# Deliverable D3.13: Implementation of closure studies for particle light scattering coefficient

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# Closure studies for particle light scattering coefficient

## 1. Motivation

In atmospheric science, closure means the comparison of either two measurements or measurement and prediction of the same physical quantity obtained by independent means, i.e. either independent observations or observation and prediction. In the case of closure between observations, the two measurements ideally use different physical principles, and are each traceable to a reference by an unbroken chain of calibrations. A closure is considered successful, i.e. closure is obtained, when both measurements or measurement and prediction agree within their ranges of uncertainty.

When comparing observations, obtaining closure requires that the measurement processes are fully understood theoretically, i.e. all sources of uncertainty are known and quantified, and that the calibration chain to the primary standard delivers its theoretical accuracy. Thus, a closure on observations is very sensitive even to small errors in the implementation of the calibration chain, calibration stability, and theoretical understanding of both measured property and measurement process. It is thus ideally suited as part of a quality control process on the observations involved.

In managing data from an observation network like ACTRIS, it is the data centres most distinguished task to curate the data for archiving and further use. The curation process "…is the active and on-going management of data through its lifecycle of interest and usefulness to scholarship, science, and education; curation activities enable data discovery and retrieval, maintain quality, add value, and provide for re-use over time." (Cragin et al., 2007). Following these principles, it is thus recommended for a data centre to make use of closure exercises as an integral part of the data quality control process.

Currently, ACTRIS distinguishes 2 types of data flow: 1) an annually updated flow where QC includes manual inspection of the data; 2) an hourly updated near-real-time (NRT) flow with automatic QC and data product generation. The particle light scattering closure scheme is intended to be used in both data flows. In implementing the scheme, priority is given to the NRT data flow since this will allow for an early detection of instrument problems as an additional service for data providers. Implementing QC at the data centre minimises the reaction time in case of problems, thus minimises the number of potential points of failure, and avoids duplication of resources in the QC chain.

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## 2. Summary of new quality control tool checking closure between calculated particle light scattering coefficient and measured particle light scattering coefficient within ACTRIS

The aerosol particle light-scattering coefficient is one of the core observation variables in ACTRIS. When considering a light-beam incident into an aerosol volume, it describes the amount of light scattered by the aerosol particles away from its original direction. The particle light-scattering coefficient is essential for describing the direct climate effect of atmospheric aerosol, i.e. its climate effect by scattering incoming solar radiation back into space before it can warm the Earth's surface. At ACTRIS surface in situ stations, the particle light-scattering coefficient is measured directly by integrating nephelometers (Heintzenberg & Charlson, 1996). The particle number size distribution (PNSD) is another ACTRIS core variable measured at the same stations. It quantifies the number of aerosol particles as a function of particle size. The PNSD is measured by Mobility Particle Size Spectrometers (MPSS) (Wiedensohler et al., 2012) in the size range of particle diameter 0.01 µm < $D_p$ < 0.8 µm. In the majority of cases, this size range covers most of the particles contributing to the particle light-scattering coefficient.

Meeting the requirements for closure exercises described above, ACTRIS has established operating procedures and traceable, independent calibration chains for both the nephelometer and MPSS systems (Wiedensohler et al., 2012). This includes thresholds for the expected accuracies, which for MPSS measurements are 3.5% deviation from the standard for particle size, and 10% for particle concentration. For nephelometers, the corresponding number is 10% deviation from the standard (Anderson et al., 1996).

For spherical and well-mixed particles of known chemical composition, the particle scattering coefficient can be calculated from theory for a given PNSD (Bohren & Huffman, 1983). The systematic uncertainty in the calculated scattering coefficient caused by assuming a particle chemical composition, i.e. refractive index real part, is typically around 13% in the ambient atmospheric boundary later (Fiebig et al., 2002), and much smaller for dried aerosol as dealt with at ACTRIS near-surface stations. Thus, deviations between scattering coefficients measured directly and calculated from MPSS will predominantly be caused by uncertainties in the measured PNSD, which includes the size range of particles larger than the upper size limit of the MPSS. However, this size range becomes relevant only for certain aerosol types with high particle concentrations in this size range, e.g. marine and dust aerosols. As a result, closure between the particle scattering coefficients measured by integrating nephelometer and calculated from the PNSD measured by the MPSS a very meaningful exercise to verify the accuracy of both measurements.

