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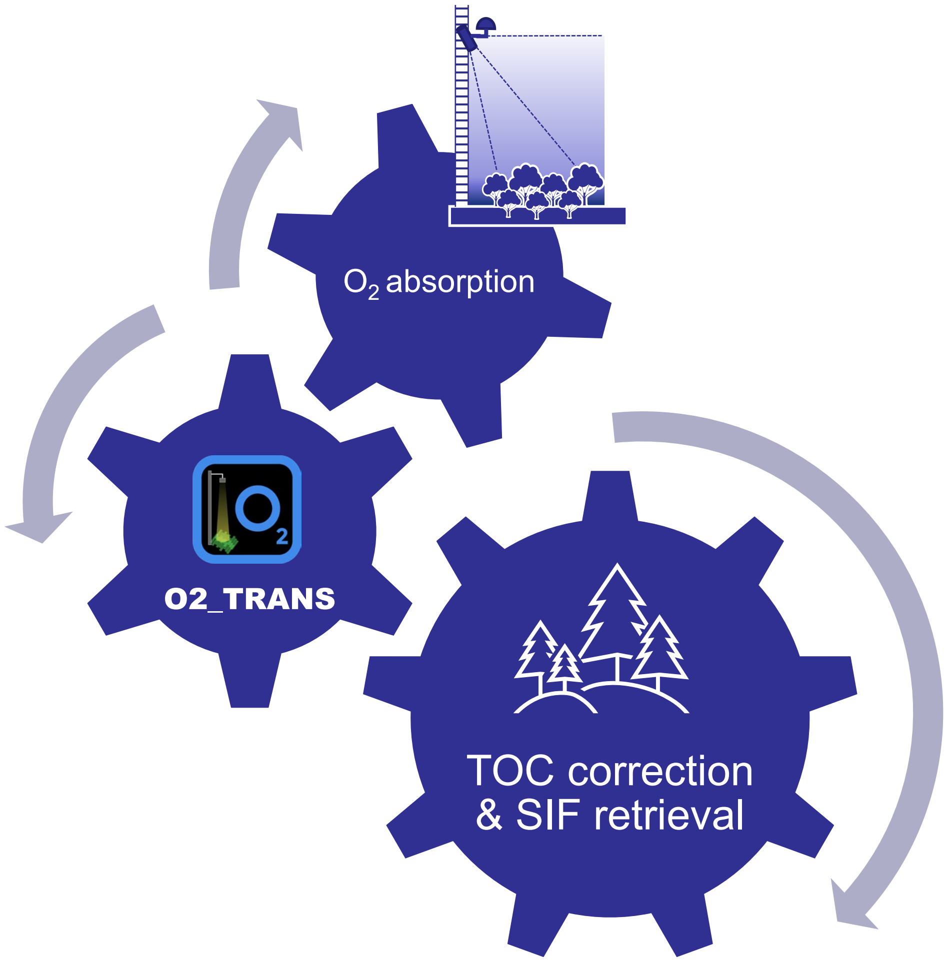
Compensating O_2 absorption effects for vegetation fluorescence retrievals at proximal sensing using the O2_TRANS software

NEUS SABATER[1], P. KOLMONEN[1], A. KUKKURAINEN[1], T.H. VIRTANEN[1], L. ALONSO[2], S. VAN WITTENBERGE[2], A. LIPPONEN[1], A. AROLA[1], T. JULITA[3], S. COGLIATI[4], A. PORCAR CASTELL[5], and J. MORENO[2]

Outline



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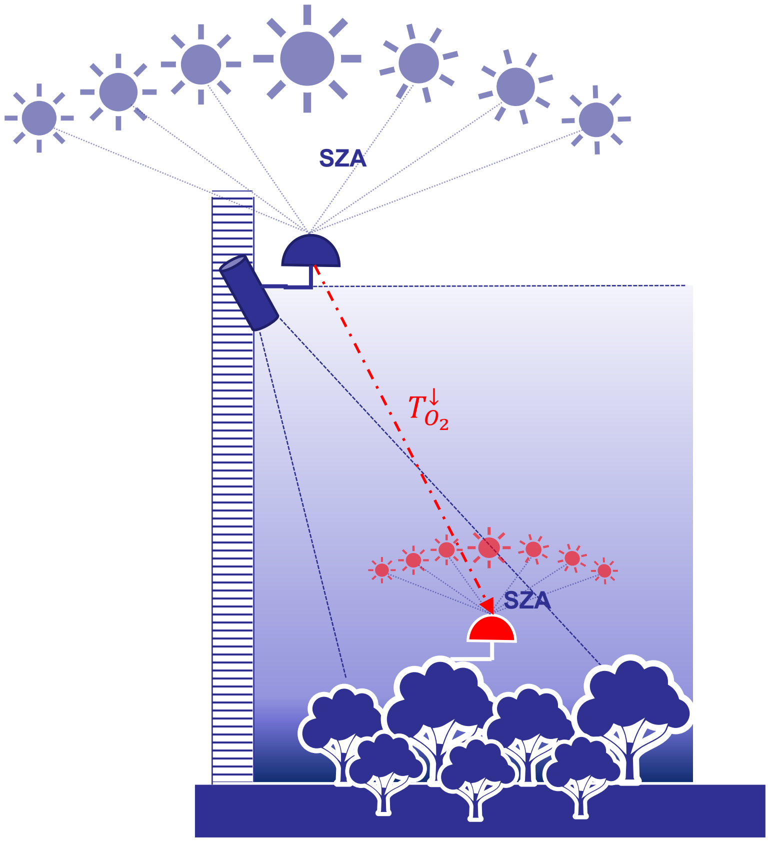
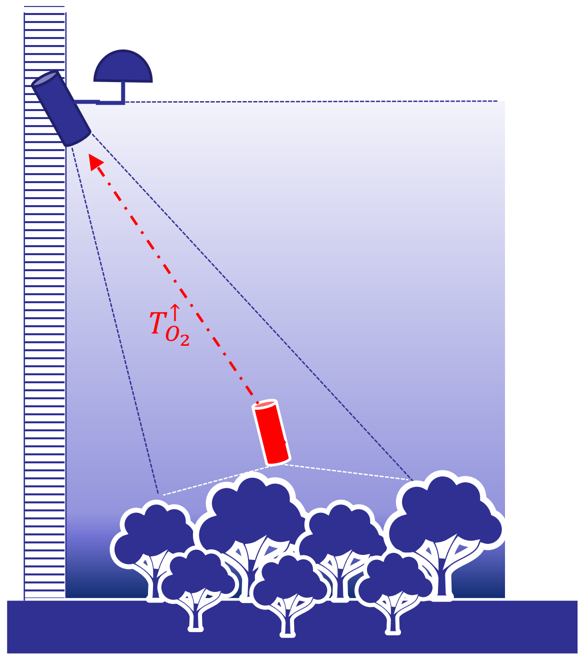
Tower-mounted measurement

