

Title: NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		Date: 03/28/2016
NEON Doc. #: NEON.DOC.002675	Author: D. Smith	Revision: A

ALGORITHM THEORETICAL BASIS DOCUMENT (ATBD)

DUST AND PARTICULATE SIZE DISTRIBUTION

PREPARED BY	ORGANIZATION	DATE
Derek Smith	FIU	05/06/2014
Josh Roberti	FIU	03/28/2016

APPROVALS	ORGANIZATION	APPROVAL DATE

RELEASED BY	ORGANIZATION	RELEASE DATE

See configuration management system for approval history.

© 2017 NEON Inc. All rights reserved.

The National Ecological Observatory Network is a project solely funded by the National Science Foundation and managed under cooperative agreement by NEON, Inc. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

<i>Title:</i> NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		<i>Date:</i> 03/28/2016
<i>NEON Doc. #:</i> NEON.DOC.002675	<i>Author:</i> D. Smith	<i>Revision:</i> A

Change Record

REVISION	DATE	ECO #	DESCRIPTION OF CHANGE
A	MM/DD/YYYY	ECO-XXXXX	Initial Release

Title: NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		Date: 03/28/2016
NEON Doc. #: NEON.DOC.002675	Author: D. Smith	Revision: A

TABLE OF CONTENTS

1 DESCRIPTION.....2

1.1 Purpose 2

1.2 Scope..... 2

2 RELATED DOCUMENTS, ACRONYMS AND VARIABLE NOMENCLATURE4

2.1 Applicable Documents 4

2.2 Reference Documents..... 4

2.3 Acronyms 4

2.4 Variable Nomenclature 5

3 DATA PRODUCT DESCRIPTION.....5

3.1 Variables Reported 5

3.2 Input Dependencies 5

3.3 Product Instances..... 6

3.4 Temporal Resolution and Extent 6

3.5 Spatial Resolution and Extent 6

4 SCIENTIFIC CONTEXT6

4.1 Theory of Measurement 7

4.2 Theory of Algorithm 9

4.2.1 Dust and Particulate Size distribution at < 50% RH 10

4.2.2 Calculating 30-minute and hourly median values 10

5 ALGORITHM IMPLEMENTATION.....10

6 UNCERTAINTY13

6.1 Uncertainty of Particulate Matter (PM) Measurements 14

6.1.1 Measurement Uncertainty..... 14

6.1.2 Uncertainty of L1, Median, Particulate Size and Distribution Data Products..... 16

7 FUTURE PLANS AND MODIFICATIONS.....16

8 BIBLIOGRAPHY16

9 CHANGELOG.....18

Title: NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		Date: 03/28/2016
NEON Doc. #: NEON.DOC.002675	Author: D. Smith	Revision: A

LIST OF TABLES AND FIGURES

Table 3-1: List of DPs used to derive L1 DPs within this ATBD. 5
 Table 5-1: Flags associated with particulate matter measurements..... 13
 Table 5-2: Information maintained in the CI data store for particulate matter. 13

1 DESCRIPTION

Sites with dust measurements include all core and relocatable sites in Domains 10, 13 and 15. The rationale for capturing dust measurements at these sites is explained in the scientific context portion of this document. Two methods will be used to study dust at NEON sites, particulate mass and particulate size. The particulate mass analyzer involves obtaining a physical sample to determine mass concentration based on gravimetric analysis, while the particulate size analyzer uses an optical technique to continuously measure different particles sizes at near real-time. The processes necessary to convert “raw” sensor measurements into meaningful scientific units and their associated uncertainties for the latter method will be described here. Dust and particulate size distribution measurements are discussed in this document.

1.1 Purpose

This document details the algorithms used for creating NEON Level 1 data products for dust and particulate size distribution measurements from Level 0 data, and ancillary data as defined in this document (such as calibration data) obtained via instrumental measurements made by the particulate size analyzer. It includes a detailed discussion of measurement theory and implementation, appropriate theoretical background, data product provenance, quality assurance and control methods used, approximations and/or assumptions made, and a detailed exposition of uncertainty resulting in a cumulative reported uncertainty for this product.

1.2 Scope

This document describes the theoretical background and entire algorithmic process for creating the NEON L1 data product for particulate matter, NEON.DOM.SITE.DP1.00017.001 from input data. It does not provide computational implementation details, except for cases where these stem directly from algorithmic choices explained here.

The particulate size analyzer consists of two main components: 1) the TSI DustTrak model: 8533EP is used to measure ambient particle concentrations, 2) a National Electrical Manufacturers Association

<i>Title:</i> NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		<i>Date:</i> 03/28/2016
<i>NEON Doc. #:</i> NEON.DOC.002675	<i>Author:</i> D. Smith	<i>Revision:</i> A

(NEMA) enclosure with an inlet to allow a pump and flow meter to sample ambient dust concentrations at 16.7 L min⁻¹, in order to meet the Environmental Protection Agency’s (EPA) guidelines for particulate sampling, and to house the DustTrak from the elements.

