NEON Algorithm Theoretical Basis Document

Terrestrial trace gas unit conversions

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1 DESCRIPTION

NEON shall measure the exchange of energy and trace gases between the earth's surface and the atmosphere. To accomplish this, NEON will operate an eddy covariance turbulent exchange subsystem (EC-TES, a summary of all notation is provided in Sect. 10), which collectively embodies a suite of sensors.

1.1 Purpose

This document describes the theoretical background and entire algorithmic process for converting the trace gas units associated with the EC-TES. The present ATBD serves to summarize all relevant trace gas unit conversions (TGUC) that will be used during the implementation of AD[02].

1.2 Scope

This ATBD is embedded in a suite of 29 existing and upcoming NEON documents, which collectively describe the acquisition, processing and quality control of data from the EC-TES (AD[02] provides an overview). As such, the scope of this ATBD is to provide all necessary processing steps between immediately preceding and succeeding documents. This document first introduces related documents, acronyms and conventions (Sect. 2). Throughout Sects. 3–7, (i) all reported variables and input dependencies are identified, (ii) theoretical background is introduced, (iii) explicit conversion algorithms are provided, (iv) uncertainty budgets are established for each reported variable, and (v) verification tests are outlined. This document does not provide computational implementation details, except for cases where these stem directly from algorithmic choices explained here.

2 RELATED DOCUMENTS

2.1 Applicable documents

AD[01]	NEON.DOC.000465	Eddy Covariance Turbulent Exchange Subsystem C^3
AD[02]	NEON.DOC.000573	FIU Plan for airshed QA/QC development
AD[03]	NEON.DOC.000785	Plan for TIS Level 1 data products uncertainty budget estimation
AD[04]	NEON.DOC.000848	NEON science commissioning and validation plan

2.2 Reference documents

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

2.3 Verb convention

"Shall" is used whenever a specification expresses a provision that is binding. The verbs "should" and "may" express non-mandatory provisions. "Will" is used to express a declaration of purpose on the part of the design activity.

3 DESCRIPTION OF VARIABLES

The algorithms in this ATBD provide generic processing steps between immediately preceding and succeeding ATBDs in a suite of NEON documents related to the EC-TES (Sect. 1.2, AD[02]). In general, the input variables of this ATBD are generated in preceding EC-TES-related documents, and the reported variables are used in succeeding documents. Which of these variables will be mapped to NEON data products (DP), as well as their corresponding IDs will be defined in succeeding documents, and are not provided in this ATBD.

3.1 Reported variables

Table 1 details the variables reported by the algorithms disclosed in this ATBD. Molar/mass density refers to the number of molecules/mass of a trace gas per volume of air (incl. water vapor). Dry mole/mass fraction refers to the number of molecules/mass of a trace gas per number of molecules/mass of dry air (excl. water vapor). Wet mole/mass fraction refers to the number of molecules/mass of a trace gas per number of molecules/mass of air (incl. water vapor).

Table 1. List of variables that are produced in this ATBD. This ATBD provides generic algorithms for the conversion of trace gas units, which are not related to particular DP IDs. Hence DP IDs are not applicable.

Variable	**Units**
Dew point temperature (T_{H2Omax})	K
Partial pressure (p_{X})	$\mathrm{Pa} \equiv \mathrm{kg\ m^{-1}\ s^{-2}}$
Saturation water vapor pressure (p_{H2Omax})	$\mathrm{Pa} \equiv \mathrm{kg\ m^{-1}\ s^{-2}}$
Relative humidity (RH)	$\mathrm{Pa\ Pa^{-1}} \cdot 100 \equiv \%$
Molar density (ρ_{mole})	$\mathrm{kmole\ m^{-3}}$
Mass density (ρ_{mass})	$\mathrm{kg\ m^{-3}}$
Dry mole fraction (FD_{mole})	$\mathrm{kmole\ kmole^{-1}}$
Wet mole fraction (FW_{mole})	$\mathrm{kmole\ kmole^{-1}}$
Dry mass fraction (FD_{mass})	$\mathrm{kg\ kg^{-1}}$
Wet mass fraction (FW_{mass})	$\mathrm{kg\ kg^{-1}}$

3.2 Input variables

Table 2 lists all input variables that are used to produce the output variables reported above.

Table 2. List of input variables that are used in this ATBD. This ATBD provides generic algorithms for the conversion of trace gas units, which are not related to particular DP IDs. Hence DP IDs are not applicable.