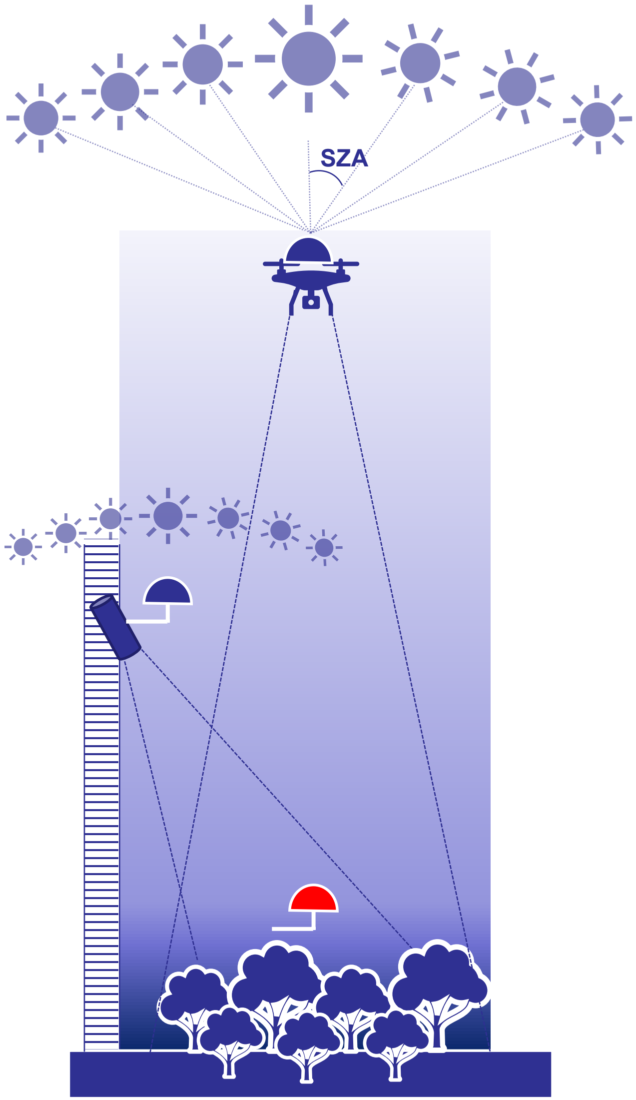


- Downward sensor-target oxygen transmittance $T^{\downarrow}_{O_2}$

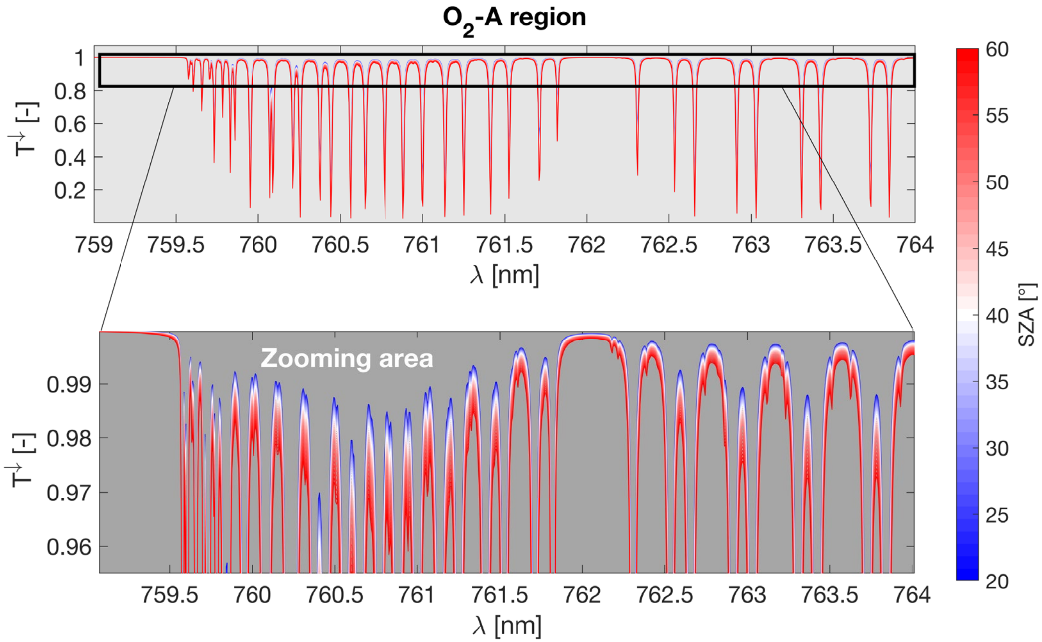


- Upward target-sensor oxygen transmittance $T^{\uparrow}_{O_2}$

Tower-mounted measurement

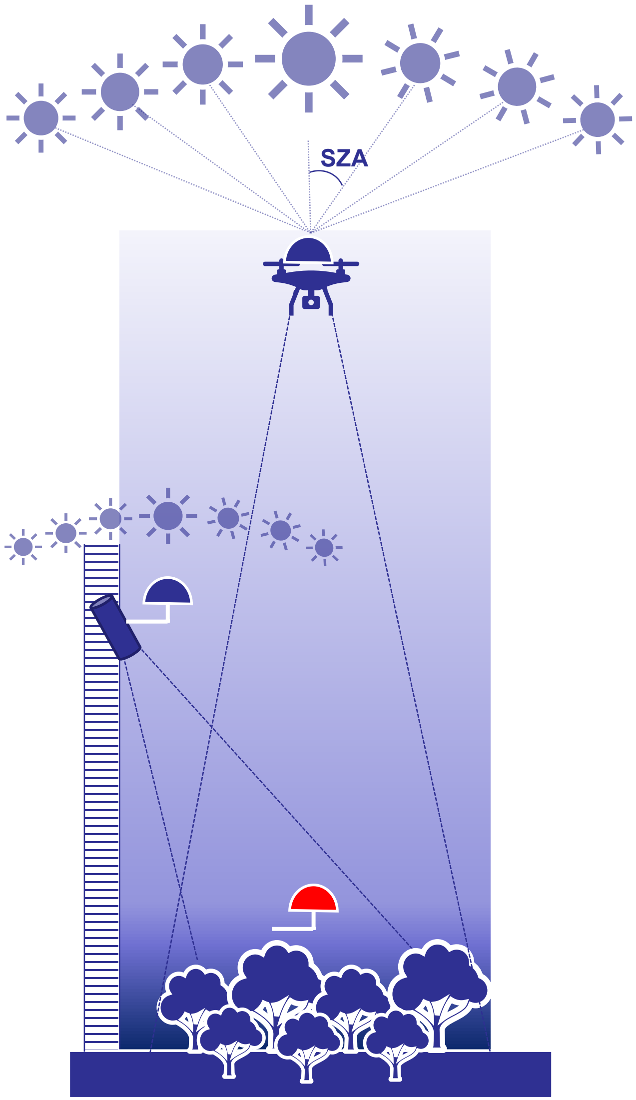


- Downward sensor-target oxygen transmittance $T^{\downarrow}$
  - ✓ Main dependency on SZA
  - ✓ Secondary dependency on (T, p)



Oxygen transmittance spectra simulated line-by-line and convolved to a fine spectral resolution of 0.1 cm−1. Different colors on T are associated to distinct SZAs. Changes in (T,p) conditions are secondary and not indicated in the figure. <u>Maximum T variation registered is around 8°C</u>

Tower-mounted measurement



- Downward sensor-target oxygen transmittance $T^{\downarrow}$
  - ✓ Main dependency on SZA
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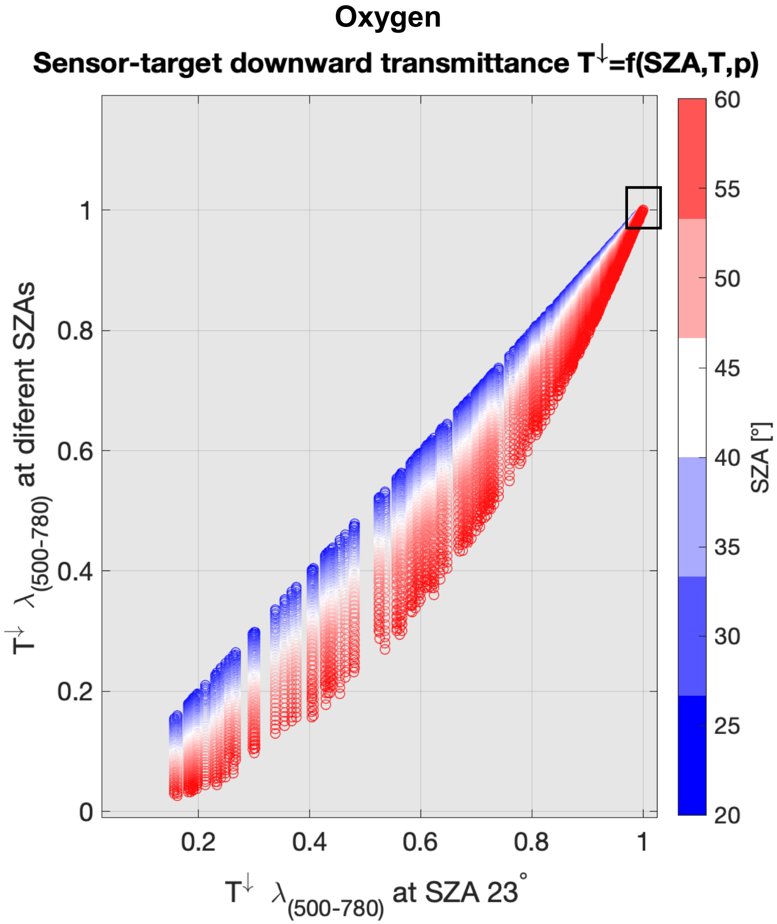
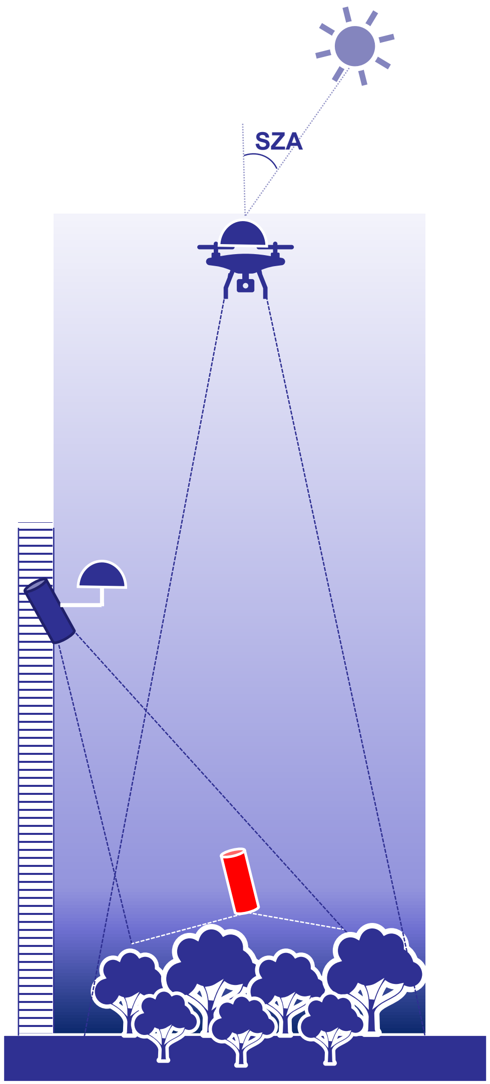
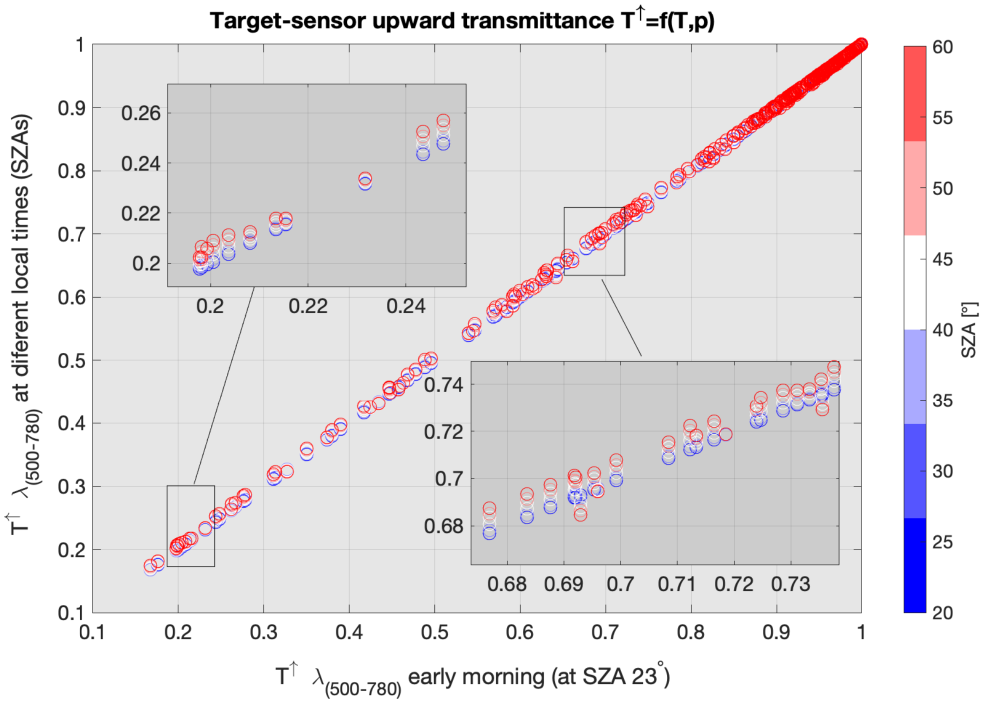


- ✓ (1,1) corresponds to the transmittance values outside the O_2 absorption regions.
- ✓ This scatter plot cover from 500-780 nm, i.e. O_2-B and O_2-A
- ✓ Is NOT a linear scaling factor that can be applied.

Tower-mounted measurement



- Upward target-sensor oxygen transmittance $T^{\uparrow}$
  - ✓ Main dependency on (T, p)



(b)

- ✓ (1,1) corresponds to the transmittance values outside the O_2 absorption regions.
- ✓ This scatter plot cover from 500-780 nm, i.e. O_2-B and O_2-A
- ✓ Is NOT a linear scaling factor but changes are more subtle that due to geometry.

Maximum T variation registered is around 8°C

(T, p) effects on oxygen regions

Temperature and pressure seasonal variation will produce a seasonal change in the O2 absorption region depth.

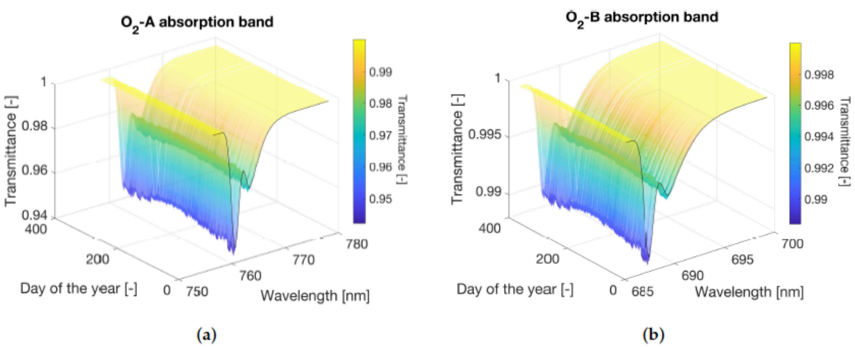


Figure 14. Spectral oxygen transmittance variation for the O_2–A (a) and O_2–B (b) absorption bands for the T and p conditions registered at 30 m tall tower at the Hyytiälä Forest Field Station in Finland.

O_2 absorption changes due to temperature and pressure seasonal variations, could have a significant impact in SIF estimates.

Sabater, N. et al. (2018). Compensation of oxygen transmittance effects for proximal sensing retrieval of canopy-leaving sun-induced chlorophyll fluorescence. *Remote Sensing*, *10*(10), 1551.