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## 3. The calculation of particle light scattering coefficient

To be suitable for the aerosol particle light scattering closure test, a station needs to operate an integrating nephelometer and a MPSS system, both following the ACTRIS operating procedures and calibration routines. For obtaining regular closure reports, both instruments need to participate in the ACTRIS near-real-time (NRT) data submission and dissemination infrastructure.

Despite some mathematical sophistication in the detail, calculating the particle light scattering coefficient from the PNSD for comparison with the nephelometer measured scattering coefficient is straight forward in principle. Sampling points are defined across the range of the measured PNSD using homogeneous logarithmic spacing in particle diameter. At the sampling points, the particle scattering cross-section is calculated by means of the Mie-scattering code of Bohren & Huffman (1983). This implies the assumption of homogeneously-mixed spherical particles. After multiplying the scattering-cross section with the particle concentration at the PNSD sampling points, the contributions of all particle sizes are summed up to yield the particle scattering coefficient. This amounts to a numerical integration of the product of particle concentration and scattering cross-section over particle size. The density of sampling points is chosen to keep the calculation uncertainty < 1% while maximising calculation speed.

For obtaining a wavelength-dependent particle refractive index to be used in the calculation, the current algorithm assumes the particles to consist of ammonium sulphate. This substance is not only abundant in atmospheric aerosol particles. Its refractive index real part, quantifying the capacity of a substance to scatter, is also close to that of many other substances commonly encountered in these particles (Fiebig et al., 2002). Water uptake by the particles would change the refractive index significantly, but can the neglected since the ACTRIS operating procedure requires drying of the aerosol to relative humidities < 40%. The closure scheme does currently not assume any absorbing substances in the aerosol in order to minimise the number of instruments and dependencies for the closure scheme. However, absorbing substances in the aerosol such as black carbon (BC) or absorbing mineral dust influence particle scattering for certain aerosol types. An extension to include particle absorption in the closure scheme, represented by BC, is therefore planned for the near future. The extended version will assume BC as absorbing component in the aerosol particle size range covered by the MPSS, represent the BC optical properties by “soot” as described by d’Almeida (1991), and constrain the BC content by collocated observations of the particle absorption coefficient.

Executable versions of the closure software will be made available on the EBAS submission website.

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# 4. Closure reports for particle light scattering coefficient

The automatic intercomparison of the measured and calculated particle light scattering coefficient is currently implemented for stations featuring the required observations and participating in the NRT data submission scheme in order to test for closure, and consists of a collection of processes and software.

The intercomparison of the measured and calculated particle light scattering coefficient is delivered as a report to data originator(s) and data submitter(s) responsible for the measurements at that station (see Appendix I as example of report). The setup, including the software and database, is hosted by NILU - Norwegian Institute for Air Research. This includes:

- Software for calculating the scattering coefficient from the MPSS particle number size distribution.
- Software for importing the data into the EBAS database as a separate data product (level 3 data)
- Software for extraction of data from EBAS, routines for plotting comparison plots of the closure variables, and automatic report generation, as well as an automatic e-mail service for regular delivery of reports.

Automatically generated reports are produced and delivered for each participating ACTRIS station, either on a monthly basis for Near-Real-Time (NRT) data, or yearly as a part of the quality control procedures performed for all stations. This will be implemented as a part of the annual data QA/QC procedures. The distribution and frequency of the reports are flexible, can be adapted to the needs and requests from the data originators, station operators or ACTRIS calibration centres. All plots and relevant metadata are consolidated into a PDF document, and then sent as an e-mail attachement. The reports are generated based on each respective dataset, and sent to the data originator(s) and/or data submitter(s), and/or instrument principal investigator(s) listed for the specific dataset.

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The report contains the following information:

- Basic information about the product, station, and time interval of the data.

**Scattering Coefficient Closure Report**

Produced by ACTRIS in-situ data center

**NO0002R August 2017**

Scattering Coefficient Closure Between Calculation from MPSS Particle Size Distribution and Nephelometer Measurement

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Station: NO0002R, Birkenes II

dmps instrument: NO01L_NILU_DMPSmodel2_BIR_NRT

nephelometer instrument: NO01L_TSI_3563_BIR_dry_NRT

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***Figure** Error! No sequence specified.:* *Basic report information*

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- Plotting of scattering coefficient measured and scattering coefficient calculated as time series, with a panel for each wavelength, both for aerosol light backscattering coefficient and aerosol light scattering coefficient.