2 RELATED DOCUMENTS, ACRONYMS AND VARIABLE NOMENCLATURE

2.1 Applicable Documents

AD[01]	NEON.DOC.000001	NEON OBSERVATORY DESIGN
AD[02]	NEON.DOC.005003	NEON Scientific Data Products Catalog
AD[03]	NEON.DOC.005004	NEON Level 1-3 Data Products Catalog
AD[04]	NEON.DOC.005005	NEON Level 0 Data Products Catalog
AD[05]	NEON.DOC.000782	ATBD QA/QC Data Consistency
AD[06]	NEON.DOC.011081	ATBD QA/QC plausibility tests
AD[07]	NEON.DOC.000783	ATBD De-spiking and time series analyses
AD[08]	NEON.DOC.000746	Evaluating Uncertainty (CVAL)
AD[09]	NEON.DOC.000785	TIS Level 1 Data Products Uncertainty Budget Estimation Plan
AD[10]	NEON.DOC.000751	CVAL Transfer of standard procedure
AD[11]	NEON.DOC.000927	NEON Calibration and Sensor Uncertainty Values ¹
AD[12]	NEON.DOC.001113	Quality Flags and Quality Metrics for TIS Data Products
AD[13]	NEON.DOC.002115	NEON Sensor Command, Control and Configuration (C3)_ Document: Particulate Analyzer - Size

2.2 Reference Documents

RD[01]	NEON.DOC.000008	NEON Acronym List
RD[02]	NEON.DOC.000243	NEON Glossary of Terms

2.3 Acronyms

Acronym	Explanation
AIS	Aquatic Instrument System
ATBD	Algorithm Theoretical Basis Document
CI	NEON Cyberinfrastructure
CVAL	NEON Calibration, Validation, and Audit Laboratory
DAS	Data Acquisition System
DP	Data Product

¹ Note that CI obtains calibration and sensor values directly from an XML file maintained and updated by CVAL in real time. This report is updated approximately quarterly such that there may be a lag time between the XML and report updates.

Title: NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		Date: 03/28/2016
NEON Doc. #: NEON.DOC.002675	Author: D. Smith	Revision: A

FDAS	Field Data Acquisition System
GRAPE	Grouped Remote Analog Peripheral Equipment
Hz	Hertz
L0	Level 0
L1	Level 1
N/A	Not Applicable
NEMA	National Electrical Manufacturers Association
NOAA	National Oceanic and Atmospheric Administration
PM	Particulate Matter
QA/QC	Quality assurance and quality control

2.4 Variable Nomenclature

N/A

3 DATA PRODUCT DESCRIPTION

3.1 Variables Reported

Dust and particulate size distribution related L1 DPs provided by the algorithms documented in this ATBD are displayed in the accompanying file, dpsd_datapub_NEONDOC002675.txt.

3.2 Input Dependencies

Table 3-1 details the dust and particulate size distribution related L0 and L1 DPs used in this ATBD.

Table 3-1: List of DPs used to derive L1 DPs within this ATBD.

Data product	Sample Frequency	Units	Data Product ID
PM 15 µm	1 Hz	mg/m ³	NEON.DOM.SITE.DP0.00017.001.01943.HOR.VE R.000
PM 10 µm	1 Hz	mg/m ³	NEON.DOM.SITE.DP0.00017.001.01942.HOR.VE R.000
PM 4 µm	1 Hz	mg/m ³	NEON.DOM.SITE.DP0.00017.001.01941.HOR.VE R.000
PM 2.5 µm	1 Hz	mg/m ³	NEON.DOM.SITE.DP0.00017.001.01940.HOR.VE R.000
PM 1 µm	1 Hz	mg/m ³	NEON.DOM.SITE.DP0.00017.001.01939.HOR.VE R.000
Relative Humidity	1 Hz	%	NEON.DOM.SITE.DP0.00098.001.01357.HOR.VE R.000
Flow Meter	1 Hz	LPM	NEON.DOM.SITE.DP0.00017.001.01946.HOR.VE

Title: NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		Date: 03/28/2016
NEON Doc. #: NEON.DOC.002675	Author: D. Smith	Revision: A

(sensor)			R.000
Flow Meter (assembly)	1 Hz	LPM	NEON.DOM.SITE.DP0.00017.001.01950.HOR.VE R.000

3.3 Product Instances

The particulate size analyzer will not be deployed at all NEON towers. TIS towers in Domains 10, 13, and 15 will be outfitted with particulate size analyzers. Only one particulate size analyzer will be deployed at these sites.

3.4 Temporal Resolution and Extent

Thirty-minute and one-hour median values for PM will be calculated to form L1 DPs.

3.5 Spatial Resolution and Extent

The particulate size analyzer will be located at the top of the tower infrastructure and therefore its measurements will represent the point in space where the measurement is taken.