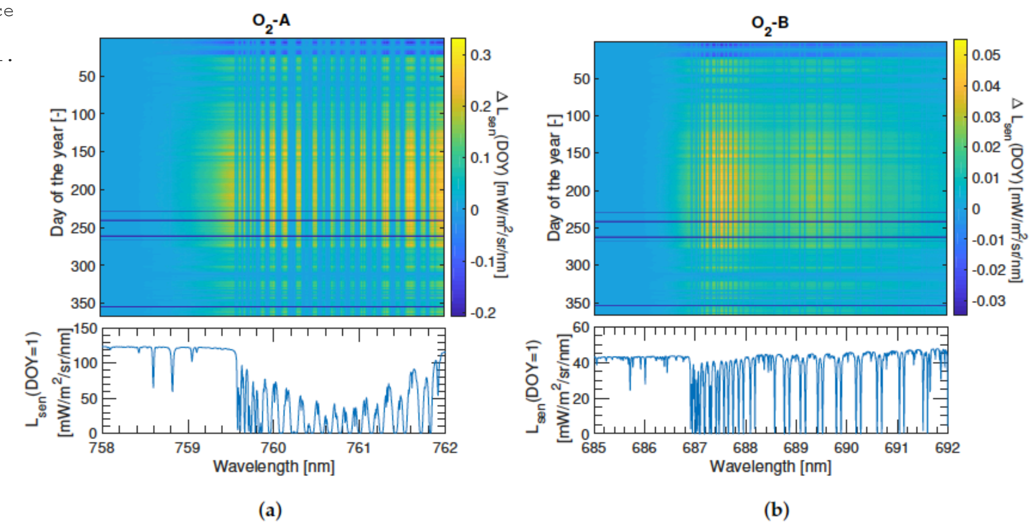


Figure 15. Variation in radiance units computed as L_{sen}(DOY)-L_{sen}(DOY=1) for the O_2–A (a) and the O_2–B (b) absorption regions. The acronym DOY refers to the Day Of Year from 1–365.

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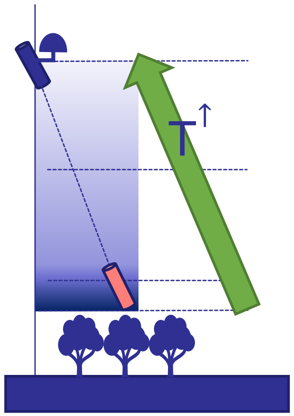
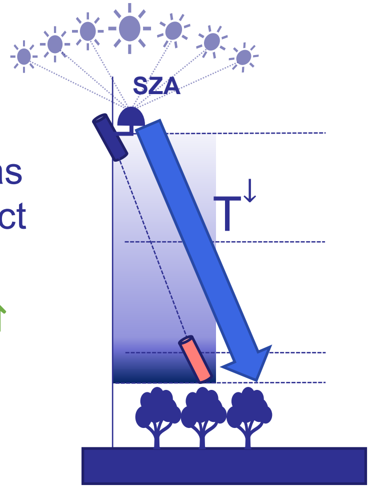
Tower-mounted measurement

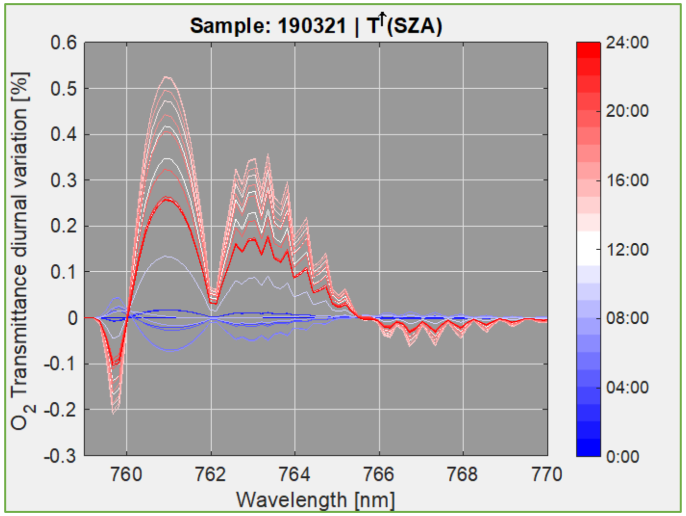
- On SIF retrievals, the correction of the upward transmittance $T^{\uparrow}$ has a larger impact than the correction of the downward transmittance $T^{\downarrow}$

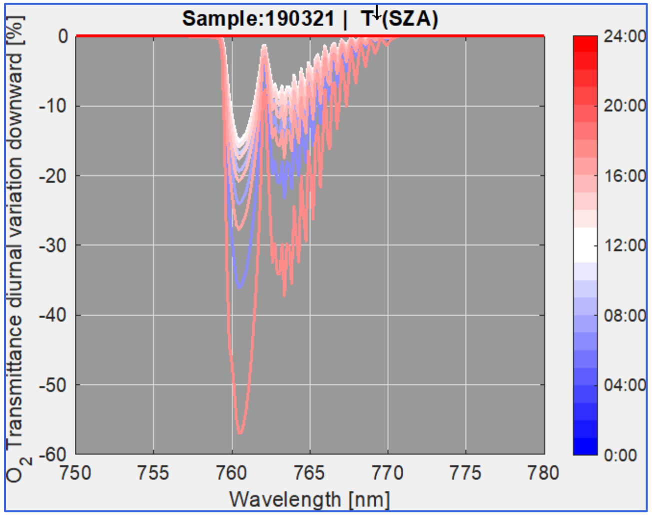


$T^{\uparrow}$ correction has a larger impact ≫ $T^{\downarrow}$ correction has a smaller impact

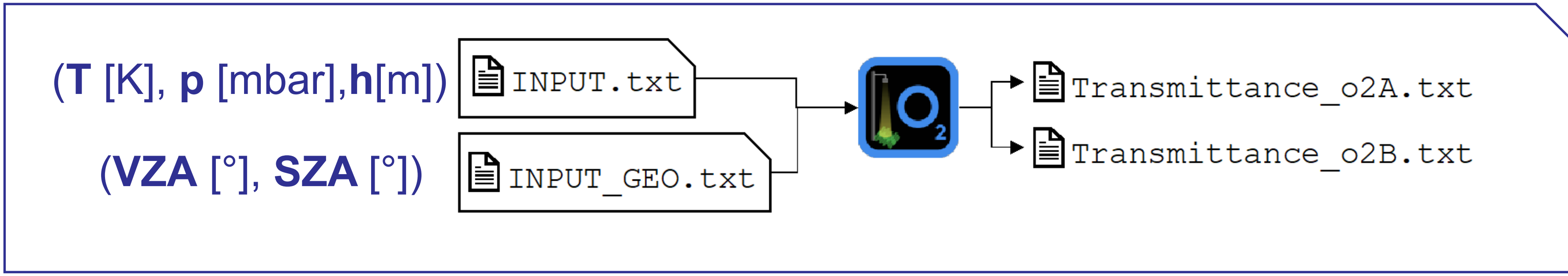
$$L_{up-sen} = (\rho L_{in-sen} T^{\downarrow} + F) T^{\uparrow}$$

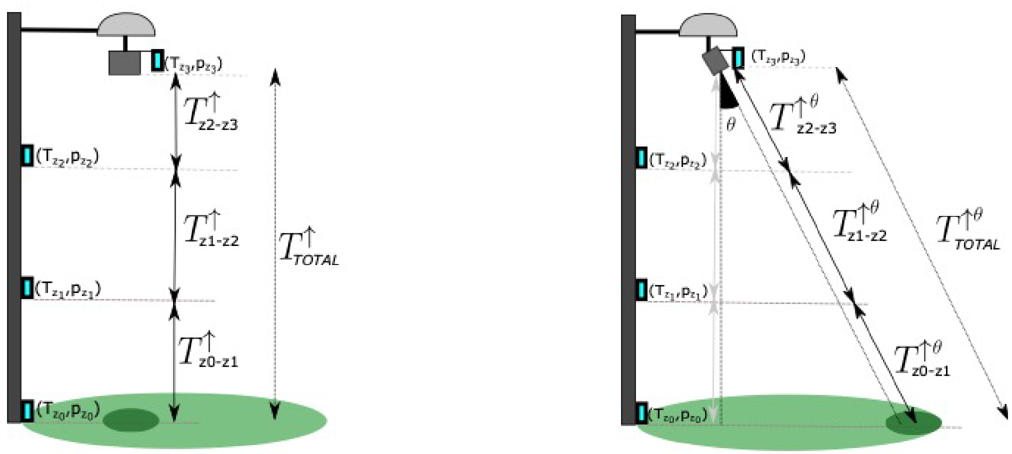






Oxygen transmittance estimation





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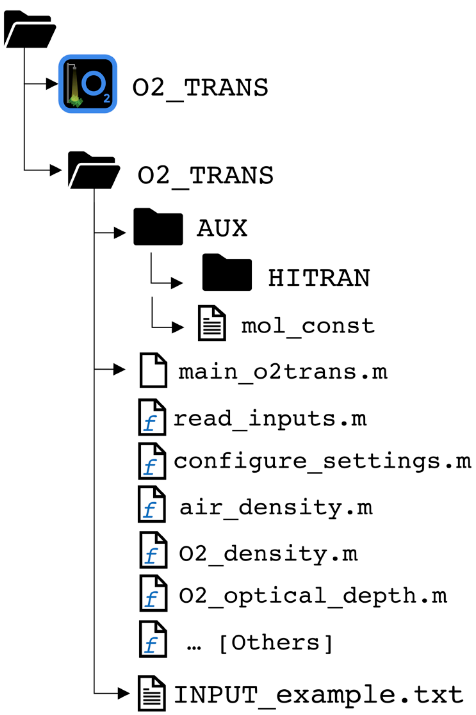
Source code: available in FMI-ISI GitHub (open after paper publication)

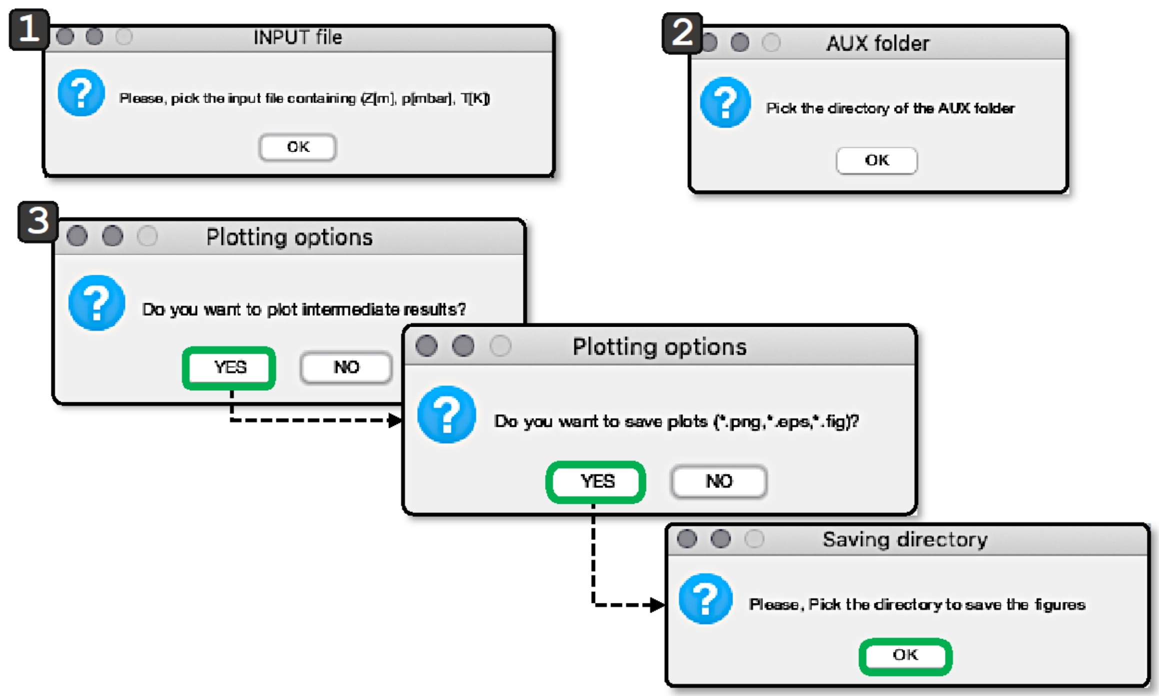
MATLAB code and binary files available to be run for non-license users

Oxygen transmittance estimation

- **O2_TRANS** tool is a set of functions (and a simple GUI) that makes use of the oxygen-related information available in **HITRAN** to compute the oxygen transmittance at a certain temperature and pressure conditions for a given optical path geometry (*dry air conditions*).

