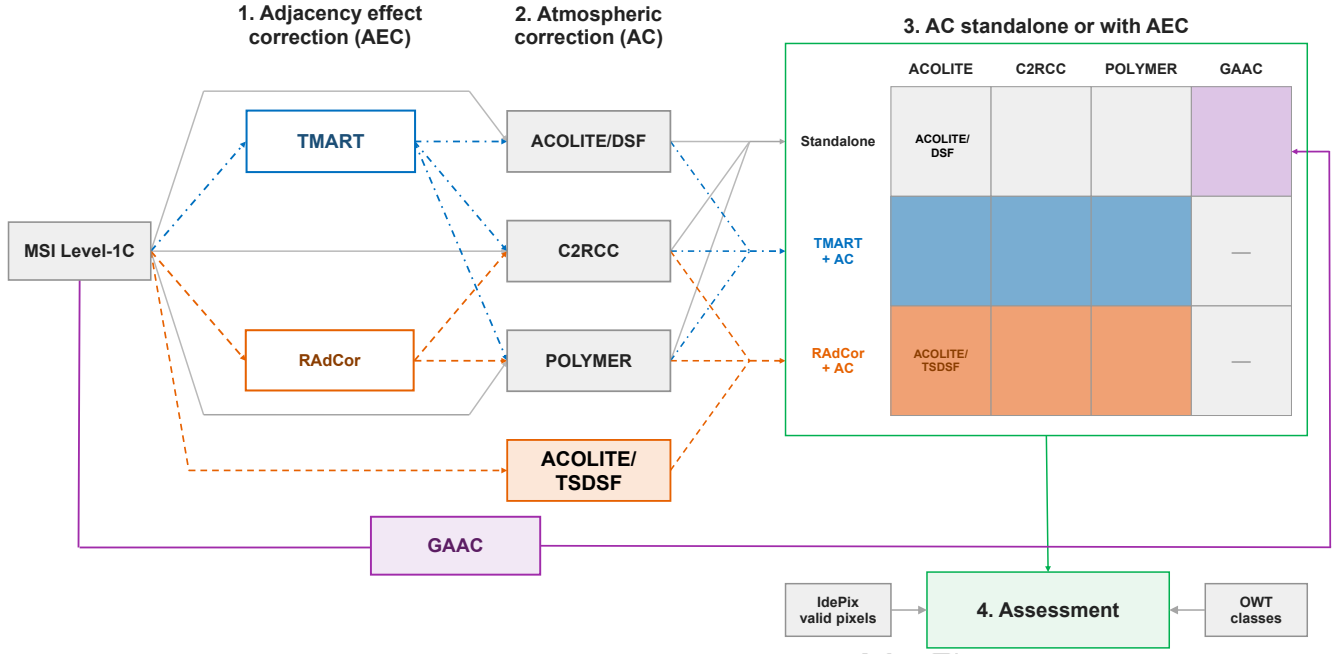


Figure 3: Sentinel-2 MSI processing scheme used to assess standalone AC and combined AEC+AC configurations. Level-1C products were processed directly by ACOLITE/DSF, C2RCC or POLYMER, or first by TMART or the Sencast implementation of RAdCor. TMART outputs were passed to all three AC approaches; modular RAdCor outputs were passed to C2RCC and POLYMER. ACOLITE/TSDSF denotes the native ACOLITE route that couples RAdCor and TSDSF. GAAC was evaluated as an integrated AEC+AC approach. Outputs were assessed on the common 20 m grid using IdePix valid pixels and OWT classes after application of the matchup criteria in Section 2.3.

3.1.2 Remote Sensing Adjacency Correction (RAdCor)

RAdCor is distributed with ACOLITE v20250114.0 as the surface reflectance retrieval component of an adjacency-corrected atmospheric correction approach (Castagna and Vanhellemont, 2025). In the native ACOLITE setting, TOA–Surface Dark Spectrum Fitting (TSDSF) first estimates a representative aerosol model and aerosol optical thickness for the processed subscene. RAdCor then uses these atmospheric parameters to retrieve surface reflectance while accounting for radiance contributed by surrounding surfaces. The spatial transport of diffuse upward radiance is represented by an atmospheric PSF, while the contribution of diffuse illumination scattered back towards the surface is represented by a spatially resolved spherical albedo function (SAF). The PSF and SAF depend on wavelength and atmospheric state and are supplied through precomputed look-up tables.

TSDSF and RAdCor therefore perform separate functions within ACOLITE: TSDSF estimates the aerosol state, and RAdCor retrieves surface reflectance using that estimate. We refer to this native sequence as ACOLITE/TSDSF throughout the figures and results (Fig. 3). This label includes the subsequent RAdCor surface reflectance retrieval.

To evaluate RAdCor with independent downstream AC approaches, we implemented an export procedure in the open source Sencast framework (see Code availability section). Sencast runs the RAdCor implementation distributed with ACOLITE on the original MSI Level-1C product and reads the adjacency-corrected TOA-equivalent `rhotc` variables from the ACOLITE Level-2R file before Level-2W aquatic products are generated. These variables are mapped deterministically to MSI band identifiers and written to a duplicate Level-1C-equivalent product that preserves the original product geometry, metadata and file structure. The resulting product can be processed independently with C2RCC or POLYMER. The corresponding AEC+AC combinations are denoted RAdCor+C2RCC and RAdCor+POLYMER.

The mapping used MSI band identifiers rather than nominal wavelengths to ensure consistent treatment of S2A, S2B and S2C. The six channels are denoted 443, 492, 560, 665, 705 and 740 nm. The B5 centre wavelength varies slightly among MSI platforms and metadata conventions and may be described near 704 or 705 nm; we use 705 nm consistently as the manuscript wavelength while mapping the channel by band identifier in the processing code.

RAdCor was run on a 20 m target grid. During write-back to the native MSI band files, B02, B03, B04 and B08 were resampled with nearest-neighbour assignment because their native resolution is 10 m. This step reproduces each corrected 20 m value on the finer file grid without introducing interpolated subpixel variation. The remaining MSI bands were written using average resampling. Native 20 m bands therefore retained the RAdCor target support,

while the corrected grid was spatially aggregated for native 60 m bands.

RAdCor exposes several processing settings whose influence on the lake matchups was not known before the assessment. Appendix 1 describes the tests used to select one configuration for processing the complete dataset.

3.1.3 Genetic Algorithm for Atmospheric Correction (GAAC)

Although GAAC was introduced as an AC approach, it embeds an explicit AE model and therefore acts as a joint AEC+AC solver. The forward model expresses TOA reflectance as the sum of (i) direct atmospheric path radiance, (ii) adjacency-scattered land radiance parameterised with a single coupling coefficient k_{AE} and a 2D exponential PSF, (iii) specular sun glint, and (iv) water-leaving radiance simulated with a two-component bio-optical approach. Seven unknowns, namely AOD₅₅₀, Ångström exponent, aerosol single-scattering albedo proxy, k_{AE} , glint reflectance, chlorophyll-specific absorption and the backscattering slope, are solved simultaneously with a genetic algorithm optimiser (population 200, 50 generations). The number of equations equals the number of VIS–NIR bands (SWIR bands are used only for Rayleigh correction), ensuring an exactly determined system (Pan and Bélanger, 2025). GAAC retrieves AE, aerosol, glint and water terms in one inversion. Its PSF mixing and coupling factors use the aerosol and transmittance state estimated within the same optimisation and operate on GAAC-internal radiometric variables. We therefore evaluated GAAC as one integrated AEC+AC configuration.

3.2 Atmospheric correction

Four AC approaches were evaluated: the Case-2 Regional CoastColour approach (C2RCC v2024.10), POLYMER v4.17, ACOLITE v20250114.0, and GAAC v20250415. C2RCC, POLYMER and ACOLITE are widely applied in inland water research and have been included in major intercomparisons (Pahlevan et al., 2021; Giardino et al., 2025; Warren et al., 2019; Werther et al., 2022b, 2025).

C2RCC couples forward and inverse neural networks trained with approximately five million radiative transfer simulations spanning atmospheric and water optical conditions (Brockmann et al., 2016). The inversion estimates inherent optical properties and water-leaving reflectance after gaseous absorption correction.

POLYMER fits atmospheric and aquatic spectral components simultaneously. A low-order polynomial represents aerosol-scattered reflectance, while a bio-optical model is fitted iteratively to the residual water signal. Its explicit sun glint term supports processing under geometries with substantial glint risk (Steinmetz et al., 2011).

ACOLITE/DSF denotes the standalone ACOLITE configuration used without RAdCor (Vanhellemont and Ruddick, 2018). After Rayleigh correction, Dark Spectrum Fitting (DSF) estimates aerosol reflectance from image-based dark targets and extrapolates it across the visible and NIR spectrum.

GAAC is described in Section 3.1.3. It retrieves atmospheric, glint, adjacency and water terms in one optimisation. Outputs were harmonised to R_{rs} according to the radiometric convention of each product. Outputs supplied as water-leaving reflectance, $\rho_w(\lambda)$, were divided by π ; outputs already expressed as R_{rs} were used directly.

3.3 Assessment statistics and paired AEC benefit

All validation statistics were calculated at the MSI validation wavelengths after spectral matching of satellite and in-situ R_{rs} . Let $R_{rs,i}^{sat}(\lambda)$ and $R_{rs,i}^{in situ}(\lambda)$ denote the satellite-derived and in-situ R_{rs} for matchup i at wavelength λ . For each valid matchup, multiplicative retrieval error was expressed as the symmetric absolute error:

$$SAE_i(\lambda) = 100 \left[\exp \left(\left| \ln \left(\frac{R_{rs,i}^{sat}(\lambda)}{R_{rs,i}^{in situ}(\lambda)} \right) \right| \right) - 1 \right]. \quad (1)$$

The median symmetric accuracy was calculated as the median SAE over the valid matchup set $\mathcal{P}_\lambda$:

$$MdSA(\lambda) = \text{median}_{i \in \mathcal{P}_\lambda} [SAE_i(\lambda)]. \quad (2)$$

Median overestimation or underestimation in satellite-derived R_{rs} was quantified with the symmetric signed percentage bias:

$$SSPB(\lambda) = 100 \text{sign}(\tilde{\delta}(\lambda)) \left[\exp \left(|\tilde{\delta}(\lambda)| \right) - 1 \right], \quad \tilde{\delta}(\lambda) = \text{median}_{i=1, \dots, n} \ln \left(\frac{R_{rs,i}^{sat}(\lambda)}{R_{rs,i}^{in situ}(\lambda)} \right). \quad (3)$$

Mean absolute error, mean bias and correlation coefficients were calculated using standard validation definitions (Seegers et al., 2018; Werther et al., 2022a). Paired AEC benefit was evaluated for six AEC+AC combinations, each compared with its corresponding standalone AC approach. Throughout the paired analyses, i indexes a matchup,

339 $j \in \{1, \dots, 6\}$ indexes one of the following six comparisons, and λ indexes one of the six MSI wavelengths, 443, 492,
340 560, 665, 705 or 740 nm:

- 341 1. TMART+ACOLITE/DSF relative to standalone ACOLITE/DSF;
- 342 2. ACOLITE/TSDSF relative to standalone ACOLITE/DSF;
- 343 3. TMART+C2RCC relative to standalone C2RCC;
- 344 4. RAdCor+C2RCC relative to standalone C2RCC;
- 345 5. TMART+POLYMER relative to standalone POLYMER; and
- 346 6. RAdCor+POLYMER relative to standalone POLYMER.

347 GAAC was not included in the paired AEC benefit analyses because it is an integrated AEC+AC approach and
348 has no corresponding standalone AC result. For matchup i , AEC+AC combination j and wavelength λ , paired AEC
349 benefit was defined as:

$$B_{i,j,\lambda} = \text{SAE}_{i,j,\lambda}^{\text{standalone}} - \text{SAE}_{i,j,\lambda}^{\text{AEC+AC}}. \quad (4)$$

350 A positive value of $B_{i,j,\lambda}$ indicates that the AEC+AC combination produced a smaller retrieval error than the
351 corresponding standalone AC approach. A negative value indicates that the error increased after AEC. The same
352 standalone-minus-AEC+AC sign convention was applied to MdSA:

$$\Delta \text{MdSA}_{j,\lambda} = \text{MdSA}_{j,\lambda}^{\text{standalone}} - \text{MdSA}_{j,\lambda}^{\text{AEC+AC}}. \quad (5)$$

353 Each paired comparison used only matchups for which both the standalone AC result and the corresponding
354 AEC+AC result were finite and positive at the same wavelength.

355 To quantify disagreement among the available AEC+AC outputs relative to the magnitude of the retrieved
356 signal, we calculated a normalised interquartile range (IQR) for each matchup and wavelength. For this calculation,
357 the seven distinct outputs were GAAC, TMART+ACOLITE/DSF, TMART+C2RCC, TMART+POLYMER,
358 ACOLITE/TSDSF, RAdCor+C2RCC and RAdCor+POLYMER. For matchup i , wavelength λ and available output
359 set $\mathcal{K}_{i,\lambda}$, the normalised interquartile range was:

$$D_{i,\lambda} = 100 \frac{Q_{75}(\{R_{\text{rs},i,\lambda,k}\}_{k \in \mathcal{K}_{i,\lambda}}) - Q_{25}(\{R_{\text{rs},i,\lambda,k}\}_{k \in \mathcal{K}_{i,\lambda}})}{\text{median}_{k \in \mathcal{K}_{i,\lambda}} |R_{\text{rs},i,\lambda,k}|}. \quad (6)$$

360 Here, k indexes the available AEC+AC outputs. A matchup–wavelength group was retained when at least six
361 outputs were finite and the median absolute R_{rs} exceeded 10^{-5} sr^{-1} . Lake- and wavelength-specific results were
362 calculated from the median and IQR of the matchup event $D_{i,\lambda}$ values. For Figs. 5–8, MdSA, MAE, SSPB and
363 Pearson’s r were calculated from all valid matchup–wavelength records at 443, 492, 560, 665, 705 and 740 nm within
364 each lake and approach. We refer to these as validation metrics calculated across all six wavelengths.

365 Validation metrics retained only records with finite, positive in-situ and satellite-derived R_{rs} ; zero, negative,
366 missing and non-finite values were excluded. For GAAC, accepted replacements were used, unresolved exact
367 lower-bound outputs of 10^{-5} sr^{-1} were set to missing and accepted near-lower-bound outputs remained eligible
368 under the same value rule (related to GAAC retrieval results, see Section 4.2). Paired AEC benefit required finite,
369 positive in-situ, standalone and corresponding AEC+AC values for the same matchup and wavelength.

370 3.4 Sensitivity analyses of AEC benefit

371 The sensitivity analyses examined how paired AEC benefit varied with optical water type, distance from shore,
372 observation geometry and regional aerosol load. They comprised an OWT analysis at the WISPstation sites, a
373 distance-to-shoreline analysis for Lake Garda and two conditional regression models. Model M1 estimated the
374 associations of SZA and OWT jointly after accounting for viewing zenith angle (VZA) and lake. Model M2 added
375 one regional aerosol quantity to the M1 model.

376 As in Section 3.3, i denotes a matchup, j denotes one of the six AEC+AC comparisons and λ denotes one of the
377 six MSI wavelengths. The response was the paired AEC benefit $B_{i,j,\lambda}$ defined in Eq. 4. A separate regression was
378 fitted for each combination of j and λ . Each model specification therefore comprised $6 \times 6 = 36$ regressions.

3.4.1 Huber M regression

Ordinary least squares regression minimises the sum of squared residuals, thus observations with very large residuals can exert disproportionate influence on the estimated coefficients. The paired AEC benefit distributions contained such values. We therefore used Huber M regression, which behaves like ordinary least squares for moderate residuals but reduces the influence of larger residuals without removing the corresponding observations. For each AEC+AC combination j and wavelength λ , the Huber estimate was:

$$\hat{\boldsymbol{\theta}}_{j,\lambda} = \arg \min_{\boldsymbol{\theta}} \sum_i \mathcal{L}_c \left(\frac{B_{i,j,\lambda} - \mathbf{x}_{i,j,\lambda}^\top \boldsymbol{\theta}}{s_{j,\lambda}} \right), \quad (7)$$

where $\mathbf{x}_{i,j,\lambda}$ contains the model variables for matchup i , including the intercept, scaled continuous variables and categorical terms in the relevant model; $\boldsymbol{\theta}_{j,\lambda}$ is the corresponding coefficient vector; and $s_{j,\lambda}$ is an estimate of the residual magnitude. The residual for matchup i was:

$$r_{i,j,\lambda} = B_{i,j,\lambda} - \mathbf{x}_{i,j,\lambda}^\top \boldsymbol{\theta}_{j,\lambda}. \quad (8)$$

At each fitting step, the residual scale was estimated as:

$$s_{j,\lambda} = \frac{\text{median}_i |r_{i,j,\lambda}|}{\Phi^{-1}(0.75)} = 1.4826 \text{ median}_i |r_{i,j,\lambda}|, \quad (9)$$

where $\Phi^{-1}(0.75) = 0.67449$ is the 75th percentile of the standard normal distribution. The factor 1.4826 places the median absolute residual centred at zero on approximately the same scale as a residual standard deviation under normally distributed errors (Rousseeuw and Croux, 1993). The Huber loss function in Eq. 7 was:

$$\mathcal{L}_c(u) = \begin{cases} \frac{1}{2}u^2, & |u| \leq c, \\ c|u| - \frac{1}{2}c^2, & |u| > c, \end{cases} \quad (10)$$

with tuning constant $c = 1.345$ (Huber, 1964). Residuals with $|u| \leq 1.345$ therefore contributed the same quadratic loss used by ordinary least squares, whereas larger residuals contributed a linear loss. The coefficients were estimated by iteratively re-weighted least squares. Residuals from one fit determined the weights for the next fit, and the procedure continued until the coefficients stabilised.

The separate Lake Garda distance-to-shoreline analysis used a Theil–Sen estimator, defined as the median slope among all pairs of observations (Sen, 1968). This estimator was used because the shoreline analysis related paired AEC benefit to one continuous variable without additional adjustment terms. Huber M regression was used for M1 and M2 because those models estimated several continuous and categorical terms simultaneously.