4 SCIENTIFIC CONTEXT

By deploying optical particulate matter analyzers at a total of 6 sites across three Domains (10, 13, and 15) NEON’s aim is to help the scientific community gain insight on the regional dust transport across the Rocky Mountain region, Figure 1. Aerosol dust can be composed of numerous inorganic and organic elements; everything from biological components such as pollen to the byproducts of incomplete combustion. All of these constituents can affect the environment in numerous ways. From a human health perspective, particulate matter (PM) or aerosols less than 10 µm have negative health effects due to their ability to be respired and reach lower regions of the respiratory tract. Aerosols also have wide reaching effects on the environment depending on their composition. One main focus area for NEON is the albedo change that can result from dust deposition. Industrialization has increased the number of anthropogenic sources that emit particulate matter, which can influence surface albedo. The primary anthropogenic particulate matter that can drive changes in surface albedo is “black carbon”. Black carbon is a byproduct of incomplete combustion of fossil fuel, biomass, and biofuels. Black carbon’s radiative properties allow it to absorb large amounts of solar radiation. In fact, by mass, black carbon has the largest radiative forcing of any PM (EPA, 2012). Thus, aerosols containing black carbon

Title: NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		Date: 03/28/2016
NEON Doc. #: NEON.DOC.002675	Author: D. Smith	Revision: A

contribute to atmospheric warming. Additionally, as black carbon accumulates on the Earth’s surface the rates at which ice and snow melt are increased. Increased snow and ice melt rates ultimately impact the Earth’s surface albedo and has far reaching impacts on the global climate. In terms of direct radiative forcing estimates, investigations have identified black carbon influence is slightly less than CH₄ and CO₂ on a global scale, while for some regional locations it can be greater than these two greenhouse gases (Panicker et al., 2010; Chung S. and J. Seinfeld, 2005; Jacobson M., 2002; Jacobson M., 2002). Additionally, the effective radiative forcing black carbon has on snow has increased roughly 6 fold over the last 200 years and black carbon is estimated to have the highest temperature impact out of any anthropogenic emissions on a time horizon less than 5 years (IPCC, 2013). Likewise, for a specific period of time, simulations have demonstrated that any reduction in global emissions of black carbon may outweigh any emission reduction in CO₂ and CH₄ with respect to a reduction in global warming (Jacobson M., 2002). Therefore, NEON has chosen to study the dust transect across the Rocky Mountain region to enable the scientific community to gain insight into questions such as, how dust transport may affect the timing of snow melt and whether this can be used as a proxy for other regions. Long-term monitoring of the dust transect across the Rocky Mountain region will allow trends to be identified overtime, which among other things will help to inform future regional and global aerosol investigations.

Another main focus of NEON’s dust measurements is how dust deposition across the Rocky Mountain region affects chemical and nutrient inputs to ecosystem. Measurements from the particulate size analyzer will provide ancillary data to answer questions related to nutrient and chemical cycling. However, filters collected from the particulate mass analyzer, which can be requested by the scientific community, are envisioned to be a greater resource to the scientific community for investigations related to this focus area. Information pertaining to the particulate mass analyzer can be found in AD [13].

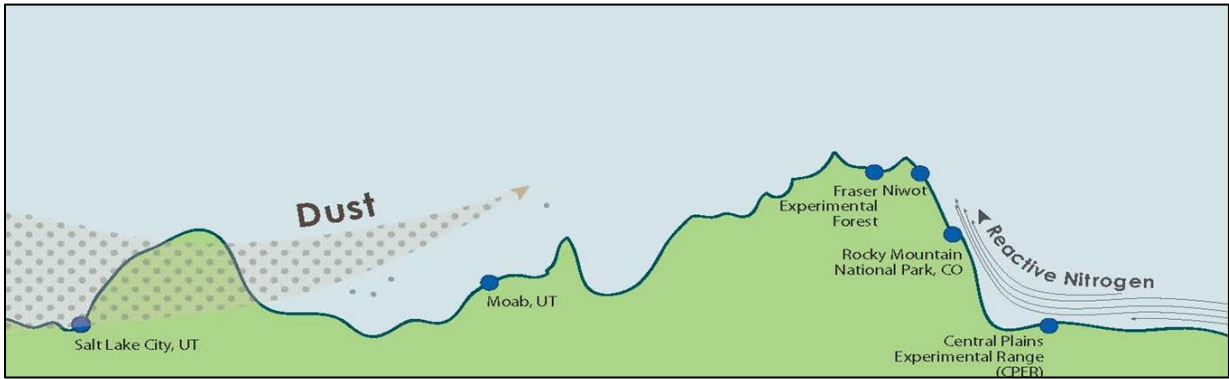


Figure 1. Depiction of the dust transect across the Rocky Mountain region that NEON tower sites will capture. The blue points indicate the relative location of the six NEON tower across the transect.