***Figure** Error! No sequence specified.:* *Line plot - Aerosol light backscattering coefficient measured and backscattering coefficient calculated*

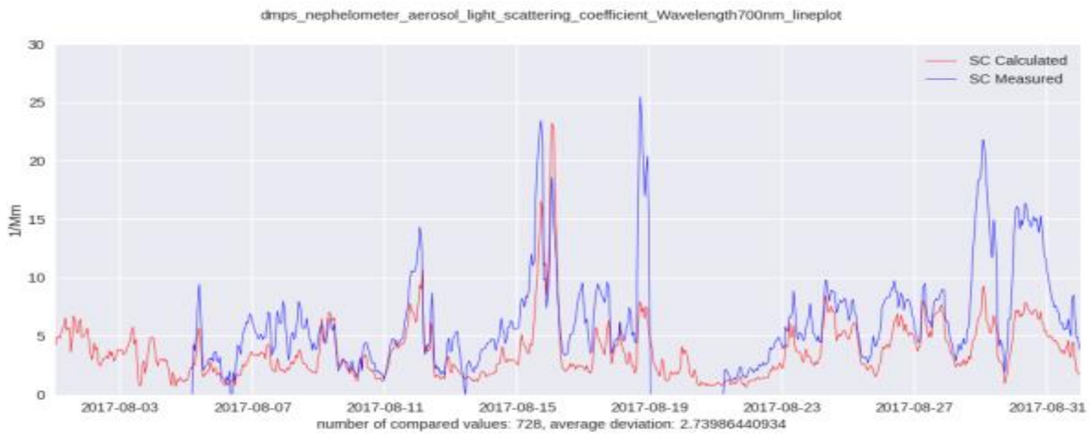


***Figure 2:*** *Line plot - Aerosol light scattering coefficient measured and scattering coefficient calculated*

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- Each data value is also plotted as points in a scatterplot with scattering coefficient calculated (y-axis) and scattering coefficient measured (x-axis), alongside with the regression line and the correlation coefficient. Also with separate panels for each wavelength

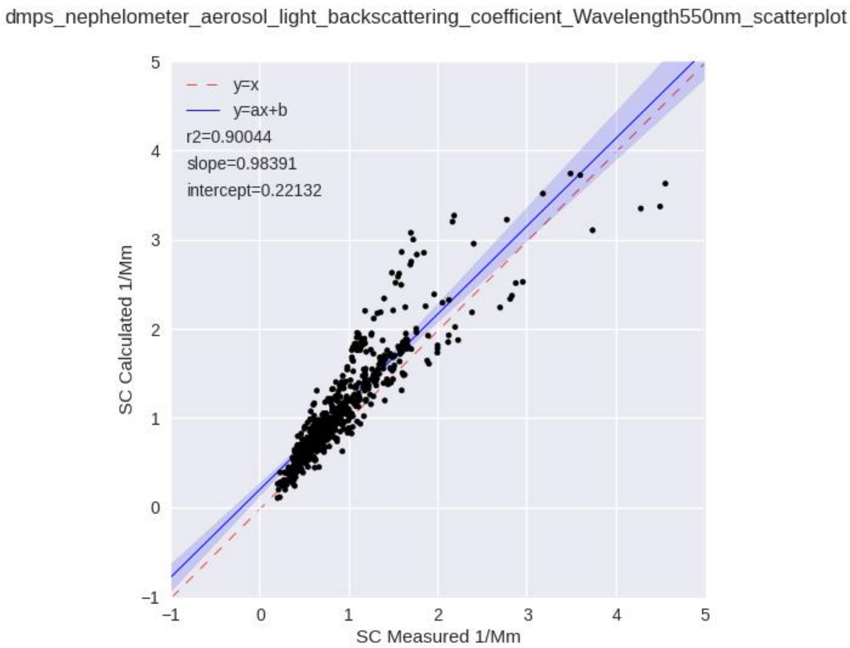


***Figure 3:*** *Scatter plot - aerosol light backscattering coefficient measured and backscattering coefficient calculated*