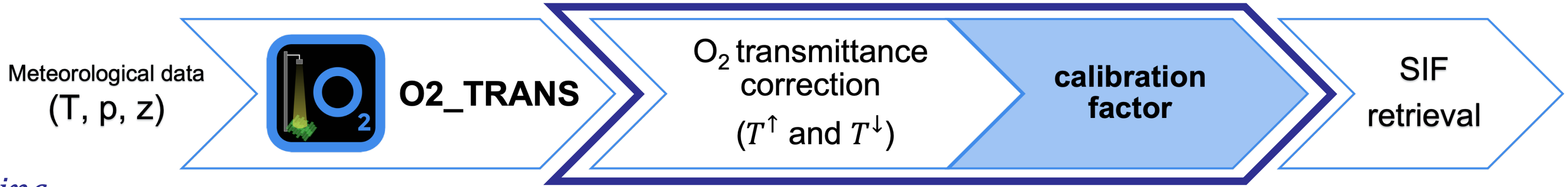
    ✓ Isotopologues O16O16, O16O17, O16O18

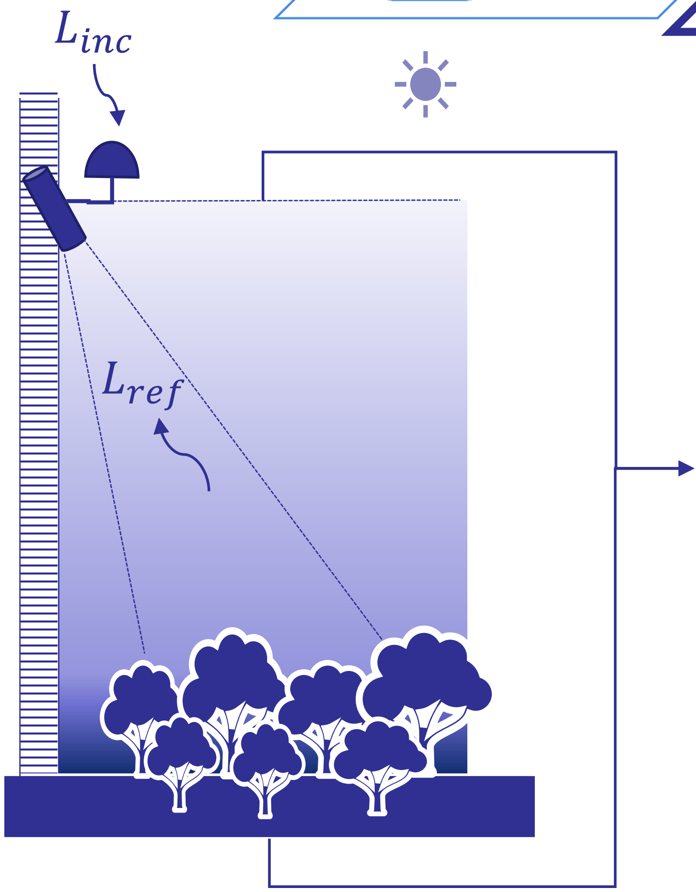




I.E. Gordon, L.S. Rothman, R.J. Hargreaves et al., "The HITRAN2020 molecular spectroscopic database", *Journal of Quantitative Spectroscopy and Radiative Transfer* **277**, 107949 (2022)

Oxygen correction





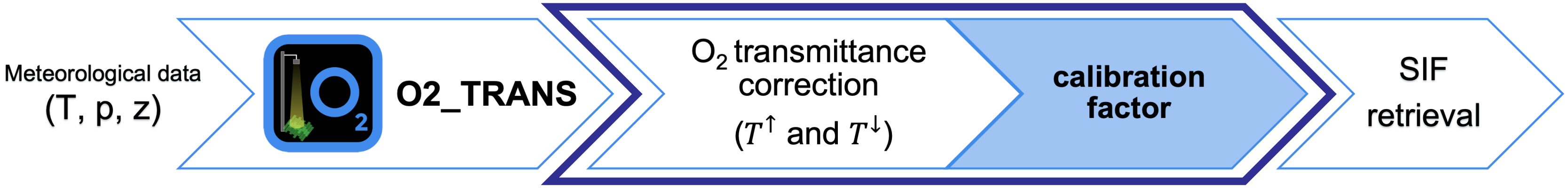
At the sensor level

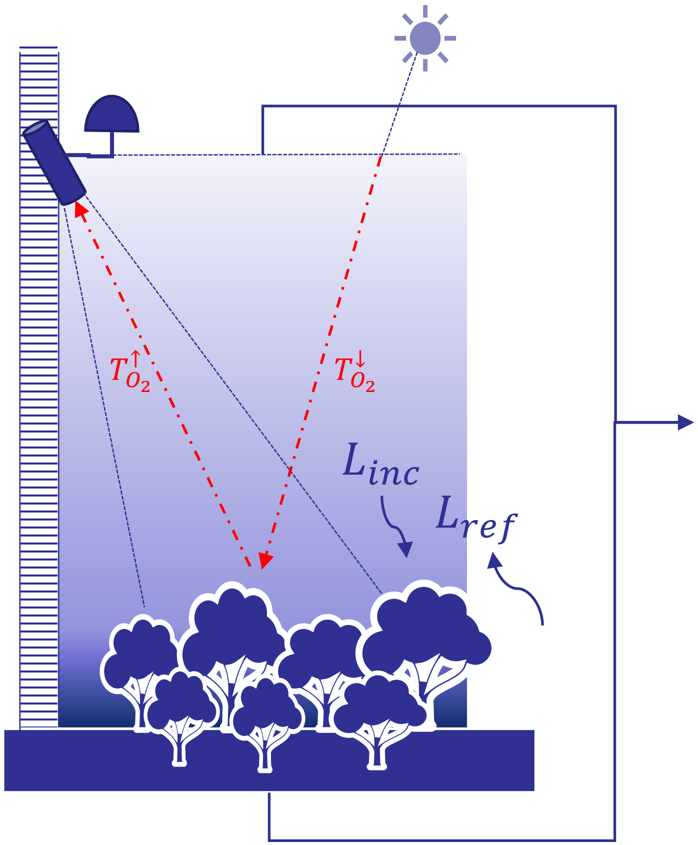
$$\rho_{app-sen} = \frac{< L_{ref-sen} >}{< L_{inc-sen} >}$$

At the Top-Of-Canopy (TOC) level

$$\rho_{app-TOC} = \frac{< L_{ref-TOC} >}{< L_{inc-TOC} >}$$

Oxygen correction





TOC level using sensor-level data

$$\hat{\rho}_{app-TOC} = \frac{\frac{<L_{ref-sen}>}{<T^{\uparrow}_{O_2}>}}{<L_{inc-sen}><T^{\downarrow}_{O_2}>}$$

- Why do we need any extra calibration correction?

$< x >$ Sensor resolution

$$< x > \cdot < y > \neq < x \cdot y >$$

Calibration correction

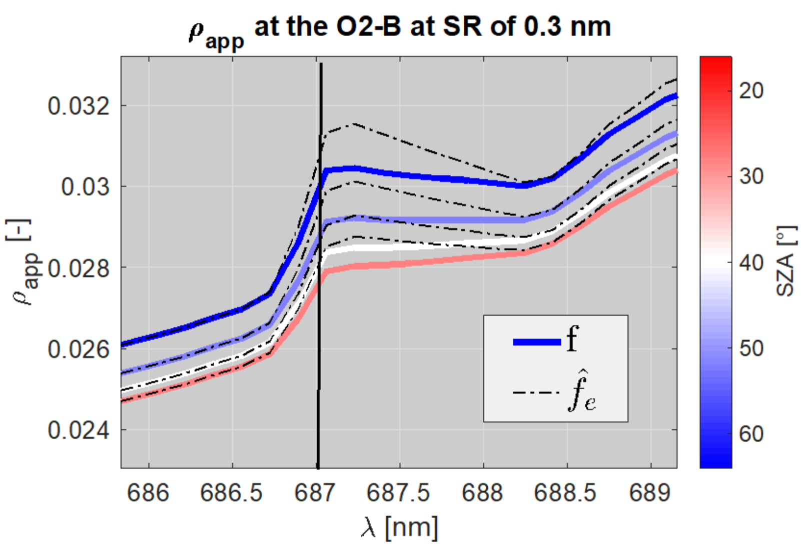
$\hat{f}_e$(error function)

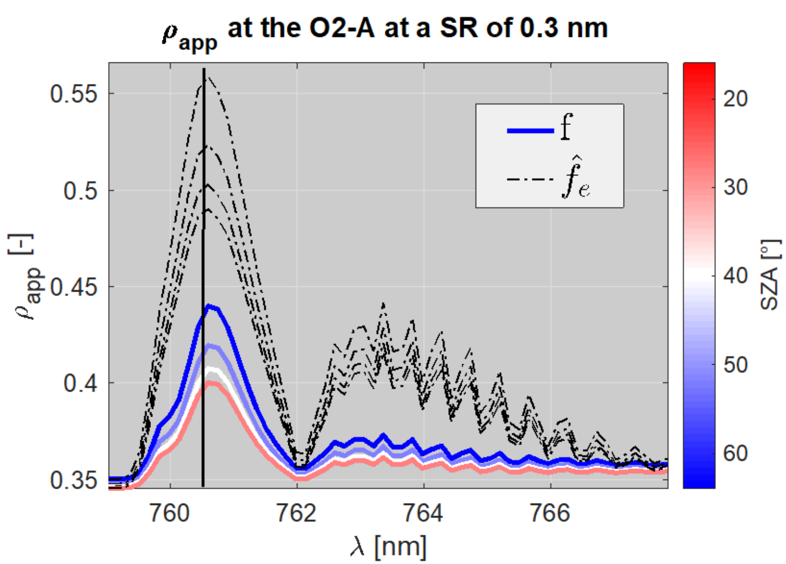
$$\hat{\rho}_{app-TOC} = \frac{\frac{<L_{ref-sen}>}{<T^{\uparrow}_{O_2}>}}{<L_{inc-sen}><T^{\downarrow}_{O_2}>}$$

f (function)

$$\rho_{app-TOC} = \frac{<L_{ref-TOC}>}{<L_{inc-TOC}>}$$

- Example of the error function $\hat{f}_e$ and f for a sensor resolution of 0.3 nm of FWHM at different illumination angles (SZA).





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Peaks are overestimated !

Calibration correction

- How to estimate the calibration correction?

  - ✓ By generating a calibration Look-up-Table (LUT), which depends mainly on the spectral resolution (SR), optical path, and ρ tabulated values.

$$\delta(\hat{\rho}_{app-TOC}) = \sqrt{\frac{\delta(<\hat{L}_{ref-TOC}>)^2}{<\hat{L}_{inc-TOC}>^2} + \frac{<\hat{L}_{ref-TOC}>^2\,\delta(<\hat{L}_{inc-TOC}>)^2}{<\hat{L}_{inc-TOC}>^4}}$$

  - ✓ Using an empirical approximation making used of the $T^{\downarrow}_{O_2}$ and $T^{\uparrow}_{O_2}$ oxygen transmittance.