4.1 Theory of Measurement

Title: NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		Date: 03/28/2016
NEON Doc. #: NEON.DOC.002675	Author: D. Smith	Revision: A

The particulate size analyzer has two main components, the DustTrak sensor and its supporting infrastructure. The supporting infrastructure for the DustTrak has two main purposes; 1) to shelter the device from extreme environmental conditions and 2) to increase the flow rate of the sample stream that the DustTrak samples from. The EPA suggests that ambient dust measurements should be taken by a sampler at a flow rate of 16.7 l min⁻¹. However, the DustTrak has a sample intake flow of 3 l min⁻¹, which is then split internal to the sensor to measure an aerosol flow of 2 l min⁻¹. Therefore the supporting infrastructure includes a separate inlet that samples ambient atmospheric conditions at a rate of 16.7 l min⁻¹, from which the DustTrak subsamples from. In order to ensure that the flow between the 16.7 l min⁻¹ sample and the DustTrak’s 3 l min⁻¹ subsample is isokinetic a custom sized inlet was designed for the DustTrak’s intake. In order to maintain the 16.7 l min⁻¹ flow the supporting infrastructure includes a flow meter, flow controller, and pump. These components along with the DustTrak are housed inside a NEMA enclosure for protection.

The DustTrak is capable of measuring different size fractions of particulate matter (PM) continuously in near real-time over a range of 0.1 to 15 µm. This range is then separated into the following size fractions, PM 1 µm, PM 2.5 µm, PM 4 µm (i.e., respirable), PM 10 µm (i.e., thoracic), and PM 15 µm. PM for each measured size fraction encompasses PM that is less than or equal to that size fraction. The DustTrak measures PM using an optical technique, which essentially relates the amount of light scattered in an optical cavity to the amount of PM present. The 3 l min⁻¹ flow that enters the DustTrak is split into a 2 l min⁻¹ flow to be sampled and a 1 l min⁻¹ flow which is filtered and then used to create a sheath flow which isolates the sample flow to minimize contamination of the optical cell path. As the sample passes through the optical cavity a laser passes through the sample, which is read by a photodetector. The photodetector’s signal and pulse height is then interpreted. This allows the sensor to identify both the total amount of light scattered, i.e., signal height, by the particles between 0.1 to 15µm in the optical cell as well as the amount of light scattered by individual particles, i.e., pulse height (Wang, 2009).

Humidity is known to bias optical measurements of PM, and since samples will not be humidity controlled two sets of data will be output. One data set representing all PM measurements and the second set representing only PM measurements collected when the ambient relative humidity was below 50%. There are two main ways that relative humidity (RH) can affect the optical properties of PM. First, because of the hygroscopic nature of PM, particle size tends to increase with increasing RH. While the relationship between particle growth and RH is mainly dependent on the chemical composition of a particle, a particle’s size can change how it’s affected by RH too. Secondly, as a particle absorbs moisture it becomes more dilute which reduces its refraction index (Tijjani B. and Uba S., 2013).

A positive correlation exists between PM and RH, however it is not linear and varies depending on the chemical makeup of the particle (Ferman M. et al., 1981; Covert et al. 1972). Thus, while generic equations exist to post-correct for humidity they each have their caveats. Generally, optical

Title: NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		Date: 03/28/2016
NEON Doc. #: NEON.DOC.002675	Author: D. Smith	Revision: A

measurements of PM are normalized to around 40% RH. The 40% RH normalization point is driven by both historical precedent in which filters analyzed by gravimetric analysis, based on first principals and serves as the reference for PM measurements, are conditioned to 30-40% RH for 24 hours prior to analysis, as well as the fact that below 40% RH humidity’s effect on PM is negligible. However, multiple investigations have found that PM throughout the region studied by NEON is typically low to non-hygroscopic in nature, and thus is generally unaffected by RH until levels reach 50% (Tijjani B. and Uba S., 2013; Jeong M.-J. et al., 2007; Zhang X., 1994; Laulainen, N., 1993; Ferman M. et al., 1981; Covert et al, 1972). Additionally, it has been suggested that DustTrak measurements are generally unaffected by RH if it is below 60% (Ramachandran G. et al., 2003). Therefore, NEON will provide two sets of data; one that uses only measurements captured when RH is less than 50% and the other that includes all measurements regardless of the RH.

4.2 Theory of Algorithm

Internal to the DustTrak particle sizes are segregated into the various size fractions and the volumetric flow rate is determined for the samples. This allows for the DustTrak to output the mass concentration per unit time at a frequency of 1 Hz. These mass concentration measurements are then aggregated to determine 30-minute and hourly estimates for each size fraction. Due to the natural variability that can exist over a short period of time when measuring dust the median value will be used instead of the mean to provide a more robust estimate of the time aggregated value.

The 30-minute medians will be determined from 1 Hz measurements taken during the 1800-second period [0, 1800), while hourly medians will be determined from measurements taken during the 3600-second period [0, 3600). Additionally, the beginning of the first averaging period in a series shall be the nearest whole minute less than or equal to the first timestamp in the series. However, before median values can be determined the data needs to be filtered to exclude erroneous data created by the auto-zeroing routine.