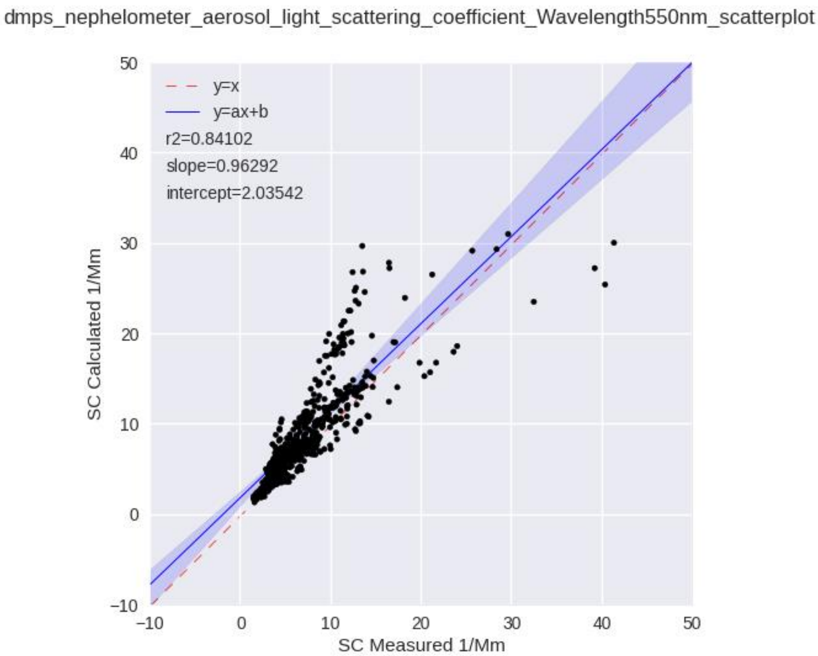


***Figure 4:*** *Scatter plot - aerosol light scattering coefficient measured and scattering coefficient calculated*

## 5. Plans and strategy for full implementation within ACTRIS

The automatic intercomparison tool has been developed using test data for a few selected stations. Implementation station by station will gradually take place from September and onwards. In September, the focus will be on implementation of the ACTRIS NRT stations, and data orginators and data submitters could already expect to see results by the start of October 2017.

Further on, the implementation will also include final data (level 2 data) and the first reports will be presented at the ACTRIS-2 WP3 meeting in Madrid in October 2017. Here we aim to collect feedback from the community.

Extension of the closure algorithm to take into account particle absorption is planned for autumn of 2017. None of the intercomparison data (level 3 data) will be made public through the EBAS database.

## 6. References

Anderson, T. L., Covert, D. S., Marshall, S. F., Laucks, M. L., Charlson, R. J., Waggoner, A. P., Ogren, J. A., Caldow, R., Holm, R. L., Quant, F. R., Sem, G. J.,Wiedensohler, A., Ahlquist, N. A., and Bates, T. S. (1996). Performance Characteristics of a High-Sensitivity, Three-Wavelength, Total Scatter/Backscatter Nephelometer, *J. Atmos. Ocean. Tech.* 13:967–986.

Bohren, Craig F.; Huffman, Donald R. (1983): Absorption and scattering of light by small particles, New York: Wiley.

*Cragin, Melissa; Heidorn, P. Bryan; Palmer, Carole L.; Smith, Linda C. (2007). "An Educational Program on Data Curation". ALA Science & Technology Section Conference. Retrieved 7 October 2013.*

d'Almeida, G., P. Koepke, and E. Shettle, Atmospheric Aerosols: Global Climatology and Radiative Characteristics, A. Deepak, Hampton, Va., 1991.

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# Appendix I

Example of report

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# Scattering Coefficient Closure Report

Produced by ACTRIS in-situ data center

## NO0002R August 2017

Scattering Coefficient Closure Between Calculation from MPSS Particle Size Distribution and Nephelometer Measurement

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Station: NO0002R, Birkenes II

