Summary of Quality of Aeolus Data Products from 4th Reprocessing Campaign covering the period from 28 June 2019 to 4 October 2022 (FM-B laser)

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The 4th reprocessing campaign with the processor baseline B16 covers for the first time the full period for the operation of the 2nd Flight-Model laser (FM-B) from 28 June 2019 to 4 October 2022. Before and after this period the instrument was operated with the first laser (FM-A). It is planned to release data products for these two FM-A periods with processor baseline B16 in early 2025 in order to provide a consistent dataset for the full mission with the latest B16 product quality; this replaces the products from the 3rd reprocessing for the first FM-A period performed with B14. The current release of the 4th reprocessing data products for this FM-B period significantly improves the data quality for the L1B, L2A, and L2B product compared to the 2nd reprocessing campaign, which was performed for a shorter period for FM-B operation and with B11 processor versions. The baseline 16 processor versions were the last versions, which were used for the near-real-time (NRT) production of the data products and was activated on 18 April 2023 for the last weeks of Aeolus operation in-orbit. In the following the major improvements in the L1B, L2A, L2B processors are listed used during reprocessing, followed by a summary of the quality of the L2B wind product and L2A aerosol product and its known limitations and known error characteristic, which might be improved in future reprocessing campaigns with the B17 processor versions, which are currently under development.

What are the main improvements with respect to the previous processing baseline B11 used for the 2nd reprocessing for the FM-B period?

The following major changes in the ground processing processor were implemented and used within the 4th reprocessing of FM-B (B16) since the 2nd reprocessing of FM-B (B11) and the NRT processing using B11 to B15 for the FM-B period.

Major changes in L1B-L2B processor (wind) for baseline B11 to B16

- B16 for the L2B product (used for NRT data production from 18 April 2023):
    - A “residual error” threshold option was included in QC (Quality Control) for the Mie Core algorithm output providing Mie cloudy winds. This helps discard gross errors from the low signal Mie winds (e.g. in aerosols), which are otherwise hard to detect as gross errors (without using the O-B (observation-background) departures from the Numerical Weather Prediction (NWP) model at ECMWF).
    - A new Rayleigh channel wind bias correction based on the Mie channel estimated emitted frequency was added. This reduces wind biases in the Rayleigh channel caused by oscillations in the pressure inside the laser housing, which impact the laser frequency. The bias caused by this pressure oscillation had a magnitude of roughly ±0.6 m/s with a period of 4.3 hr at the end of 2022 (for the FM-A laser, thought to be less important in other periods).
    - A correction was applied for start/stop latitude/longitude values for the geolocation. The new calculation adds half a measurement length to the reported accumulation to give a better estimate of the accumulated region. This also solves the problem of having identical start/stop locations in case a wind is derived from a single measurement, which became

more common when using the N=5, P=114 setting (N: number of measurements per observation accumulated in the on-ground processing, P: number of laser pulse returns accumulated on-board the instrument detector per measurement) after 4 April 2022.

- B16 for the L1B product (used for NRT data production from 18 April 2023):
    - L1B Rayleigh signal-to-noise-ratio (SNR) calculation was updated to be more realistic: The detection chain offset and read-out noise are included in the L1B Rayleigh SNR calculation. As a result, the L2B HLOS wind estimated error for Rayleigh-clear winds increased by ~8% on average in 2019 (and relatively even more as the useful signal continuously decreased until October 2022).
    - New detection chain offset (DCO) correction in L1B using orbital means for this parameter: This improved the random errors of the L2B wind products by ~1-2%.
- B15 for the L2B product (used for NRT data production from 13 September 2022):
    - A new threshold check was added to catch gross errors on measurement level Rayleigh response, i.e. if one of the channels A or B has an abnormally high signal and the other does not (likely due to cosmic rays affecting the ACCD), then we consider this an artefact that is not related to atmospheric winds and we flag the resulting measurement invalid so it is not used in the wind retrieval. This improves the standard deviation of L2B Rayleigh-clear O-B significantly by reducing gross errors.
    - A climatological sanity check on the reported L2B wind values was added, to ensure unrealistic high wind results will be flagged invalid (after some outliers with very large wind speeds were noticed).
- B14 for the L2B product (used for NRT data production from 29 March 2022):
    - A switch was added so that moon-blinding of the satellite´s star tracker does not lead to L1B measurements being flagged as invalid and therefore can be used for the L2B wind retrieval, but in case the moon-blinding has occurred, the resulting L2B wind result can be flagged invalid. This means the wind results during moon-blinding are still available for use if one ignores the validity flag.
    - The wind bias correction for L2B products (AUX_TEL_generator) was modified to also allow the correction of harmonic (sinusoidal) biases with argument of latitude (orbit phase). The L2B processor was adapted to allow using these harmonic factors for wind bias correction. This corrects for opposing biases (< 0.5 m/s magnitude) in ascending and descending orbits that was evident in October and March in previous reprocessing campaigns (possibly related to the angle of the sun on the satellite resulting in some thermal distortions).
- B14 for the L1B product (used for NRT data production from 29 March 2022):
    - Corrections to remove a longitudinal offset (0.075° ~8 km at the equator) in the geolocation of all Aeolus products, which were discovered by the comparison with precise on-ground laser track measurements by the Auger observatory for cosmic rays.
- B13 for the L2B product (used for NRT data production from 6 December 2021):
    - A new parameterization to correct the Rayleigh response as a function of (collocated) L1B (Mie channel) scattering ratio was added. The parameters are derived via NWP-based calibration. This improves the O-B statistics of the Rayleigh cloudy winds.
    - Ground detection algorithms were extended for detection if the surface is near (but not intersecting with) the bottom of the range bin. This can be used to account for inaccuracies