Variable	**Units**
Absolute air temperature (T_{air})	K
Air pressure (p_{air})	$\mathrm{Pa} \equiv \mathrm{kg\ m^{-1}\ s^{-2}}$
Dew point temperature (T_{H2O})	K
Partial pressure (p_{X})	$\mathrm{Pa} \equiv \mathrm{kg\ m^{-1}\ s^{-2}}$

Variable	**Units**
Saturation water vapor pressure (p_{H2Omax})	Pa ≡ kg m^{-1} s^{-2}
Relative humidity (*RH*)	%
Molar density (ρ_{mole})	kmole m^{-3}
Mass density (ρ_{mass})	kg m^{-3}
Dry mole fraction (FD_{mole})	kmole kmole^{-1}
Wet mole fraction (FW_{mole})	kmole kmole^{-1}
Dry mass fraction (FD_{mass})	kg kg^{-1}
Wet mass fraction (FW_{mass})	kg kg^{-1}

4 SCIENTIFIC CONTEXT

A variety of trace gas units are used during the calculation of the exchange of energy and matter between the earth's surface and the atmosphere from turbulence observations.

4.1 Theory of algorithm

The majority of the trace gas units derived in this ATBD are based on the ideal gas law;

$$p_{\mathrm{X}} = \rho_{\mathrm{mole,X}}\, R\, T_{\mathrm{air}}, \tag{1}$$

where p_{X} is the partial pressure of gas X, $\rho_{\mathrm{mole,X}}$ is its molar density, R is the universal gas constant, and T_{air} is the air temperature. Mass density $\rho_{\mathrm{mass,X}}$ and molar density $\rho_{\mathrm{mole,X}}$ are related by the molar mass M_{X} of gas X;

$$\rho_{\mathrm{mass,X}} = \rho_{\mathrm{mole,X}}\, M_{\mathrm{X}}. \tag{2}$$

To distinguish, e.g. between ambient air (including water vapor) and dry air as denominator of trace gas units, Dalton's law of partial pressures is used;

$$p_{\mathrm{air}} = p_{\mathrm{dry}} + p_{\mathrm{H2O}}, \tag{3}$$

with the partial pressures of dry air p_{dry} and water vapor p_{H2O}. Moreover, in the special case of water vapor, the dew point temperature T_{H2O} is also used as a measure of concentration. The partial pressure of water vapor p_{H2O} is related to T_{H2O} through the Clausius-Clapeyron relation, which requires knowledge of the latent heat of condensation. The latent heat of condensation is taken into account, herein, by using the parameterization for water vapor pressure by Buck (1981);

$$p_{\mathrm{H2O}} = Y\, c_1\, e^{\left(\frac{c_2\,(T_{\mathrm{H2O}}+T_{\mathrm{zero}})}{c_3+T_{\mathrm{H2O}}+T_{\mathrm{zero}}}\right)}, \tag{4}$$

with the enhancement factor $Y = 1 + c_4 + c_5\, p_{\mathrm{air}}$, the coefficients c_1–c_5 in Table 3 (which are different over water and over ice), and the absolute zero temperature, T_{zero}. Within the specified ranges, the maximum deviation of this parameterization from the Clausius-Clapeyron relation is insignificant (≤0.5‰), and not further considered in Sect. 6.

Table 3. Coefficients for relation of water vapor pressure and temperature according to Buck (1981).

Coefficient	**Temperature range**	c_1	c_2	c_3	c_4	c_5
Over ice	223.15–273.15 K	611.15	22.452	272.55	$3 \cdot 10^{-4}$	$4.18 \cdot 10^{-8}$
Over water	273.15–323.15 K	611.21	17.368	238.88	$7 \cdot 10^{-4}$	$3.46 \cdot 10^{-8}$

5 ALGORITHM IMPLEMENTATION

Eq. (1)–(4) are combined and recast in order to enable (i) converting from any trace gas unit (Sect. 3) into partial pressure (Table 4), and (ii) converting from partial pressure into any trace gas unit (Table 5). In the cases of molar/mass fractions the algorithms apply to water vapor and other air constituents differently, and are marked accordingly. The difference originates from the definition of the denominators in the molar/mass fractions, which explicitly exclude or include the water vapor fraction (i.e. dry vs. wet). In the special case of water vapor, the following synonyms are commonplace; mass density ≡ absolute humidity, dry mole fraction ≡ molar mixing ratio, dry mass fraction ≡ mass mixing ratio, wet mass fraction ≡ specific humidity.

