Sentinel-5 Precursor + Innovation: Sentinel-5 Precursor Ocean Color (S5POC) S5P diffuse attenuation (K_d) product in Sentinel-5-p (S5p) Productive Algorithm Laboratory (PAL)

Product User Manual (S5POC-PAL-PUM)

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Change log

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1.0	Mar 6, 2025	PUMv1.0	Revised according to S&T feedback
1.1	Aug 25, 2025	PUMv1.1	New variables added

Contents

List of Figures

List of Abbreviations

AWI Alfred Wegener Institute Helmholtz Centre for Polar and Marine Research

blue DOAS fit window in ultraviolet-A from 390 to 423 nm

DOAS Differential Optical Absorption Spectroscopy

IUP Institute of Environmental Physics

K_d Diffuse attenuation coefficient

MODIS-Aqua Moderate Resolution Imaging Spectroradiometer-Aqua

OC-CCI Ocean Colour Climate Change Initiative

OLCI Ocean and Land Colour Instrument

PhytoDOAS DOAS applied for retrieval of phytoplankton biomass

RMS Root mean square

RMSD Root mean square difference

S5P Sentinel-5 Precursor

S5POC Sentinel-5 Precursor Ocean Color

TROPOMI Tropospheric Monitoring Instrument

UV Ultraviolet

UVA DOAS fit window in ultraviolet-A from 356.5 to 390 nm

UVAB DOAS fit window in ultraviolet-A from 312.5 to 338.5 nm

VIIRS Visible/Infrared Imager Radiometer Suite

VRS Vibrational Raman Scattering

AOT Aerosol optical thickness

WS Wind speed (surface roughness term)

QA Quality assessment flag (0–1 after scaling)

List of Related Documents

[RD1] Bracher A., Oelker J., Bellido Rosas A. J., Richter A. (2024) Exploitation of Sentinel-5-p (S5p) for Ocean Colour Products (S5POC) - S5p diffuse attenuation (K_d) product in Sentinel-5-p (S5p) Productive Algorithm Laboratory (PAL): Algorithm Theoretical Base Document (S5POC-PAL-K_d-ATBD) Version 1.0, 20 Dec 2024, S5POC_PAL_K_d_ATBD_v1.0_20122024.pdf.

[RD2] Losa S. N., Brotas V., Brito A., Costa M., Dinter T., Favareto L., Gomes M., Oelker J., Rio M.-H., Sa C., Soppa M.S., Suseelan V. P., Bracher A. (2022) Sentinel-5P Ocean Colour: Data Pool and Auxiliary User Manual 2 (DP + AUM2; S5POC_DP-D2_AUM2-D8). Version 1.2, 13 May 2022. https://www.awi.de/fileadmin/user_upload/AWI/Forschung/Klimawissenschaft/Physikalische_Ozeanographie_der_Polarmeere/S5POC_DP-D02_AUM2-D08_v1.2_13052022_signed.pdf

[RD3] Bracher A., Losa S. N. (2024) Exploitation of Sentinel-5-p (S5p) for Ocean Colour Products (S5POC) - S5p diffuse attenuation (K_d) product in Sentinel-5-p (S5p) Productive Algorithm Laboratory (PAL): Validation Report (S5POC-PAL-K_d-VR). Version 1.0, 13 May 2024. S5POC_VR_D05_v3.0_13052022.pdf

[RD4] Bracher A., Alvarado A., Richter A., Rio M.-H., Brotas V., Brito A., Costa M. (2022) Sentinel-5P Ocean Colour: Impact Assessment Report. S5POC-IAR-D09 v3.1. 13 May 2022. S5POC_IAR_D05_v3.1_13052022.pdf

[RD5] Oelker J., Losa S. N., Richter A., Bracher A. (2022) TROPOMI-retrieved underwater light attenuation in three spectral regions in the ultraviolet to blue. Frontiers in Marine Science 9. 787992. doi: 10.3389/fmars.2022.787992

1 Introduction

1.1 Purpose and Objective

This document describes the technical characteristics of the TROPOMI S5POC level 2 products developed within the Sentinel-5 Precursor (S5P) + Innovation project, theme 7 S5P Ocean Color (S5POC). The purpose of this document is to provide product users with a brief description of the underlying retrieval, a summary of the product validation, recommendations for flagging, and a detailed description of the data file format.