3.4.2 Variable scaling and categorical terms

Continuous variables were rescaled so that their coefficients represented interpretable changes. SZA was divided by 5° , thus its coefficient gives the change in paired AEC benefit associated with a 5° increase in SZA. VZA was divided by its observed interquartile range. Its coefficient gives the change associated with a one-IQR increase in VZA. Each aerosol quantity was divided by its own product-specific IQR, calculated once for the corresponding analysis and then held fixed across its 36 regressions.

OWT and lake were represented as categorical variables. The model therefore estimated separate terms for the observed OWT classes and lakes instead of imposing a numerical order or continuous relationship among them. OWT 3a and Lake Garda were used as reference categories. This parameterisation determines how the intercept and category coefficients are written but does not change the fitted values, the continuous variable coefficients or the pairwise comparisons among OWT classes.

3.4.3 Uncertainty and hypothesis tests

Several matchups could originate from the same Sentinel-2 acquisition and therefore share atmospheric conditions, observation geometry and image processing characteristics. Such matchups are statistically dependent. The complete Sentinel-2 scene identifier defined an independent cluster, and all matchups from the same acquisition remained together in every resampling step.

Confidence intervals (CIs) for the SZA and aerosol coefficients were obtained with a scene-pairs bootstrap. For each of 9,999 bootstrap replicates, scene identifiers were sampled with replacement, all matchups belonging to each

selected scene were retained together, and the complete Huber model was refitted. The 2.5th and 97.5th percentiles of the resulting coefficient distribution defined the 95% CI.

Two-sided hypothesis tests used a null-imposed Rademacher wild-scene bootstrap- t procedure (Cameron et al., 2008). For each coefficient, the model was first fitted under the null hypothesis that the coefficient equalled zero. All residuals belonging to one scene were then multiplied by the same randomly selected sign, either +1 or -1, and the model was refitted. This procedure was repeated 9,999 times. The unadjusted two-sided p value was the proportion of bootstrap statistics at least as extreme as the observed statistic. A finite +1 correction was applied to the numerator and denominator, therefore no resampling-based p value was described as zero.

Each SZA or aerosol analysis contained 36 simultaneous coefficient tests, corresponding to the six AEC+AC combinations at the six MSI wavelengths. Testing many coefficients increases the probability of obtaining low unadjusted p values by chance. We therefore corrected for multiple testing separately within each predefined analysis family. The 36 SZA coefficients formed one family, the 36 MERRA-2 aerosol coefficients formed a second family, and the 36 CAMS aerosol coefficients formed a third family.

Benjamini–Hochberg (BH) correction was applied independently within each family to control the false discovery rate, defined as the expected proportion of false positives among the coefficients identified as supported (Benjamini and Hochberg, 1995). A coefficient was classified as BH-supported when its BH-adjusted value was below 0.05.

The tests within each family were not independent because the same matchups contributed to several wavelengths and AEC+AC combinations. Benjamini–Yekutieli (BY) adjusted values were therefore also calculated independently within each family (Benjamini and Yekutieli, 2001). The BY procedure provides a more conservative correction when dependence among the tests is present. A coefficient was classified as BY-supported when its BY-adjusted value was below 0.05. Let:

$$f \in \{\text{SZA, MERRA, CAMS}\}$$

identify the analysis family. For AEC+AC combination j and wavelength λ ,

$$p_{j,\lambda}^{(f)},$$

denotes the unadjusted two-sided p value, while:

$$q_{j,\lambda}^{\text{BH},(f)} \quad \text{and} \quad q_{j,\lambda}^{\text{BY},(f)},$$

denote the corresponding BH- and BY-adjusted values. Thus, $q_{j,\lambda}^{\text{BH},(\text{SZA})}$ refers to the BH-adjusted SZA result, whereas $q_{j,\lambda}^{\text{BH},(\text{MERRA})}$ and $q_{j,\lambda}^{\text{BH},(\text{CAMS})}$ refer to the two aerosol analyses.

CI exclusion, BH support and BY support were described separately. The CIs quantify coefficient uncertainty using the scene-pairs bootstrap distribution. The unadjusted p values test the null hypothesis that the corresponding coefficient equals zero using the null-imposed wild-scene bootstrap. The q values additionally account for the 36 simultaneous tests within the relevant analysis family. A CI can therefore exclude zero even when the coefficient does not retain BH or BY support after multiple testing correction.

3.4.4 Optical water type and shoreline analyses

OWT classification was used to examine whether paired AEC benefit differed among water optical regimes. Each matchup was assigned an OWT from its in-situ R_{rs} spectrum using pyOWT (Bi and Hieronymi, 2024). The full pyOWT scheme defines ten classes. Five classes occurred in the dataset: 3a ($n = 59$), 3b ($n = 19$), 4a ($n = 73$), 4b ($n = 174$) and 5a ($n = 3$) (Fig. 4); one spectrum could not be classified.

OWT 3a denotes waters with low to moderate phytoplankton, detritus and coloured dissolved organic matter, while OWT 3b is its brighter, more strongly scattering counterpart. OWT 4a represents waters with elevated biomass and low short-wavelength reflectance caused by particle and coloured dissolved organic matter absorption, while OWT 4b is a brighter, green and more strongly scattering variant. OWT 5a represents substantially higher phytoplankton biomass and elevated reflectance near 560 nm and in the red-to-near-infrared range.

The WISPstation sites at Greifensee, Lake Geneva and Lake Trasimeno were analysed separately from Lake Garda because they provided repeated observations at constant local shoreline geometry. For each site s , OWT class c , AEC+AC combination j and wavelength λ , paired ΔMdSA was calculated using the sign convention in Eq. 5. The site-specific values were then combined using the number of valid matchups in each site-specific group as weights:

$$\Delta\text{MdSA}_{c,\lambda,j}^{\text{weighted}} = \frac{\sum_s n_{s,c,\lambda,j} \Delta\text{MdSA}_{s,c,\lambda,j}}{\sum_s n_{s,c,\lambda,j}}, \quad (11)$$

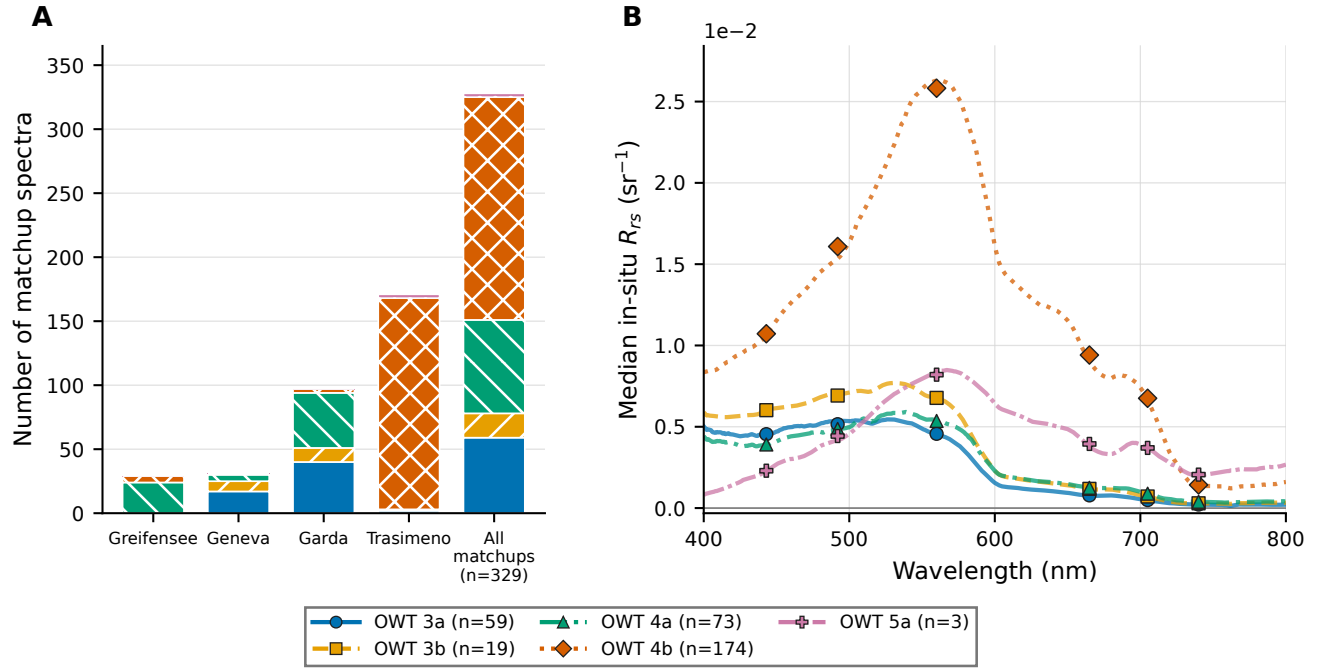


Figure 4: OWT composition and median in-situ reflectance spectra for the matchup dataset. Panel A gives retained matchup counts by lake and OWT class. Panel B shows class median hyperspectral R_{rs} curves, with symbols at the six MSI wavelengths.

where $n_{s,c,\lambda,j}$ is the number of valid matchups contributing to the corresponding site, OWT class, wavelength and AEC+AC combination.

Lake Garda was evaluated separately because its campaign locations span a broader distance-to-shoreline gradient. This distance analysis used RAdCor+POLYMER relative to standalone POLYMER and was fitted separately for each wavelength. A Theil–Sen slope related $B_{i,j,\lambda}$ to distance from the nearest shoreline and was expressed in percentage points of paired AEC benefit per kilometre. Two-sided 95% CIs were obtained from 9,999 scene-cluster bootstrap resamples. Within each wavelength, represented Sentinel-2 acquisition scenes were sampled with replacement, all valid matchups from each sampled scene were retained together and the Theil–Sen slope was recalculated. The 2.5th and 97.5th percentiles defined the interval. The analysis is described in Appendix 3.

3.4.5 Solar geometry and optical water type model (M1)

Model 1 (M1) estimated the associations of SZA and OWT simultaneously while accounting for VZA and lake. SZA and OWT were included in the same model because their distributions were not independent in the dataset. Particular OWT classes occurred more frequently in some lakes and under some illumination geometries than in others. A model containing SZA without OWT could therefore attribute differences among water types to SZA. Conversely, an OWT comparison without SZA could attribute differences in illumination geometry to OWT.

M1 addressed two complementary questions. The SZA coefficient estimated how paired AEC benefit changed with SZA when VZA, OWT class and lake were held constant. This is the OWT-adjusted SZA association. Differences among the fitted OWT terms estimated how paired AEC benefit differed among OWT classes when SZA, VZA and lake were held constant. These are the SZA-adjusted OWT contrasts.

For each AEC+AC combination j and wavelength λ , M1 was:

$$B_{i,j,\lambda} = \alpha_{j,\lambda}^{(1)} + \beta_{j,\lambda}^{SZA} \left(\frac{SZA_i}{5^\circ} \right) + \beta_{j,\lambda}^{VZA} \left(\frac{VZA_i}{IQR_{VZA}} \right) + \gamma_{OWT(i),j,\lambda} + \delta_{lake(i),j,\lambda} + \varepsilon_{i,j,\lambda}^{(1)} \quad (12)$$

Here, the coefficient $\beta_{j,\lambda}^{SZA}$ is the estimated change in paired AEC benefit per 5° increase in SZA after accounting for VZA, OWT and lake. The coefficient $\beta_{j,\lambda}^{VZA}$ accounts for variation associated with viewing geometry. The terms $\gamma_{OWT(i),j,\lambda}$ allow the modelled level of paired AEC benefit to differ among OWT classes, and $\delta_{lake(i),j,\lambda}$ accounts for persistent differences among the four lakes.

OWT 3a and Lake Garda were the reference categories. This choice affects the intercept and the way individual category coefficients are written but does not affect fitted values, SZA or VZA coefficients, or pairwise OWT comparisons.

For example:

$$\gamma_{\text{OWT } 4b,j,\lambda} - \gamma_{\text{OWT } 4a,j,\lambda}, \quad (13)$$

compares paired AEC benefit between OWT 4b and OWT 4a for observations with comparable SZA, VZA and lake. The M1 model includes lake as a categorical term and therefore accounts for average differences in paired AEC benefit among the four lakes. It nevertheless estimates one common SZA coefficient from the complete dataset. We used two exploratory analyses to examine whether that coefficient adequately represented the individual lakes.

First, each of the 36 M1 analyses was extended by adding interactions between SZA and lake. These interaction terms allowed the SZA coefficient to differ among lakes. A joint test of the three lake-by-SZA interaction terms evaluated the null hypothesis that the SZA association was the same in all four lakes. The 36 joint tests formed a separate exploratory family for BH and BY correction. Support for a lake-by-SZA interaction indicates that at least one lake had a different SZA association and that one common coefficient did not describe all four lakes equally well.

Second, the RAdCor+POLYMER SZA models were refitted four times, each time omitting all matchups from one lake. These leave-one-lake-out refits assessed whether the coefficient estimated from all four lakes depended strongly on the contribution of an individual lake. They were evaluated descriptively from the coefficient estimates and scene-pairs bootstrap CIs. No p values, q values or significance classifications were assigned. A large change in coefficient magnitude or sign indicates sensitivity to lake composition.

Five observed OWT classes yield ten pairwise OWT contrasts within each of the 36 M1 regressions, giving 360 contrasts. All 360 estimates were retained descriptively. Formal inference was limited to contrasts for which each OWT class was represented by at least ten independent Sentinel-2 scenes and at least one lake contained five independent scenes from each class. This support criterion was applied to the contrast inference only; it did not remove observations from the fitted M1 regressions.

For each contrast eligible for formal inference under the independent-scene criterion, the standard error was calculated from the scene-clustered covariance matrix of the fitted Huber model. The 95% CI was the contrast estimate plus or minus 1.96 times its scene-clustered standard error, and the unadjusted two-sided p value used the corresponding normal approximation. These OWT contrasts formed a separate multiplicity family to which BH and BY correction were applied. These scene-clustered CIs differ from the scene-pairs bootstrap CIs used for the SZA coefficients.

3.4.6 Aerosol load model (M2)

Model 2 (M2) added one regional aerosol quantity to the SZA, VZA, OWT and lake terms in M1. MERRA-2 and CAMS were analysed in separate models. As in M1, a separate regression was fitted for each of the six AEC+AC combinations and six MSI wavelengths:

$$\begin{aligned} B_{i,j,\lambda} = & \alpha_{j,\lambda}^{(2,d)} + \beta_{j,\lambda}^{\text{aer},d} \left(\frac{A_{i,d}}{\text{IQR}(A_d)} \right) + \beta_{j,\lambda}^{\text{SZA},d} \left(\frac{\text{SZA}_i}{5^\circ} \right) \\ & + \beta_{j,\lambda}^{\text{VZA},d} \left(\frac{\text{VZA}_i}{\text{IQR}_{\text{VZA}}} \right) + \gamma_{\text{OWT}(i),j,\lambda}^d + \delta_{\text{lake}(i),j,\lambda}^d + \varepsilon_{i,j,\lambda}^{(2,d)}, \end{aligned} \quad (14)$$

where $d \in \{\text{MERRA}, \text{CAMS}\}$ identifies the aerosol dataset, $A_{i,d}$ is the corresponding aerosol quantity for matchup i and the product-specific interquartile range $\text{IQR}(A_d)$. The IQR was calculated once for the corresponding aerosol analysis and held fixed across its 36 regressions. The primary aerosol analysis used MERRA-2 total aerosol scattering optical thickness at 550 nm:

$$A_{i,\text{MERRA}} = \tau_{\text{sca},i}^{\text{aer}}(550 \text{ nm}), \quad (15)$$

from TOTSCATAU. Its matchup event IQR was 0.08609. The coefficient $\beta_{j,\lambda}^{\text{aer},\text{MERRA}}$ is the estimated change in paired AEC benefit associated with one MERRA-2 scattering AOT IQR after accounting for SZA, VZA, OWT and lake. The secondary aerosol analysis used CAMS EAC4 total aerosol optical depth at 550 nm:

$$A_{i,\text{CAMS}} = \text{AOD}_{550,i}. \quad (16)$$

Its matchup event IQR was 0.13325. The coefficient $\beta_{j,\lambda}^{\text{aer},\text{CAMS}}$ is the corresponding change in paired AEC benefit per CAMS AOD_{550} IQR after accounting for the same model variables. For each aerosol product, M1 was refitted using the same matchups and OWT specification as M2. The difference between these M1 and M2 estimates for

the same sample therefore measures the change associated with adding the aerosol quantity instead of a change in data availability. The primary M2 analysis retained all five observed OWT classes. As a sensitivity analysis, M2 and its corresponding M1 fit for the same sample were repeated using only OWT 3a, 4a and 4b, the three classes represented by at least 20 matchups. The product-specific aerosol IQR was recalculated for this restricted analysis. The primary MERRA-2 M2 regressions were also refitted four times in a leave-one-lake-out analysis, each time omitting one lake while retaining the aerosol IQR over the entire sample. A direction was retained only when the coefficient sign matched the sign over the full dataset after every individual lake omission.

4 Results

4.1 Remote-sensing reflectance matchups

The ten approaches produced different validation rankings across the four lakes. RAdCor+POLYMER achieved the lowest MdSA in Greifensee, Lake Geneva and Lake Trasimeno, whereas TMART+POLYMER produced the lowest MdSA in Lake Garda (Figs. 5–8). The unweighted mean of the four lake-specific MdSA values was 46.9% for standalone POLYMER and 30.8% for RAdCor+POLYMER. The corresponding difference was 16.1 %pt., equivalent to 34.3% of the standalone POLYMER value.