Table 4. Conversion to partial pressure from;

Convert from	**Algorithm**	**Eq.**
Dew point temperature (T_{H2O})	$p_{\mathrm{H2O}} = Y\, c_1\, e^{\left(\frac{c_2\,(T_{\mathrm{H2O}}+T_{\mathrm{zero}})}{c_3+T_{\mathrm{H2O}}+T_{\mathrm{zero}}}\right)}$	(5)
Air temperature (T_{air})	$p_{\mathrm{H2Omax}} = Y\, c_1\, e^{\left(\frac{c_2\,(T_{\mathrm{air}}+T_{\mathrm{zero}})}{c_3+T_{\mathrm{air}}+T_{\mathrm{zero}}}\right)}$	(6)
Relative humidity (RH)	$p_{\mathrm{H2O}} = \frac{p_{\mathrm{H2Omax}}\, RH}{100}$	(7)
Molar density (ρ_{mole})	$p_{\mathrm{X}} = \rho_{\mathrm{mole,X}}\, R\, T_{\mathrm{air}}$	(8)
Mass density (ρ_{mass})	$p_{\mathrm{X}} = \frac{\rho_{\mathrm{mass,X}}}{M_{\mathrm{X}}}\, R\, T_{\mathrm{air}}$	(9)
Dry mole fraction (FD_{mole})	$p_{\mathrm{H2O}} = \frac{p_{\mathrm{air}}\, FD_{\mathrm{mole,H2O}}}{1+FD_{\mathrm{mole,H2O}}}$ (water vapor), $p_{\mathrm{X}} = FD_{\mathrm{mole,X}}\,(p_{\mathrm{air}} - p_{\mathrm{H2O}})$ (other air constituents)	(10) (11)
Wet mole fraction (FW_{mole})	$p_{\mathrm{X}} = FW_{\mathrm{mole,X}}\, p_{\mathrm{air}}$	(12)
Dry mass fraction (FD_{mass})	$p_{\mathrm{H2O}} = \frac{p_{\mathrm{air}}\, FD_{\mathrm{mass,H2O}}}{\varepsilon+FD_{\mathrm{mass,H2O}}}$ (water vapor), $p_{\mathrm{X}} = \frac{M_{\mathrm{dry}}}{M_{\mathrm{X}}}\, FD_{\mathrm{mass,X}}\,(p_{\mathrm{air}} - p_{\mathrm{H2O}})$ (all air constituents)	(13) (14)
Wet mass fraction (FW_{mass})	$p_{\mathrm{H2O}} = \frac{p_{\mathrm{air}}}{1+\frac{\varepsilon}{FW_{\mathrm{mass,H2O}}}-\varepsilon}$ (water vapor), $p_{\mathrm{X}} = FW_{mass,\mathrm{X}} \frac{p_{\mathrm{H2O}}\, M_{\mathrm{H2O}}+(p_{\mathrm{air}}-p_{\mathrm{H2O}})\, M_{\mathrm{dry}}}{M_{\mathrm{X}}}$ (all air constituents)	(15) (16)

Table 5. Conversion from partial pressure to;

Convert to	**Algorithm**	**Eq.**
Dew point temperature (T_{H2O})	$T_{\mathrm{H2O}} = \frac{c_3 \ln(\frac{p_{\mathrm{H2O}}}{Y\, c_1})}{c_2 - \ln(\frac{p_{\mathrm{H2O}}}{Y\, c_1})} - T_{\mathrm{zero}}$	(17)
Air temperature (T_{air})	$T_{\mathrm{air}} = \frac{c_3 \ln(\frac{p_{\mathrm{H2Omax}}}{Y\, c_1})}{c_2 - \ln(\frac{p_{\mathrm{H2Omax}}}{Y\, c_1})} - T_{\mathrm{zero}}$	(18)

