NEON ALGORITHM THEORETICAL BASIS DOCUMENT (ATBD): HOMOGENEITY AND STATIONARITY

PREPARED BY	ORGANIZATION	DATE
Natchaya Pingintha-Durden	FIU	03/01/2014
Stefan Metzger	FIU	02/26/2014
Jeff Taylor	FIU	03/01/0214

APPROVALS	ORGANIZATION	APPROVAL DATE
Kate Thibault	SCI	05/26/2022

RELEASED BY	ORGANIZATION	RELEASE DATE
Tanisha Waters	CM	05/26/2022

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1 DESCRIPTION

The theoretical assumptions underlying the eddy-covariance (EC) technique can have far reaching implications, especially at sites located in non-homogenous terrain. For assuring the validity of NEON's ecosystem exchange data products (DPs), a dedicated quality assessment and quality control framework (the flux QA/QC) is used. This framework consists of various QA/QC analyses that are applied to NEON's ecosystem exchange DPs (AD[01] provides an overview). The present algorithm theoretical basis document (ATBD) details one of the QA/QC analyses, the testing of the time series for homogeneity and stationarity.

1.1 Purpose

Homogeneity and stationarity of the flow field is one of the flux QA/QC used to test on fulfillment of the theoretical requirements for EC measurements (AD[01]). This document describes the theoretical background and entire algorithmic process for homogeneity and stationarity test.

1.2 Scope

Information presented here relates to the homogeneity and stationarity test for the flux QA/QC. This document first introduces related documents (Sect. 2). Throughout Sects. 3–5, (i) all reported variables and input dependencies are identified, (ii) theoretical background is provided, and (iii) explicit algorithm descriptions are given. This document does not provide computational implementation details, except for cases where these stem directly from algorithmic choices explained here.

2 RELATED DOCUMENTS AND ACRONYMS

2.1 Applicable Documents

Applicable documents contain information that shall be applied in the current document. Examples are higher level requirements documents, standards, rules and regulations.

AD[01]	NEON.DOC.000573	FIU Plan for airshed QA/QC development
AD[02]	NEON.DOC.000823	Calculation of variances and covariance ATBD
AD[03]	NEON.DOC.000852	Terrestrial trace gas unit conversion ATBD
AD[04]	NEON.DOC.000465	Eddy-covariance turbulent exchange subsystem C^3
AD[05]	NEON.DOC.000807	Eddy-covariance turbulent exchange subsystem level 0 to level 1 data products ATBD
AD[06]	NEON.DOC.000853	Coordinate rotations ATBD
AD[07]	NEON.DOC.001044	Calculation of eddy-covariance momentum, heat, water vapor and carbon dioxide fluxes ATBD

2.2 Reference Documents

Reference documents contain information complementing, explaining, detailing, or otherwise supporting the information included in the current document.

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

2.3 External References

External references contain information pertinent to this document, but are not NEON configuration-controlled. Examples include manuals, brochures, technical notes, and external websites.

ER [01]	
ER [02]	
ER [03]	

2.4 Acronyms

Acronym	Description
ATBD	Algorithm Theoretical Basis Document
C^3	Command, control, and configuration document
CI	NEON Cyberinfrastructure project team
CO_2	Carbon dioxide
DP	Data Product
DPS	Data Products (NEON project team)
EC	Eddy covariance
EC-TES	Eddy-covariance turbulent exchange subsystem

F_{90}	Spatial extent containing 90% of the contributions to a measurement
H_2O	Water vapor
L0	Level 0
L1	Level 1
NA	Not available/not applicable
NEON	National Ecological Observatory Network
QA/QC	Quality Assurance/Quality Control
TIS	Terrestrial Instrument System

3 DESCRIPTION OF DATA PRODUCTS

3.1 Reported Variables

Table 1 details the variables reported by the algorithms disclosed in this ATBD.

Table 1. List of variables that are produced in this ATBD.