Greifensee showed the largest response to prior AEC (Fig. 5). The standalone approaches produced MdSA values between 82.1 and 89.2%, whereas GAAC, RAdCor+C2RCC and RAdCor+POLYMER reduced MdSA to 45.9, 37.4 and 32.6%, respectively. RAdCor+POLYMER therefore had an MdSA 49.5 %pt. lower than standalone

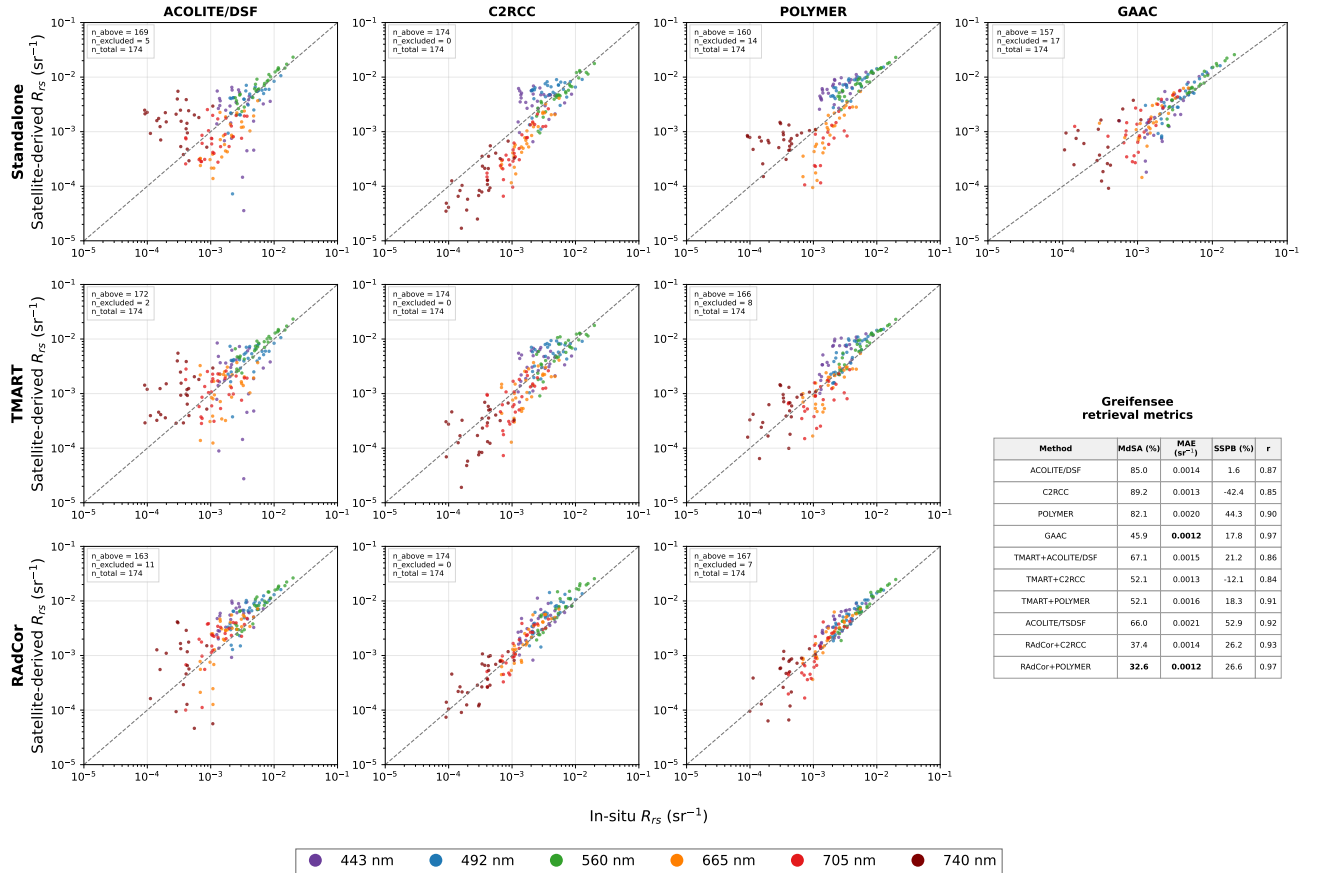


Figure 5: Satellite-in-situ R_{rs} comparison and retrieval metrics for Greifensee WISPstation matchups. Columns show ACOLITE/DSF, C2RCC, POLYMER and GAAC; rows show standalone, TMART and RAdCor approaches. Point colours identify the six MSI wavelengths and the dashed line is the 1:1 relation. Panel annotations use one common denominator within each lake: n_{total} is the number of possible lake matchups multiplied by six MSI wavelengths, n_{above} counts R_{rs} outputs above $1.05 \times 10^{-5} \text{ sr}^{-1}$ and $n_{excluded} = n_{total} - n_{above}$.

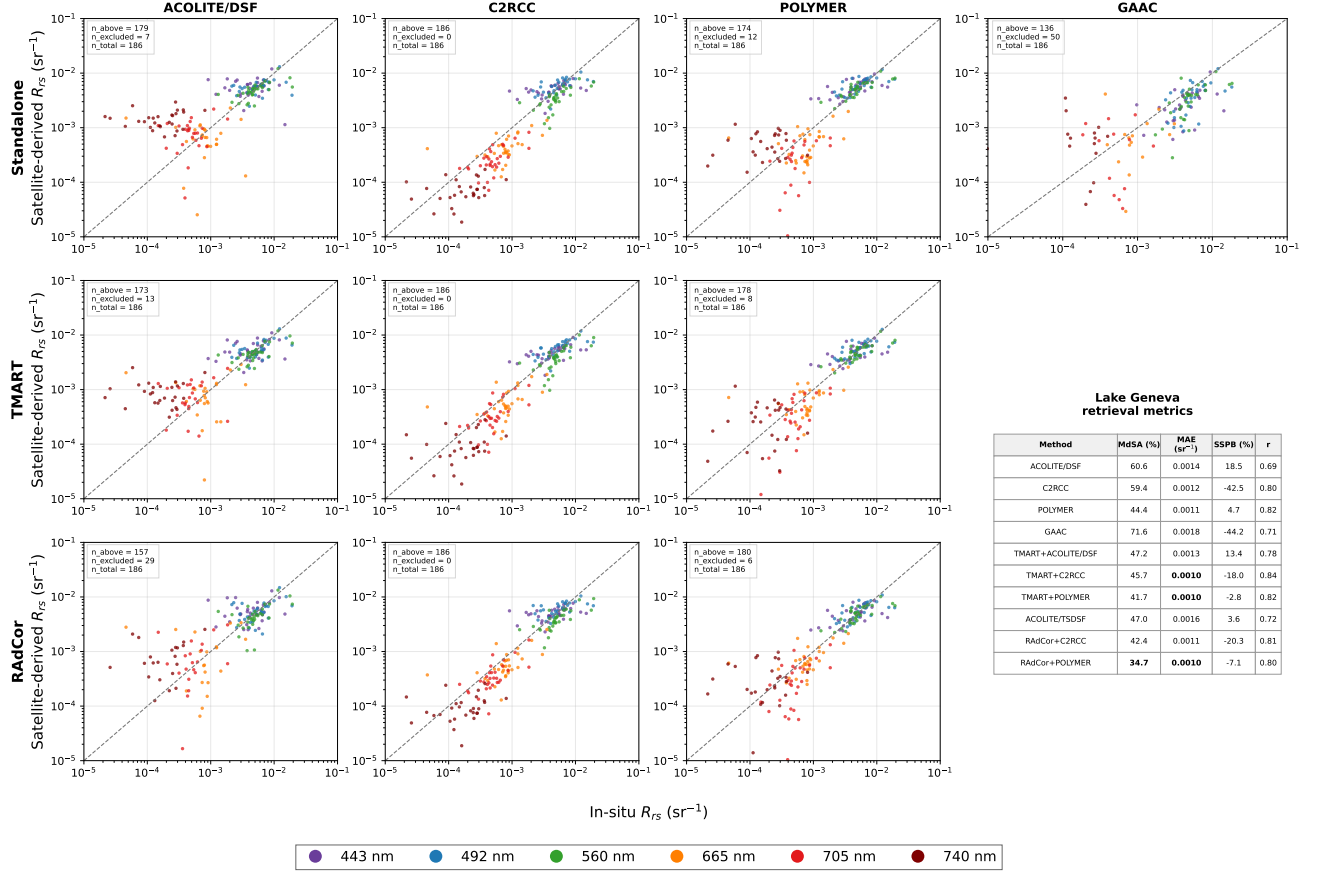


Figure 6: Satellite-in-situ R_{rs} comparison and retrieval metrics for Lake Geneva WISPstation matchups. Columns show ACOLITE/DSF, C2RCC, POLYMER and GAAC; rows show standalone, TMART and RAdCor approaches. Point colours identify the six MSI wavelengths and the dashed line is the 1:1 relation. Panel annotations use one common denominator within each lake: n_{total} is the number of possible lake matchups multiplied by six MSI wavelengths, n_{above} counts R_{rs} outputs above $1.05 \times 10^{-5} \text{ sr}^{-1}$ and $n_{excluded} = n_{total} - n_{above}$.

POLYMER. RAdCor+POLYMER and GAAC also produced the lowest MAE values at this site and both reached a Pearson correlation of 0.97. The SSPB results showed that prior AEC altered not only error magnitude but also retrieval bias. For example, the negative SSPB of standalone C2RCC was reduced by TMART+C2RCC, whereas RAdCor+C2RCC changed the sign of the bias.

Lake Geneva showed the same overall ranking. Standalone POLYMER was the most accurate of the three standalone AC approaches, with an MdSA of 44.4%, and RAdCor+POLYMER produced the lowest MdSA overall, at 34.7% (Fig. 6). TMART+POLYMER, RAdCor+C2RCC and TMART+C2RCC formed a second group with MdSA values between 41.7 and 45.7%. The ACOLITE-based AEC+AC approaches produced similar MdSA values of approximately 47%, whereas GAAC had the largest retrieval error at this site. Within the POLYMER branch, prior AEC reduced both MdSA and the magnitude of SSPB, with TMART+POLYMER producing an SSPB close to zero and RAdCor+POLYMER producing a small negative SSPB.

Lake Trasimeno produced the lowest retrieval errors overall. RAdCor+POLYMER, GAAC and TMART+POLYMER all achieved MdSA below 20%, while standalone POLYMER remained close at 22.8%. Differences among these four approaches were therefore much smaller than those observed in Greifensee (Fig. 7). The same pattern occurred within the C2RCC branch, where both AEC combinations reduced MdSA relative to standalone C2RCC and reduced the magnitude of the negative SSPB. The three ACOLITE-based approaches were more closely grouped and all produced MdSA values between 32.6 and 33.5%.

Lake Garda differed from the three WISPstation sites. The three POLYMER-based results were nearly identical, with MdSA values of 37.9% for TMART+POLYMER, 38.1% for RAdCor+POLYMER and 38.3% for standalone POLYMER. Their MAE, SSPB and Pearson correlation values were also similar (Fig. 8). The C2RCC-based approaches showed only small differences in MdSA, whereas the ACOLITE branch showed a clearer separation:

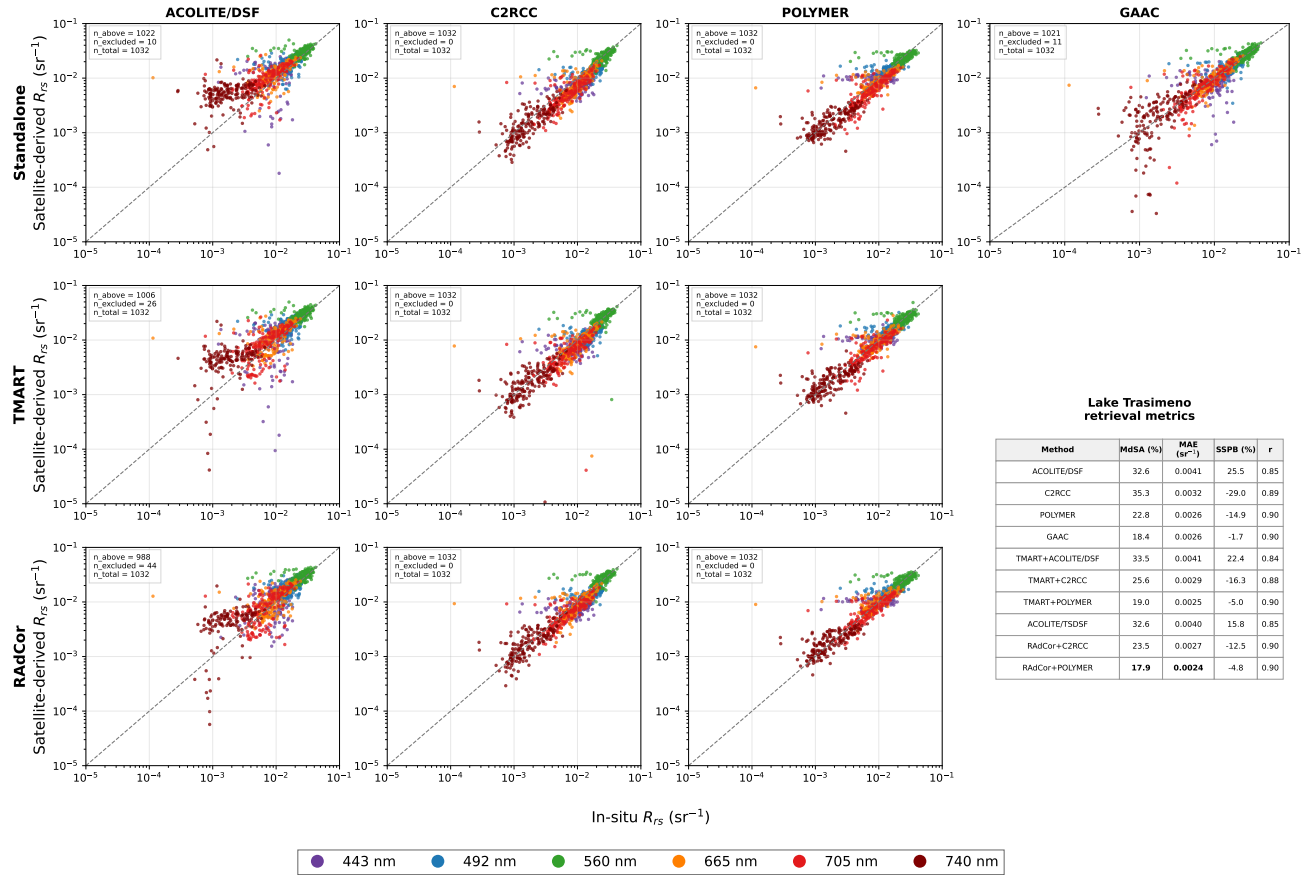


Figure 7: Satellite-in-situ R_{rs} comparison and retrieval metrics for Lake Trasimeno WISPstation matchups. Columns show ACOLITE/DSF, C2RCC, POLYMER and GAAC; rows show standalone, TMART and RadCor approaches. Point colours identify the six MSI wavelengths and the dashed line is the 1:1 relation. Panel annotations use one common denominator within each lake: n_{total} is the number of possible lake matchups multiplied by six MSI wavelengths, n_{above} counts R_{rs} outputs above $1.05 \times 10^{-5} \text{ sr}^{-1}$ and $n_{excluded} = n_{total} - n_{above}$.

standalone ACOLITE/DSF had an MdSA of 65.9%, TMART+ACOLITE/DSF had an MdSA of 74.5%, and ACOLITE/TSDF had an MdSA of 94.5%. Thus, prior AEC did not produce a consistent lake-wide improvement in Lake Garda, and the result depended strongly on the downstream AC approach.

The wavelength analysis compared each AEC+AC result with the corresponding standalone AC result (Fig. 9). Prior AEC reduced MdSA in 98 of the 144 lake, approach and wavelength comparisons, corresponding to 68%. Positive changes were least frequent at 560 nm and became increasingly common towards longer wavelengths. Prior AEC reduced MdSA in 19 of 24 comparisons at 665 nm, 22 of 24 at 705 nm and 21 of 24 at 740 nm. By contrast, positive changes occurred in 14 of 24 comparisons at 443 nm, 13 of 24 at 492 nm and only 9 of 24 at 560 nm.

The frequency of positive changes also differed among lakes. Greifensee showed the largest number of improvements, followed by Lake Trasimeno and Lake Geneva, whereas Lake Garda showed the fewest. Every AEC+AC combination reduced MdSA at 443, 665 and 705 nm in Greifensee, at 705 and 740 nm in Lake Geneva, and at 740 nm in Lake Trasimeno. Across all four lakes, improvements were therefore concentrated at 665–740 nm, while changes at 560 nm were smaller and less consistently positive.

Agreement among the seven AEC+AC approaches also depended strongly on wavelength (Fig. 10). The analysis retained all 1,974 event-wavelength groups from the 329 matchup events. Median normalised disagreement was lowest at 560 nm, at 15.9%, and increased towards longer wavelengths, reaching 48.1% at 705 nm and 104.4% at 740 nm. The same wavelength dependence occurred in all four lakes. At 740 nm, the lake-specific median disagreement was 143.3% in Lake Garda, 142.4% in Lake Geneva, 93.7% in Greifensee and 72.5% in Lake Trasimeno. Lake Trasimeno generally showed the smallest disagreement among AEC+AC approaches, whereas Lake Garda and Lake Geneva showed the largest disagreement at 705 and 740 nm. These results show that the choice of AEC+AC approach had relatively little effect at 560 nm but produced substantially different retrievals at the longer MSI wavelengths.