    - ❖ Implicit dependency on (T, p) on the geometry (height, SZA)
    - ❖ Only requires outputs from **O2_TRANS**
    - ❖ This approximation results convenient but not as accurate as a dedicated LUT. Optimization results for a SR of 0.3 nm results in $x \approx 2.5$

$$f_{cal} = \left(\frac{T^{\downarrow}_{O_2(SZA)}}{T^{\uparrow}_{O_2}}\right)^x$$

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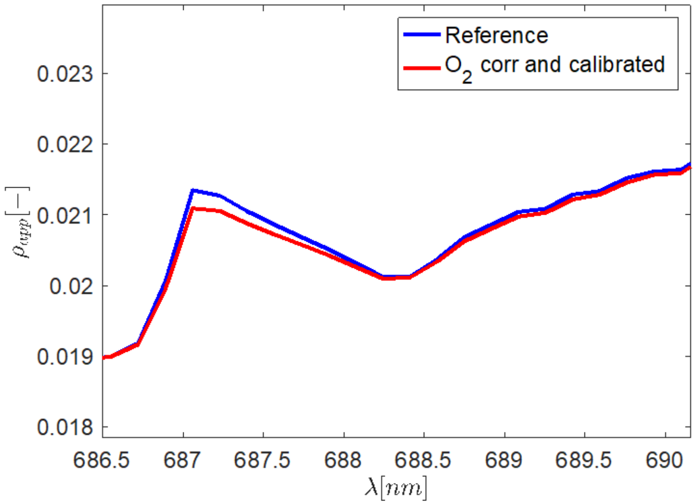
Calibration correction

- How to estimate the calibration correction?
  - ✓ Using an empirical approximation making used of the $T_{O_2}^{\downarrow}$ and $T_{O_2}^{\uparrow}$ oxygen transmittance.

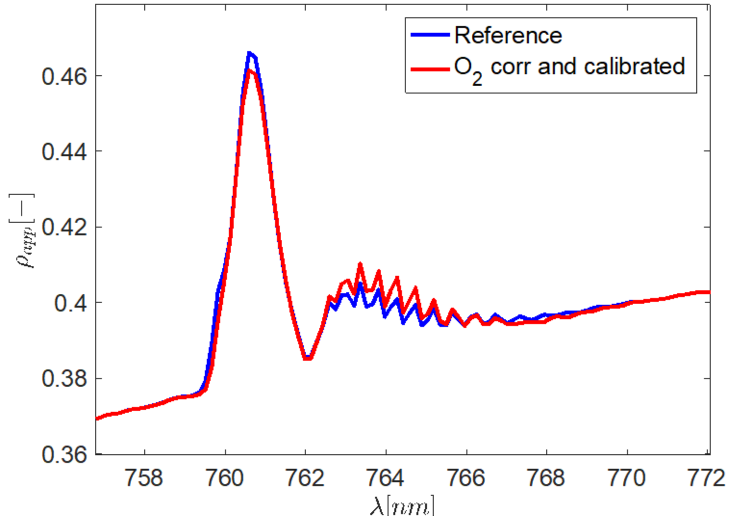
$$f_{cal} = \left(\frac{T^{\downarrow}_{O_2(SZA)}}{T^{\uparrow}_{O_2}} \right)^{x}$$

  - ✓ Simulated reference $\boldsymbol{f} = \rho_{app-TOC}$ and oxygen corrected and calibrated $\hat{f}_e = \hat{\rho}_{app-TOC} \cdot f_{cal}$

O_2-B

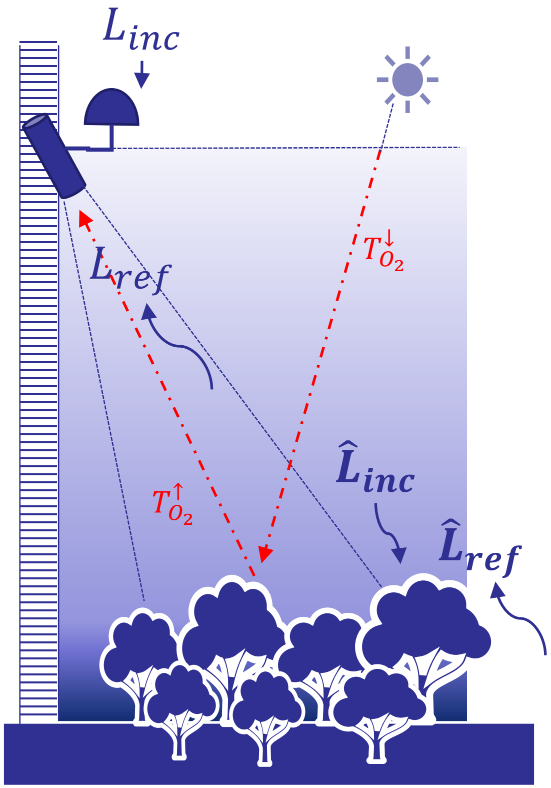


O_2-A



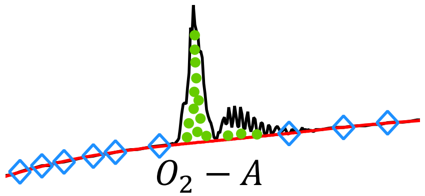
Impact on SIF retrievals

- Accuracy level achieved on the oxygen correction and calibration of the acquired signal ($\hat{L}_{inc}$, $\hat{L}_{ref}$) will distinctly propagate in SIF estimates depending on the retrieval strategy used.



Two family-methods evaluated:

- Differential absorption technique - **Peak Height method -**
  - Relating the SIF contribution to the Peak Height in apparent reflectance taking as a reference the lower envelope of $\hat{\rho}_{app}$



Ø oxygen free

$\hat{\rho}_{app}$ oxygen corrected (as TOC) and calibrated

- Spectral fitting technique – Minimizing the fitting between simulated and measured ρ_{app} in the full fluorescence interval 650-780 nm

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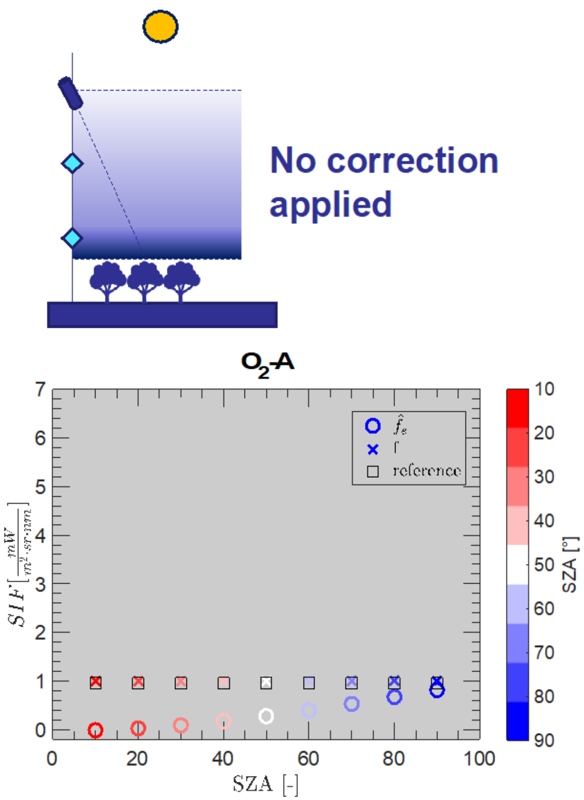
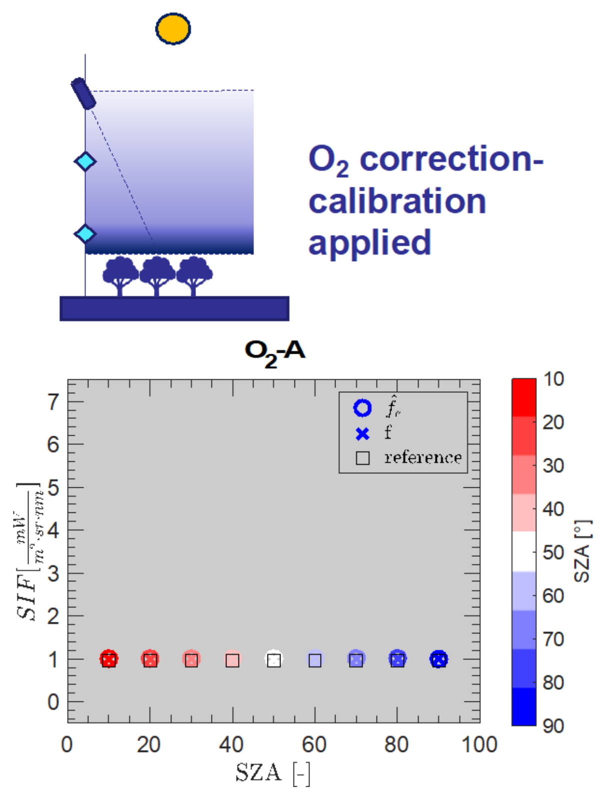
Impact on SIF retrievals

Peak height method SIF_λ

- SIF estimates from the **Peak Height** method evaluated against a constant simulated □ reference of 1 mW/m²·sr·nm
- Comparison of three scenarios: (a) No correction, (b) Oxygen and calibration correction



(a)



(b)

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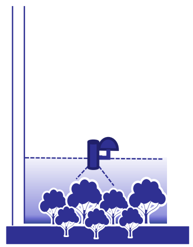
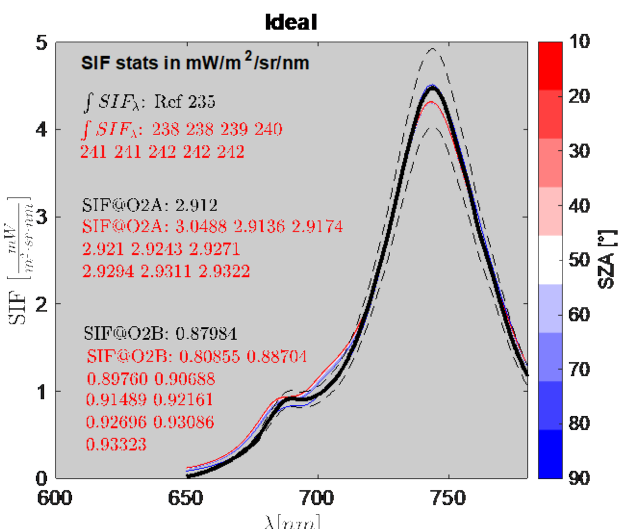
Impact on SIF retrievals

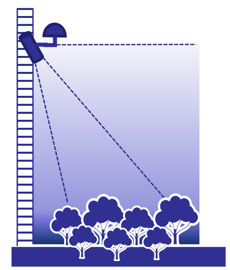
Spectra fitting method

- SIF estimates from the **spectral fitting** method evaluated against a constant simulated reference (black solid line) $\pm 10\%$ (black dashed line)
- SIF estimates under distinct illumination conditions (blue-red color bar)