DP	Sample Frequency	Units	Data Product ID NEON.DOM.SIT.DPL.PRN.REV.SPN.SPR.TMR
Results for stationarity test according to Vickers and Mahrt (1997): $RES_{\mathrm{STA,1}}$			
Friction velocity ($RES_{\mathrm{STA,1,u_*}}$)	30 minute	percentage	The DPs ID will be updated and assigned later accordance with the other EC-TES documents.
Along and vertical wind covariance ($RES_{\mathrm{STA,1,\overline{u'w'}}}$)	30 minute	percentage	
Cross and vertical wind covariance ($RES_{\mathrm{STA,1,\overline{v'w'}}}$)	30 minute	percentage	
Vertical wind and air temperature covariance ($RES_{\mathrm{STA,1,}\overline{w'T'_{\mathrm{air}}}}$)	30 minute	percentage	
Vertical wind and H_2O dry mole fraction covariance ($RES_{\mathrm{STA,1,}\overline{w'FD'_{\mathrm{mole,H2O}}}}$)	30 minute	percentage	
Vertical wind and CO_2 dry mole fraction covariance ($RES_{\mathrm{STA,1,}\overline{w'FD'_{\mathrm{mole,CO2}}}}$)	30 minute	percentage	
Results for stationarity test according to Foken and Wichura (1997): $RES_{\mathrm{STA,2}}$			
Friction velocity ($RES_{\mathrm{STA,2,u_*}}$)	30 minute	percentage	
Along and vertical wind covariance ($RES_{\mathrm{STA,2,\overline{u'w'}}}$)	30 minute	percentage	
Cross and vertical wind covariance ($RES_{\mathrm{STA,2,\overline{v'w'}}}$)	30 minute	percentage	
Vertical wind and air temperature covariance ($RES_{\mathrm{STA,2,}\overline{w'T'_{\mathrm{air}}}}$)	30 minute	percentage	

Vertical wind and H_2O dry mole fraction covariance ($RES_{\mathrm{STA,2},\overline{w'FD'_{\mathrm{mole,H2O}}}}$)	30 minute	percentage	
Vertical wind and CO_2 dry mole fraction covariance ($RES_{\mathrm{STA,2},\overline{w'FD'_{\mathrm{mole,CO2}}}}$)	30 minute	percentage	

3.2 Input Variables

A summary of the inputs variables that required producing the output variables reported above are shown in **Table 2**.

Table 2. List of input variables that are used in this ATBD.

DP	Sample Frequency	Units	Data Product ID NEON.DOM.SIT.DPL.PRN.REV.SPN.SPR.TMR
Along-axis, cross-axis, and vertical axis wind components (u, v, w)	20 *Hz*	m s^{-1}	The DPs ID will be updated and assigned later accordance with the other EC-TES documents.
Sonic Temperature (T_{SONIC})	20 *Hz*	K	
H_2O dry mole fraction ($FD_{\mathrm{mole,H2O}}$)	20 *Hz*	kmole kmol e^{-1}	
CO_2 dry mole fraction ($FD_{\mathrm{mole,CO2}}$)	20 *Hz*	kmole kmol e^{-1}	
Along axis and vertical axis wind covariance ($\overline{u'w'}$)	30 min	(m s^{-1})^2	
Along axis and vertical axis wind covariance ($\overline{v'w'}$)	30 min	(m s^{-1})^2	
Vertical axis wind and H_2O dry mole fraction covariance ($\overline{w'FD'_{\mathrm{mole,H20}}}$)	30 min	kmole kmol e^{-1} m s^{-}	
Vertical axis wind and CO_2 dry mole fraction covariance ($\overline{w'FD'_{\mathrm{mole,CO2}}}$)	30 min	kmole kmol e^{-1} m s^{-}	
Vertical axis wind and air temperature covariance ($\overline{w'T'_{\mathrm{air}}}$)	30 min	K m s^{-1}	

3.3 Product Instances

All sites across the NEON observatory own a single individual instance of the reported variables in **Table 1**.

3.4 Temporal Resolution and Extent

The temporal resolution/extent of all reported variables in **Table 1** shall be similar to the fundamental averaging period of data products derived from the EC-TES, i.e. 30 min.