Convert to	**Algorithm**	**Eq.**
Relative humidity (*RH*)	$RH = \frac{p_{\mathrm{H2O}}}{p_{\mathrm{H2Omax}}} 100$	(19)
Molar density (ρ_{mole})	$\rho_{\mathrm{mole,X}} = \frac{p_{\mathrm{X}}}{R\, T_{\mathrm{air}}}$	(20)
Mass density (ρ_{mass})	$\rho_{\mathrm{mass,X}} = \frac{p_{\mathrm{X}} M_{\mathrm{X}}}{R\, T_{\mathrm{air}}}$	(21)
Dry mole fraction (FD_{mole})	$FD_{\mathrm{mole,X}} = \frac{p_{\mathrm{X}}}{p_{\mathrm{air}} - p_{\mathrm{H2O}}}$	(22)
Wet mole fraction (FW_{mole})	$FW_{\mathrm{mole,X}} = \frac{p_{\mathrm{X}}}{p_{\mathrm{air}}}$	(23)
Dry mass fraction (FD_{mass})	$FD_{\mathrm{mass,H2O}} = \varepsilon \frac{p_{\mathrm{H2O}}}{p_{\mathrm{air}} - p_{\mathrm{H2O}}}$ (water vapor), $FD_{\mathrm{mass,X}} = \frac{M_{\mathrm{X}}}{M_{\mathrm{dry}}} \frac{p_{\mathrm{X}}}{(p_{\mathrm{air}} - p_{\mathrm{H2O}})}$ (all air constituents)	(24) (25)
Wet mass fraction (FW_{mass})	$FW_{\mathrm{mass,H2O}} = \varepsilon \frac{p_{\mathrm{H2O}}}{p_{\mathrm{air}} - (1-\varepsilon)\, p_{\mathrm{H2O}}}$ (water vapor), $FW_{\mathrm{mass,X}} = \frac{M_{\mathrm{X}}}{M_{\mathrm{dry}}} \frac{p_{\mathrm{X}}}{(p_{\mathrm{air}} - p_{\mathrm{H2O}}) + M_{\mathrm{H2O}} p_{\mathrm{H2O}}}$ (all air constituents)	(26) (27)

6 UNCERTAINTY

Uncertainty of measurement is inevitable (International Organization for Standardization, 1995, Taylor, 1997). It is imperative that uncertainties are identified and quantified to determine statistical interpretations about mean quantity and variance structure; both are needed to construct higher level data products (i.e., L1 DP, etc.) and to model processes. This portion of the document serves to identify, evaluate, and quantify sources of uncertainty relating to L1 DPs associated with TGUC. It is a reflection of the information described in AD[03], and is explicitly described for TGUC variables in the following sections.

6.1 Uncertainty of trace gas unit conversions

In the following, algorithms for the propagation of uncertainty into each of the reported variables are provided (Table 6). These uncertainty estimates are provided per-quantity. If several of these quantities are used in a calculation, it is required to: (i) combine Eqs. (5)–(27) appropriately, (ii) take the partial derivatives of the resulting function, and (iii) propagate individual, standard uncertainties into a combined uncertainty.

6.2 Combined Uncertainty

Here, the combined uncertainties U_c for each quantity are derived. **NOTE**: All derivations shall be computed by CI ($\#_{CI}$).

Table 6. Algorithms for the propagation of individual, standard uncertainties, *U*, through the TGUC Eqs. (5)–(27). The final result is a combined uncertainty U_c.

TGUC Eq.	Algorithm	Eq.
(5)	$U_{\mathrm{c}}(p_{\mathrm{H2O}}) = \left(\left(\frac{c_1\, c_2\, c_3 (1 \,+\, c_4 \,+\, c_5\, p_{\mathrm{air}})}{(c_3 + T_{\mathrm{H2O}} + T_{\mathrm{zero}})^2}\, e^{\left(\frac{c_2\,(T_{\mathrm{H2O}} + T_{\mathrm{zero}})}{c_3 + T_{\mathrm{H2O}} + T_{\mathrm{zero}}}\right)}\, U(T_{\mathrm{H2O}}) \right)^2 + \left(c_1 c_5\, e^{\left(\frac{c_2\,(T_{\mathrm{H2O}} + T_{\mathrm{zero}})}{c_3 + T_{\mathrm{H2O}} + T_{\mathrm{zero}}}\right)}\, U(p_{\mathrm{air}}) \right)^2 \right)^{\frac{1}{2}}$	(28)
(6)	$U_{\mathrm{c}}(p_{\mathrm{H2Omax}}) = \left(\left(\frac{c_1\, c_2\, c_3 (1 \,+\, c_4 \,+\, c_5\, p_{\mathrm{air}})}{(c_3 + T_{\mathrm{air}} + T_{\mathrm{zero}})^2}\, e^{\left(\frac{c_2\,(T_{\mathrm{air}} + T_{\mathrm{zero}})}{c_3 + T_{\mathrm{air}} + T_{\mathrm{zero}}}\right)}\, U(T_{\mathrm{air}}) \right)^2 + \left(c_1 c_5\, e^{\left(\frac{c_2\,(T_{\mathrm{air}} + T_{\mathrm{zero}})}{c_3 + T_{\mathrm{air}} + T_{\mathrm{zero}}}\right)}\, U\left(p_{\mathrm{air}}\right) \right)^2 \right)^{\frac{1}{2}}$	(29)
(7)	$U_{\mathrm{c}}(p_{\mathrm{H2O}}) = \left(\left(\frac{RH}{100}\, U(p_{\mathrm{H2Omax}}) \right)^2 + \left(\frac{p_{\mathrm{H2Omax}}}{100}\, U(RH) \right)^2 \right)^{\frac{1}{2}}$	(30)
(8)	$U_{\mathrm{c}}(p_{\mathrm{X}}) = \left(\left(R\, T_{\mathrm{air}}\, U(\rho_{\mathrm{mole,X}}) \right)^2 + \left(R\, \rho_{\mathrm{mole,X}}\, U(T_{\mathrm{air}}) \right)^2 \right)^{\frac{1}{2}}$	(31)
(9)	$U_{\mathrm{c}}(p_{\mathrm{X}}) = \left(\left(\frac{R}{M_{\mathrm{X}}} T_{\mathrm{air}}\, U(\rho_{\mathrm{mass,X}}) \right)^2 + \left(\frac{R}{M_{\mathrm{X}}} \rho_{\mathrm{mass,X}}\, U(T_{\mathrm{air}}) \right)^2 \right)^{\frac{1}{2}}$	(32)