Every three hours the DustTrak will run an auto-zero routine to minimize instrument drift. The auto-zero routine lasts for approximately 100 seconds, during which no data will be reported from the analyzer. However, the first data point after the completion of the auto-zeroing routine will have a zero reading for mass concentration and thus needs to be excluded from the data set. Since it is highly unlikely that PM concentrations will be zero in ambient atmospheric conditions, all zero values from the DustTrak must be removed prior to any other treatment of the data. Following the removal of zero values, the DustTrak data shall then be subset for measurements captured when RH was less than 50% according to Section 4.2.1, while median values can be computed for the data set that includes all data regardless of RH according to Section 4.2.2.

Title: NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		Date: 03/28/2016
NEON Doc. #: NEON.DOC.002675	Author: D. Smith	Revision: A

4.2.1 Dust and Particulate Size distribution at < 50% RH

Level 0 relative humidity (RH) data, i.e, NEON.DOM.SITE.DP0.00098.001.01357.HOR.VER.000, shall be temporally aligned with the L0 DustTrak observations [AD 14]. At every time point when RH is greater than 50%, the corresponding L0 DustTrak observations will be omitted from calculation of the L1 subproduct for <50% RH. If RH data are missing, the L0 DustTrak data will likewise be omitted from calculation of the L1 subproducts for <50% RH. The remaining L0 DustTrak data, corresponding to time points when RH is known to be below 50%, shall then be used to determine 30-minute and hourly median values according to Section 4.2.2.

4.2.2 Calculating 30-minute and hourly median values

The median value for a given time interval and PM size fraction will be determined by sorting all the associated data points from smallest to largest. If the number of samples collected over the time interval is odd then the median will be represented by the middle value. Alternatively, if the number of samples collected over the time interval is even then the median will be represented by the average of the two middle numbers. Accompanying the median value shall be a count of the number of points that were used in determining its value.

5 ALGORITHM IMPLEMENTATION

Data flow for signal processing of L1 DPs will be treated in the following order.

1. Data observed immediately following the auto-zero routine shall be removed from the data
2. QA/QC Plausibility tests will be applied to the data stream in accordance with AD[06], details are provided below.
3. A new data set from the DustTrak data will be generated, representing measurements captured when the ambient RH was below 50%, i.e., Section 4.2.1.
4. 30-minute and hourly PM medians will be calculated for the various PM size fractions for the two data sets, i.e., one representing all DustTrak measurements and one representing DustTrak measurements captured when the ambient RH was below 50%, i.e. Section 4.2.2.
5. For the two data sets descriptive statistics, i.e. number of points used, minimum, maximum, median and median absolute deviation from the median (Eq. (1)), will be determined for the thirty-minute and hourly medians.
6. QA/QC Summary (Qsum) will be produced for the two data sets according to AD[12].

Title: NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		Date: 03/28/2016
NEON Doc. #: NEON.DOC.002675	Author: D. Smith	Revision: A

Equation (1) displays the median absolute deviation; it is assumed that the data are sorted in ascending order prior to calculating (Huber 1981).

$$MAD = M_i(|x_i - M_j(x_j)|) \quad (1)$$

Where,

M_i = median of the series

x_i = individual observation

$M_j(x_j)$ = residuals (deviations) of each observation from the data's median

QA/QC Procedure:

1. **Plausibility Tests AD[06]** – All plausibility tests will be determined for the particulate size analyzer. Test parameters will be provided by FIU and maintained in the CI data store. All plausibility tests will be applied to the sensor's converted L0 DPs and associated quality flags (QFs) will be generated for each test.
2. **Sensor Flags** – Sensor flags are derived from L0 data products identified in the C³ document (AD[13]).

- a. Sensor Flow Rate: [denoted as *sensorFlowRate* in *dpsd_datapub_NEONDOC002675.txt*]

$$QF_{SF} = \begin{cases} 0 & \text{if } 2.85 < SF < 3.15 \\ 1 & \text{otherwise} \end{cases}$$

Where:

SF = Sensor Flow rate (LPM)

- b. Assembly Flow Rate: [denoted as *assemblyFlowRate* in *dpsd_datapub_NEONDOC002675.txt*]

$$QF_{AF} = \begin{cases} 0 & \text{if } 15.84 < AF < 17.51 \\ 1 & \text{otherwise} \end{cases}$$

Title: NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		Date: 03/28/2016
NEON Doc. #: NEON.DOC.002675	Author: D. Smith	Revision: A

Where:

AF = Assembly Flow rate (LPM)

The flow rate flag indicates whether the exhaust flow from the DustTrak is adequate. A flow outside $\pm 5\%$ of the nominal DustTrak exhaust flow, indicates that the DustTrak is no longer operating normally. Data during these times will be flagged. The flow information will help identify the cause for the sensor malfunction, e.g., a low flow may indicate a filter that has become fouled.