3.5 Spatial Resolution and Extent

The spatial resolution and extent of the variables reported in this ATBD is a function of several factors such as measurement height $d_{z,m}$, displacement height $d_{z,d}$, wind speed and wind direction, atmospheric stability and surface roughness. From dispersion modeling (e.g., Schmid, 1994, Vesala et al., 2008) it is found that ≈10 $(d_{z,m}-d_{z,d}) < d_{x,FP90} < 100 (d_{z,m}-d_{z,d})$, where $d_{x,FP90}$ is the cross-wind integrated upwind extent from within which 90% of a measured flux value is sourced.

4 SCIENTIFIC CONTEXT

4.1 Theory of Measurement/Observation

If environmental conditions yield a horizontally homogeneous flow field, horizontal (turbulent and advective) flux divergence terms are negligible in EC flux calculations (AD[01]). The validity of this condition is difficult to test, because EC is measured at a single point and does not provide spatial information. However Taylor's hypothesis (Taylor, 1915, Taylor, 1938), itself assuming homogeneity, suggests that turbulent eddies can be considered frozen as they are carried with the mean wind speed past a fixed point. This means that the measurement at a certain point as a function of the time gives a result similar to a spontaneous spatial measurement. This hypothesis is applied as a substitute for a true spatial measurement, and consequently the test of spatial homogeneity translates into a test of temporal stationarity at the measurement location (e.g., Foken and Wichura, 1996). Therefore, a process is said to be covariance-stationary if its first and second moments are time invariant.

Non-stationary conditions are typically indicated by changes in meteorological variables. Examples for typical causes are the diurnal radiation cycle, changes in weather patterns, significant mesoscale variability, or changes of the phase of atmospheric waves relative to the measuring point (Foken et al., 2004). The latter may occur because of source area variability, changing internal boundary layers (especially internal thermal boundary layers in the afternoon), or due to the presence of gravity waves (Foken et al., 2004). Several stationarity tests have been developed, and failure of these tests is interpreted as a violation in one or more of the assumptions of steady state, homogeneity, or the neglect of subsidence or convection. In such cases, the removal of respective terms in the flux calculations cannot be justified, and resultant fluxes must be interpreted with much care. Therefore, these tests provide an important measure of the overall suitability of when to apply the eddy-covariance method (AD[01]).

4.2 Theory of Algorithm

Stationarity in the first moment is tested by comparing the covariances of the original time series with the covariance of the detrended time series (Vickers and Mahrt, 1997):

$$RES_{\mathrm{STA,1}} = \left| \frac{\overline{X'Y'} - \overline{X'_{\mathrm{tr}}Y'_{\mathrm{tr}}}}{\overline{X'Y'}} \right| \cdot 100 \tag{1}$$

where: X is a wind component (u, v, w)

Y is a scalar quantity (CO_2, H_2O, temperature)

$\overline{X'Y'}$ is the covariance of the original time series over a time period t_{a}

$\overline{X'_{\mathrm{tr}}Y'_{\mathrm{tr}}}$ is the covariance of the detrended time series over a period t_{a}

In the case of detrending, the fluctuations are obtained by subtracting a signal (X_{t}) from a base state ($X_{\mathrm{base,t}}$) at time t, which is given by the linear regression line over the time period $t_{\mathrm{a}} = N\Delta t$,

$$X_{\mathrm{base,t}} = c_1 \cdot t + c_2, \tag{2}$$

where: c_1 is the regression slope
c_2 is the intercept
t is time

The regression slope and intercept are determined by applying the least-squares criterion:

$$c_1 = \frac{N\sum(tX_{\mathrm{t}}) - \sum t \sum X_{\mathrm{t}}}{N\sum(t^2) - (\sum t)^2}, \tag{3}$$

and

$$c_2 = \frac{\sum X_{\mathrm{t}} - c_1 \sum t}{N}, \tag{4}$$

where $t = i\Delta t$ and the summation is made over $i = 1, 2, \dots \dots .., N$ (Rannik and Vesala, 1999). The covariance of the detrended time series can be calculated as:

$$\overline{X'_{\mathrm{tr}}Y'_{\mathrm{tr}}} = \frac{1}{N-1}\sum_{i=1}^{N}\left(X_{\mathrm{t}} - X_{\mathrm{base,t}}\right)\cdot\left(Y_{\mathrm{t}} - Y_{\mathrm{base,t}}\right) \tag{5}$$

where: X_{t} is a wind component at time t

Y_{t} is a scalar quantity at time t

$X_{\mathrm{base,t}}$ is the instantaneous base state of wind components X at time t