dmps instrument: NO01L_NILU_DMPSmodel2_BIR_NRT

nephelometer instrument: NO01L_TSI_3563_BIR_dry_NRT

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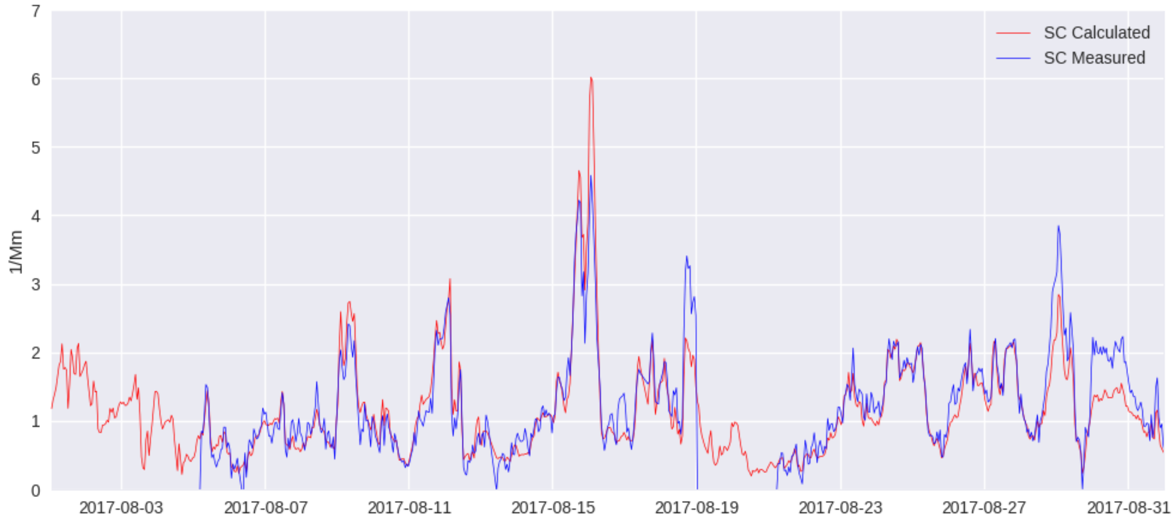
## aerosol light backscattering coefficient measured and calculated

dmps_nephelometer_aerosol_light_backscattering_coefficient_Wavelength450nm_lineplot




number of compared values: 728, average deviation: 0.368738104396

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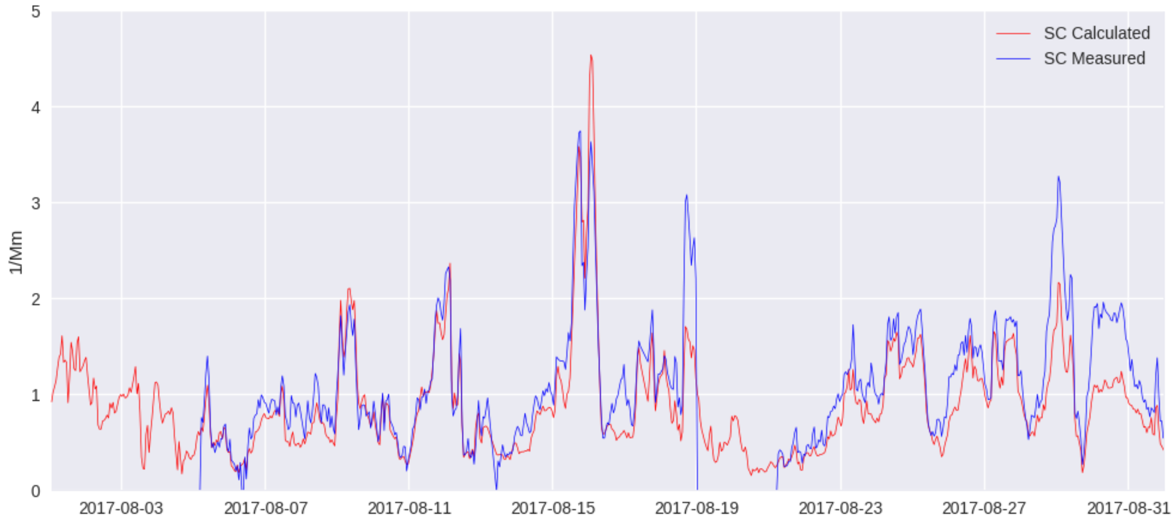