- Measurement Validity** – This QA/QC analysis interprets the validity of the data by comparing the different PM size fractions to one another from the L0 data. If the logic fails a measurement validity flag (i.e., QF_MV) will be set high and otherwise remain low. If a validity flag is set high, then all data with a corresponding timestamp will not be used to calculate L1 DPs. This flag is denoted as *measurementValidity* in *dpsd_datapub_NEONDOC002675.txt*

$$QF_MV = \begin{cases} 1 & \text{if } PM_{15} < PM_{10} \text{ OR } PM_{10} < PM_4 \text{ OR } PM_4 < PM_{2.5} \text{ OR } PM_{2.5} < PM_1 \\ 0 & \text{otherwise} \end{cases}$$

Where:

PM_{15} = PM 15 μm (mg/m^3)
 PM_{10} = PM 10 μm (mg/m^3)
 PM_4 = PM 4 μm (mg/m^3)
 $PM_{2.5}$ = PM 2.5 μm (mg/m^3)
 PM_1 = PM 1 μm (mg/m^3)

- Signal Despiking** – Time segments and threshold values for the automated despiking QA/QC routine will be specified by FIU and maintained in the CI data store. QFs from the despiking analysis will be applied according to AD[07].
- Consistency Analysis** – Currently, a consistency analysis will not be run on the L1 DPs. However, consistency analysis on the time series may be explored in the future.
- Quality Flags (QFs) and Quality Metrics (QMs) AD[12]** – If a datum has one of the following flags raised, then it will not be used to create a L1 DP, **QF_R , QF_P , and QF_MV** . α and β QFs and QMs will be determined for all of the external flags, Table 3. All L1 DPs will have an associated final quality flag, QF_FINAL , and quality summary, $Qsum$, as detailed in AD[12]. Flags that may

Title: NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		Date: 03/28/2016
NEON Doc. #: NEON.DOC.002675	Author: D. Smith	Revision: A

be associated with DustTrak’s measurements, as well as information maintained in the CI data store can be found below in Tables 3, 4 and 5.

Table 5-1: Flags associated with particulate size measurements.

Tests	Flags
Range (hard)	QF_R
Persistence	QF_P
Step (hard)	QF_S
Null	QF_N
Gap	QF_G
Sensor Tests AD[13]	QF_SF, QF_AF
Measurement Validity	QF_MV
Final quality flag	QF_FINAL

Table 5-2: Information maintained in the CI data store for particulate matter.

Tests/Values	CI Data Store Contents
Range	Minimum and maximum values
Persistence	Window size, threshold values and maximum time length
Step	Threshold values
Null	Test limit
Gap	Test limit
Signal Despiking	Time segments and threshold values
Uncertainty	AD[11]
Sensor Tests	QF_SF and QF_AF
Measurement validity	QF_MV
Final Quality Flag	AD[12]

6 UNCERTAINTY

Uncertainty of measurement is inevitable; therefore, measurements should be accompanied by a statement of their uncertainty for completeness (JCGM 2008; Taylor 1997). To do so, it is imperative to identify all sources of measurement uncertainty related to the quantity being measured. Quantifying the uncertainty of TIS measurements will provide a measure of the reliability and applicability of individual measurements and TIS data products. This portion of the document serves to identify, evaluate, and quantify sources of uncertainty relating to individual, calibrated pressure measurements as well as L1 DPs. It is a reflection of the information described in AD[10], and is explicitly described for the particulate size assembly in the following sections.

Title: NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		Date: 03/28/2016
NEON Doc. #: NEON.DOC.002675	Author: D. Smith	Revision: A

6.1 Uncertainty of Particulate Matter (PM) Measurements

Uncertainty of the particulate size assembly is discussed in this section. This section discusses two topics. The first informs the sources of *measurement* uncertainty, i.e., those associated with *individual measurements*. The second details uncertainties associated with L1 data products. The L1 data products are not temporally averaged data, but are median values of aggregated measurements.

6.1.1 Measurement Uncertainty

The following subsections present the uncertainties associated with *individual particulate matter observations*. It is important to note that the uncertainties presented in the following subsections are *measurement uncertainties*, that is, they reflect the uncertainty of an *individual* measurement. These uncertainties should not be confused with those presented in Section 6.1.2. We urge the reader to refer to AD[11] for further details concerning the discrepancies between quantification of measurement uncertainties and L1 uncertainties.

Nominally, NEON calculates measurement uncertainties according to recommendations of the Joint Committee for Guides in Metrology (JCGM) 2008. In essence, if a measurand y is a function of n input quantities

x_i ($i = 1, \dots, n$), i.e., $y = f(x_1, x_2, \dots, x_n)$, the combined measurement uncertainty of y , assuming the inputs are independent, can be calculated as follows:

$$u_c(y) = \left(\sum_{i=1}^N \left(\frac{\partial f}{\partial x_i} \right)^2 u^2(x_i) \right)^{\frac{1}{2}} \quad (2)$$

Where,

$\frac{\partial f}{\partial x_i}$ = partial derivative of y with respect to x_i

$u(x_i)$ = combined standard uncertainty of x_i .