1.2 Document overview

Section 2 gives an overview of the products, including a description of available flags and their recommended usage, a summary of the validation results, and information on data distribution. Section 3 contains details on the data file format.

2 Overview of the S5POC products

2.1 Product overview

The S5POC product consists of diffuse attenuation coefficients (K_d) at different spectral ranges in the UV and blue spectral range from TROPOMI. The retrieval is based on Differential Optical Absorption Spectroscopy (DOAS) extended to the ocean domain (PhytoDOAS). Fit results from the DOAS retrieval are converted into physical quantities using look-up-tables which were established with radiative transfer modeling.

The S5POC K_d product consists of three variables - the mean diffuse attenuation coefficient (K_d) of the downwelling plane irradiance over the first optical depth and over three different wavelength regions: 390 - 423 nm (K_d-blue), 356.5 - 390 nm (K_d-UVA), and 312.5 - 338 nm (K_d-UVAB). The spectral dependent K_d are derived from the Vibrational Raman Scattering (VRS) signal of the ocean which is retrieved by a DOAS fit in three different fit windows. K_d-blue corresponds to a DOAS VRS fit in the wavelength region 450 - 493 nm, K_d-UVA to 405 - 450 nm, and K_d-UVAB to 349.5 - 382 nm. VRS fit factors in the blue fit window (450 - 493 nm) were offset corrected (an offset of 0.186 was added to the VRS fit factor of all processed S5P ground pixels). Derived K_d-blue are otherwise unrealistically high. The offset was determined with the help of K_d data at 490 nm from the Ocean and Land Color Instrument (OLCI) onboard Sentinel-3A.

Details on the algorithms can be found in the Algorithm Theoretical Baseline Document (ATBD, [RD1]) which is based on Oelker et al. 2022 [RD5].

2.1.1 Quality assurance

All TROPOMI ground pixels are processed globally. Valid ocean pixels are those that are not on land or ice, have a very low cloud, and acceptable total uncertainty. The product provides: (i) cloud fraction from the S5P NO_2 CRB product, (ii) land/water and snow–ice flags, and (iii) a per–channel overall QA flag (qa_value_blue, qa_value_UVA, qa_value_UVAB).

2.1.1.1 Definition of qa_value_* (autoscaled to 0–1).

Define

$$\mathrm{QA}_{\mathrm{cloud}}(\mathrm{cloud}) = \begin{cases} 1, & \mathrm{cloud} \le 0.01, \\ \dfrac{0.10 - \mathrm{cloud}}{0.09}, & 0.01 < \mathrm{cloud} < 0.10, \\ 0, & \mathrm{cloud} \ge 0.10. \end{cases}$$

Let $\sigma_{\mathrm{tot},\%}$ be the total uncertainty per channel in percent (see Eq. (1)). Then the QA flag (shown to users on the 0-1 scale) is

$$\mathrm{QA} = \begin{cases} 0, & \text{if not open ocean or } K_d \text{ is NaN}, \\ 0, & \text{if } \sigma_{\mathrm{tot},\%} > 50, \\ \mathrm{QA}_{\mathrm{cloud}}(\mathrm{cloud}), & \text{otherwise.} \end{cases}$$

2.1.1.2 Practical filters.

Strict: `qa_value_* == 1.0` (equivalent to cloud ≤ 0.01, total uncertainty $\le 50\%$, open ocean).
Lenient: `qa_value_* >= 0.9`.

2.1.1.3 Encoding note.

qa_value_* are stored as unsigned byte 0–100 with `scale_factor=0.01`, `add_offset=0`, fill=255. Most tools auto-apply the scale and display 0–1.

The product files also contain the root mean square (RMS) of the DOAS fit residual for advanced interpretation of the retrieval results.

2.1.2 Product validation results

K_d validation results

S5POC TROPOMI K_d data was compared to field measurements of spectral K_d obtained during three ship campaigns in the Atlantic (C) and polar regions (D). In-situ data was either obtained from radiometric profiles measured at stations or measured by a ship-towed undulating system. Using a loose match-up criterion of ±2 days and a radius of 5.5 km, 25 in-situ measurements could be matched in total (only 3 match-ups for polar regions). Bias of -0.023 (K_d-UVAB), -0.011 (K_d-UVA), and -0.009 (K_d-blue), and RMSD of 0.029 (K_d-UVAB), 0.028 (K_d-UVA), 0.016 (K_d-blue) were found. Pearson correlation coefficient is around 0.68 for K_d-UVAB and K_d-blue, and 0.4 for K_d-UVA.