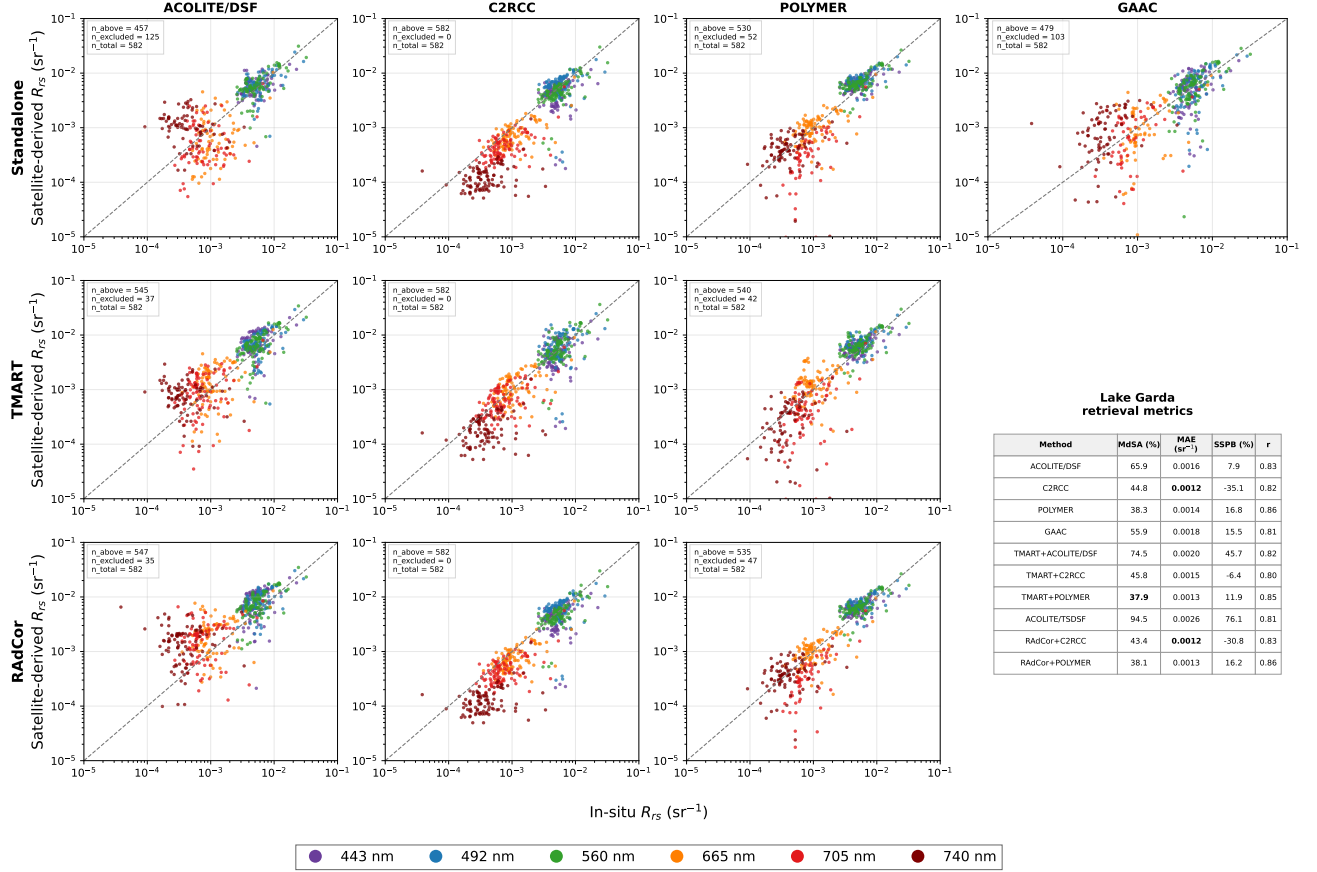


Figure 8: Satellite-in-situ R_{rs} comparison and retrieval metrics for the Lake Garda matchups acquired from 12 September 2015 to 9 July 2024. Columns show ACOLITE/DSF, C2RCC, POLYMER and GAAC; rows show standalone, TMART and RAdCor approaches. Point colours identify the six MSI wavelengths and the dashed line is the 1:1 relation. Panel annotations use one common denominator within each lake: n_{total} is the number of possible lake matchups multiplied by six MSI wavelengths, n_{above} counts R_{rs} outputs above $1.05 \times 10^{-5} \text{ sr}^{-1}$ and $n_{excluded} = n_{total} - n_{above}$.

4.2 GAAC lower-bound remote-sensing reflectance retrieval

Some GAAC matchup spectra reached the approach lower bound for R_{rs} , which appeared as exactly $R_{rs} = 1 \times 10^{-5} \text{ sr}^{-1}$. These instances were investigated with a custom procedure and were not interpreted as physically meaningful near-zero water-leaving reflectance. The procedure recovered 16 flagged GAAC values where investigation supported correction and masked 169 unresolved exact lower-bound values from GAAC validation statistics. The lower-bound behaviour was consistent with GAAC correction terms driving the pre-clipped water-leaving reflectance below zero, mainly through aerosol/sky path closure and residual glint sensitivity. The complete investigation and accepted recovery rules are detailed in Appendix 2.

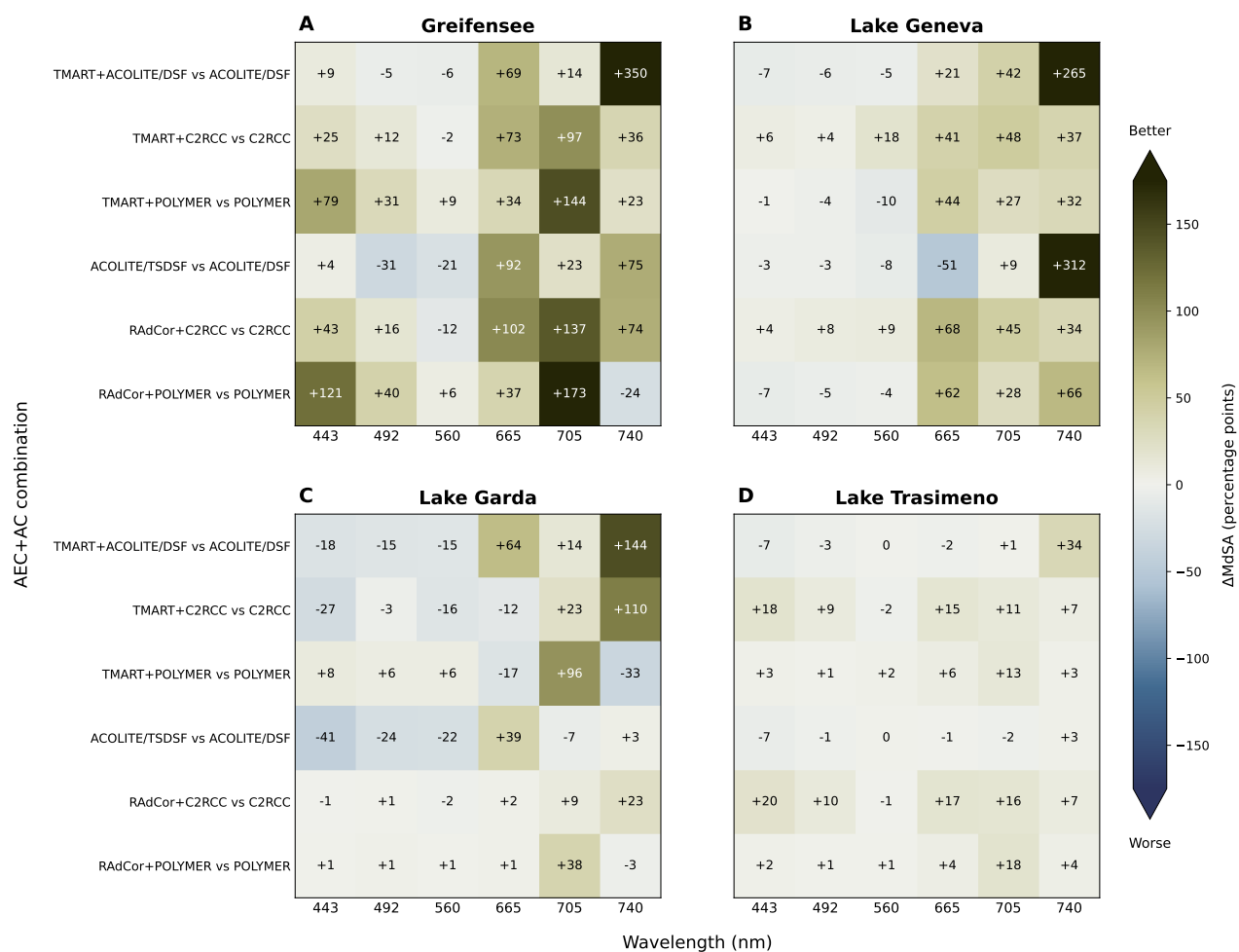


Figure 9: Change in match-up agreement after prior AEC. Panels show Greifensee (A), Lake Geneva (B), Lake Garda (C) and Lake Trasimeno (D). Each heatmap entry describes $\Delta\text{MdSA} = \text{MdSA}(\text{standalone AC}) - \text{MdSA}(\text{AEC} + \text{the same AC})$ for one wavelength, prior AEC method and downstream AC approach. Positive values indicate lower MdSA after AEC. The colour scale is centred at zero and saturated at ± 175 %pt.; printed values retain their full magnitude.

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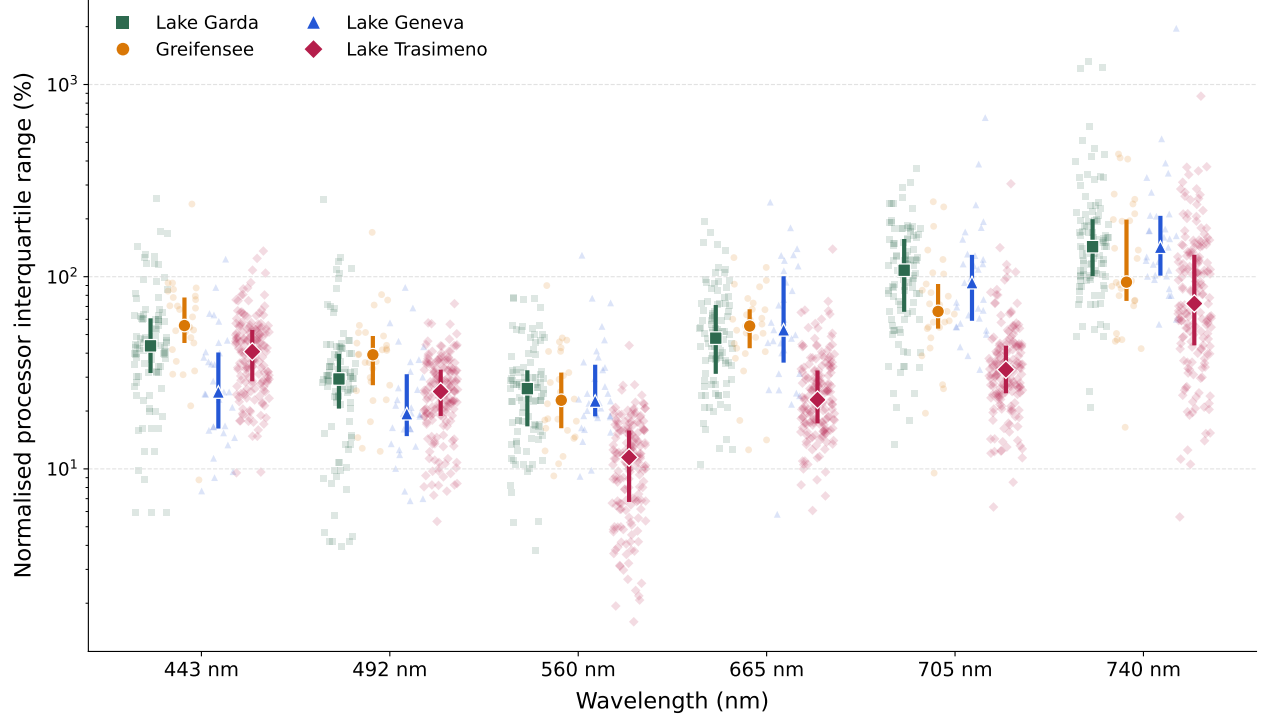


Figure 10: Normalised disagreement among AEC+AC approaches. Each translucent point is one retained matchup event–wavelength group containing at least six outputs drawn from GAAC, TMART+ACOLITE/DSF, TMART+C2RCC, TMART+POLYMER, ACOLITE/TSDSF, RAdCor+C2RCC and RAdCor+POLYMER. The value is 100 times the output interquartile range divided by the median absolute R_{rs} for the same matchup event and wavelength, which was required to exceed 10^{-5} sr^{-1} . Large symbols show lake-specific medians and vertical bars show the corresponding matchup event interquartile ranges.

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4.3 Sensitivity analyses

The sensitivity analyses examined whether paired AEC benefit differed among OWTs, changed with distance from shore or varied with regional aerosol load and solar geometry. The WISPstation observations provided comparisons among OWT classes under constant site geometry, whereas the spatially distributed Lake Garda observations were used to examine distance from shore. M1 estimated the SZA and OWT associations jointly after adjustment for VZA and lake, and M2 added one regional aerosol quantity to the same model structure. Together, these analyses separated the broad patterns observed at the fixed sites from associations estimated after accounting for observation geometry and lake.

4.3.1 Optical water type and shoreline distance

At the WISPstation sites, the reduction in retrieval error produced by AEC differed strongly among OWT classes and wavelengths (Fig. 11). Across the displayed AEC+AC combinations and wavelengths, mean weighted paired Δ MdSA was 79.9 %pt. for OWT 4a and 5.3 %pt. for OWT 4b. The mean response also increased towards the longer MSI wavelengths. Averaged across OWT classes and AEC+AC combinations, weighted paired Δ MdSA was 38.7 %pt. at 665 nm, 57.8 %pt. at 705 nm and 119.6 %pt. at 740 nm, whereas the mean responses at 492 and 560 nm were small. Thus, the largest mean AEC benefits occurred in OWT 4a and at 665–740 nm.

The response also differed among AEC+AC combinations. The C2RCC-based combinations produced positive Δ MdSA in most OWT–wavelength combinations, indicating lower MdSA after AEC in most of these strata. The ACOLITE- and POLYMER-based validation response depended more strongly on OWT class and wavelength.

After adjustment for SZA, VZA and lake in M1, the evidence for systematic differences among OWT classes was more limited. Of the 121 contrasts with sufficient independent-scene support, 9 had 95% scene-clustered CIs that lay entirely above or below zero, and one contrast had both BH- and BY-adjusted values below 0.05. Most adjusted OWT contrasts therefore did not establish a clear difference in paired AEC benefit between classes.

The supported contrast occurred for RAdCor+POLYMER relative to standalone POLYMER at 443 nm. Paired AEC benefit was 31.5 %pt. lower in OWT 4b than in OWT 4a (95% CI: –37.9 to –25.1 %pt.). For observations with

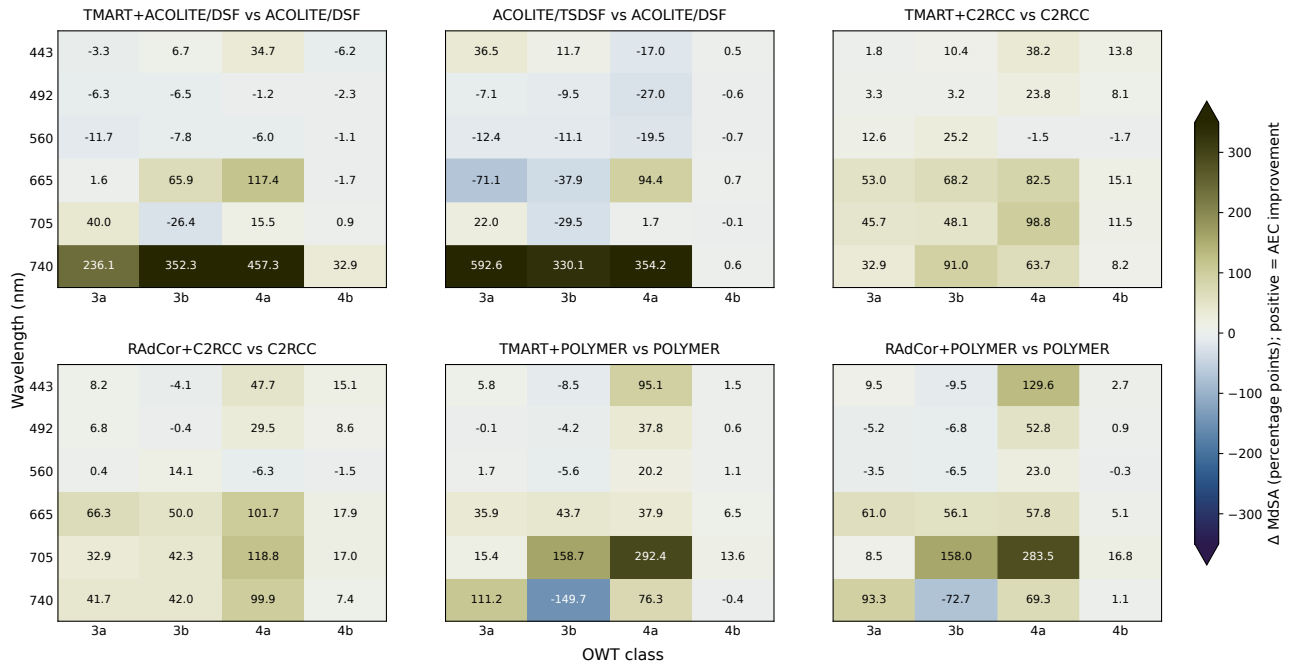


Figure 11: OWT-stratified benefit of prior AEC at the three WISPstation sites. Values are weighted paired Δ MdSA across Greifensee, Lake Geneva and Lake Trasimeno, with site weights equal to the number of valid matchups in the corresponding site-specific group. Positive values indicate lower MdSA after AEC, whereas negative values indicate higher MdSA. The colour scale is centred at zero and saturated at ± 400 %pt.; printed values keep their full magnitude. Lake Garda is analysed separately by shoreline distance in Appendix 3. OWT 5a was excluded from this visualisation because of its low abundance (n=3).

comparable SZA, VZA and lake, RAdCor therefore reduced POLYMER retrieval error more strongly in OWT 4a than in OWT 4b at 443 nm.

In Lake Garda, paired AEC benefit did not show a consistent dependence on distance from shore. While most wavelength-specific slopes were negative, indicating a tendency for AEC benefit to decrease with increasing distance from shore, only the 492 nm scene-cluster bootstrap interval excluded zero (-0.28 %pt. km^{-1} , 95% CI: -0.72 to -0.01 %pt. km^{-1}). The largest estimated decline occurred at 705 nm (-4.24 %pt. km^{-1}), but its uncertainty was substantially larger and the interval included zero, as did those at 443, 560, 665 and 740 nm. Following exploratory BH and BY adjustment across the six wavelength-specific shoreline tests, no distance-to-shoreline association remained supported (see Appendix 3 for more details).

4.3.2 Regional aerosol loading

Both aerosol reanalyses identified the same principal result: higher regional aerosol load was associated mainly with larger AEC benefits for the RAdCor-based combinations, particularly at 705 nm. The coefficient signs agreed between MERRA-2 and CAMS in 35 of the 36 analyses defined by the six AEC+AC combinations and six wavelengths. Eight positive RAdCor associations had $q_{j,\lambda}^{\text{BH,(MERRA)}} < 0.05$ and $q_{j,\lambda}^{\text{BH,(CAMS)}} < 0.05$ for the same AEC+AC combination and wavelength (Fig. 12). The aerosol response was therefore concentrated in selected RAdCor combinations and wavelengths and not shared by all 36 analyses.