$Y_{\mathrm{base,t}}$ is the instantaneous base state of scalar quantities Y at time t

Stationarity in the second moment is tested by comparing the covariances determined for the averaging period ($\overline{X'Y'}$) and for shorter intervals ($\overline{X'Y'}_S$) within this period (Foken and Wichura, 1996). For example, the time series for the determination of the covariance of the measured signals X and scalar Y over period t_a (i.e. 30 minutes duration) will be divided into short S intervals. The sample covariances of x and scalar y for each of the short intervals ($j = 1, 2, \dots \dots .., S$) are computed as:

$$\left(\overline{X'Y'}\right)_j = \frac{1}{M-1}\sum_{k=1}^{M}\left(X_{\mathrm{k}} - \overline{X}_j\right)\cdot\left(Y_{\mathrm{k}} - \overline{Y}_j\right) \tag{6}$$

where: M is the number of measurement points in the short interval (i.e. if a 30 min averaging period is divided into S = 6 intervals, M = 6,000 for 20 Hz data acquisition frequency over a 5 minute interval)

S is the number of short interval over averaging period

$\overline{X}_j$ is the mean of the wind component over j interval

$\overline{Y}_j$ is the mean of the scalar quantity over j interval

Then the covariances for shorter intervals have to be averaged over the dataset as:

$$\overline{X'Y'}_S = \frac{1}{S}\sum_{j=1}^{S}\left(\overline{X'Y'}\right)_j. \tag{7}$$

Finally, the result is compared to the covariances computed for the whole period:

$$RES_{\mathrm{STA,2}} = \left|\frac{\overline{X'Y'} - \overline{X'Y'}_S}{\overline{X'Y'}}\right| \cdot 100. \tag{8}$$

4.3 Special Considerations

Meteorological measurements fulfill stationary conditions only roughly for typical averaging periods up to one hour. Because of differing source areas and strength of stationarity, Eqs. (1) – (8) must be evaluated individually for each quantity under consideration (Table 3). Per the current design, there is no measurement of air temperature at high frequency (20 Hz). A conversion of sonic temperature shall be applied according to AD[02] to yield means, variances and, covariances of air temperature.

Table 3. Homogeneity / stationarity test for the different quantities.

Homogeneity / stationarity test	$\mathbf{u}_*$	Wind component covariances		Temperature	H_2O	CO_2
$RES_{\mathrm{STA,1}}$	$\left(\overline{u'w'}^2 + \overline{v'w'}^2\right)^{\frac{1}{4}}$	$\overline{u'w'}$	$\overline{v'w'}$	$\overline{w'T'_{\mathrm{air}}}$	$\overline{w'FD'}_{\mathrm{mole,H2O}}$	$\overline{w'FD'}_{\mathrm{mole,CO2}}$
$RES_{\mathrm{STA,2}}$	$\left(\overline{u'w'}^2 + \overline{v'w'}^2\right)^{\frac{1}{4}}$	$\overline{u'w'}$	$\overline{v'w'}$	$\overline{w'T'_{\mathrm{air}}}$	$\overline{w'FD'}_{\mathrm{mole,H2O}}$	$\overline{w'FD'}_{\mathrm{mole,CO2}}$

The results from this ATBD will be combined with other QA/QC metrics, flags for sensor operation, and statistical QA/QC, resulting in a final quality metric for each flux datum as detailed in AD[01].

5 ALGORITHM IMPLEMENTATION

The implementation of Eqs. (1) – (8) results in the reported variables in Table 1, and is realized in the following order. Note that the overall EC data processing sequence is outlined in AD[01], and details are provided in AD[02]–AD[07]. In particular, the general algorithmic implementation provided in AD[07] is required for producing the output variables reported in this ATBD.