S5POC K_d-blue was compared to wavelength-converted K_d490 from the multispectral sensor Sentinel-3A Ocean and Land Colour Instrument (OLCI) and the merged Ocean Color Climate Change Initiative (OC-CCI) version 4 product which contains data from VIIRS and MODIS-Aqua. Data sets were compared as gridded data (0.083°) on a daily basis. Pearson correlation coefficients greater than 0.7 are reached, if data sets are restricted to K_d < 0.3 m^{-1} (<0.5 m^{-1} for polar regions) which covers more than 95% of the world ocean. Absolute differences between the three data sets are generally smaller than the uncertainties provided by the OC-CCI K_d490 product as RMSD on a pixel-by-pixel basis. (Note that the biases between the three data sets are particularly low, because OLCI K_d490 data was used for offset-correcting VRS fit factors from which K_d-blue product was derived. Comparisons were considered to estimate the random error and regional differences.) More details can found in S5POC-VR [RD-3] and Oelker et al. 2022 [RD-5].

3 Product Format Specifications

3.1 File format

The S5POC PAL K_d data are provided as netCDF-4/HDF5 files.

3.2 Filename convention

The file name format follows the convention used for operational level 2 TROPOMI products. File name example:

`S5P_PAL__L2__KD_____20180728T073812_20180728T091942_04085_03_010000_20241220T194647.nc`

- The first field corresponds to the mission name, always `S5P`;
- The second field corresponds to the file class, `PAL`;
- The third field corresponds to the product level, here `L2__`;
- The fourth field corresponds to the product name, for KD_____;
- The fifth field corresponds to the start of granule in UTC as `YYYYMMDDTHHMMSS` with "T" as a fixed character;
- The sixth field corresponds to the end of the granule in UTC as `YYYYMMDDTHHMMSS` with "T" as a fixed character;

- The seventh field is the orbit number;
- The eighth field is the collection number;
- The ninth field corresponds to the processor version number as MMmmpp, with MM the major version number, mm the minor version number, and pp the patch level;
- The tenth field corresponds to the time of data file creation as YYYYMMDDTHHMMSS with "T" as a fixed character;
- The file name extension is nc for netCDF-4/HDF5.

3.3 Structure of S5POC data files

The structure of the S5POC data files follows the operational TROPOMI level 2 data files. Data are organized into groups as follows (FIg. 1), as provided in the K_d product:

- PRODUCT: This group contains information on dimensions and their corresponding variables time, scanline, ground_pixel, corner. The main variables are the variables of the TROPOMI S5POC product variables (K_d_blue, K_d_UVA, K_d_UVAB), delta_time, quality values (qa_value_blue, qa_value_UVAB, qa_value_UVA) and the central latitude and longitude coordinates.
- PRODUCT/SUPPORT_DATA/GEOLOCATIONS: This group contains information on viewing geometries (viewing_zenith_angle, viewing_azimuth_angle, relative_azimuth_angle, solar_zenith_angle, solar_azimuth_angle), satellite position variables and all four corner coordinates of the TROPOMI ground pixels (longitude_bounds, latitude_bounds).
- PRODUCT/SUPPORT_DATA/DETAILED_RESULTS: This group contains the VRS fit factors in three different fit windows (VRS_fit_factor_blue, VRS_fit_factor_shortblue, VRS_fit_factor_UV), fit errors and the corresponding RMS of the retrieval residual (RMS_blue, RMS_UV, RMS_shortblue).
- PRODUCT/SUPPORT_DATA/INPUT_DATA: This group contains information on cloud coverage (cloud_fraction_crb_nitrogendioxide_window) and flags for land (land_flag) and ice-covered pixels (snow_ice_flag).
- META_DATA/ALGORITHM_SETTINGS/DOAS_RETRIEVAL/: This group contains a description of detailed settings for the DOAS retrieval which are valid for all three DOAS fits and the specific setting for the current fit.