In the primary MERRA-2 analysis, positive associations were retained for RAdCor+C2RCC at 560, 665, 705 and 740 nm and for RAdCor+POLYMER at 492, 560, 665, 705 and 740 nm. Across all 36 coefficients, the median association was $+0.237$ %pt. per MERRA-2 scattering AOT IQR, and the coefficients ranged from -4.757 to $+17.328$ %pt. per IQR. Thirteen 95% scene-pairs bootstrap CIs lay entirely above or below zero. Of the 36 MERRA-2 coefficients, 10 had $q_{j,\lambda}^{\text{BH,(MERRA)}} < 0.05$, and 8 had $q_{j,\lambda}^{\text{BY,(MERRA)}} < 0.05$.

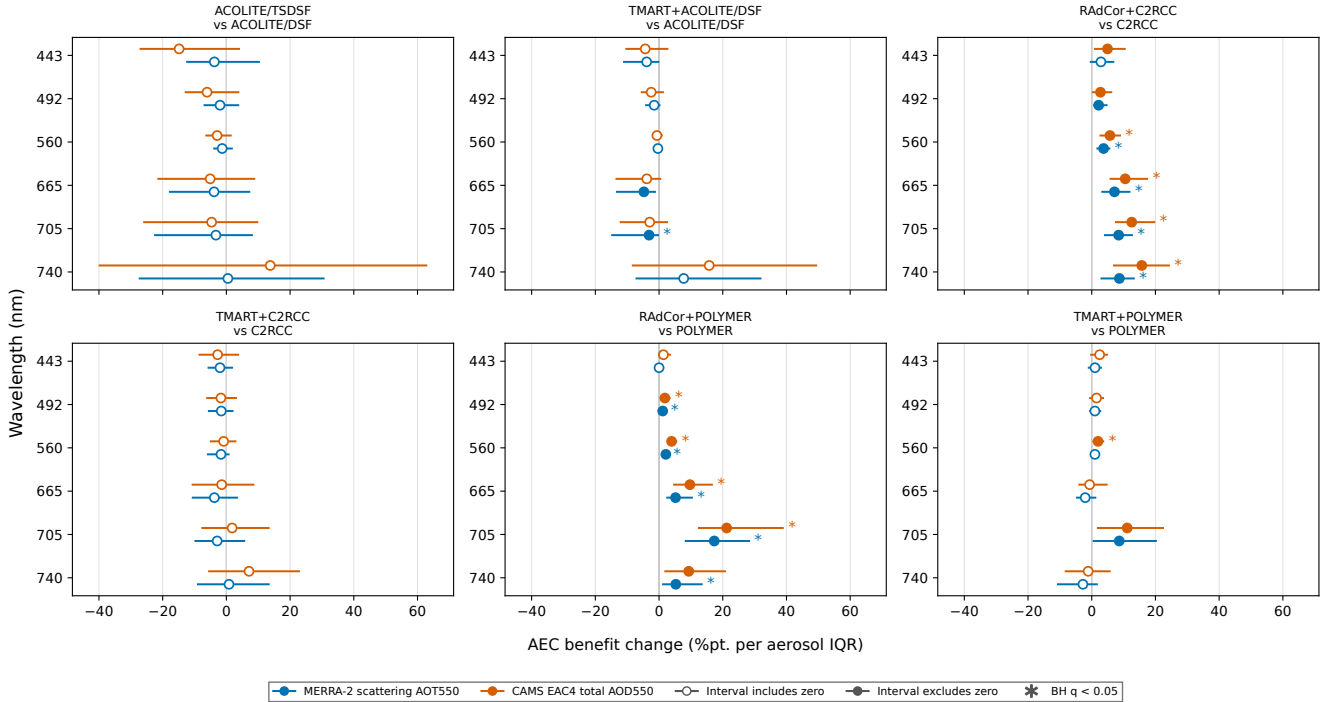


Figure 12: Conditional associations between regional aerosol load and AEC benefit from M2. The six panels show the six AEC+AC combinations, each compared with its corresponding standalone AC approach. Positive coefficients indicate that AEC benefit increased with aerosol load, whereas negative coefficients indicate that it decreased. Blue points show coefficients per IQR of MERRA-2 total aerosol scattering optical thickness at 550 nm, and orange points show coefficients per IQR of CAMS EAC4 total aerosol optical depth at 550 nm. The two aerosol products were fitted separately, with adjustment for SZA, VZA, OWT class and lake. Horizontal lines are 95% scene-pairs bootstrap CIs, and filled points identify intervals that do not include zero. Asterisks identify MERRA-2 coefficients with $q_{j,\lambda}^{\text{BH,(MERRA)}} < 0.05$ and CAMS coefficients with $q_{j,\lambda}^{\text{BH,(CAMS)}} < 0.05$.

The largest MERRA-2 coefficient occurred for RAdCor+POLYMER at 705 nm. A one-IQR increase in MERRA-2 scattering AOT was associated with a 17.33 %pt. larger reduction in retrieval error from adding RAdCor before POLYMER (95% CI: 8.07 to 28.56 %pt. per IQR). The only supported negative MERRA-2 association occurred for TMART+ACOLITE/DSF at 705 nm. In that analysis, a one-IQR increase in scattering AOT was associated with a 3.14 %pt. smaller AEC benefit (coefficient: -3.14 %pt. per IQR; 95% CI: -15.01 to -0.03 %pt. per IQR).

The separate CAMS analysis reproduced the main directional pattern. The CAMS coefficients had a median of +1.651 %pt. per CAMS AOD₅₅₀ IQR and ranged from -14.829 to +21.223 %pt. per IQR. Thirteen CIs lay entirely above or below zero. Of the 36 CAMS coefficients, 9 had $q_{j,\lambda}^{BH,(CAMS)} < 0.05$, and 7 had $q_{j,\lambda}^{BY,(CAMS)} < 0.05$. Eight positive associations were supported with both products: RAdCor+C2RCC at 560, 665, 705 and 740 nm, and RAdCor+POLYMER at 492, 560, 665 and 705 nm. MERRA-2 additionally supported RAdCor+POLYMER at 740 nm and the negative TMART+ACOLITE/DSF association at 705 nm, whereas CAMS additionally supported a positive TMART+POLYMER association at 560 nm.

The two products therefore identified the same principal RAdCor response, although the numerical coefficient sizes differed. Across the eight RAdCor associations supported by both products, the CAMS coefficient was numerically larger in every case. For RAdCor+POLYMER, the CAMS and MERRA-2 coefficients were 1.82 and 1.15 %pt. per IQR at 492 nm and 21.22 and 17.33 %pt. per IQR at 705 nm, respectively. These magnitudes cannot be compared as measurements of the same physical increment because MERRA-2 and CAMS represent different aerosol quantities and were scaled by different product-specific IQRs.

Regional aerosol load also covaried with SZA in the available observations. Higher SZA values tended to occur with lower aerosol values: Pearson's r was -0.356 for MERRA-2 scattering optical thickness and -0.424 for CAMS AOD₅₅₀. When M1 was refitted using the same events as the MERRA-2 model, adding the aerosol term changed the sign of 9 of the 36 SZA coefficients, with a median absolute change of 0.320 %pt. per 5°.

For RAdCor+POLYMER at 705 nm, the SZA coefficient changed from -1.957 %pt. per 5° in M1 to +0.123 %pt. per 5° in M2. The estimated decrease in AEC benefit with SZA was therefore reduced to a value close to zero after regional aerosol load was included. At 740 nm, the coefficient increased from +1.007 to +1.692 %pt. per 5°. In contrast, the direction of 142 of 144 directly parameterised OWT coefficients relative to OWT 3a was unchanged after the aerosol term was added. The aerosol adjustment therefore altered several SZA estimates but had little effect on the direction of these coefficients.

Restricting the analysis to the more frequently represented OWT 3a, 4a and 4b classes preserved the main aerosol result. Within this sensitivity analysis, eight coefficients for each aerosol product had BH-adjusted values below 0.05, and only three product-specific BH decisions changed relative to the analysis with all OWT classes. The positive RAdCor associations identified by both MERRA-2 and CAMS remained present.

4.3.3 Solar geometry

SZA was associated with paired AEC benefit in a subset of the analyses, but the direction and magnitude of the association differed among AEC+AC combinations and wavelengths. Higher SZA corresponded to greater AEC benefit in some cases and smaller AEC benefit in others.

M1 produced 12 of 36 scene-pairs bootstrap CIs excluding zero. Of the 36 SZA coefficients, 8 had $q_{j,\lambda}^{BH,(SZA)} < 0.05$, and 4 had $q_{j,\lambda}^{BY,(SZA)} < 0.05$. The median association was +0.224 %pt. of paired AEC benefit per 5° increase in SZA, with a range from -8.118 to +1.889 %pt. per 5°. The coefficients with $q_{j,\lambda}^{BH,(SZA)} < 0.05$ spanned both signs and several AEC+AC combinations: RAdCor+C2RCC at 665 and 705 nm; RAdCor+POLYMER at 560 and 705 nm; TMART+ACOLITE/DSF at 740 nm; and TMART+POLYMER at 492, 560 and 705 nm. Thus, the analysis identified supported SZA associations for selected AEC+AC combinations and wavelengths, but no single positive or negative response described all 36 analyses.

The RAdCor+POLYMER results illustrate this wavelength dependence (Fig. 13). At 560 nm, paired AEC benefit increased by 0.437 %pt. for each 5° increase in SZA. At 705 nm, paired AEC benefit decreased by 1.937 %pt. for each 5° increase in SZA. For both coefficients, $q_{j,\lambda}^{BH,(SZA)} < 0.05$. Higher SZA was therefore associated with greater RAdCor+POLYMER benefit at 560 nm but smaller benefit at 705 nm.

At 443, 492, 665 and 740 nm, the analysis did not establish a clear SZA association for RAdCor+POLYMER because the CIs included zero or $q_{j,\lambda}^{BH,(SZA)} \geq 0.05$. Panel A of Fig. 13 also shows broad distributions of paired AEC benefit at 665–740 nm and substantial overlap among lakes across the sampled SZA range. The RAdCor+POLYMER response therefore varied by wavelength without a common SZA relationship.

To assess whether one SZA coefficient adequately represented all four lakes, exploratory versions of M1 allowed the SZA association to differ by lake. The joint lake-by-SZA interaction tests had BH-adjusted values below 0.05 in 11 of the 36 analyses and BY-adjusted values below 0.05 in 9 analyses. For these analyses, the association between

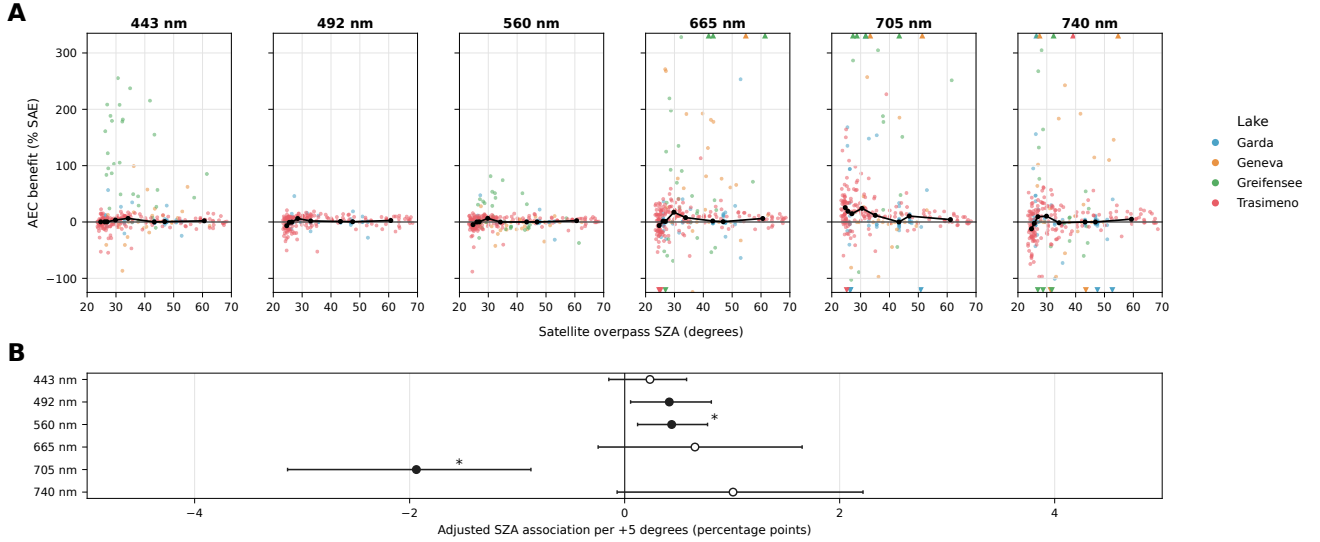


Figure 13: SZA analysis for RAdCor+POLYMER relative to standalone POLYMER. Panel A shows observed paired AEC benefit by wavelength and lake. Triangles at the upper and lower boundaries denote observations outside the displayed benefit range; black points and connecting lines are medians in SZA quantile bins containing at least eight observations. Panel B shows the M1 Huber SZA coefficient at each wavelength after adjustment for VZA, OWT class and lake, expressed per 5° increase. Positive coefficients indicate that paired AEC benefit increased with SZA, whereas negative coefficients indicate that paired AEC benefit decreased with SZA. Horizontal lines are 95% scene-pairs bootstrap CIs, and filled points have CIs excluding zero. Asterisks identify coefficients with $q_{j,\lambda}^{BH,(SZA)} < 0.05$ within the family of 36 M1 SZA coefficients.

SZA and paired AEC benefit differed among lakes, thus the coefficient estimated from the complete dataset did not describe every lake equally well.

The leave-one-lake-out refits show how the RAdCor+POLYMER estimates depended on lake composition. At 705 nm, the coefficient estimated from all four lakes was -1.937 %pt. per 5°. Omitting Lake Trasimeno changed the estimate to $+2.359$ %pt. per 5°, with a wide CI from -19.24 to $+22.47$ %pt. per 5°. The refit without Lake Trasimeno therefore did not establish whether paired AEC benefit increased or decreased with SZA. The change in sign shows that the estimate from the four lakes was sensitive to the observations and SZA–OWT distribution contributed by Lake Trasimeno.

Overall, SZA was related to paired AEC benefit for selected AEC+AC combinations and wavelengths, while the direction and strength of the relationship varied among wavelengths and, for some models, among lakes.

4.4 Spatial analysis

RAdCor+POLYMER was selected for the spatial analysis because it had the lowest MdSA calculated across all six wavelengths in both Lake Geneva and Lake Trasimeno and produced the most consistent validation performance across the four lakes. The spatial analysis therefore compared RAdCor+POLYMER with standalone POLYMER. GAAC was included in the Lake Trasimeno map as an additional integrated AEC+AC result.

4.4.1 Lake Geneva

The Lake Geneva case study used a Sentinel-2 MSI acquisition from 8 August 2025 and examined a shoreline-to-open-water transect through the inner Geneva bay and Petit Lac. Differences between RAdCor+POLYMER and standalone POLYMER were small over most of the open water section and larger in the inner bay and near shoreline margins (Fig. 14). Median absolute relative differences remained below 10% at 665, 705 and 740 nm, and the corresponding 95th-percentile values remained below 20%. The largest relative differences occurred at 740 nm.

The direction of the difference varied among wavelengths. RAdCor+POLYMER generally produced higher R_{rs} than standalone POLYMER at 665 nm. At 705 nm, standalone POLYMER frequently produced negative or near-zero values in the inner bay and near shoreline sections, whereas RAdCor+POLYMER produced higher values. At 740 nm, RAdCor+POLYMER generally produced lower R_{rs} . The difference did not follow a monotonic change

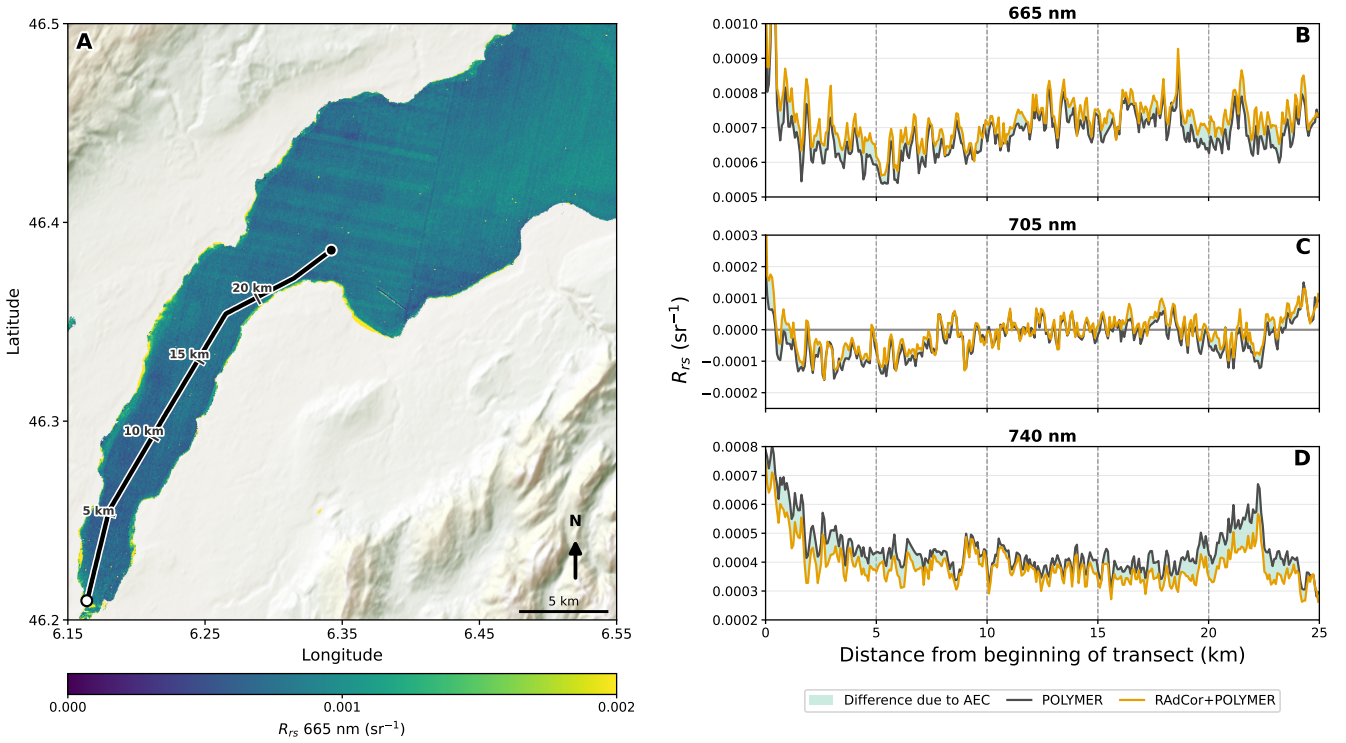


Figure 14: Lake Geneva west-bay transect for the Sentinel-2 MSI acquisition on 8 August 2025. Panel A shows RADCor+POLYMER R_{rs} at 665 nm and the shoreline-to-open-water transect through the inner Geneva bay and Petit Lac. Panels B–D compare standalone POLYMER and RADCor+POLYMER at 665, 705 and 740 nm. Shading shows the signed difference $\Delta R_{rs} = R_{rs, \text{RADCor+POLYMER}} - R_{rs, \text{standalone POLYMER}}$. The mean absolute relative difference along the same transect was 2.2% across the omitted 443, 492 and 560 nm products.

from the shoreline towards open water. Across the omitted 443, 492 and 560 nm products, the mean absolute relative difference was 2.2%.