in the Digital Elevation Model (DEM) and for the range bin signal overlap (cross-talk between range bins) which may result in wrong winds close to the surface. In addition, a new check was added based on the digital elevation model (DEM) value provided via the AUX_MET_12 file.

- B12 for the L2B product (used for NRT data production from 26 May 2021):
    - Step changes in L2B Rayleigh wind bias were detected and found to be associated with noise/jumps in the Rayleigh channel internal reference signal in December 2020. To avoid this the internal Rayleigh response can be not used via a switch to apply a fixed internal reference value. Switches were added for both Rayleigh and Mie channels.
    - The new moon-blinding flag from the L1B measurements can be used to avoid moon-blinding affected measurements from being used in the L2B wind retrieval. This avoid biases occurring for parts of the orbit of up to 4 m/s, due to moon-blinding affecting the satellite pointing due to its effect on the star-trackers.
    - An array of Mie non-linear response corrections can be provided via the AUX_PAR_2B (input parameter file for the L2B processor) for use in correcting the issue of "wiggling" biases with wind speed due to uncertainty in the Mie calibration non-linearity. NWP-based calibration to derive the Mie-nonlinearity array can be applied to derive these Mie non-linearity correction parameters.
- B12 for the L1B product (used for NRT data production from 26 May 2021):
    - Several additional Attitude and Orbit Control System (AOCS) flags (e.g. moon blinding status, eclipse status, star tracker status) were added to the L1B product for better quality control.
    - Negative signal counts in Mie spectral data were no longer set to zero in order to avoid biasing the signal statistics. Those negative signal counts could occur, as several corrections are applied to the Mie spectral data (e.g. DCO, dark current in memory zone, solar background), which themselves are of noisy nature.

Major changes in L2A processors (aerosol)

- Implementation of the Maximum Likelihood Estimation (MLE) at sub-BRC (Basic Repeat cycle corresponding to one observation) level, i.e. accumulated measurements per sub profile depending on settings for the number of accumulated laser pulses P per measurement and number of measurement N per observation. Addition of corresponding Quality Check (QC) flags, the thresholds being aligned with BRC level retrievals. These datasets are flagged invalid in operational NRT product, but now flagged valid for the reprocessing.
- Fine-tuning of the MLE number of iterations and Quality Check flags for both BRC level and sub-BRC level retrievals.
- Correction of the SCA (Standard Correct Algorithm) group product mid-bin height assignment and L1B flagging for Rayleigh and Mie observed and simulated signals to be used for L2A radiometric correction of K_{Ray} and K_{Mie} coefficients.
- The Aeolus feature mask (AEL-FM) and Aeolus Profile (AEL-PRO) extinction coefficient and lidar-ratio profiles are available in the 4th reprocessing and flagged valid. All products are provided at the Mie measurement altitude grid and, although the "background'' thin ice clouds and aerosols are representative of the observation scale.

What are further improvements for L1B, L2A and L2B with respect to NRT data products, which were implemented during reprocessing?

- The use of the wind-bias correction for the L2B products is performed in NRT with NWP model data from the previous day, while it is performed for the reprocessing campaign using global O-B departures from the same day, which improves the L2B quality compared to NRT production.
- The correction for hot-pixel anomalies (steps in dark current rates) can be performed in NRT only with measured dark current maps (from the instrument mode DUDE (Down Under Dark Experiment)), which was performed 4-8 times per day during FM-B period. During reprocessing a major effort is performed in L1B level to detect dark current steps in time between measurements and correct it for each orbit file (mostly around 90 minutes); with this approach more than 4000 hot-pixel jumps were corrected for the FM-B period. As the correction of hot-pixel jumps can be performed only with constant dark-current rates for each orbit level file, sub-orbital variations and jumps can not be corrected with this method also during reprocessing.
- Activation of the Maximum Likelihood Estimation (MLE) at sub-BRC level product including error estimates and corresponding Quality Check (QC) flags.
- Fine-tuning of the Horizontal_Sampling_Factor (i.e. set on value 5) for MLE at sub-BRC level. This allows homogeneous horizontal resolution of about 18 km per sub-profile, independent of varying number of measurements accumulated because of N/P settings.
- It is the first time that valid AEL-FM and AEL-PRO L2A products are available for the FM-B period, as those were only flagged valid with the B16 version.