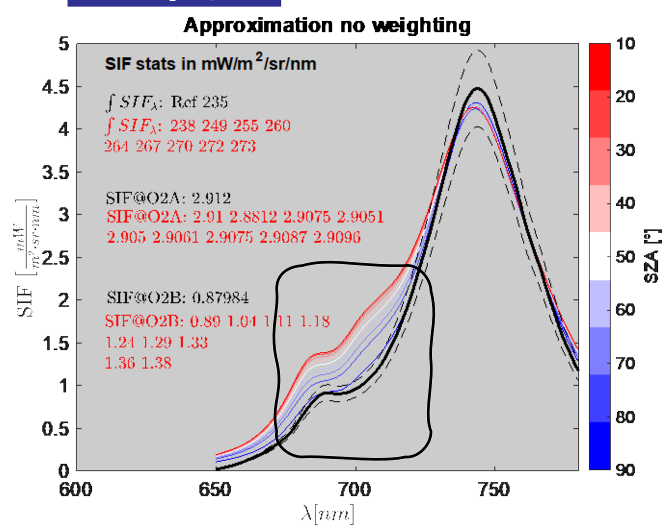


Ideal





Tower corrected



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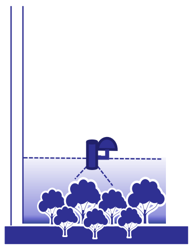

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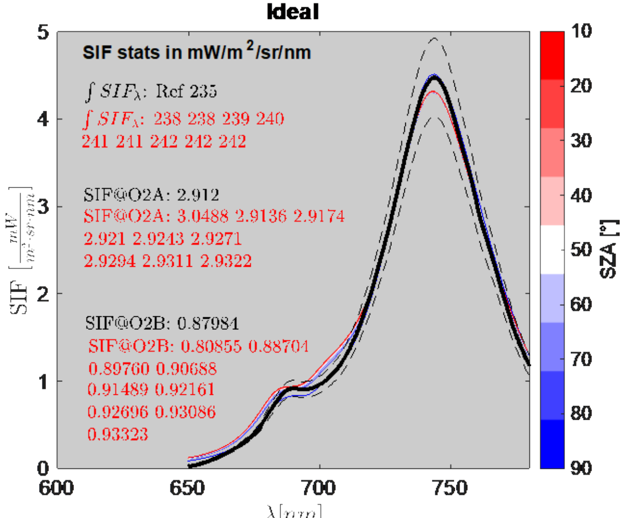
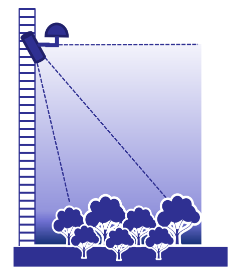
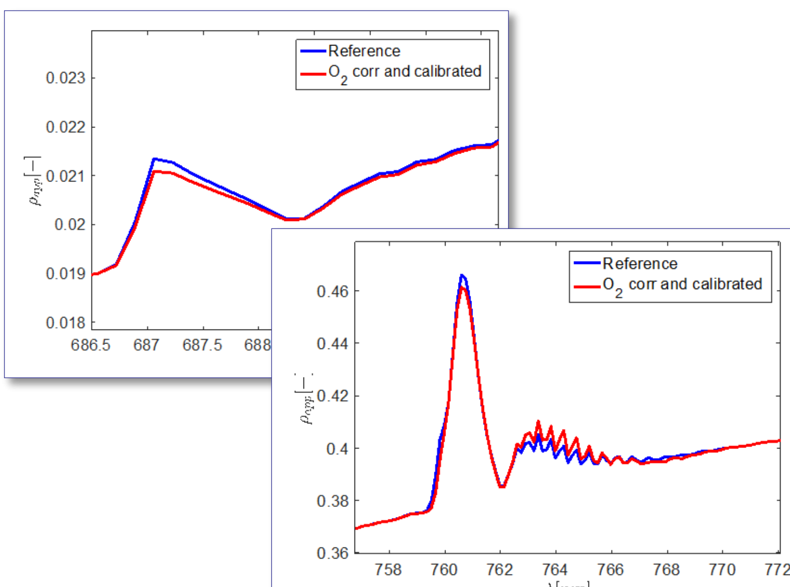




Tower corrected



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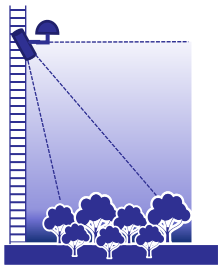
Impact on SIF retrievals

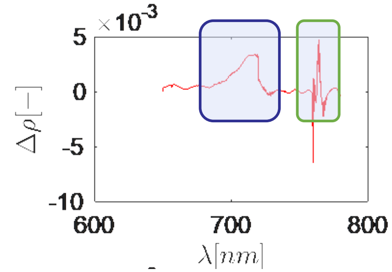
Spectra fitting method

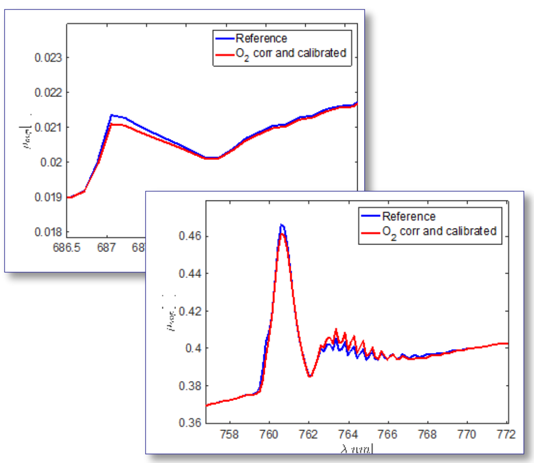
- SIF estimates from the **spectral fitting** method evaluated against a simulated **reference** (black solid line) $\pm 10\%$ (black dashed line)
- The SFM can be optionally weighted by the inverse of the reflectance as a weighting in the optimization routine

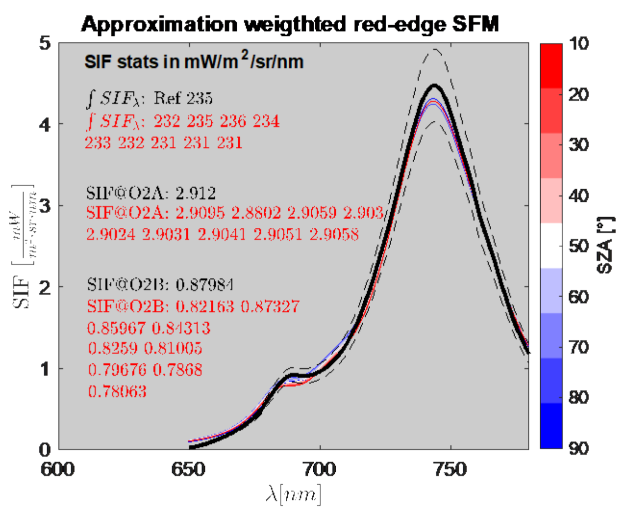


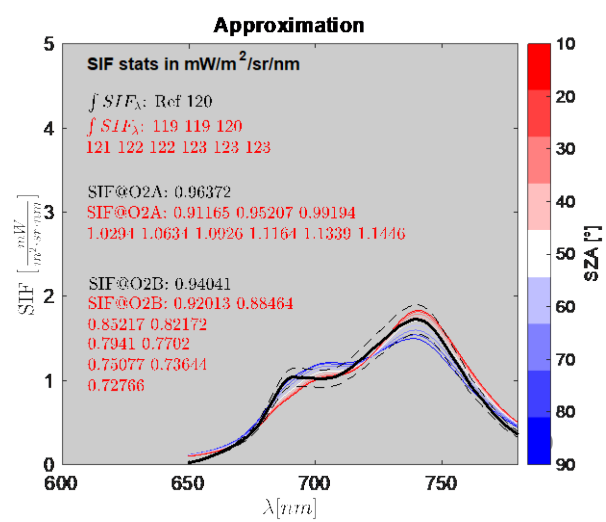
Tower corrected

weighted in the SFM with: 1/ reflectance









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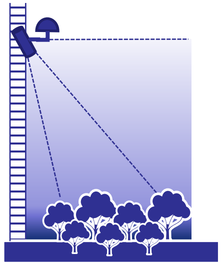
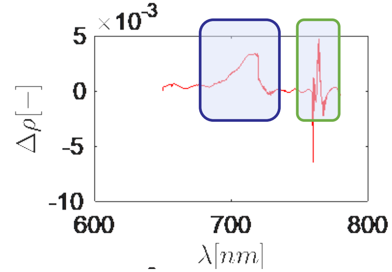
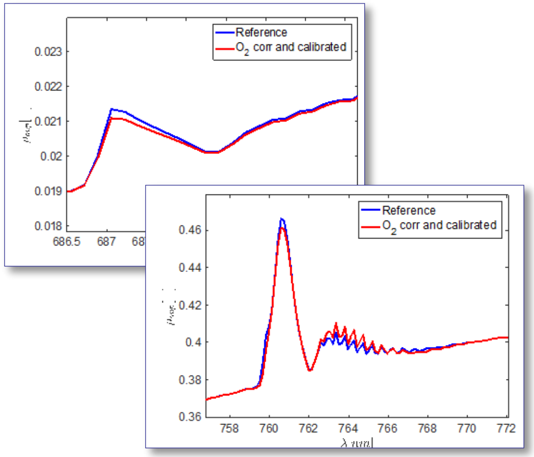
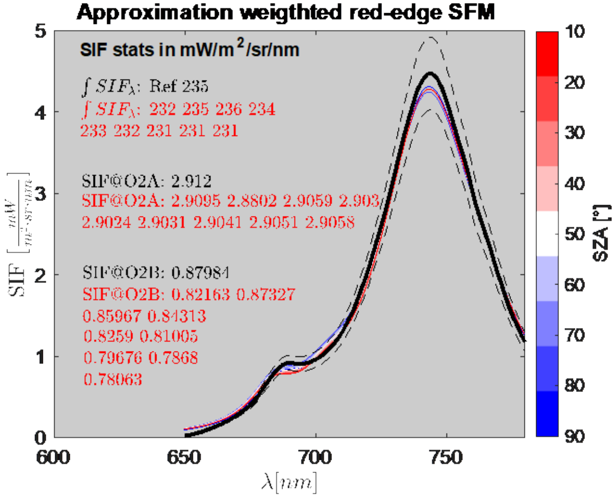


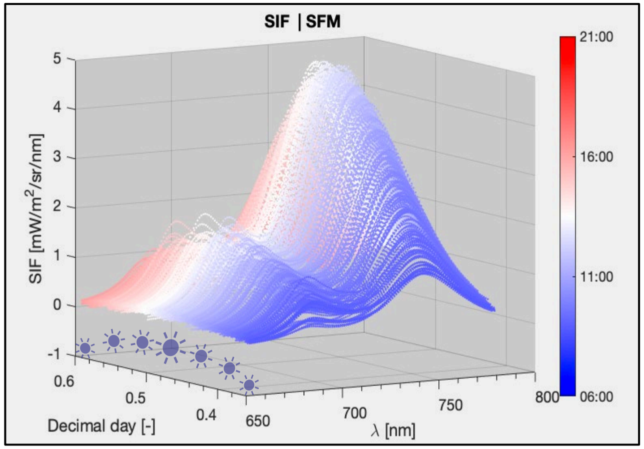
Tower corrected

weighted in the SFM with: 1/ reflectance









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Oxygen correction planned work…

- Measuring non-vegetated targets under different illumination conditions
  - ✓ Using the top roof facilities of FMI headquarters to validate TOC oxygen absorption correction. Measurements using FLOX.
  - ✓ Complementary atmospheric measurements available (if required for validation)

- Conduct seasonal measurements focus on Nordic ecosystems (TBD) in Hyytiälä and/or Sodankylä, thanks to the close collaboration with
  - ✓ FMI Greenhouse Gases and Satellite Methods group *(Prof. Hannakaisa Lindqvist)*
  - ✓ University of Helsinki Optics of Photosynthesis Laboratory *(Prof. Albert Porcar)*

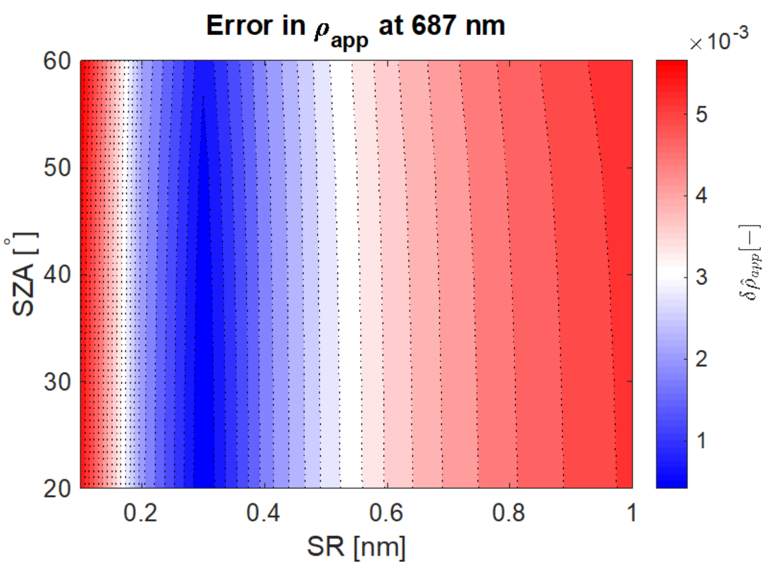
- Processing some datasets in the frame of FLEX campaign activities
  - ✓ Assessment of the TOC oxygen correction for fluorescence retrievals. Intercomparison between three alternative TOC strategies for SIF retrievals.