TGUC Eq.	Algorithm	Eq.
(10)	$U_c(p_{\mathrm{H2O}}) = \left(\left(\frac{FD_{\mathrm{mole,H2O}}}{1 + FD_{\mathrm{mole,H2O}}} \, U(p_{\mathrm{air}}) \right)^2 + \left(\frac{p_{\mathrm{air}}}{\left(1 + FD_{\mathrm{mole,H2O}}\right)^2} \, U(FD_{\mathrm{mole,H2O}}) \right)^2 \right)^{\frac{1}{2}}$	(33)
(11)	$U_{\mathrm{c}}(p_{\mathrm{X}}) = \left(\left((p_{\mathrm{air}} - p_{\mathrm{H2O}}) \, U(FD_{\mathrm{mole,X}}) \right)^2 + \left(FD_{\mathrm{mole,X}} \, U(p_{\mathrm{air}}) \right)^2 + \left(-FD_{\mathrm{mole,X}} \, U(p_{\mathrm{H2O}}) \right)^2 \right)^{\frac{1}{2}}$	(34)
(12)	$U_{\mathrm{c}}(p_{\mathrm{X}}) = \left(\left(p_{\mathrm{air}} \, U(FW_{\mathrm{mole,X}}) \right)^2 + \left(FW_{\mathrm{mole,X}} \, U(p_{\mathrm{air}}) \right)^2 \right)^{\frac{1}{2}}$	(35)
(13)	$U_{\mathrm{c}}(p_{\mathrm{H2O}}) = \left(\left(\frac{FD_{\mathrm{mass,H2O}}}{\varepsilon + FD_{\mathrm{mass,H2O}}} \, U(p_{\mathrm{air}}) \right)^2 + \left(\frac{p_{\mathrm{air}} \, \varepsilon}{\left(\varepsilon + FD_{\mathrm{mass,H2O}}\right)^2} \, U(FD_{\mathrm{mass,H2O}}) \right)^2 \right)^{\frac{1}{2}}$	(36)
(14)	$U_{\mathrm{c}}(p_{\mathrm{X}}) = \left(\left(\varepsilon (p_{\mathrm{air}} - p_{\mathrm{H2O}}) \, U(FD_{\mathrm{mass,X}}) \right)^2 + \left(\varepsilon \, FD_{\mathrm{mass,X}} \, U(p_{\mathrm{air}}) \right)^2 + \left(-\varepsilon \, FD_{\mathrm{mass,X}} \, U(p_{\mathrm{H2O}}) \right)^2 \right)^{\frac{1}{2}}$	(37)
(15)	$U_{\mathrm{c}}(p_{\mathrm{H2O}}) = \left(\left(\frac{1}{1 + \frac{\varepsilon}{FW_{\mathrm{mass,H2O}}} - \varepsilon} \, U(p_{\mathrm{air}}) \right)^2 + \left(\frac{\frac{\varepsilon}{{FW_{\mathrm{mass,H2O}}}^2} \, p_{\mathrm{air}}}{\left(1 + \frac{\varepsilon}{FW_{\mathrm{mass,H2O}}} - \varepsilon\right)^2} \, U(FW_{\mathrm{mass,H2O}}) \right)^2 \right)^{\frac{1}{2}}$	(38)