Figure 1: General structure of the S5P K_d L2 file

A detailed overview of the example file's structure and description of its variable dimensions and attributes can be found below for the S5P K_d:

Table 1: List of variables in the PRODUCT group

Product			
Names	Units	Dimensions	Description
time	s	1	seconds since 2010-01-01 00:00:00
scanline	1	number of scans	defines the indices along the track
ground_pixel	1	ground pixels = 450	defines the indices across the track
corner	1	corners = 4	defines the indices for the pixel corners
delta_time	ms	time x scanline	offset from reference start time of measurement
latitude	°N	time x scanline x ground_pixel	pixel center latitude
longitude	°E	time x scanline x ground_pixel	pixels center longitude
KD_blue	m^{-1}	time x scanline x ground_pixel	KD region 390 - 423 nm
KD_UVA	m^{-1}	time x scanline x ground_pixel	KD region 356.5 - 390 nm
KD_UVAB	m^{-1}	time x scanline x ground_pixel	KD region 312.5 - 338.5 nm
qa_value_blue	1	time x scanline x ground_pixel	Overall quality flag (0–1 after scaling). Stored as byte 0–100 with `scale_factor=0.01` (`_FillValue`=255). 1.0 corresponds to cloud ≤ 0.01 and total uncertainty $\leq 50\%$ over open ocean.
qa_value_UVA	1	time x scanline x ground_pixel	Overall quality flag (0–1 after scaling). Stored as byte 0–100 with `scale_factor=0.01` (`_FillValue`=255). 1.0 corresponds to cloud ≤ 0.01 and total uncertainty $\leq 50\%$ over open ocean.
qa_value_UVAB	1	time x scanline x ground_pixel	Overall quality flag (0–1 after scaling). Stored as byte 0–100 with `scale_factor=0.01` (`_FillValue`=255). 1.0 corresponds to cloud ≤ 0.01 and total uncertainty $\leq 50\%$ over open ocean.

Table 2: List of variables in the SUPPORT_DATA/GEOLOCATIONS group

Geolocations			
Names	Units	Dimensions	Description
latitude_bounds	°N	time x scanline x ground_pixel x corner	The four latitude boundaries of each ground pixel.
longitude_bounds	°E	time x scanline x ground_pixel x corner	The four longitude boundaries of each ground pixel.
relative_azimuth_angle	°	time x scanline x ground_pixel	Relative azimuth angle between the solar azimuth and the viewing azimuth of the satellite measured at the ground pixel location
viewing_azimuth_angle	°	time x scanline x ground_pixel	Azimuth angle of the satellite measured at the ground pixel location
viewing_zenith_angle	°	time x scanline x ground_pixel	Zenith angle of the satellite measured at the ground pixel location
solar_zenith_angle	°	time x scanline x ground_pixel	Zenith angle of the sun at the ground pixel location
solar_azimuth_angle	°	time x scanline x ground_pixel	Azimuth angle of the sun at the ground pixel location
satellite_altitude	1	time x scanline	Altitude of the satellite
satellite_orbit_phase	1	time x scanline	Orbit phase of the satellite
satellite_latitude	°N	time x scanline	Latitude of the satellite on the reference ellipsoid
satellite_longitude	°E	time x scanline	Longitude of the satellite on the reference ellipsoid

Table 3: List of variables in the SUPPORT_DATA/DETAILED_RESULTS group

Detailed Results			
Names	Unit	Dimensions	Description
VRS_fit_factor_blue	1	time x scanline x ground_pixel	VRS fit factor from DOAS fit in window 450 - 493 nm
VRS_fit_factor_shortblue	1	time x scanline x ground_pixel	VRS fit factor from DOAS fit in window 405 - 450 nm
VRS_fit_factor_UV	1	time x scanline x ground_pixel	VRS fit factor from DOAS fit in window 349.5 - 382.0 nm
VRS_fit_factor_error_blue	%	time x scanline x ground_pixel	VRS fit factor error from DOAS fit in window 450 - 493 nm
VRS_fit_factor_error_shortblue	%	time x scanline x ground_pixel	VRS fit factor error from DOAS fit in window 405 - 450 nm
VRS_fit_factor_error_UV	%	time x scanline x ground_pixel	VRS fit factor error from DOAS fit in window 349.5 - 382.0 nm
RMS_blue	1	time x scanline x ground_pixel	RMS fit residual from DOAS fit in window 450 - 493 nm
RMS_shortblue	1	time x scanline x ground_pixel	RMS fit residual from DOAS fit in window 405 - 450 nm
RMS_UV	1	time x scanline x ground_pixel	RMS fit residual from DOAS fit in window 349.5 - 382.0 nm
total_uncertainty_blue	%	time x scanline x ground_pixel	Total 1σ uncertainty for KD_blue in percent (0–100); quadrature of target (fit), AOT, WS, and ocean RMS terms (Eq. 1).
total_uncertainty_UVA	%	time x scanline x ground_pixel	Total 1σ uncertainty for KD_UVA in percent (0–100); quadrature of target (fit), AOT, WS, and ocean RMS terms (Eq. 1).
total_uncertainty_UVAB	%	time x scanline x ground_pixel	Total 1σ uncertainty for KD_UVAB in percent (0–100); quadrature of target (fit), AOT, WS, and ocean RMS terms (Eq. 1).