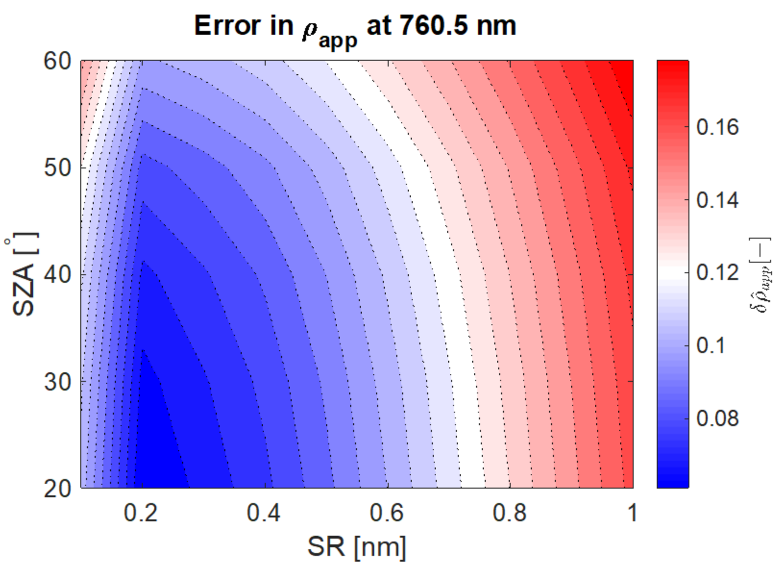
Thanks

Calibration correction

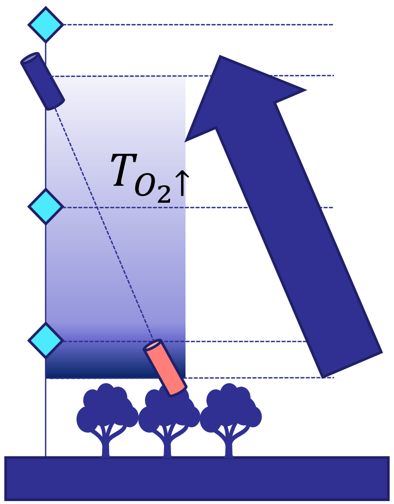
- Following the error propagation formula and neglecting correlations between variables, error in $\rho_{app-TOC}$ results for different sensor resolutions and different illumination angles (SZA) at the O_2-B and O_2-A regions.

$$\delta(\hat{\rho}_{app-TOC}) = \sqrt{\frac{\delta(<\hat{L}_{ref-TOC}>)^2}{<\hat{L}_{inc-TOC}>^2} + \frac{<\hat{L}_{ref-TOC}>^2\,\delta(<\hat{L}_{inc-TOC}>)^2}{<\hat{L}_{inc-TOC}>^4}}$$



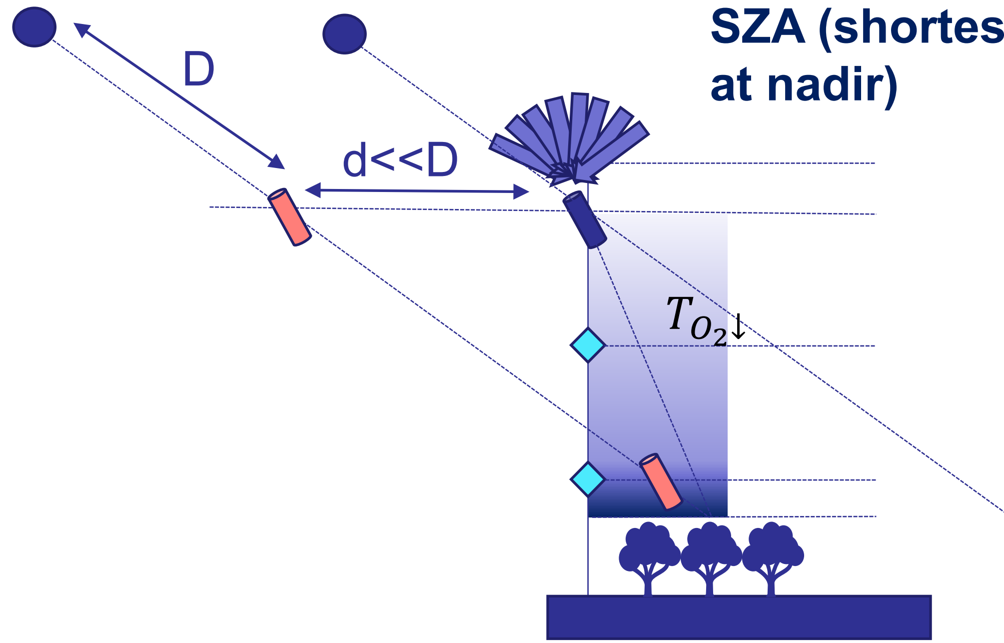


Fixed VZA (dependency on the air density)

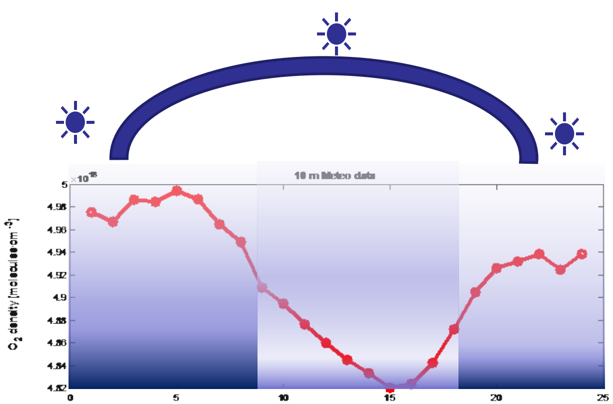


This variability is lower but affects the L_{ref}

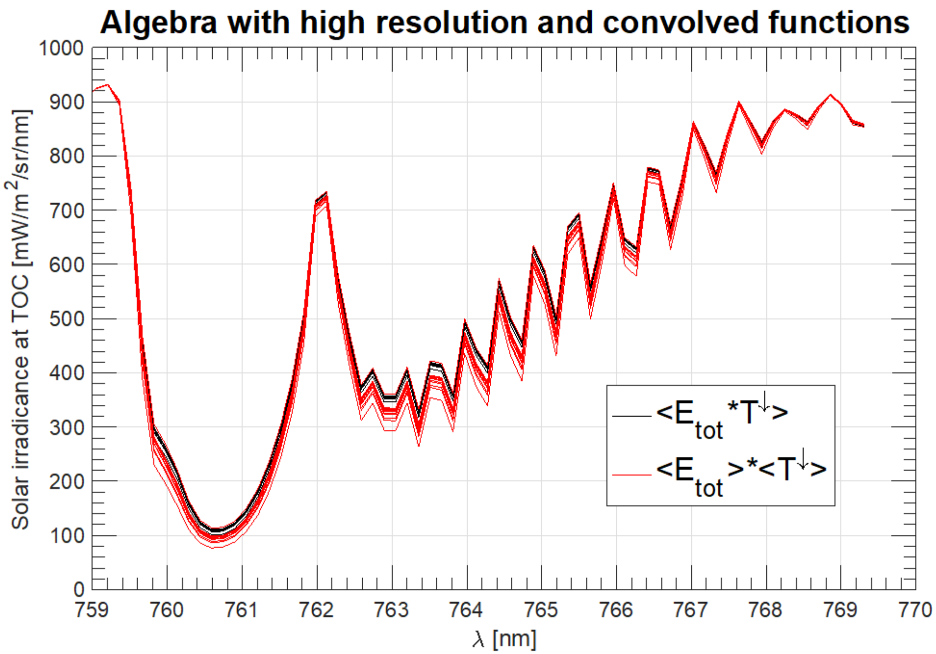
SZA (shortest path at nadir)



This variability is higher but affects the L_{inc}



Calibration correction



Ideally,

$$\rho_{app\_TOC\{HR\}} = < \frac{L_{ref}}{L_{inc}\cdot T_{O_2\downarrow}\cdot T_{O_2\uparrow}} >$$

Our computation,

$$\rho_{app\_TOC} = \frac{< L_{ref} >}{< L_{inc} > \cdot < T_{O_2\downarrow}\cdot T_{O_2\uparrow} >}$$

$$\rho_{app\_TOC\{HR\}} = \rho_{app\_TOC}\cdot f_{cal\{HR\}}$$

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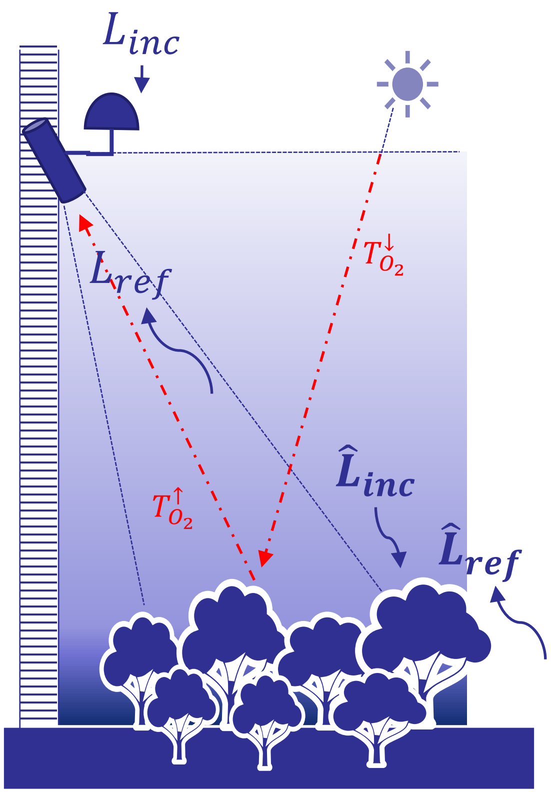
Impact on SIF retrievals

- Accuracy level achieved on the oxygen correction and calibration of the acquired signal ($\hat{L}_{inc}$, $\hat{L}_{ref}$) will distinctly propagate in SIF estimates depending on the retrieval strategy used.