What is the quality of the L2B wind data product?

- A significant improvement in the Rayleigh-clear HLOS wind noise is evident. The standard deviation of O-B for the 4th reprocessing is improved relative to the 2nd reprocessing by ~15% in July 2019 and ~25% in October 2020. The profile average estimated HLOS wind error standard deviation is ~5 m/s in 2019 increasing to ~7-8 m/s in 2022 (N.B. absolute values are very sensitive to QC thresholds). At best it was ~ 4 m/s in the free troposphere in 2019.
- The Mie-cloudy noise is also improved with the 4th reprocessing compared to the 2nd reprocessing by ~9%, whilst the data count increased. The profile average estimated HLOS wind error standard deviation is ~3.3 m/s throughout the period.
- The L2B global wind bias is well constrained (close to 0 m/s) for the Rayleigh-clear and Mie-cloudy winds and the bias has smaller variability from orbit to orbit compared to the 2nd reprocessing.
- The Mie-cloudy and Rayleigh-clear wind-speed-dependent bias is improved in the 4th reprocessing compared to the 2nd reprocessing. Particularly for the Mie-cloudy, due to a new Mie non-linearity correction.
- The Rayleigh-cloudy winds also show a large improvement (~25%) in noise compared to the 2nd reprocessing, and improved bias thanks to the new parameterised correction based on scattering ratio. The profile average estimated HLOS wind error standard deviation is ~8 m/s in 2019 increasing to ~9 m/s in 2022 (N.B. applying stricter QC thresholds than here leads to more reasonable noise).
- The issue in the 2nd reprocessing of opposing sign biases for Rayleigh-clear for ascending and descending orbits in October 2019 and March 2020 has been resolved with the 4th reprocessing.
- The 4th reprocessing improves upon the NRT dataset (B13 to B15) in terms of bias and standard deviation of O-B for all L2B wind types.

- The 4th reprocessing has improved the Rayleigh-clear hot-pixel related wind biases compared to NRT dataset in 2021 and 2022 for range-bins 5, 9, 22 and 24.
- Based on an initial assessment of the L2B wind product and its error estimates using DLR´s airborne wind-lidar campaign data from September 2019 around Iceland and September 2021 around Cap Verde we recommend to re-assess the use of Mie and Rayleigh error estimates for instrument comparison and Cal/Val. For Mie-cloudy winds, the error estimate slightly increased (< 1 m/s) in average and fewer gross errors are now more symmetrically distributed, such that the bias validation is less dependent on the error estimates-based QC-threshold. The number of valid Mie-cloudy winds has substantially increased (up to +50%), and also Rayleigh-clear winds coverage has gained (~ +20%). For Rayleigh-clear the error estimate significantly increased (by up to ~ 2 m/s in average, depending on SNR), such that the number of values passing the QC is substantially reduced, when keeping the error estimate-threshold used in the validation of earlier baselines. The low number of gross errors and their homogeneous distribution leads to the recommendation to use the modified Z-score as QC-criterion for discarding gross outliers for the Mie and Rayleigh clear products.

What is the quality of the L2A aerosol data product?

- Radiometric coefficients K_{Ray} and K_{Mie} have been corrected using primary mirror M1 temperatures-based regression and provided per observation. They show continuous decrease from 2019 to 2022 partially compensated with N/P settings adjustment (i.e. switch from 30/19 to 15/38 on 2021-12-13, switch from 15/38 to 5/114 on 2022-04-04).
- Both MLE and MLEsub show valid scores despite higher error estimates. Compared to SCA and SCAMid the MLE and MLEsub show no negative outliers by concept, lower amount of non-processed bins and positive outliers except for very low altitude bins.
- The AEL-FM and AEL-PRO products are consistent with the corresponding products from the prototype processors. The feature mask shows clear features of aerosols and clouds. The AEL-PRO extinction coefficients are comparable to the extinction coefficients from the lidar on-board NASA´s lidar mission CALIPSO. This is checked with collocated orbits for some desert dust aerosols.
- We suggest using the lidar ratio when the extinction coefficient is greater than 10^{-5} m^{-1} for the AEL-PRO. All retrieved extinction coefficients and lidar ratios are provided.
- The most reliable extinction coefficients are between 10^{-6} m^{-1} and 10^{-2} m^{-1}. Valid lidar ratios are between 10 and 200 sr. The user should examine the estimated errors and the classification variable in order to appropriately screen the data for the purpose at hand.
- Classification between aerosols and clouds are not always reliable, especially in the areas when clouds are directly on top of aerosol layers.
- The particle effective area radius can be used for ice clouds, not for aerosols. This is not a main product. It has to be used with caution.