Thus, the uncertainty of the measurand can be found by summing the input uncertainties in quadrature. However, measurement uncertainties of the DustTrak will not follow Eq. (2). The justification behind this is detailed in the sections below.

6.1.1.1 Understanding Uncertainties of Particulate Mass Size and Distribution

The DustTrak combines photometry and optical particle sizing in a single device (TSI 2014). Photometry and optical particle counter measurements are based heavily on assumptions that can influence the accuracy of particulate matter measurements (details below). Additionally, as mentioned in Section 4.1,

Title: NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		Date: 03/28/2016
NEON Doc. #: NEON.DOC.002675	Author: D. Smith	Revision: A

particulate size distributions are sensitive to relative humidity due to the hygroscopicity of the particles (propensity of the particles to take on water).

The DustTrak sensors are calibrated by TSI using the industry standard (ISO 12103-1; A1-dust), ultrafine, Arizona Road Dust (ARD; TSI 2014). By calibrating to this standard, it is assumed the DustTrak will be monitoring aerosols of similar characteristics to A1-dust when deployed. If the sensor is installed in an environment where the aerosols are much different than A1-dust, it is important to apply corrections appropriate to the composition of the expected aerosols of the local environment (TSI 2014). Even with corrections applied, however, large uncertainties are still common. This is due to the temporal and spatial distributions of aerosols varying greatly as a function of the aerosols’ origin (Wang *et al.* 2009a).

Photometry, which the DustTrak uses to monitor PM_{2.5} mass concentration, is affected by many factors. These include:

- 1) humidity levels affecting the refraction index of the aerosol (Gobeli *et al.* 2008),
- 2) aerosol morphology,
- 3) particle size distribution,
- 4) scattering angle (Hinds 1999), and
- 5) the density of the aerosol being sampled (Wang *et al.* 2009a).

In addition to photometry, the DustTrak uses an optical particle counter (OPC) to monitor mass distributions for particles > 1 µm (TSI 2014). Optical particle counters are accurate when particulate mass concentrations are small; however, they share the same uncertainties as photometers with the exception of scattering angle (Wang *et al.* 2009a).

Due to constraints, the DustTrak sensors deployed throughout the NEON Observatory will not be calibrated to site-specific (local) environments. The sensors will operate using the calibration associated with A1-dust and thus the measurement uncertainty associated with monitoring purely A1-dust will be provided as 15% (TSI 2014). Given the amount of unquantified uncertainties listed above, and the complex interactions of these uncertainties on aerosol quantification, it is not practical to provide dynamic uncertainty estimates for individual particulate size and distribution measurements. NEON’s objective for monitoring particulate mass and distributions is to determine the temporal and spatial transport of dust throughout NEON Domains 15, 13, and 10. Although uncertainty estimates will not be fully characterized, aerosol transport trends can still be quantified in terms of relative mass concentrations throughout the region of interest.

6.1.1.2 Calibration

Uncertainties introduced by the calibration process are not provided.

Title: NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		Date: 03/28/2016
NEON Doc. #: NEON.DOC.002675	Author: D. Smith	Revision: A

6.1.1.3 Field DAS

This aerosol monitor has an internal A/D converter and outputs data in digital form. Because of this, uncertainty introduced by the field DAS is considered negligible.

6.1.2 Uncertainty of L1, Median, Particulate Size and Distribution Data Products

Level 1 uncertainty will be represented by the median absolute deviation (from the data’s median; MAD) of particulate size and distribution median data products. Although this approach does not quantify the uncertainties listed in Section 6.1.1.1, it does provide the end-user with a metric of particulate size and distribution variance during the aggregated time-span that the samples were collected (See Eq. (1)).

7 FUTURE PLANS AND MODIFICATIONS

Future system flags may be incorporated into the data stream and included in the QA/QC summary. Additionally, individual calibrated and QA/QC’d measurements with their respective uncertainties may become a common data output in the future.

Details concerning the evaluation and quantification of Sensor and Field DAS drift will be added to the uncertainty section.

8 BIBLIOGRAPHY

- Chung, S.H., and J.H. Seinfeld. (2005) Climate response of direct radiative forcing of anthropogenic black carbon. *Journal of Geophysical Research*. 110, pp. 25, DOI: 10.1029/2004JD005441.
- Covert, D.S., Charlson, R.J., and N.C. Ahlquist. (1972) A study of the relationship of chemical composition and humidity to light scattering by aerosols. *Journal of Applied Meteorology*. 11, pp. 968-976.
- EPA. (2012) Report to congress on black carbon: Chapter 2 black carbon and its effects on climate. United States Environmental Protection Agency. Technical Report. EPA-450/R-12-001, pp. 50, [Online] Available: <http://www.epa.gov/blackcarbon/2012report/Chapter2.pdf> [July, 2014].
- Ferman, M.A., Wolff, G.T., and N.A. Kelly. (1981) The nature and sources of haze in the Shenandoah valley/blue ridge mountains area. *Journal of the Air Pollution Control Association*, 31(10), pp. 1074-1082, DOI: 10.1080/00022470.1981.10465329.
- Gobeli, D., Schloesser, H., and T., Potterberg (2008) Met One instruments BAM-1020 beta attenuation mass monitor US-EPA PM 2.5 federal equivalent method field test results. Met One Inst. Inc. [Available online at: <http://www.metone.com/documents/AWMA2008-Final-2.pdf>]