Two family-methods evaluated:

- Differential absorption technique - **Peak Height method -**
  - Relating the SIF contribution to the Peak Height in apparent reflectance taking as a reference the lower envelope of

$$F = \frac{1}{\pi}\left(\hat{\rho}_{app} - \hat{\rho}_{app,\emptyset}\right)\frac{\hat{E}_{TOC,\emptyset} \cdot \hat{E}_{TOC}}{\hat{E}_{TOC,\emptyset} - \hat{E}_{TOC}}$$

$\emptyset$ oxygen free
$\hat{x}$ oxygen corrected (as TOC) and calibrated

- Spectral fitting technique – Minimizing the fitting between simulated and measured ρ_{app} in the full fluorescence interval 650-780 nm

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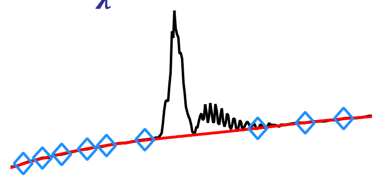
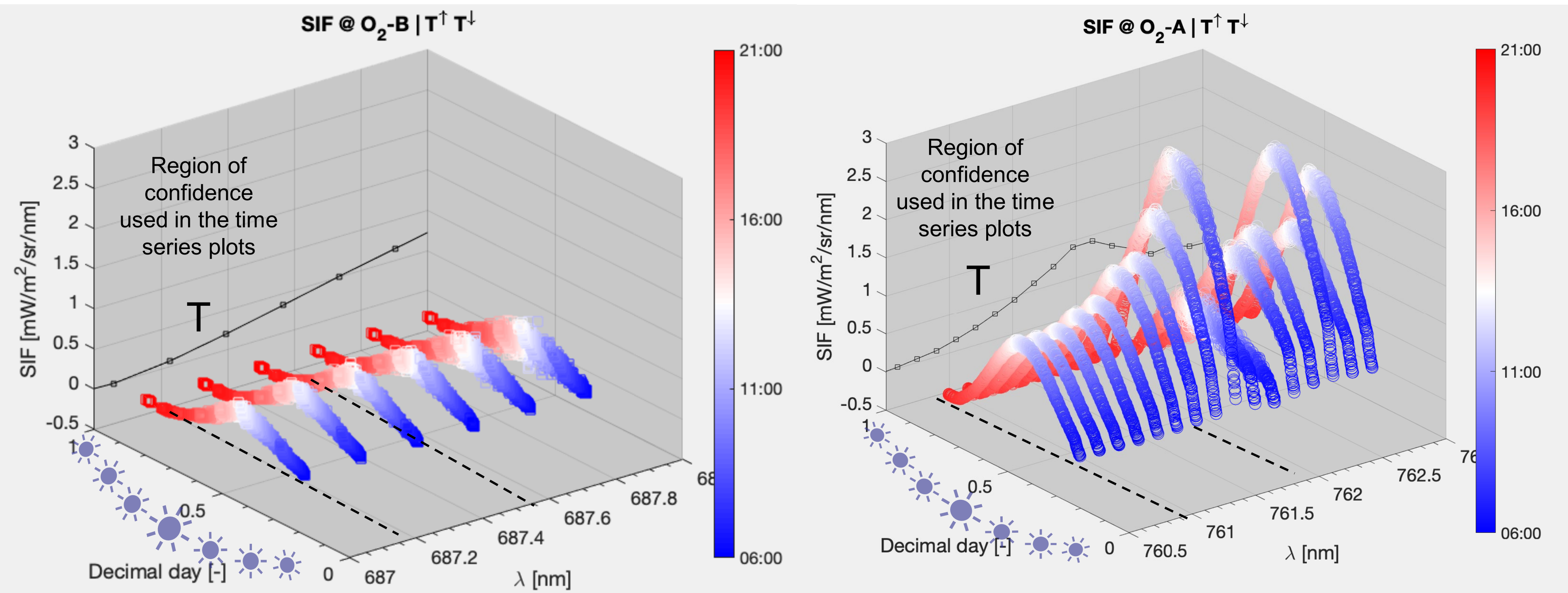
Impact on SIF retrievals

Peak height method SIF_λ



$$F = \frac{1}{\pi}\left(\hat{\rho}_{app} - \hat{\rho}_{app,\emptyset}\right)\frac{\hat{E}_{TOC,\emptyset} \cdot \hat{E}_{TOC}}{\hat{E}_{TOC,\emptyset} - \hat{E}_{TOC}}$$

$\emptyset$ oxygen free
$\hat{x}$ oxygen corrected (as TOC) and calibrated

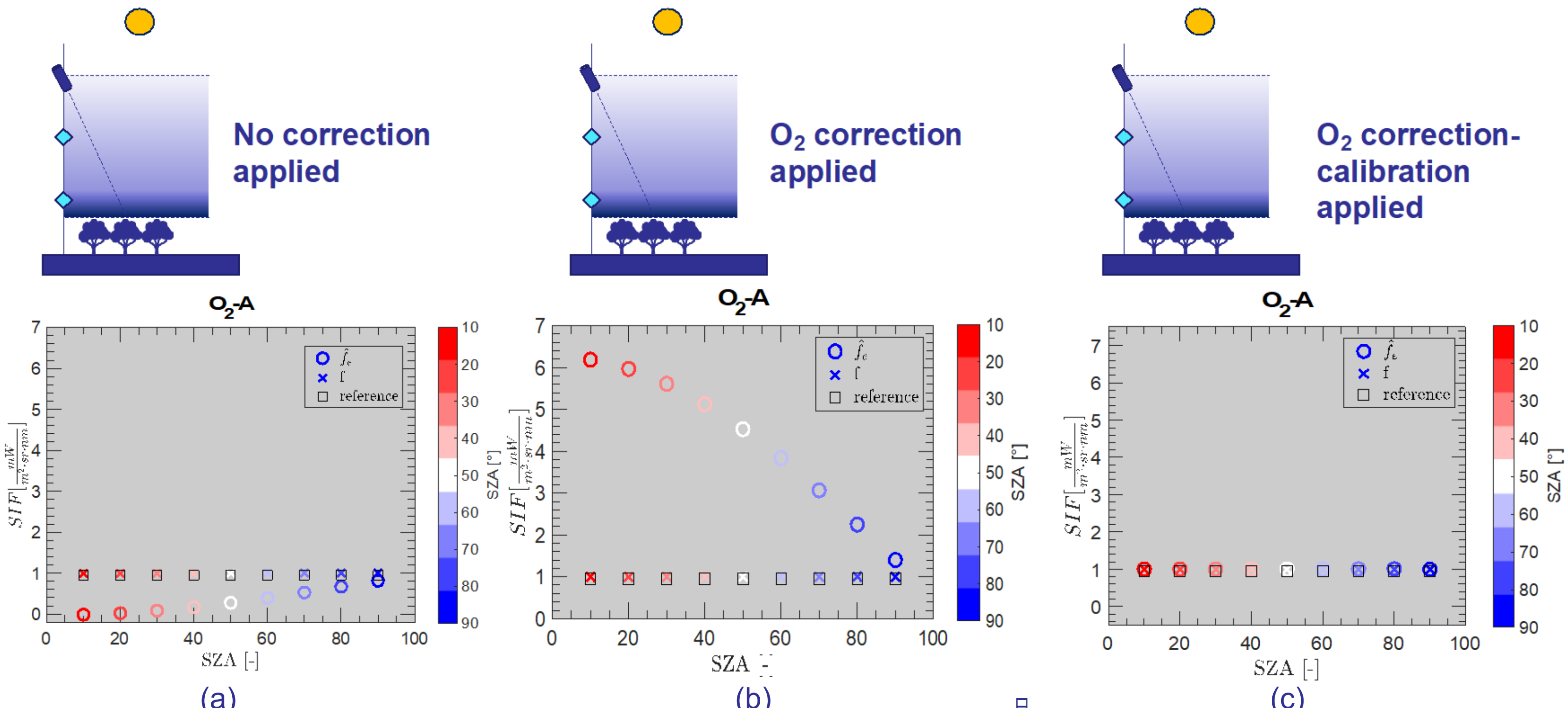


- The **Peak Height** method estimates SIF at each individual wavelength within the oxygen absorption feature.
- Channels more sensitive to pressure changes or noise are discarded.
- $\tilde{\rho}_{app,\lambda}$ and $\tilde{E}_{TOC,\lambda}$ estimated through interpolation using the absorption vicinities

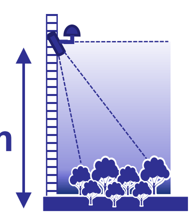
Impact on SIF retrievals

Peak height method SIF_λ

- SIF estimates from the **Peak Height** method evaluated against a constant simulated □ reference of 1 $mW/m^2{\cdot}sr{\cdot}nm$
- Comparison of three scenarios: (a) No correction, (b) Oxygen correction, (c) Oxygen and calibration correction

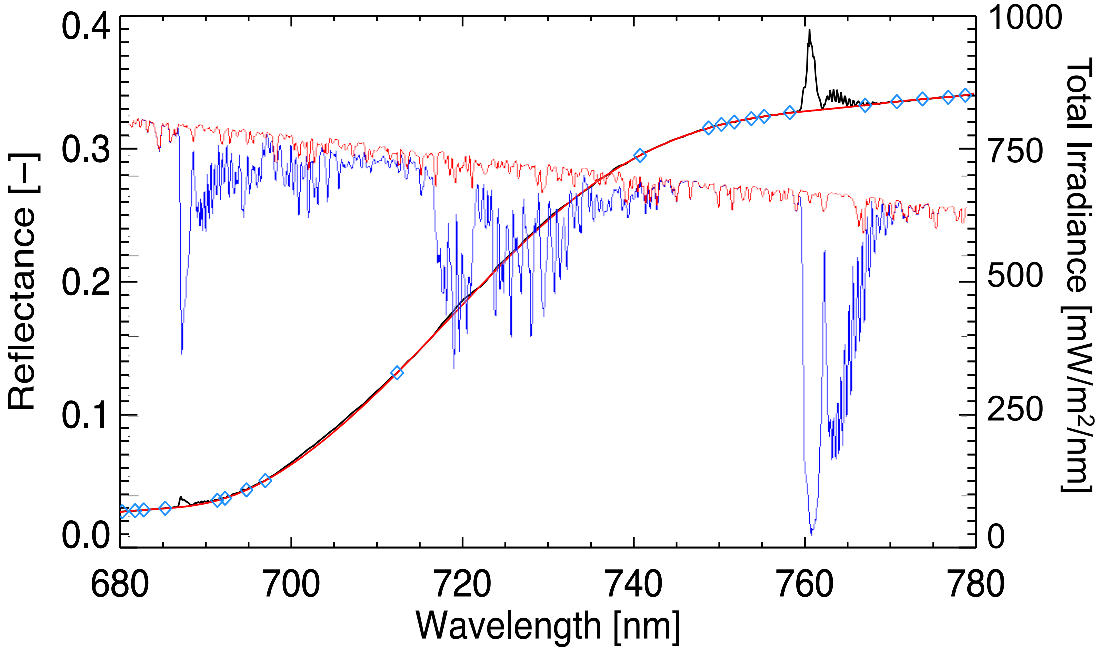


Simulated Tower height 90 m



Impact on SIF retrievals

Peak height method SIF_λ



$\hat{\rho}_{app}(O_2)$

$\hat{\rho}_{app,\emptyset}(no\ O_2)$

◇ Interpolation points

$\hat{E}_{TOC}(O_2)$

$\hat{E}_{TOC,\emptyset}(no\ O_2)$

$$F = \frac{1}{\pi}\left(\hat{\rho}_{app} - \hat{\rho}_{app,\emptyset}\right)\frac{\hat{E}_{TOC,\emptyset} \cdot \hat{E}_{TOC}}{\hat{E}_{TOC,\emptyset} - \hat{E}_{TOC}}$$

$\emptyset$ oxygen free

$\hat{x}$ oxygen corrected (as TOC) and calibrated

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