1. The 20 *Hz* instantaneous base state ($X_{\mathrm{base,t}}$ and $Y_{\mathrm{base,t}}$) for each wind component (u, v, and w) and scalar (T_{SONIC}, $FD_{\mathrm{mole,H20}}$, and $FD_{\mathrm{mole,CO2}}$), shall be determined by the linear best fit over the period t_{a} (period in this ATBD depends on averaging period defined in AD[02], which is 30 minutes) accoding to Eq. (2) to Eq. (4).
2. The covariance of the detrended time series of different quantities in Table 3 shall be calculated according to Eq. (5).
3. Stationarity tests according to Vickers and Mahrt (1997) for the different quantities in Table 3 shall be determined according to Eq. (1).
4. The covariances of quantities detailed in Table 3 for every one of the S intervals over period t_{a} shall be computed according to Eq. (6).
5. The covariances of the S intervals resulting from step 4 shall be averaged over period t_{a} according to Eq. (7).
6. Stationarity tests according to Foken and Wichura (1996) for different quantities in Table 3 shall be determined according to Eq. (8).

6 ALGORITHM VERIFICATION

The algorithms specified in Sect. 4.2, and implemented by CI shall be verified against those algorithms written and used by FIU in the course of developing the present ATBD. For this purpose both algorithms shall be evaluated using the site depiction data as outlined in AD[01]. During subsequent comparisons, the maximum deviation resulting from algorithmic differences shall not exceed 1% for all L1 DPs in **Table 1**.

7 UNCERTAINTY

N/A

8 FUTURE PLANS AND MODIFICATIONS

This ATBD will be version controlled, i.e. future developments might results in modifications to this ATBD, which will be documented accordingly.

9 BIBLIOGRAPHY

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APPENDIX A FUNCTIONS, PARAMETERS, AND SUBSCRIPTS

Table 4. Functions

Function	Description
$\overline{X}$	Short-term (i.e., 5 and 30 min) arithmetic mean of atmospheric quantity *X*
$\overline{Y}$	Short-term (i.e., 5 and 30 min) arithmetic mean of atmospheric quantity *Y*
$\overline{X'Y'}$	Short-term (i.e., 5 and 30 min) sample covariance of atmospheric quantities *X* and *Y*

Table 5. Subscripts

Subscript	Description
air	Air (sum of dry air and water vapor)
CO2	Carbon dioxide
H2O	Water vapor
i	Running index
j	Running index
k	Running index
SONIC	Sonic anemometer/thermometer
STA	Stationarity test
t	Time
tr	Detrending sample
u_*	Friction velocity
X	Scalar quantity
Y	Scalar quantity

Table 6. Variables

Variable	Description	Units
d	Distance/length/height	m
$d_{\mathrm{x,FP90}}$	Cross-wind integrated upwind extent from within which 90% of an observed value is sourced	m
$d_{\mathrm{z,0}}$	Roughness length	m
$d_{\mathrm{z,d}}$	Displacement height	m
$d_{\mathrm{z,m}}$	Measurement height	m
FD_{mole}	Dry mole fraction	$\mathrm{kmole\ kmole^{-1}}$
i, j, k	Running index	Dimensionless (count)
$RES_{\mathrm{STA,1}}$	Stationarity test according to Vickers and Mahrt (1997)	Percentage
$RES_{\mathrm{STA,2}}$	Stationarity test according to Foken and Wichura (1996)	Percentage
t	Time	s
t_{a}	Averaging period	Hours (h)

T	Absolute temperature	K
u, v, w	Along-, cross- and vertical wind speed	m s^{-1}
u_*	Friction velocity	m s^{-1}
X	Scalar quantity	Depending on unit of atmospheric quantity
X_{base}	Instantaneous base state of scalar quantities	Depending on unit of atmospheric quantity
Y	Scalar quantity	Depending on unit of atmospheric quantity
Y_{base}	Instantaneous base state of scalar quantities	Depending on unit of atmospheric quantity