R_{rs} for the entire scene followed the same wavelength-dependent response as the transect (Fig. 15). RADCor+POLYMER increased R_{rs} over nearly all valid pixels at 665 nm. Differences at 705 nm included both positive and negative values, while RADCor+POLYMER decreased R_{rs} over most valid pixels at 740 nm.

The largest differences occurred in the inner bay and along shoreline margins. Pixels in the central Petit Lac generally changed less. The 95th-percentile absolute relative difference was 17.9% at 665 nm, 22.3% at 705 nm and 22.7% at 740 nm, and the mean absolute relative difference across the omitted 443, 492 and 560 nm products was 4.2%. The Lake Geneva case study therefore showed a spatially coherent but moderate RADCor response whose direction depended on wavelength.

4.4.2 Lake Trasimeno

The Lake Trasimeno case study used a Sentinel-2 MSI acquisition from 9 April 2024. The transect crossed the western part of the lake near Isola Polvese, while the lake-wide comparison showed the complete spatial distribution of the differences among standalone POLYMER, RADCor+POLYMER and GAAC.

The Lake Trasimeno transect showed larger differences between RADCor+POLYMER and standalone POLYMER than the Lake Geneva transect, particularly at 665, 705 and 740 nm (Fig. 16). Median absolute relative differences were approximately 3–5% at 443, 492 and 560 nm and 16–28% at 665, 705 and 740 nm. The largest median difference occurred at 705 nm.

The first kilometre of the transect showed larger differences than the more open water section, especially at 665 and 705 nm. Within the 1–4 km section crossing the high R_{rs} feature west of Isola Polvese, RADCor+POLYMER produced lower R_{rs} than standalone POLYMER at 443 nm and higher R_{rs} from 492 to 740 nm. At 740 nm, the median signed difference relative to RADCor+POLYMER in this section was 42.1%. These differences extended beyond the selected transect (Fig. 17). RADCor+POLYMER generally produced lower R_{rs} than standalone POLYMER near shoreline areas at 443 and 492 nm. It produced higher R_{rs} over extensive parts of the lake at 560, 665 and 705 nm, while differences at 740 nm included both positive and negative values.

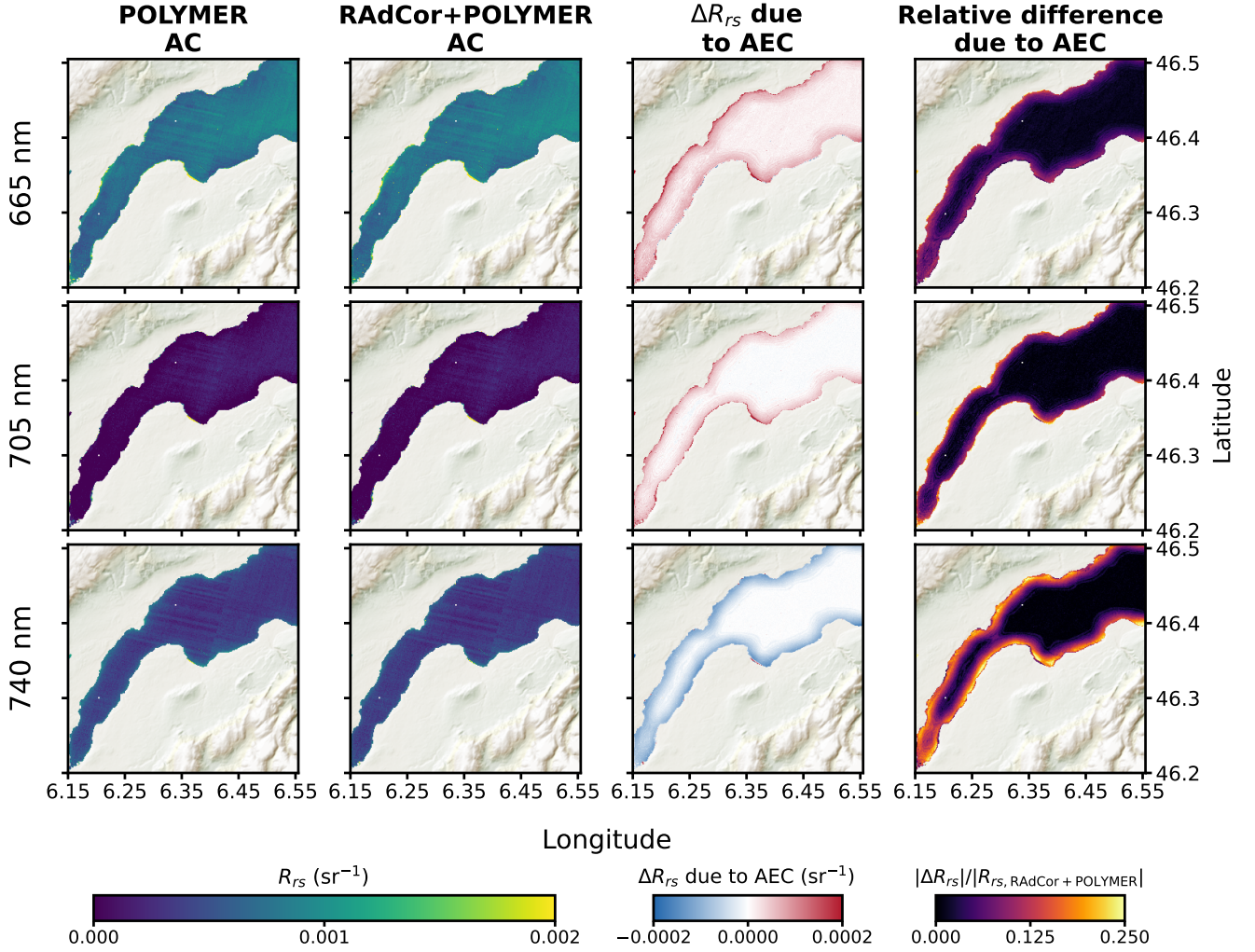


Figure 15: Spatial comparison over the Lake Geneva west bay on 8 August 2025. Rows show 665, 705 and 740 nm. Columns show standalone POLYMER, RAdCor+POLYMER, the signed difference ΔR_{rs} , and the absolute relative difference $|\Delta R_{rs}|/|R_{rs, \text{RAdCor+POLYMER}}|$. The mean absolute relative difference over valid lake pixels was 4.2% across the omitted 443, 492 and 560 nm products.

Across the complete scene, median absolute relative differences were approximately 2–4% at 443–560 nm and 11–18% at 665–740 nm. The largest differences occurred at 705 and 740 nm, with substantial positive differences also present at 665 nm. Positive differences at 665 and 705 nm occurred around Isola Polvese, over the western high R_{rs} feature, across parts of the south-eastern shallow water region and along several shoreline sections.

GAAC produced R_{rs} values that differed substantially from both standalone POLYMER and RAdCor+POLYMER, particularly at 665, 705 and 740 nm. The Lake Trasimeno case study therefore showed larger and more spatially extensive differences among AEC+AC approaches than the Lake Geneva case study.

Across the two selected scenes, Lake Geneva showed moderate differences concentrated in the inner bay and near shoreline margins. Lake Trasimeno showed larger differences across broader areas of the lake, particularly at 665–740 nm. In both scenes, the sign and magnitude of the difference varied among wavelengths.

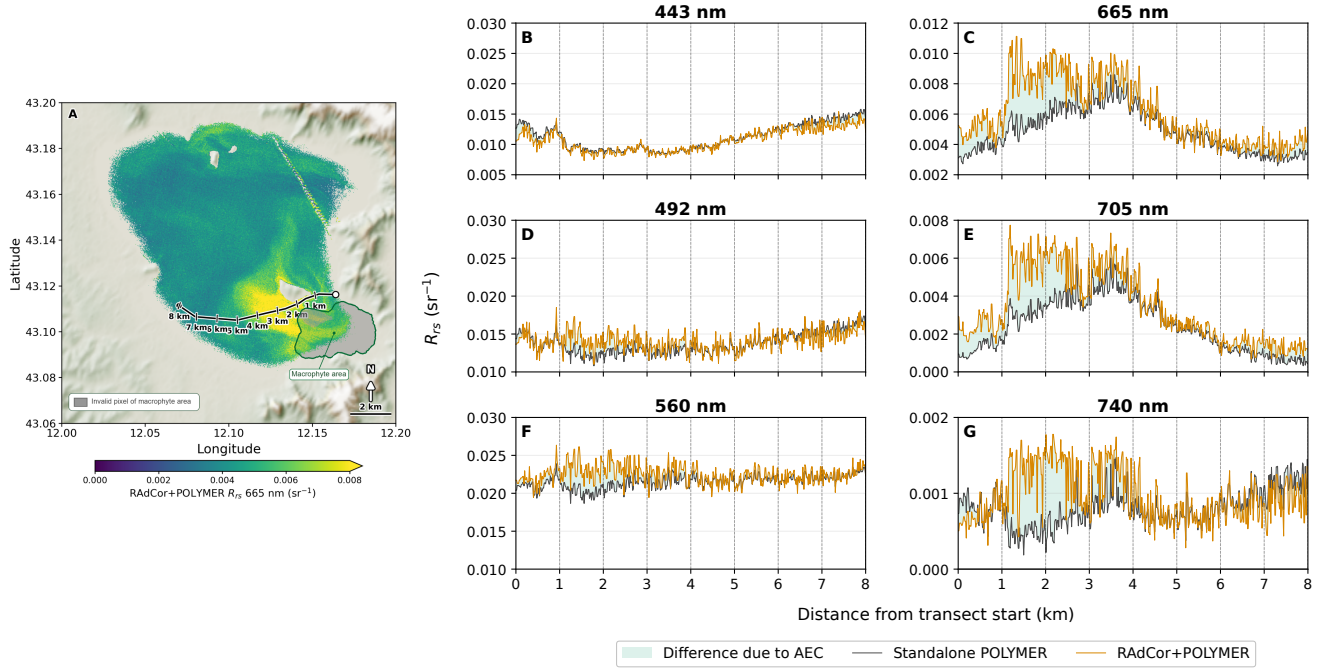


Figure 16: Lake Trasimeno transect for the Sentinel-2 MSI acquisition on 9 April 2024. Panel A shows RADCor+POLYMER R_{rs} at 665 nm, the 8 km transect, 1 km distance markers and a contextual macrophyte area polygon supplied by CNR-IREA. Grey pixels within the polygon are invalid under the IdePix mask; other pixels retain the 665 nm colour scale. Panels B–G compare standalone POLYMER and RADCor+POLYMER at 443, 492, 560, 665, 705 and 740 nm. Shading shows ΔR_{rs} .

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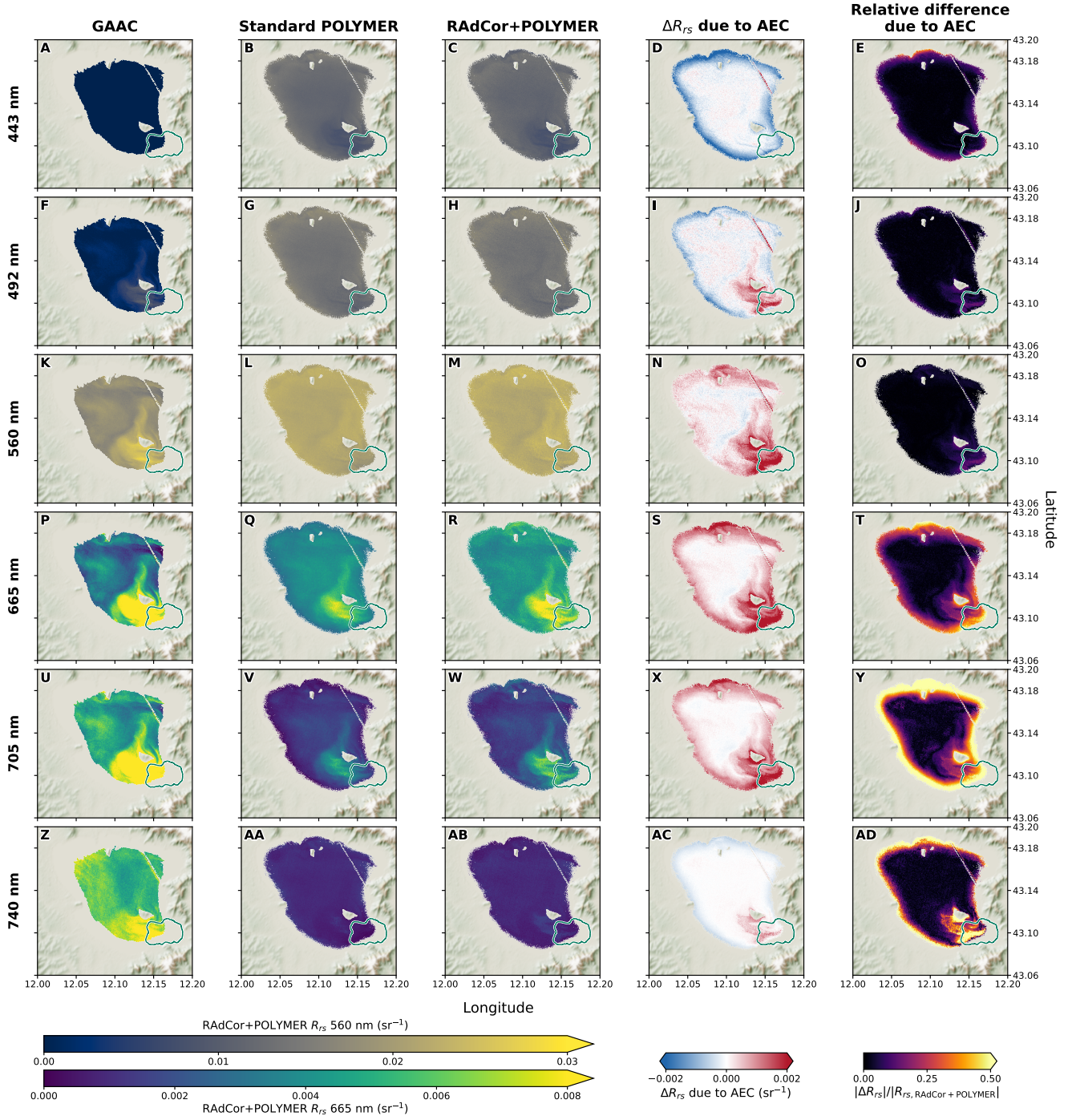


Figure 17: Lake Trasimeno spatial comparison for the Sentinel-2 MSI acquisition on 9 April 2024. Rows show 443, 492, 560, 665, 705 and 740 nm. Columns show GAAC, standalone POLYMER, RAdCor+POLYMER, signed ΔR_{rs} , and the absolute relative difference $|\Delta R_{rs}|/|R_{rs, \text{RAdCor+POLYMER}}|$. Blue and red in the signed difference column indicate decreases and increases after RAdCor, respectively. GAAC uses its internal validity mask; the remaining columns use an IdePix valid pixel mask. The narrow north-eastern diagonal stripe is a masked Sentinel-2 Level-1C product processing seam.

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5 Discussion

5.1 Adjacency effect correction results and interaction with downstream atmospheric correction

Prior AEC changed both MSI-derived R_{rs} and its agreement with in-situ measurements. Applying the same upstream AEC approach before different downstream AC approaches produced different retrieval responses. TMART estimates and removes the adjacency contribution before AC, RAdCor retrieves surface reflectance using atmospheric PSF and spherical albedo terms, and GAAC estimates adjacency together with aerosol, glint and water terms (Wu et al., 2024; Castagna and Vanhellemont, 2025; Pan and Bélanger, 2025). ACOLITE/DSF, C2RCC and POLYMER then partition the corrected TOA signal differently among atmospheric path radiance, surface reflection, glint and water-leaving components. The resulting R_{rs} therefore depends on the complete AEC+AC combination. Our results across the approaches extend earlier radiative transfer and method-specific studies by quantifying that dependence for identical lake matchups (Tanre et al., 1981; Reinersman and Carder, 1995; Bulgarelli et al., 2014; Bulgarelli and Zibordi, 2018).

RAdCor+POLYMER produced the lowest method-specific MdSA calculated across the six MSI wavelengths in Greifensee, Lake Geneva and Lake Trasimeno. In Lake Garda, its MdSA was 38.1%, compared with 37.9% for TMART+POLYMER. The unweighted mean of the four method-specific lake MdSA values was 46.9% for standalone POLYMER and 30.8% for RAdCor+POLYMER. The largest difference occurred in Greifensee, where standalone POLYMER had the largest error and strongest positive SSPB among the four lake-specific POLYMER results. Differences were smaller in Lake Geneva, Lake Trasimeno and Lake Garda, where standalone POLYMER already agreed more closely with the field measurements. In this sequence, RAdCor first accounts for radiance contributed by the spatially heterogeneous surroundings, after which POLYMER fits the remaining atmospheric, glint and water-leaving spectral components (Steinmetz et al., 2011; Castagna and Vanhellemont, 2025).