TGUC Eq.	Algorithm	Eq.
(16)	$U_\mathrm{c}(p_\mathrm{X}) = \left(\left(\frac{p_\mathrm{H2O}\, M_\mathrm{H2O} + (p_\mathrm{air} - p_\mathrm{H2O})M_\mathrm{dry}}{M_\mathrm{X}}\, U(FW_\mathrm{mass,X})\right)^2 + \left(\frac{FW_\mathrm{mass,X}(M_\mathrm{H2O} - M_\mathrm{dry})}{M_\mathrm{X}}\, U(p_\mathrm{H2O})\right)^2 + \left(\frac{FW_\mathrm{mass,X}\, M_\mathrm{dry}}{M_\mathrm{X}}\, U(p_\mathrm{air})\right)^2\right)^{\frac{1}{2}}$	(39)
(17)	$U_\mathrm{c}(T_\mathrm{H2O}) = \left(\left(\frac{c_2\, c_3}{p_\mathrm{H2O}\left(c_2 - \ln\left(\frac{p_\mathrm{H2O}}{\mathrm{c}_1(1\, +\, c_4\, +\, c_5\, p_\mathrm{air})}\right)\right)^2}\, U(p_\mathrm{H2O})\right)^2 + \left(-\frac{c_2\, c_3}{c_1\left(c_2 - \ln\left(\frac{p_\mathrm{H2O}}{\mathrm{c}_1(1\, +\, c_4\, +\, c_5\, p_\mathrm{air})}\right)\right)^2}\, U(p_\mathrm{air})\right)^2\right)^{\frac{1}{2}}$	(40)
(18)	$U_\mathrm{c}(T_\mathrm{air}) = \left(\left(\frac{c_2\, c_3}{p_\mathrm{H2O}\left(c_2 - \ln\left(\frac{p_\mathrm{H2Omax}}{\mathrm{c}_1(1\, +\, c_4\, +\, c_5\, p_\mathrm{air})}\right)\right)^2}\, U(p_\mathrm{H2Omax})\right)^2 + \left(-\frac{c_2\, c_3}{c_1\left(c_2 - \ln\left(\frac{p_\mathrm{H2Omax}}{\mathrm{c}_1(1\, +\, c_4\, +\, c_5\, p_\mathrm{air})}\right)\right)^2}\, U(p_\mathrm{air})\right)^2\right)^{\frac{1}{2}}$	(41)
(19)	$U_\mathrm{c}(RH) = \left(\left(\frac{100}{p_\mathrm{H2Omax}}\, U(p_\mathrm{H2O})\right)^2 + \left(\frac{-100\, p_\mathrm{H2O}}{p_\mathrm{H2Omax}^2}\, U(p_\mathrm{H2Omax})\right)^2\right)^{\frac{1}{2}}$	(42)