number of compared values: 728, average deviation: 0.34999043956

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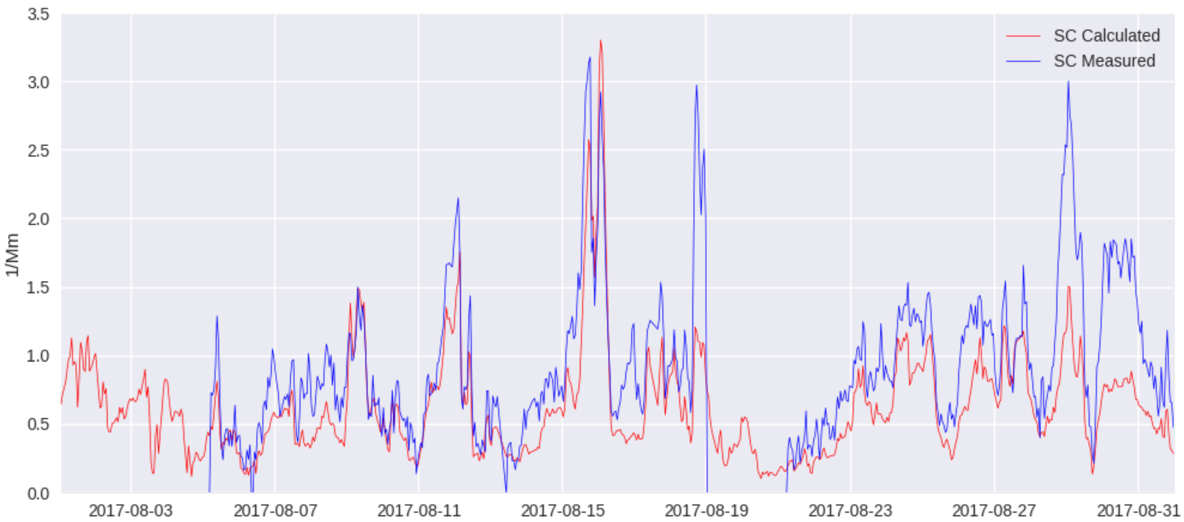
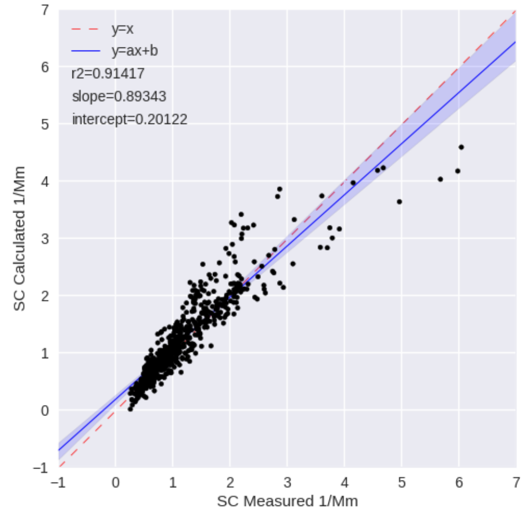


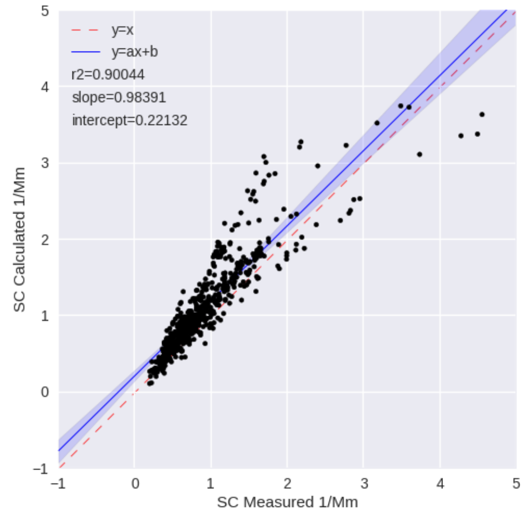

number of compared values: 728, average deviation: 0.357415164835

## aerosol light backscattering coefficient measured and calculated

dmps_nephelometer_aerosol_light_backscattering_coefficient_Wavelength450nm_scatterplot




dmps_nephelometer_aerosol_light_backscattering_coefficient_Wavelength550nm_scatterplot