Title: NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		Date: 03/28/2016
NEON Doc. #: NEON.DOC.002675	Author: D. Smith	Revision: A

- Hinds, W.C. (1999) Aerosol technology: properties, behavior, and measurement of airborne particles. 2nd Edition, John Wiley and Sons, Toronto, CA. pp. 483
- Huber, P. J. (1981). Robust statistics. New York: John Wiley
- IPCC. (2013) Climate change 2013: the physical science basis. Contribution of Working Group I to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change [Stocker, T.F., D. Qin, G.-K. Plattner, M. Tignor, S.K. Allen, J. Boschung, A. Nauels, Y. Xia, V. Bex and P.M. Midgley (eds.)] Cambridge, United Kingdom and New York, NY USA, pp. 1535
- Jacobson, M.Z. (2002) Control of fossil-fuel particulate black carbon and organic matter, possibly the most effective method of slowing global warming. *Journal of Geophysical Research*. 107, DOI: 10.1029/2001JD001376, 2002.
- Jacobson, M.Z. (2001) Strong radiative heating due to the mixing state of black carbon in atmospheric aerosols. *Nature*. 409, pp. 695-697.
- JCGM (2012) International vocabulary of metrology – Basic and general concepts and associated terms (VIM). 3rd Edition. pp. 92.
- Jeong, M.-J., Zhanqing, L., Andrews, E., and S.-C. Tsay. (2007) Effect of aerosol humidification on the column aerosol optical thickness over the atmospheric radiation measurement southern Great Plains site. *Journal of Geophysical Research*. 112, DOI: 10.1029/2006JD007176.
- Joint Committee for Guides in Metrology (JCGM) (2008) Evaluation of measurement data – Guide to the expression of uncertainty in measurement. pp. 120.
- Laulainen, N.S. (1993) Summary of conclusions and recommendations from a visibility science workshop. SciTech Connect. Pacific Northwest Laboratory. DOI: 10.2172/10149541.
- Panicker, A.S., Pandithurai, G., Safai, P.D., Dipu, S., and D.-I. Lee. (2010) On the contribution of black carbon to the composite aerosol radiative forcing over an urban environment. *Atmospheric Environment*. 44, pp. 3066-3070, DOI: 10.1016/j.atmosenv.2010.04.047.
- Ramachandran, G., Adgate, J.L., Pratt, G.C. and K. Sexton. (2010) Characterizing indoor and outdoor 15 minute average PM 2.5 concentrations in urban neighborhoods. *Aerosol Science and Technology*, 37(1), pp. 33-45, DOI: 10.1080/02786820300889.
- Smith, D.E. (2014) DustTrak comparison to Federal Equivalent Method [in Appendix].
- Taylor, J. R. (1997) An Introduction to Error Analysis: The Study of Uncertainties in Physical Measurements. University Science Books, Mill Valley, California. 2nd Ed. pp. 327.
- Tijjani, B.I., and S. Uba. (2013) The effect of hygroscopic growth on desert aerosols. *Advances in*

Title: NEON Algorithm Theoretical Basis Document (ATBD) – Dust and Particulate Size Distribution		Date: 03/28/2016
NEON Doc. #: NEON.DOC.002675	Author: D. Smith	Revision: A

Applied Science Research, 4(4), pp. 465-478.

TSI Incorporated (2014) DustTrak DRX aerosol monitor model 8533/8534/8533EP: operations and service manual. Revision L. pp. 85.

Wang, X.L., Chancellor, G., Evenstad, J., Farnsworth, J.E., Hase, A., Olsen, G.M., Sreenath, A., and Agarwal, J.K. (2009a) A novel optical instrument for estimating size segregated aerosol mass concentration in real time. *Aerosol Science and Technology*, 43(9), pp. 939-950.

Wang, X.L., Hase, A., Olson, G., Sreenath, A., and J. Agarwal. (2009b) Response of the DustTrak DRX to aerosols of different materials. AAAR 2009, Minneapolis [Online] Available: http://www.tsi.com/uploadedFiles/_Site_Root/Products/Literature/Posters/AAAR_2009_DRX_Poster.pdf [July, 2014].

Zhang, X., Turpin, B.J., McMurry, P.H., Hering, S.V., and M.R. Stolzenburg. (1994) Mie theory evaluation of species contributions to 1990 wintertime visibility reductions in the Grand Canyon. *Journal of Air and Waste Management Association*. 44, pp. 153-162.

9 CHANGELOG