3.3.1 Per–channel total uncertainty

The total (1σ) uncertainty used by the QA gate is computed as percent

$$\begin{aligned}\sigma_{\text{tot},\%} = \Big[&\min\big(\sigma_{\text{target},\%},\,20\big)^2 \\ &+ \max\big(|\sigma_{\text{AOT},\%-}|,\,|\sigma_{\text{AOT},\%+}|\big)^2 \\ &+ \max\big(|\sigma_{\text{WS},\%-}|,\,|\sigma_{\text{WS},\%+}|\big)^2 + |\sigma_{\text{RMS},\%}|^2\Big]^{1/2}.\end{aligned} \tag{1}$$

Here, the target (fit) term is capped at 20% to avoid overweighting noisy fits; AOT and WS contributions use the larger magnitude of their minus/plus bounds; the ocean term is taken as the absolute RMS-derived contribution in percent. In figure 2 can be observed a bar plot with valid total uncertainty values (the quality assurance value was set at 1) on 18.07.2018 for each of the Kd products.

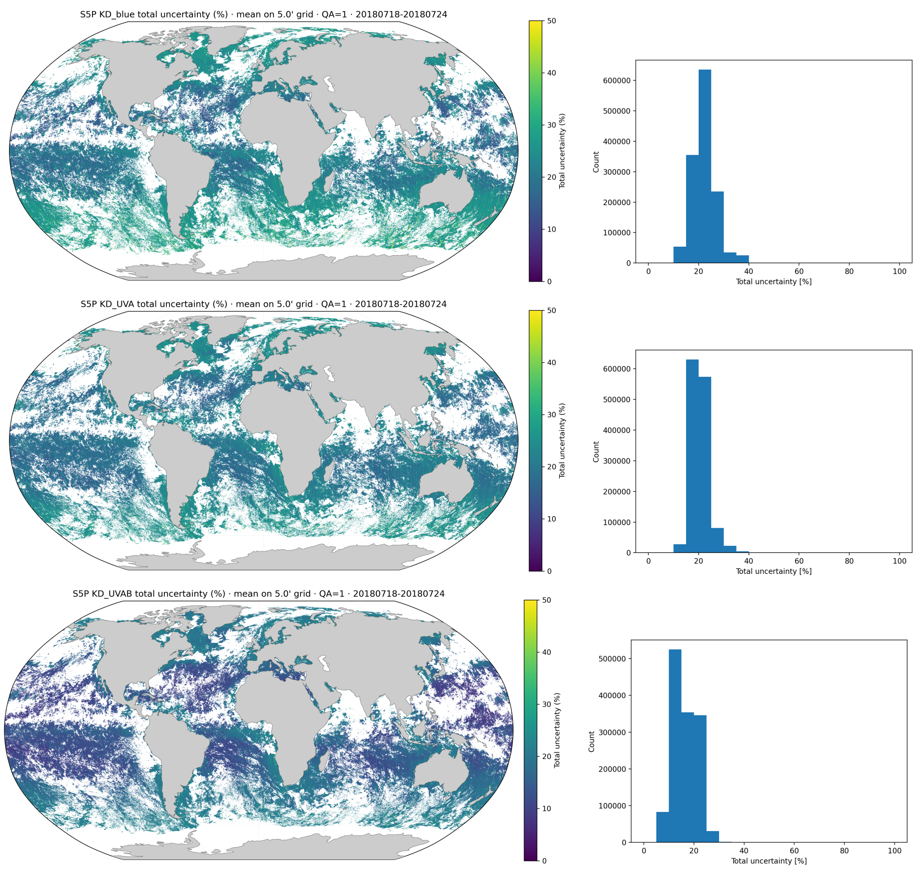

Figure 2: Total uncertainty global map calculated with the equation 1. Only valid values were used, the quality assurance value was set to 1.