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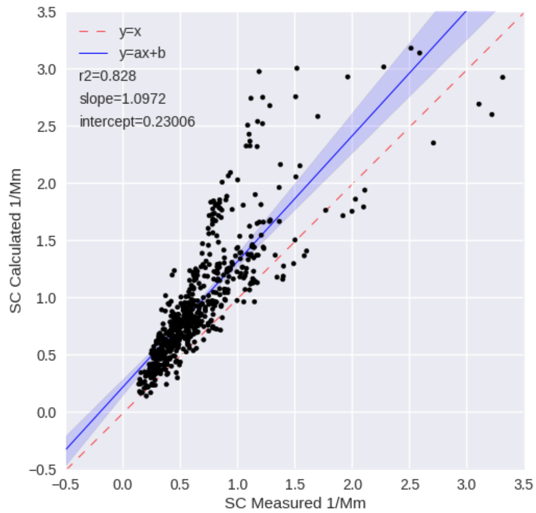
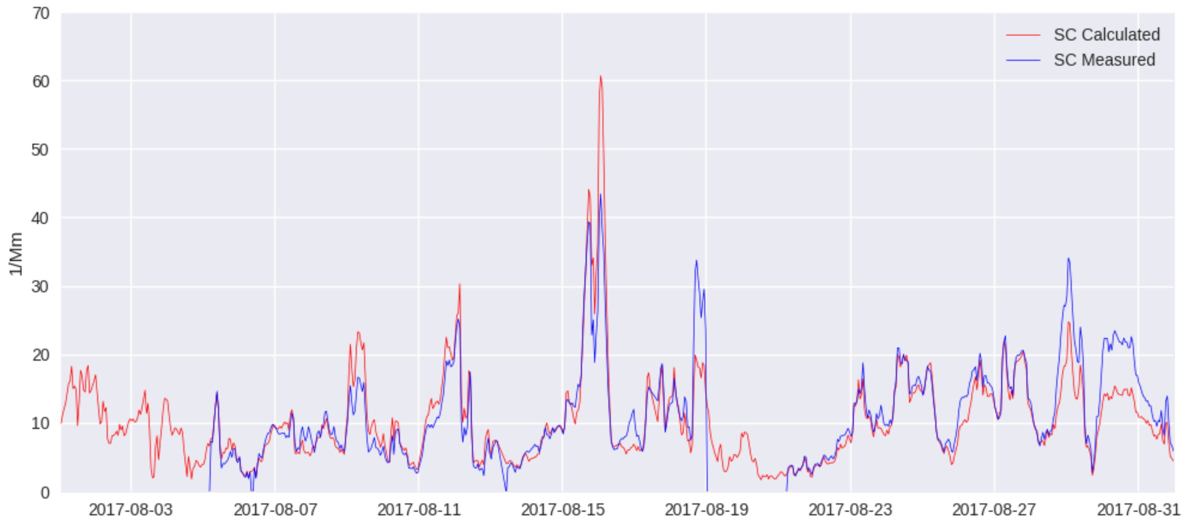


## aerosol light scattering coefficient measured and calculated

dmps_nephelometer_aerosol_light_scattering_coefficient_Wavelength450nm_lineplot

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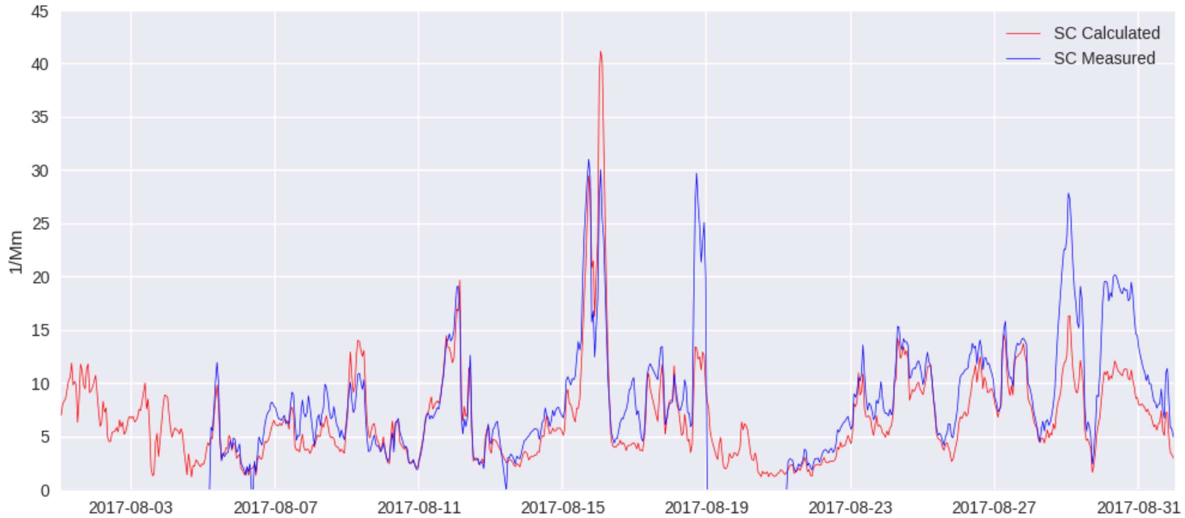