TGUC Eq.	**Algorithm**	**Eq.**
(20)	$U_\mathrm{c}(\rho_\mathrm{mole,X}) = \left(\left(\frac{1}{R\,T_\mathrm{air}}\,U(p_\mathrm{X})\right)^2 + \left(-\frac{p_\mathrm{X}}{R\,T_\mathrm{air}^2}\,U(T_\mathrm{air})\right)^2\right)^{\frac{1}{2}}$	(43)
(21)	$U_\mathrm{c}(\rho_\mathrm{mass,X}) = \left(\left(\frac{M_\mathrm{X}}{R\,T_\mathrm{air}}\,U(p_\mathrm{X})\right)^2 + \left(-\frac{p_\mathrm{X}\,M_\mathrm{X}}{R\,T_\mathrm{air}^2}\,U(T_\mathrm{air})\right)^2\right)^{\frac{1}{2}}$	(44)
(22)	$U_\mathrm{c}(FD_\mathrm{mole,X}) = \left(\left(\frac{1}{p_\mathrm{air} - p_\mathrm{H2O}}\,U(p_\mathrm{X})\right)^2 + \left(-\frac{p_\mathrm{X}}{(p_\mathrm{air} - p_\mathrm{H2O})^2}\,U(p_\mathrm{air})\right)^2 + \left(\frac{p_\mathrm{X}}{(p_\mathrm{air} - p_\mathrm{H2O})^2}\,U(p_\mathrm{H2O})\right)^2\right)^{\frac{1}{2}}$	(45)
(23)	$U_\mathrm{c}(FW_\mathrm{mole,X}) = \left(\left(\frac{1}{p_\mathrm{air}}\,U(p_\mathrm{X})\right)^2 + \left(-\frac{p_\mathrm{X}}{p_\mathrm{air}^2}\,U(p_\mathrm{air})\right)^2\right)^{\frac{1}{2}}$	(46)
(24)	$U_\mathrm{c}(FD_\mathrm{mass,H2O}) = \left(\left(\frac{\varepsilon\,p_\mathrm{air}}{(p_\mathrm{air} - p_\mathrm{H2O})^2}\,U(p_\mathrm{H2O})\right)^2 + \left(-\frac{\varepsilon\,p_\mathrm{H2O}}{(p_\mathrm{air} - p_\mathrm{H2O})^2}\,U(p_\mathrm{air})\right)^2\right)^{\frac{1}{2}}$	(47)
(25)	$U_\mathrm{c}(FD_\mathrm{mass,X}) = \left(\left(\frac{M_\mathrm{X}}{M_\mathrm{dry}(p_\mathrm{air} - p_\mathrm{H2O})}\,U(p_\mathrm{X})\right)^2 + \left(-\frac{M_\mathrm{dry}\,M_\mathrm{X}\,p_\mathrm{X}}{\left(M_\mathrm{dry}(p_\mathrm{air} - p_\mathrm{H2O})\right)^2}\,U(p_\mathrm{air})\right)^2 + \left(\frac{M_\mathrm{dry}\,M_\mathrm{X}\,p_\mathrm{X}}{\left(M_\mathrm{dry}(p_\mathrm{air} - p_\mathrm{H2O})\right)^2}\,U(p_\mathrm{H2O})\right)^2\right)^{\frac{1}{2}}$	(48)
(26)	$U_\mathrm{c}(FW_\mathrm{mass,H2O}) = \left(\left(\frac{\varepsilon\,p_\mathrm{air}}{(p_\mathrm{air} - (1-\varepsilon)\,p_\mathrm{H2O})^2}\,U(p_\mathrm{H2O})\right)^2 + \left(\frac{\varepsilon\,p_\mathrm{H2O}}{(p_\mathrm{air} - (1-\varepsilon)\,p_\mathrm{H2O})^2}\,U(p_\mathrm{air})\right)^2\right)^{\frac{1}{2}}$	(49)

TGUC Eq.	**Algorithm**	**Eq.**
(27)	$U_{\mathrm{c}}(FW_{\mathrm{mass,X}}) = \left(\left(\frac{M_{\mathrm{X}}}{M_{\mathrm{dry}}(p_{\mathrm{air}} - p_{\mathrm{H2O}}) + M_{\mathrm{H2O}}p_{\mathrm{H2O}}} U(p_{\mathrm{X}})\right)^2 + \left(-\frac{M_{\mathrm{dry}}\, M_{\mathrm{X}}\, p_{\mathrm{X}}}{\left(M_{\mathrm{dry}}(p_{\mathrm{air}} - p_{\mathrm{H2O}}) + M_{\mathrm{H2O}}p_{\mathrm{H2O}}\right)^2} U(p_{\mathrm{air}})\right)^2 + \left(\frac{\left(M_{\mathrm{dry}} - M_{\mathrm{H2O}}\right) M_{\mathrm{X}}\, p_{\mathrm{X}}}{\left(M_{\mathrm{dry}}(p_{\mathrm{air}} - p_{\mathrm{H2O}}) + M_{\mathrm{H2O}}p_{\mathrm{H2O}}\right)^2} U(p_{\mathrm{H2O}})\right)^2\right)^{\frac{1}{2}}$	(50)