3.3.2 Provenance of AOT, WS, and ocean RMS terms

3.3.2.1 Sensitivity framework.

The atmospheric and oceanic uncertainty are derived from coupled radiative–transfer sensitivity experiment. The following subchapters summarize the experiments which are described in detail in the ATBD [RD1]. For each spectral window, solar/ viewing geometry, and VRS scale, the DOAS fit is run on perturbed scenarios and the retrieved $\hat{K}_d$ is compared to the expected K_d from unperturbed scenarios. Relative deviation (in percent) is

$$\varepsilon \;=\; \frac{K_d - \hat{K}_d}{K_d} \times 100\,. \tag{2}$$

Results are summarized in dedicated LUTs for each error source and channel.

3.3.2.2 Aerosol optical thickness (AOT).

Main K_d LUTs use $\tau_{\mathsf{lut}} = 0.1$. Error LUTs provide deviations at $\tau_- = 0.05$ and $\tau_+ = 0.2$. Assuming local linearity, the AOT–induced relative error at an arbitrary τ is

$$\varepsilon_{\mathsf{AOT}}(\tau) \;=\; \begin{cases} \varepsilon_{\mathsf{lut}}(2\tau_{\mathsf{lut}})\,\dfrac{\tau - \tau_{\mathsf{lut}}}{\tau_{\mathsf{lut}}}, & \tau > \tau_{\mathsf{lut}}, \\ 2\,\varepsilon_{\mathsf{lut}}(\frac{\tau_{\mathsf{lut}}}{2})\,\dfrac{\tau_{\mathsf{lut}} - \tau}{\tau_{\mathsf{lut}}}, & \tau < \tau_{\mathsf{lut}}. \end{cases} \tag{3}$$

Here $\varepsilon_{\mathsf{lut}}(2\tau_{\mathsf{lut}})$ and $\varepsilon_{\mathsf{lut}}(\tau_{\mathsf{lut}}/2)$ are read from the AOT error LUT for the pixel's geometry and VRS scale.

3.3.2.3 Wind speed (WS).

Main LUTs use $v_{\mathsf{lut}} = 4.1\,\mathrm{m\,s^{-1}}$; error LUTs provide $\varepsilon_{\mathsf{lut}}(v_-)$ at $v_- = 2\,\mathrm{m\,s^{-1}}$ and $\varepsilon_{\mathsf{lut}}(v_+)$ at $v_+ = 8\,\mathrm{m\,s^{-1}}$. With the same linearity assumption,

$$\varepsilon_{\mathsf{WS}}(v) \;=\; \begin{cases} \varepsilon_{\mathsf{lut}}(v_+)\,\dfrac{v - v_{\mathsf{lut}}}{v_+ - v_{\mathsf{lut}}}, & v > v_{\mathsf{lut}}, \\ \varepsilon_{\mathsf{lut}}(v_-)\,\dfrac{v_{\mathsf{lut}} - v}{v_{\mathsf{lut}} - v_-}, & v < v_{\mathsf{lut}}. \end{cases} \tag{4}$$

3.3.2.4 Ocean RMS term.

To capture sensitivity to CDOM magnitude/slope variants, five ocean perturbations are considered. For a given geometry and VRS scale, the per-case relative errors ε_i are combined as an RMS:

$$\varepsilon_{\mathsf{RMS}} \;=\; \sqrt{\frac{1}{N}\sum_{i=1}^{N}\varepsilon_i^2}\,, \qquad N = 5. \tag{5}$$

These RMS values are tabulated in the ocean error LUT and accessed by interpolation like the main K_d LUT.