number of compared values: 728, average deviation: 2.94109663462

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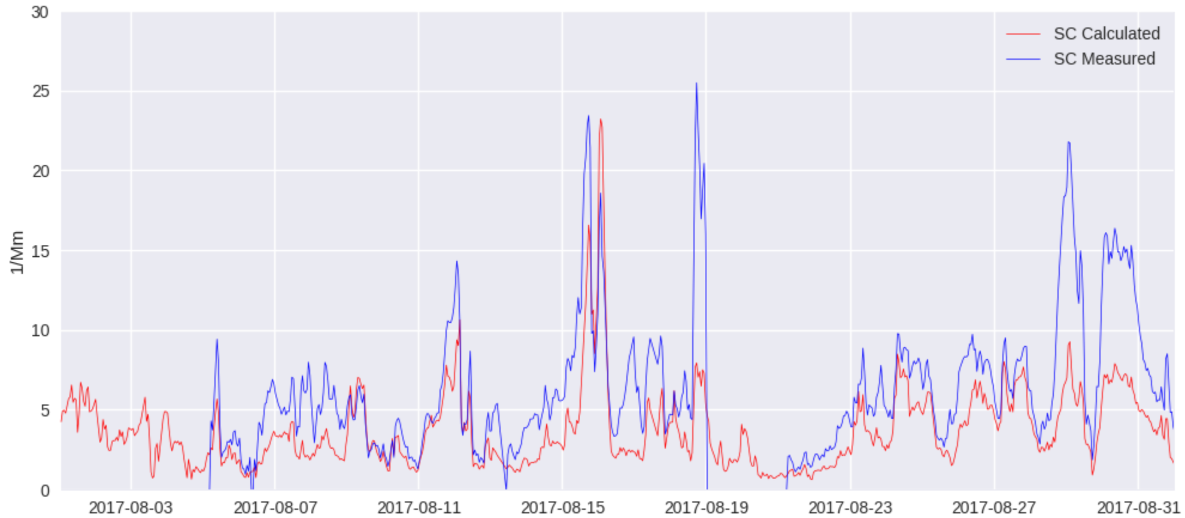


number of compared values: 728, average deviation: 2.73986440934

## aerosol light scattering coefficient measured and calculated

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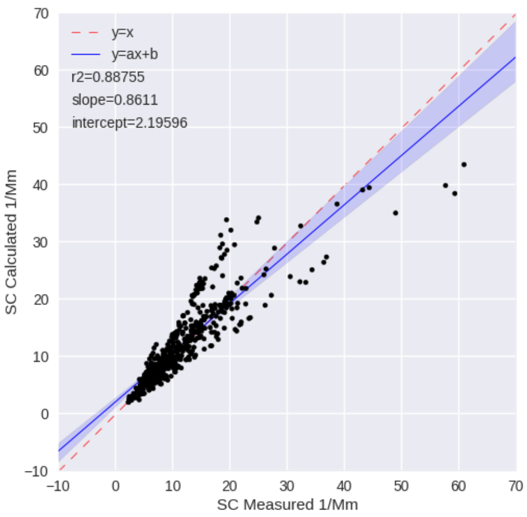
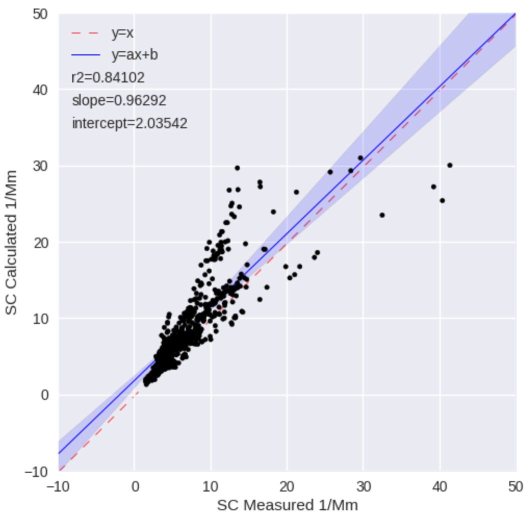



dmps_nephelometer_aerosol_light_scattering_coefficient_Wavelength550nm_scatterplot




dmps_nephelometer_aerosol_light_scattering_coefficient_Wavelength700nm_scatterplot