What are the known limitations of the L2B wind data product?

- There were two long periods without L2B data due to the instrument not measuring winds:
    - From 2021-03-22T02:56:59 until 2021-04-01T15:09:32, due to the FM-B laser switching off automatically (Survival Mode).
    - From 2021-10-22T13:46:32 until 2021-10-29T07:56:41, due to the FM-B laser switching off automatically (Survival Mode).

- Twelve (shorter) periods occurred where the L2B winds were deliberately flagged invalid due to poor data quality which were related to instrumental tests or adjustments.
- Altitude varying Rayleigh-clear HLOS wind bias is present from June 2019 to March 2021, with a negative bias (-0.7 m/s) in the lower troposphere and a positive bias (+0.4 m/s) in the upper troposphere. This bias was also present in the 2nd reprocessing and is caused by the current choice of the calibration files. We aim at improving this for the next reprocessing.
- An increasing fraction of hot-pixel related wind biases is present for the Rayleigh-clear particularly in 2021 and 2022, as the number of hot pixels increased with time and the useful signal levels decreased. Range-bins 3, 5, 11, 13 and 22 are most strongly affected.
- The Mie-cloudy HLOS winds are slightly more negatively biased for ascending orbits compared to descending orbits in the troposphere and there is a tendency for more negative bias towards the surface more generally.
- Noise increases with time for the Rayleigh-clear winds due to a gradual decline in atmospheric path useful signal during this period. The profile, daily average Rayleigh-clear standard deviation (O-B) started at ~4.8 m/s in July 2019 and increased to 7-8 m/s by September 2022.
- The Mie-cloudy data counts decreased with time due to declining useful signal – fewer low backscatter (e.g. aerosol, cirrus) Mie winds.
- Rayleigh-cloudy HLOS winds are positively biased in the global average, up to 1.5 m/s in 2021, which we aim to improve for the next reprocessing.

What are the known limitations of the L2A aerosol data product?

- The L2A SCA and MLE products still show some limitations for isolated orbits with specific conditions linked to special operations (e.g. ALADIN instrument internal delay test, M1 telescope thermal test). The radiometric correction is degraded when top range bin is set below 16 km altitude (e.g. range-bin settings during October 2019). Both SCA and MLE products are also affected by signal attenuation above top range bin, e.g. early 2022 with Hunga volcanic aerosols spreading in southern hemisphere above up to 80 km altitudes. Moreover, the SCA appears degraded when top profile encompasses high altitude clouds or aerosols (i.e. the a-priori hypothesis of particles free condition being made for top first bin when calculating the extinction coefficient).
- The SCA product is affected by uncorrected hot pixel jumps but not the SCAmid, MLE and MLEsub.
- The assessment of the L2A SCA mid-bin data product quality was performed using the COMPO-IFS model (at ECMWF). The data seems to have similar characteristics to the 2nd reprocessing dataset and NRT data in 2022. As the ALADIN instrument only detects the co-polar component of the backscattered signal, it is underestimating the total backscatter coefficient in polarizing scenes used as model parameter in COMPO-IFS, e.g. during desert dust events. Thus, the co-polar backscatter coefficient shows lower values compared to the model in areas where desert dust is known to be present (via MODIS) and where the COMPO-IFS model contains dust plumes. For example, it is difficult to see any enhanced backscatter (above the noise) for the Godzilla event in June 2020 (in monthly average plots of the L2A observation backscatter compared to COMPO-IFS background equivalent, for which the enhanced backscatter is very obvious). Areas of enhanced backscatter associated with central African wildfire smoke are however evident. It remains difficult to screen out areas of enhanced backscatter due to ice/water clouds, making it difficult to use the product for atmospheric composition applications.

- No imposed cut-off in extinction coefficients for extreme large and small values for the AEL-PRO product. This will be improved for the next reprocessing.
- Some hotpixel jumps are still present in the reprocessed data. It shows up as high values in the parameters attenuated_mie_backscatter_msp close to surrounding values and low values in attenuated_rayleigh_backscatter_msp.
- The retrieved lidar calibration constant is set to zero and will be added in next version.