The sign of the retrieved R_{rs} change varied among wavelengths, scenes and downstream AC approaches. Every downstream inversion re-estimates its atmospheric, glint and water terms after the TOA signal has been corrected. A positive R_{rs} change can occur when the standalone fit assigned part of the adjacency-contaminated signal to atmospheric or glint terms. A negative change can occur when surrounding radiance remained in the standalone water term. The spatial case studies contained both responses. In Lake Geneva, RAdCor+POLYMER generally increased R_{rs} at 665 nm, produced positive and negative differences at 705 nm and decreased R_{rs} at 740 nm. In Lake Trasimeno, differences were generally negative near shore at 443 and 492 nm, positive over extensive areas at 560–705 nm and spatially mixed at 740 nm. Correction sign therefore records how the downstream spectral inversion responds to the corrected TOA signal. Correction sign alone cannot quantify the amount of adjacency radiance removed.

The Lake Geneva comparison identified a recurring spectral feature of the POLYMER retrieval. We processed three additional same-orbit acquisitions from 29 June, 9 July and 12 July 2025 with the same standalone POLYMER and RAdCor+POLYMER settings used for the displayed 8 August scene. Median R_{rs} at 740 nm exceeded median R_{rs} at 705 nm for both POLYMER approaches on all four dates. RAdCor increased the 705 nm median and decreased the 740 nm median in every scene, while the wavelength ordering remained. The four acquisitions therefore establish that this ordering recurred across dates. POLYMER retained it before and after RAdCor, which associates the pattern with the downstream POLYMER retrieval under weak water-leaving signals at 705 and 740 nm. Small residual path radiance or spectral fit errors can occupy a large fraction of R_{rs} in this spectral region (Steinmetz et al., 2011; Warren et al., 2019; Pahlevan et al., 2021). Spatially coincident field spectra were unavailable, therefore the absolute local spectral ordering remains unvalidated. Shallow water and benthic contributions may also affect individual nearshore sections.

Prior AEC reduced MdSA in 98 of the 144 comparisons defined by four lakes, six AEC+AC combinations and six wavelengths, with the most frequent improvements at 705 and 740 nm. At 560 nm, 9 comparisons improved and 15 deteriorated. The median normalised IQR increased from 15.9% at 560 nm to 104.4% at 740 nm. At 740 nm, the interquartile spread among AEC+AC combinations was therefore approximately equal to the retrieved signal magnitude for a typical matchup event. AEC+AC combination selection is consequently a major source of uncertainty for products that depend on 740 nm R_{rs} . The 560 nm result demonstrates that agreement among the combinations and validation accuracy are separate properties: relative AEC+AC combination disagreement was smallest at this wavelength, while prior AEC increased MdSA in most paired comparisons.

5.2 Water type, aerosol load, solar geometry and shoreline context

The WISpstation OWT analysis identified large differences in AEC benefit among optical regimes. Mean weighted paired ΔMdSA was 79.9 %pt. for OWT 4a and 5.3 %pt. for OWT 4b, with the largest mean responses at 665–740 nm. After M1 accounted for SZA, VZA and lake, only one OWT contrast retained support after both BH and BY correction: RAdCor+POLYMER produced a larger 443 nm benefit in OWT 4a than in OWT 4b. These results therefore identify a strong OWT pattern, while the adjusted analysis establishes one class difference that can be separated clearly from the sampled geometry and lake composition. Optical regime alters the magnitude and spectral structure of the water signal used by the downstream AC approach. OWT describes this water type state, but it does not represent the surrounding land radiance field that supplies the adjacency contribution (Moore et al., 2014; Spyrakos et al., 2018; Uudeberg et al., 2019; Bi and Hieronymi, 2024).

The two aerosol reanalyses identified the same principal RAdCor response. MERRA-2 and CAMS coefficient signs agreed in 35 of the 36 analyses defined by the six AEC+AC combinations and six wavelengths, and both products supported eight positive RAdCor associations. These common associations occurred for RAdCor+C2RCC at 560, 665, 705 and 740 nm and for RAdCor+POLYMER at 492, 560, 665 and 705 nm. Higher regional aerosol load was therefore associated with larger RAdCor benefit in these specific wavelength and downstream AC combinations. Atmospheric scattering transfers radiance from surrounding surfaces into the target field of view, therefore the common MERRA-2 and CAMS pattern agrees with radiative transfer estimates of aerosol-dependent adjacency radiance (Bulgarelli et al., 2014; Bulgarelli and Zibordi, 2018). Eight of the ten BH-supported MERRA-2 coefficient directions were retained after every individual lake omission. The two failures occurred when omitting Lake Trasimeno moved the coefficient across zero: RAdCor+C2RCC vs C2RCC at 560 nm changed from +3.7176 to -0.0803 %pt. per IQR, and RAdCor+POLYMER vs POLYMER at 665 nm changed from +5.1689 to -0.3085 %pt. per IQR. Most of the primary MERRA-2 pattern therefore remained stable when each lake was omitted in turn.

The two aerosol products quantify different atmospheric properties. MERRA-2 supplied total aerosol scattering optical thickness, whereas CAMS supplied total aerosol optical depth. Each coefficient was scaled by a product-specific IQR. Agreement in coefficient direction across AEC+AC combinations and wavelengths therefore provides the direct cross-product comparison while numerical coefficient magnitudes represent different aerosol increments. Both reanalyses also describe regional atmospheric conditions on grids that are much coarser than the lake scenes. They cannot resolve local aerosol gradients, shoreline microclimates or residual sub-pixel cloud contamination (Gelaro et al., 2017; Randles et al., 2017; Inness et al., 2019).

SZA was associated with paired AEC benefit in selected analyses, and the direction varied among wavelengths and AEC+AC combinations. For RAdCor+POLYMER, higher SZA was associated with greater benefit at 560 nm and smaller benefit at 705 nm. The other four RAdCor+POLYMER wavelengths did not retain BH support. Lake-by-SZA tests and leave-one-lake-out refits further showed that some coefficients fitted to the complete dataset depended on the lakes represented in the analysis. The SZA associations therefore describe the sampled combination of AEC method, downstream AC approach, wavelength and lake conditions. No common increase or decrease in AEC benefit with SZA described all analyses.

Regional aerosol load also changed several SZA estimates. Adding the MERRA-2 term changed the sign of 9 of the 36 SZA coefficients. For RAdCor+POLYMER at 705 nm, the negative M1 coefficient moved to a value close to zero in M2. MERRA-2 scattering optical thickness and SZA were correlated in the matchup dataset, thus M2 estimated the SZA association at comparable regional aerosol load. The resulting coefficient changes show that selected M1 SZA associations were sensitive to aerosol context. This wavelength- and combination-specific response agrees with radiative transfer descriptions in which illumination geometry acts together with viewing geometry, aerosol scattering, water optical state and land–water contrast (Bulgarelli and Zibordi, 2018; Wu et al., 2024).

Nearest distance to shore captured only part of the spatial variation in AEC benefit. In Lake Garda, the scene-cluster bootstrap interval excluded zero only at 492 nm, but exploratory BH and BY adjustment across the six shoreline tests retained no slope. The 705 nm point estimate was strongly negative, but its interval included zero after accounting for observations shared within acquisition scenes. The percentile intervals included zero at the other wavelengths. The Lake Geneva and Lake Trasimeno maps showed spatial organisation around bays, islands, shoreline curvature, and shallow water areas. Atmospheric scattering integrates radiance from the full surrounding field through a wavelength- and atmosphere-dependent PSF. Two-dimensional measures of shoreline geometry, surrounding land fraction and land–water radiometric contrast therefore correspond more directly to this source term than nearest-shore distance alone (Reinersman and Carder, 1995; Bulgarelli et al., 2014).

5.3 Implications for operational processing and downstream products

The validation results justify explicit AEC as a default component of Sentinel-2 MSI lake processing for lakes with sizes, optical conditions and shoreline settings comparable to those studied here. The strongest case applies to small or narrow lakes and to products that use 665, 705 and 740 nm. Operational implementation should treat the AEC approach and downstream AC approach as one combination because both determine R_{TS} . RAdCor+POLYMER provided the strongest validated combination in this dataset. The mixed 560 nm response and the differences among ACOLITE-, C2RCC- and POLYMER-based combinations require wavelength-specific validation before a configuration is transferred to another lake type or processing system.

Band-dependent changes in R_{TS} propagate directly into downstream products. Phytoplankton chlorophyll-*a*, cyanobacteria and suspended matter algorithms often use spectral ratios or features near 665 and 705 nm, and sun-induced fluorescence retrieval depends on small red and near-infrared signals (Warren et al., 2019; Pahlevan et al., 2021; Gupana et al., 2025). In Lake Trasimeno, RAdCor+POLYMER altered the 665–740 nm spatial structure across extensive parts of the lake. Products derived from these wavelengths can therefore change even where the blue-green correction remains small. Existing MSI products generated without AEC should be reassessed where nearby land, islands or shallow margins contribute materially to the TOA signal.

OWT-dependent processing systems require an additional consistency assessment. OWT classification uses spectral shape, therefore wavelength-dependent AEC changes can move a spectrum across a class boundary. Systems that select or blend retrieval algorithms from OWT membership may then change both the input R_{TS} and the subsequent algorithm pathway (Moore et al., 2014; Spyarakos et al., 2018; Uudeberg et al., 2019). Where OWT is derived from satellite R_{TS} , operational systems should evaluate class membership from the AEC-corrected spectrum and document its sensitivity to the selected AEC+AC combination.

The evidence in this study applies to near-nadir MSI observations over four mid-latitude lakes. Transfer to larger lakes, strongly CDOM-dominated waters or substantially different shoreline settings requires additional validation. Wider-swath and off-nadir sensors, including the Sentinel-3 Ocean and Land Cover Instrument, also sample larger viewing angle ranges and different atmospheric path lengths, scattering geometries, surface anisotropy and projected adjacency footprints (Bulgarelli and Zibordi, 2018). Their AEC performance should be assessed with sensor-specific geometry. Further work should evaluate complete AEC+AC combinations across additional lake types, aerosol regimes and acquisition geometries and should quantify the uncertainty caused by aerosol inputs, PSFs, masks and downstream AC settings.

6 Conclusions

This study evaluated ten Sentinel-2 MSI AC and AEC+AC approaches using 329 satellite-in-situ matchups from Greifensee, Lake Geneva, Lake Garda and Lake Trasimeno. Prior AEC improved retrieval agreement in most paired comparisons and substantially changed the ranking of AC approaches. RAdCor+POLYMER achieved the lowest method-specific MdSA in Greifensee, Lake Geneva and Lake Trasimeno, whereas TMART+POLYMER performed marginally better in Lake Garda. Across the four lakes, the method-specific mean MdSA decreased from 46.9% for standalone POLYMER to 30.8% for RAdCor+POLYMER, corresponding to a relative difference of 34.3%. Improvements occurred in 98 of the 144 paired comparisons and were most consistent at 665, 705 and 740 nm, whereas responses at 560 nm were mixed.

AEC benefit depended on environmental and processing context instead of a single controlling variable. Larger validation gains were most frequently observed for OWT 4a (elevated biomass concentration and low short-wavelength reflectance), longer wavelengths and several RAdCor-based combinations under higher aerosol loading. In contrast, SZA and distance to shore did not provide general indicators of R_{TS} retrieval benefit across lakes, wavelengths or AEC+AC combinations. Together, these results show that the performance of current AEC approaches depends on the complete combination of water type, atmospheric conditions, observation geometry, wavelength and downstream AC.

Differences among AEC+AC approaches also increased towards longer wavelengths. Median processor disagreement relative to the retrieved signal was lowest at 560 nm (15.9%), increased to 48.1% at 705 nm and reached 104.4% at 740 nm, where disagreement frequently exceeded the retrieved signal itself. The spatial analyses further showed that AEC effects could extend well beyond the immediate shoreline and influence larger parts of a lake.

Overall, these results support routine inclusion of AEC in Sentinel-2 MSI lake processing, particularly for small and narrow lakes and for products using wavelengths ≥ 665 nm. At the same time, the magnitude, direction and benefit of AEC remain approach-, wavelength- and environment-dependent, and cannot yet be generalised across inland waters. Future work should focus on both methodological refinement and broader validation across

911 more diverse lake types, shoreline configurations, aerosol conditions and observation geometries, with evaluation of
912 complete AEC+AC combinations instead of individual components.

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924 CRediT author statement

925 Conceptualisation: MW, DO
926 Data curation: MW, MB, CG
927 Methodology: MW, DO, AIR, LM
928 Formal analysis: MW, DO
929 Investigation: MW, DO, MB, CG
930 Software: MW, JR
931 Visualisation: MW
932 Writing – Original Draft: MW
933 Writing – Review & Editing: All authors

934 8 Code availability

935 The RAdCor, TMART, C2RCC, POLYMER, ACOLITE and IdePix methods are available through Sencast:
936 <https://github.com/eawag-surface-waters-research/sencast>. GAAC is available upon request from the
937 authors of the original study. WISPstation in-situ measurements from Greifensee and Lake Geneva are continuously
938 updated and available on: <https://www.datalakes-eawag.ch>, and for Lake Trasimeno and Lake Garda are available
939 upon request. The 3C JAX implementation is available on: https://gitlab.com/pgroetsch/rrs_model_3C/-/tree/werther_jax_version.

Appendix 1: Determination of RAdCor processing settings

We carried out an additional RAdCor area of interest (AOI) analysis to identify a processing geometry that could be used consistently for the matchup analysis. The purpose of this analysis was to evaluate a common set of AOI, buffer and kernel settings across representative platform cases. This was necessary because RAdCor requires sufficient spatial context around the target water pixel. If the processed footprint is too small relative to the requested correction kernel, the correction cannot be completed and no valid Level-2 reflectance product is produced.

The assessment used two selected dates for each of the three WISPs stations: Greifensee, the Lake Geneva LÉXPLORE platform and Lake Trasimeno. For each site and date, we processed the same family of RAdCor configurations. Five AOI sizes were considered: an AOI centred on the station (denoted as “small”), one point-spread-function (PSF) footprint, two PSF footprints, a 3 km box, and a 5 km box. These AOIs were combined with different RAdCor limit buffer settings and kernel radii. The limit buffer (lb) expands the processing domain around the AOI, while the kernel radius (kr) defines the neighbourhood used by the RAdCor correction.

To avoid configurations where the requested kernel was not supported by the buffered footprint after cropping around the centre, combinations with an active kernel were filtered before processing:

$$L_{\text{eff}} \geq 2R,$$

where

$$L_{\text{eff}} = L_{\text{base}} + 2B.$$

Here, L_{eff} is the effective footprint edge length in kilometres after applying buffer B (km) to a base footprint of edge length L_{base} (km), and R is the kernel radius (km). The factor of two arises because the kernel radius must be supported on both sides of the target pixel, so the minimum required footprint width is the kernel diameter, $2R$. The buffer also contributes on both sides of the base AOI, giving $L_{\text{eff}} = L_{\text{base}} + 2B$.

Starting from a factorial grid of $5 \times 4 \times 3 = 60$ combinations with an active kernel, the geometric criterion was applied to the buffered configurations. The 15 unbuffered active kernel configurations were retained as controls. For the five base AOI edge lengths used here, $L_{\text{base}} = 0.22, 0.75, 1.5, 3$ and 5 km, the criterion retained only $R = 2$ km for $B = 2$ km, retained $R = 2$ and $R = 5$ km for $B = 5$ km and retained all three tested radii for $B = 10$ km. This gave $15 + 5 + 10 + 15 = 45$ active kernel configurations including the unbuffered controls. Five reference runs with the kernel switched off were then added, yielding 50 runs per site and date.

Each configuration was assessed separately for the two dates at each site. A run was considered feasible when it produced a valid ACOLITE/TSDSF Level-2 product from which a R_{rs} spectrum centred on the station could be extracted. Runs that stopped because the scene was too small, or that failed to produce the required output product, were classified as infeasible. The resulting feasibility counts are given in Table 1.

The feasibility pattern was highly consistent across the three sites. For each site, 31 of the 50 configurations were feasible on both selected dates, while 19 configurations were not feasible on either selected date. No configuration showed a mixed result between the two dates within a site. The cases that were not feasible were associated with insufficient scene size for the requested RAdCor settings. In particular, unbuffered configurations with an active kernel generally failed for the smaller AOIs, while buffered configurations succeeded when the buffer was large enough for the requested kernel radius. The largest 5 km AOI allowed the unbuffered 2 km kernel case to succeed, but larger unbuffered kernels remained infeasible.

After the feasibility assessment, we compared the feasible retrievals with the field spectra for the six site-date cases shown in Fig. 18. Among the feasible settings, the AOI centred on the station with a 2 km limit buffer and a 2 km kernel radius produced the closest overall statistical agreement with the field spectra across these six cases. The final configuration was therefore selected after examining agreement for these six scenes and was then applied to all matchups. We used base AOIs with a 200 m edge length, together with the 2 km limit buffer and 2 km kernel radius.

Table 1: Feasibility of the 50 tested RAdCor AOI configurations across the two selected dates for each site. Entries describe the number of feasible runs out of the two selected dates for Greifensee, Lake Geneva and Lake Trasimeno. Values of 2/2 denote feasible processing for both selected dates at a given site, whereas 0/2 denotes not feasible processing for both selected dates. The selected date pairs are Greifensee: 2022-05-11 and 2022-07-18; Lake Geneva: 2025-07-17 and 2025-08-18; Lake Trasimeno: 2018-07-30 and 2024-04-09.