3.3.2.5 From LUT errors to $\sigma_{\mathrm{tot},\%}$.

The per-pixel contributions used in Eq. (1) are taken as

- $\sigma_{\mathsf{AOT},\%-} = \varepsilon_{\mathsf{AOT}}(\tau_-)$, $\sigma_{\mathsf{AOT},\%+} = \varepsilon_{\mathsf{AOT}}(\tau_+)$, then $\sigma_{\mathsf{AOT},\%} = \max\big(|\sigma_{\mathsf{AOT},\%-}|, |\sigma_{\mathsf{AOT},\%+}|\big)$;
- $\sigma_{\mathsf{WS},\%-} = \varepsilon_{\mathsf{WS}}(v_-)$, $\sigma_{\mathsf{WS},\%+} = \varepsilon_{\mathsf{WS}}(v_+)$, then $\sigma_{\mathsf{WS},\%} = \max\big(|\sigma_{\mathsf{WS},\%-}|, |\sigma_{\mathsf{WS},\%+}|\big)$;
- $\sigma_{\mathsf{RMS},\%} = |\varepsilon_{\mathsf{RMS}}|$ from the ocean error LUT.

The target (fit) term $\sigma_{\mathsf{target},\%}$ is capped at 20% before quadrature as stated under Eq. (1).

Note. Ozone-column and phytoplankton absorption perturbations were also analyzed. Since their sensitivities were rather low (¡5%), they were not combined into $\sigma_{\mathrm{tot},\%}$ in this product release.

3.3.3 Interpolation from look-up tables (LUTs)

The conversion from DOAS fit output to K_d and error terms is obtained by interpolating precomputed LUTs in a four-dimensional space:

$$\mathbf{x} = \big(\,\mathrm{SZA},\ \mathrm{ZEN},\ \mathrm{AZM},\ \mathrm{VRS}_{\mathrm{eff}}\,\big).$$

Here $\mathrm{VRS}_{\mathrm{eff}}$ is the fit factor mapped onto the LUT axis via the per-channel affine transform used in the processor;

$$\mathrm{VRS}_{\mathrm{eff}} \;=\; -\,\mathrm{target} \times \mathrm{factor} \;+\; \mathrm{offset}.$$

3.3.3.1 Inverse-distance weighting (IDW).

By default we use local Shepard-type inverse-distance weighting over the k nearest LUT nodes (with $k = 8$). Let $\mathcal{N}_k(\mathbf{x})$ be the k nearest LUT nodes $\{\mathbf{x}_i\}$ to a query point $\mathbf{x}$ (Euclidean distance in the raw coordinates), with distances $d_i = \|\mathbf{x} - \mathbf{x}_i\|_2$. If $\min_i d_i = 0$, the value at the exact node is returned. Otherwise, weights are

$$w_i \;=\; \frac{d_i^{-p}}{\sum_{j\in\mathcal{N}_k(\mathbf{x})} d_j^{-p}}, \qquad \text{with power } p = 2,$$

and the estimate for any LUT field f (K_d or an error component) is

$$\widehat{f}(\mathbf{x}) \;=\; \sum_{i\in\mathcal{N}_k(\mathbf{x})} w_i\, f(\mathbf{x}_i).$$

For vector-valued LUTs (e.g. the four error components in the error LUT), this is applied component-wise. The method is local and smooth; it exactly recovers node values and provides a reasonable approximation between nodes.

3.3.3.2 Notes and assumptions.

- Distances are computed in the native units of each axis; no axis normalization is applied.
- $k = 8$ and $p = 2$ were chosen as a practical trade-off between locality and smoothness.
- IDW provides mild extrapolation near domain edges (using the nearest nodes), while the piecewise-linear fallback does not extrapolate beyond the LUT hull.

Table 4: List of variables in the SUPPORT_DATA/INPUT_DATA group

Input Data			
Names	Units	Dimensions	Description
cloud_fraction_crb _nitrogendioxide_window	1	time x scanline x ground_pixel	cloud fraction from NO_2 RPRO product
land_flag	1	time x scanline x ground_pixel	flag indicating land/water-type of ground pixel, such as land, ocean, lake and pond (0, 1, 2, 3)
snow_ice_flag	1	time x scanline x ground_pixel	flag indicating snow/ice at center of ground pixel, such as snow free land, permanent ice, dry snow, wet snow, mixed pixels at coastlines, suspect ice value, ocean (0, 101, 103, 104, 252, 253, 255)

3.3.4 Data product examples

Figure 3 shows as an example example global coverage from the period of 18.07.2018 - 24.07.2018, the K_d [m^{-1}] data from the example file. It was plotted on a 5-minute grid where non-valid pixels were removed.