Run	Size	LB	KR	Greifensee	Lake Geneva	Lake Trasimeno	Note
1	small	none	2	0/2	0/2	0/2	Scene too small
2	small	none	5	0/2	0/2	0/2	Scene too small
3	small	none	10	0/2	0/2	0/2	Scene too small
4	small	2km	2	2/2	2/2	2/2	-
5	small	5km	2	2/2	2/2	2/2	-
6	small	5km	5	2/2	2/2	2/2	-
7	small	10km	2	2/2	2/2	2/2	-
8	small	10km	5	2/2	2/2	2/2	-
9	small	10km	10	2/2	2/2	2/2	-
10	PSF	none	2	0/2	0/2	0/2	Scene too small
11	PSF	none	5	0/2	0/2	0/2	Scene too small
12	PSF	none	10	0/2	0/2	0/2	Scene too small
13	PSF	2km	2	2/2	2/2	2/2	-
14	PSF	5km	2	2/2	2/2	2/2	-
15	PSF	5km	5	2/2	2/2	2/2	-
16	PSF	10km	2	2/2	2/2	2/2	-
17	PSF	10km	5	2/2	2/2	2/2	-
18	PSF	10km	10	2/2	2/2	2/2	-
19	2×PSF	none	2	0/2	0/2	0/2	Scene too small
20	2×PSF	none	5	0/2	0/2	0/2	Scene too small
21	2×PSF	none	10	0/2	0/2	0/2	Scene too small
22	2×PSF	2km	2	2/2	2/2	2/2	-
23	2×PSF	5km	2	2/2	2/2	2/2	-
24	2×PSF	5km	5	2/2	2/2	2/2	-
25	2×PSF	10km	2	2/2	2/2	2/2	-
26	2×PSF	10km	5	2/2	2/2	2/2	-
27	2×PSF	10km	10	2/2	2/2	2/2	-
28	3km	none	2	0/2	0/2	0/2	Scene too small
29	3km	none	5	0/2	0/2	0/2	Scene too small
30	3km	none	10	0/2	0/2	0/2	Scene too small
31	3km	2km	2	2/2	2/2	2/2	-
32	3km	5km	2	2/2	2/2	2/2	-
33	3km	5km	5	2/2	2/2	2/2	-
34	3km	10km	2	2/2	2/2	2/2	-
35	3km	10km	5	2/2	2/2	2/2	-
36	3km	10km	10	2/2	2/2	2/2	-
37	5km	none	2	2/2	2/2	2/2	-
38	5km	none	5	0/2	0/2	0/2	Scene too small
39	5km	none	10	0/2	0/2	0/2	Scene too small
40	5km	2km	2	2/2	2/2	2/2	-
41	5km	5km	2	2/2	2/2	2/2	-
42	5km	5km	5	2/2	2/2	2/2	-
43	5km	10km	2	2/2	2/2	2/2	-
44	5km	10km	5	2/2	2/2	2/2	-
45	5km	10km	10	2/2	2/2	2/2	-
46	small	none	off	0/2	0/2	0/2	Scene too small
47	PSF	none	off	0/2	0/2	0/2	Scene too small
48	2×PSF	none	off	0/2	0/2	0/2	Scene too small
49	3km	none	off	0/2	0/2	0/2	Scene too small
50	5km	none	off	0/2	0/2	0/2	Scene too small

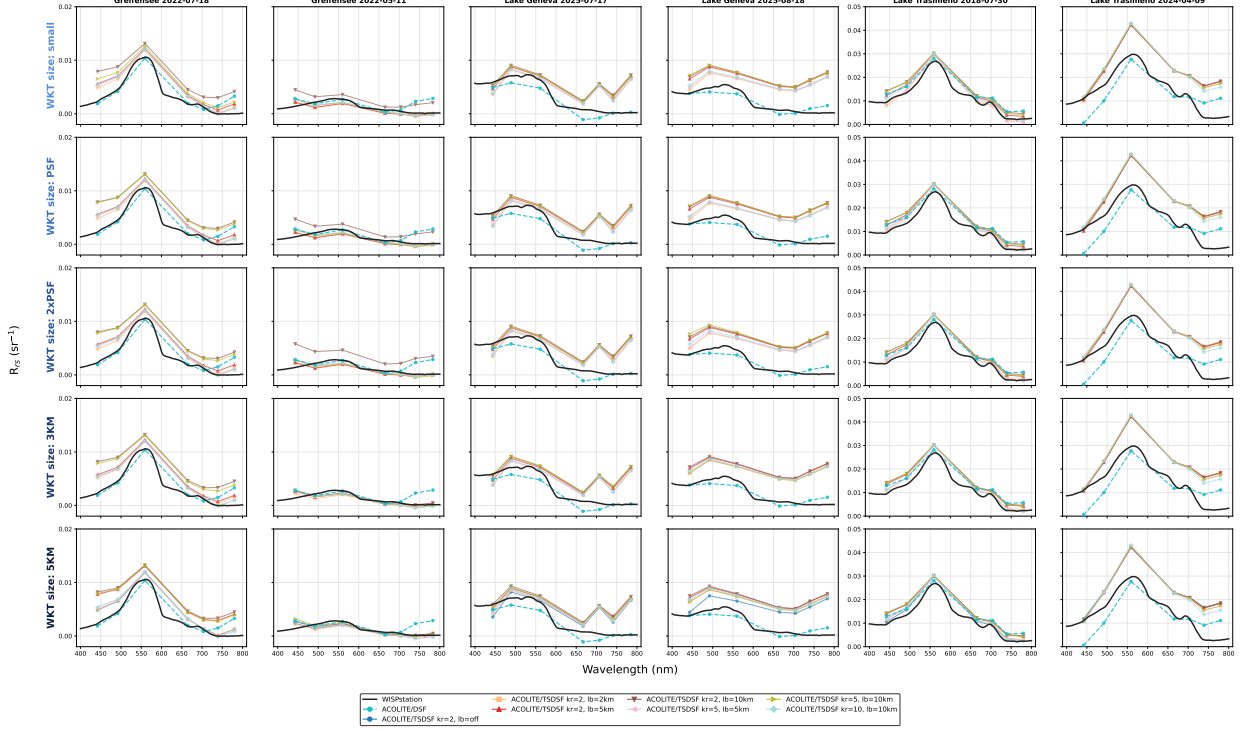


Figure 18: Feasible ACOLITE/TSDSF processing configurations for Greifensee, Lake Geneva at L XPLORE and Lake Trasimeno. Columns are the two selected dates at each site; rows are the small, PSF, 2 PSF, 3 km and 5 km AOI extents defined in Appendix 1. Curves show in-situ spectra, standalone ACOLITE/DSF and feasible ACOLITE/TSDSF combinations; **kr** and **lb** denote kernel radius and limit buffer. Configurations absent from a panel failed the feasibility criteria summarised in Table 1.

Appendix 2: GAAC investigation of lower-bound remote-sensing reflectance retrieval

GAAC retrieves water-leaving reflectance after subtracting estimated atmospheric path, sky reflection, adjacency and residual glint contributions from the observed signal. Before applying the minimum permitted output value, the water-leaving reflectance can be written schematically as:

$$\rho_{w,pre}(\lambda) = \frac{\rho_{obs}(\lambda) - \rho_{atm}(\lambda) - \rho_{sky}(\lambda) - \rho_{adj}(\lambda) - \rho_{glint}(\lambda)}{T^{\uparrow}(\lambda)T^{\downarrow}(\lambda)}, \quad (17)$$

where ρ_{obs} is the observed reflectance after the initial sensor and gas treatment; ρ_{atm} , ρ_{sky} , ρ_{adj} and ρ_{glint} are the atmospheric path, sky reflection, adjacency and residual glint contributions; and $T^{\uparrow}$ and $T^{\downarrow}$ are the upward and downward atmospheric transmittances. The numerator is the residual signal assigned to the water component.

A lower-bound retrieval occurs when the combined non-water terms exceed the observed signal:

$$\rho_{atm}(\lambda) + \rho_{sky}(\lambda) + \rho_{adj}(\lambda) + \rho_{glint}(\lambda) > \rho_{obs}(\lambda), \quad (18)$$

which makes $\rho_{w,pre}(\lambda)$ negative or smaller than the permitted output minimum. GAAC then writes:

$$\rho_{w,out}(\lambda) = \max[\rho_{w,pre}(\lambda), \rho_{w,min}], \quad (19)$$

with:

$$\rho_{w,min} = \pi \times 10^{-5}. \quad (20)$$

Because $R_{rs}(\lambda) = \rho_w(\lambda)/\pi$, this lower bound appears as:

$$R_{rs,min} = 10^{-5} \text{ sr}^{-1}. \quad (21)$$

995 Repeated values of exactly 10^{-5} sr^{-1} therefore identify the GAAC output limit rather than independently retrieved
 996 low water-leaving signals. Values close to the limit were retained as flagged near-lower-bound cases unless the
 997 intermediate products supported a specific correction or exclusion.

998 2.1 GAAC investigation design

999 The investigation addressed two questions: which fitted terms produced the lower-bound values, and which affected
 1000 matchup values could be recovered without using the in-situ spectra to select settings. Decisions used only information
 1001 from the GAAC products and ancillary data, including pre-lower-bound water reflectance, exact and near-lower-bound
 1002 masks, atmospheric and adjacency terms, residual glint, matchup window statistics, atmospheric metadata and
 1003 acquisition geometry. The analysis comprised four stages:

1004 **Stage 1:** The original products were compared with products generated from larger areas of interest around the
 1005 matchup location. This test assessed whether limited land–water context caused the lower-bound retrieval.
 1006 For each target 3×3 window, we recorded the area size, land–water context, exact lower-bound count,
 1007 negative pre-lower-bound count and fitted correction terms.

1008 **Stage 2:** A 6 km spatial context was held fixed while deterministic optimisation pixel choices were varied. This test
 1009 assessed whether the solution depended on an optimisation pixel affected by local masks, shoreline mixing
 1010 or invalid water classification.

1011 **Stage 3:** For unresolved scenes, we tested a bounded set of physically motivated changes to residual glint treatment,
 1012 fit band weighting, AOD bounds and aerosol model constraints. A revised result was accepted only when
 1013 the target window contained neither exact lower-bound values nor negative pre-lower-bound values.

1014 **Stage 4:** The remaining cases were evaluated from the fitted reflectance components. The final 329-event GAAC
 1015 matchup dataset contained 184 exact lower-bound scene–wavelength retrievals and 13 near-lower-bound
 1016 retrievals. Sixteen were recovered: six exact lower-bound retrievals through accepted scene settings, eight
 1017 through supported residual glint updates, one by recomputing the 3×3 statistic from valid pixels, and one
 1018 near-lower-bound retrieval through a wavelength-specific update. The remaining 169 exact lower-bound
 1019 retrievals were set to missing. The remaining 12 near-lower-bound retrievals were retained with flags
 1020 because the intermediate products did not support a change.

1021 The component budgets showed that the lower-bound cases occurred when the fitted atmospheric, sky reflection,
 1022 adjacency and residual glint contributions left a negative pre-lower-bound water signal. The most frequent pattern
 1023 involved large aerosol and sky terms combined with residual glint. Local window contamination contributed in
 1024 some cases. Optimised AOD by GAAC at 550 nm was often higher than CAMS EAC4 AOD₅₅₀ and the MERRA-2
 1025 scattering AOT variables. These products represent different aerosol quantities. Therefore, the comparison was used
 1026 only to identify unusually large GAAC aerosol estimates. In 31 investigation runs, GAAC AOD at 550 nm exceeded
 1027 CAMS EAC4 AOD₅₅₀ by more than 0.15.

1028 2.1.1 Rules used for GAAC matchup handling

1029 Final GAAC matchup values were selected with a fixed hierarchy. Valid original retrievals were retained unchanged.
 1030 Exact lower-bound values were replaced only when an accepted scene or wavelength-specific result removed both the
 1031 lower-bound value and the negative pre-lower-bound water signal without using in-situ spectra for selection. Where
 1032 a 3×3 target window contained both lower-bound and valid pixels, the matchup statistic was recomputed from
 1033 the valid pixels only when at least five of the nine pixels remained and their pre-lower-bound water signals were
 1034 positive. Changes to residual glint treatment were accepted only when the intermediate products showed that the
 1035 change removed the lower-bound behaviour. Exact lower-bound retrievals that did not meet these criteria were set
 1036 to missing.

1037 These rules recovered 15 exact lower-bound retrievals and one near-lower-bound retrieval. The remaining 169
 1038 exact lower-bound retrievals were excluded from the GAAC validation statistics, and 12 near-lower-bound retrievals
 1039 were retained. The statistics of this paper therefore exclude values imposed by the GAAC output limit while
 1040 retaining low R_{rs} values that were supported by the intermediate products.

2.1.2 GAAC lower-bound interpretation

The investigation identified a GAAC-specific closure problem in the affected retrievals: the fitted non-water contributions exceeded the observed signal and left a negative water component before the output limit was applied. Increasing the spatial context or changing the optimisation pixel resolved only a subset of cases. Targeted settings, supported residual glint updates and wavelength-level window checks recovered 16 retrievals. The remaining exact lower-bound values were excluded, and the standard global GAAC parametrisation was retained for the full assessment. This handling prevents the output limit from biasing the comparison among AC and AEC+AC approaches while preserving GAAC retrievals supported by the component-level evidence.

Appendix 3: Lake Garda distance-to-shoreline sensitivity

The Lake Garda campaign stations span a distance-to-shore gradient that is absent from the WISPs station records. We therefore analysed the association between shoreline distance and paired AEC benefit separately for each wavelength. The Theil-Sen estimator defined in Section 3.4 was used because this was a univariate analysis without the multivariable adjustment required in M1 and M2. To preserve dependence among matchups from the same acquisition, two-sided 95% CIs were calculated from 9,999 scene-cluster bootstrap resamples. For each wavelength, the represented Sentinel-2 sensing times were sampled with replacement and all valid matchups belonging to each selected scene were retained. The Theil-Sen slope was recalculated for every resample, and the 2.5th and 97.5th percentiles formed the interval. There were 19 represented scenes at 443, 492, 560, 665 and 740 nm and 13 at 705 nm.

For RAdCor+POLYMER relative to standalone POLYMER, AEC benefit generally decreased with increasing distance from shore, but the relationship was weak and inconsistent among wavelengths. The only scene-cluster bootstrap interval that excluded zero occurred at 492 nm, where the Theil-Sen slope was $-0.276 \text{ \%pt. km}^{-1}$ and the 95% CI ranged from -0.717 to $-0.009 \text{ \%pt. km}^{-1}$. The largest estimated decline occurred at 705 nm, with a slope of $-4.237 \text{ \%pt. km}^{-1}$, but the interval was wide and included zero. The intervals at 443, 560, 665 and

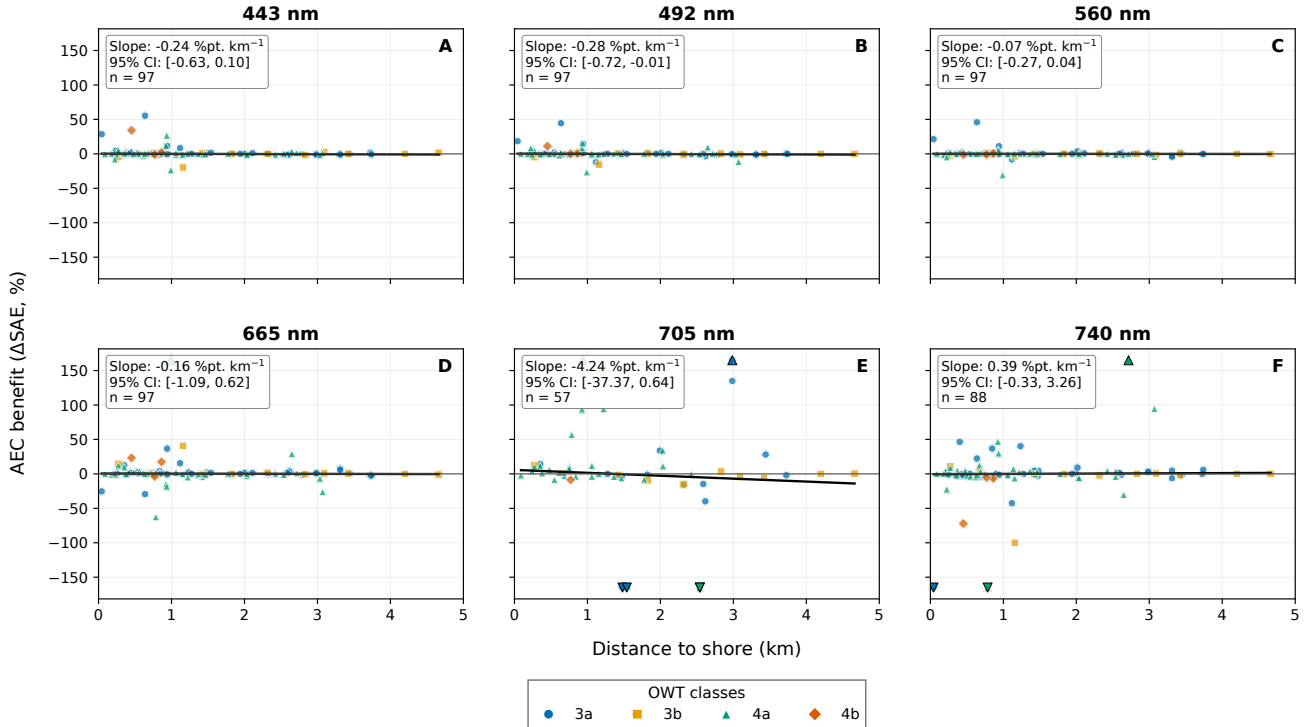


Figure 19: Lake Garda distance-to-shoreline sensitivity of paired AEC benefit for RAdCor+POLYMER relative to standalone POLYMER in the Lake Garda matchup dataset. Points are valid matchups coloured by OWT class; OWT 5a did not occur among the valid Lake Garda shoreline records. Boxes describe Theil-Sen slopes in $\text{\%pt. km}^{-1}$, two-sided 95% percentile-bootstrap CIs from 9,999 scene-cluster bootstrap resamples and wavelength-specific valid counts.

1063 740 nm also included zero. After exploratory BH and BY adjustment across the six wavelength-specific tests, no
1064 distance-to-shoreline association remained supported. Distance to shore therefore did not provide a consistent
1065 explanation of RAdCor+POLYMER benefit across wavelengths. The full wavelength-specific slopes, intervals and
1066 sample counts are shown in Fig. 19.

UNDER REVIEW

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