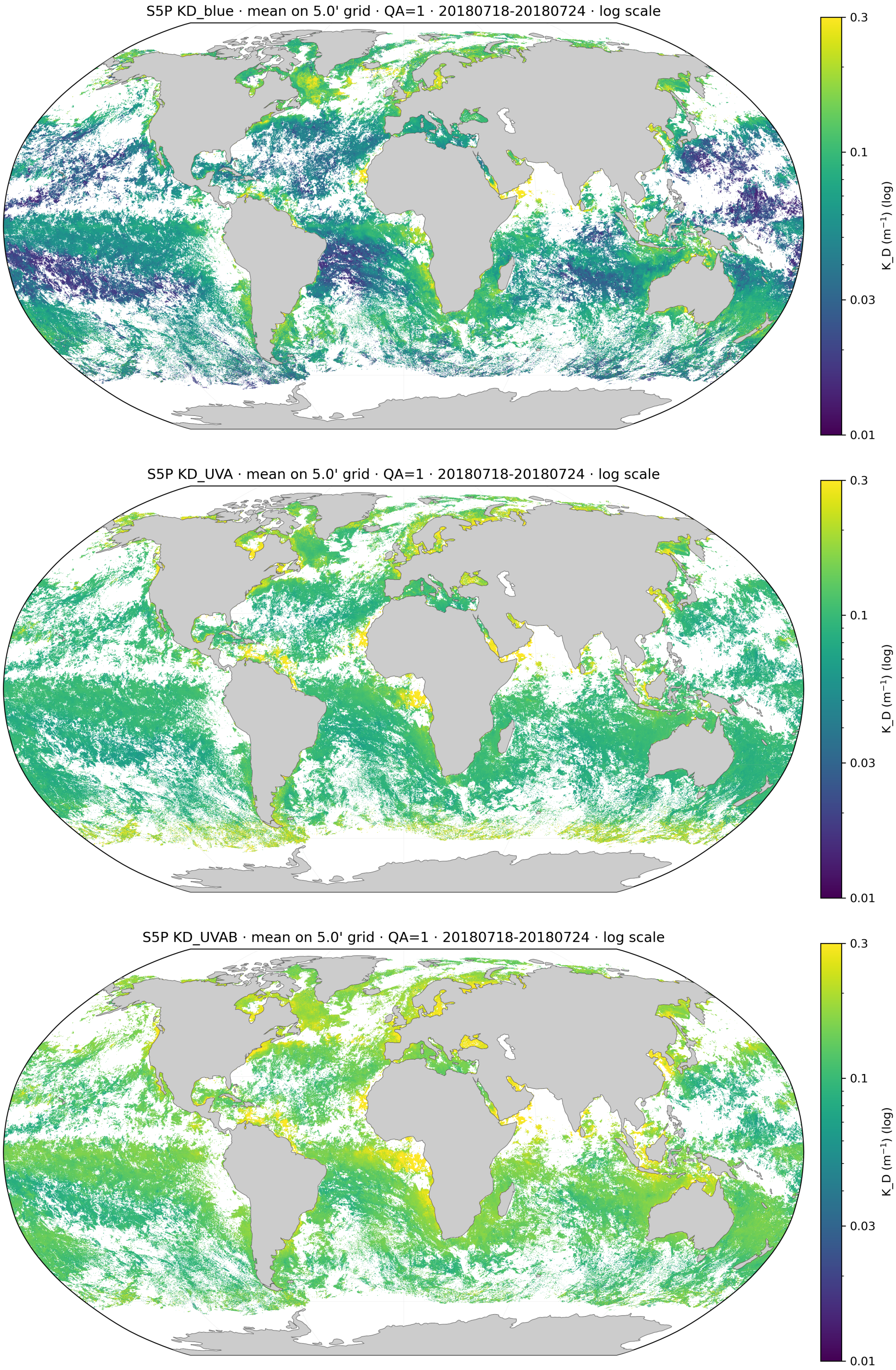

Figure 3: Gridded plot (5 minutes) of K_d data [m^{-1}] within example file from the period of 18.07.2018 - 24.07.2018. Only valid pixels of the example data set are shown, the quality assurance value was set to 1.