6.3 Expanded Uncertainty

The equation for effective degrees of freedom (*DF*DF_{eff}, AD[03]) will vary based on the variables that are being considered. For instance, DF_{eff} for calculating $FW_{\mathrm{mass,H2O}}$ will be different from that of $FW_{\mathrm{mass,X}}$, because the functions that are used to calculate them contain different terms. As an example, the effective degrees of freedom for aforementioned variables are calculated here, thus serving as a reference for the derivation of DF_{eff} for other variables (i.e. *RH*, T_{H2O}, T_{air}, *etc.*). The effective degree of freedom for $FW_{\mathrm{mass,H2O}}$ is:

$$DF_{\mathrm{eff}}(FW_{\mathrm{mass,H2O}}) = \frac{U^4(FW_{\mathrm{mass,H2O}})}{\frac{\left(\frac{\varepsilon\, p_{\mathrm{air}}}{(p_{\mathrm{air}} - (1-\varepsilon)\, p_{\mathrm{H2O}})^2} U(p_{\mathrm{H2O}})\right)^4}{DF(p_{\mathrm{H2O}})} + \frac{\left(\frac{\varepsilon\, p_{\mathrm{H2O}}}{(p_{\mathrm{air}} - (1-\varepsilon)\, p_{\mathrm{H2O}})^2} U(p_{\mathrm{air}})\right)^4}{DF(p_{\mathrm{air}})}} \qquad (51)$$

And that of $FD_{\mathrm{mass,X}}$ is:

$$DF_{\mathrm{eff}}(FD_{\mathrm{mass,X}}) = \frac{U^4(FD_{\mathrm{mass,X}})}{\frac{\left(\frac{M_{\mathrm{X}}}{M_{\mathrm{dry}}(p_{\mathrm{air}} - p_{\mathrm{H2O}}) + M_{\mathrm{H2O}}p_{\mathrm{H2O}}} U(p_{\mathrm{X}})\right)^4}{DF(p_{\mathrm{X}})} + \frac{\left(-\frac{M_{\mathrm{dry}}\, M_{\mathrm{X}}\, p_{\mathrm{X}}}{\left(M_{\mathrm{dry}}(p_{\mathrm{air}} - p_{\mathrm{H2O}}) + M_{\mathrm{H2O}}p_{\mathrm{H2O}}\right)^2} U(p_{\mathrm{air}})\right)^4}{DF(p_{\mathrm{air}})} + \frac{\left(\frac{(M_{\mathrm{dry}} -}{(M_{\mathrm{dry}}(p_{\mathrm{air}} - p}\right.}{}}$$

where DF represents the degrees of freedom for each variable. As atmospheric pressure p_{air} is measured at each site, $U(p_{\mathrm{air}})$ is derived from a Type A analysis, and its degrees of freedom, $DF(p_{\mathrm{air}})$, shall be $N-1$, where N is the number of observations made during the averaging period. This applies to all quantities that are directly measured at NEON sites. However, those that are not measured directly (e.g. p_{H2O}) are considered Type B analyses, and degrees of freedom from these shall always be 100 (refer to AD[03]). The effective degrees of freedom are used to determine the corresponding expansion factor (k) for a given level of confidence (95%, AD[03]). The expanded uncertainty can then be calculated at 95% confidence via Eq. (53)and (54) and with the aid of Table 5 of AD [11].

$$U_{95}(FW_{\mathrm{mass,H2O}}) = k_{95}\, U_c(FW_{\mathrm{mass,H2O}}) = \#_{CI}, \tag{53}$$

$$U_{95}(FW_{\mathrm{mass,X}}) = k_{95}\, U_c(FW_{\mathrm{mass,X}}) = \#_{CI}. \tag{54}$$

The resulting data product shall be displayed twice, once accompanied by a value of combined uncertainty, and again with an expanded uncertainty value. Effective degrees of freedom and the *coverage* factor (k) for each computed L1 DP will also be stored in the CI data store.

7 ALGORITHM VERIFICATION

Verification of the algorithms disclosed in this ATBD shall follow the procedures outlined in AD[04]. During the implementation of AD[02], DPs will be derived from the present algorithms, and DP verification and validation will be specified accordingly.

8 SCIENTIFIC AND EDUCATIONAL APPLICATIONS

The conversion of trace gas units is the basis for data processing of trace gas measurements into calibrated, quality-controlled, and observatory-vetted DPs with ecological relevance. The present ATBD details all TGUCs and uncertainty propagation related to instrument readings within the EC-TES. During the implementation of AD[02], data will continue to be processed into higher-level DPs. Ecologically relevant high-level DPs generated using inputs of the EC-TES include the exchange of heat, water vapor and CO_2 between the land surface and the atmosphere. These DPs are then used for constraining, calibrating and validating process-based land surface models (e.g., Rastetter et al., 2010). This shall enable the detection of continental scale ecological change and the forecasting of its impacts.

Standardized and transparent documentation intends to foster reproducibility of all data processing steps. For this purpose, it is planned to make all processing steps available as open-source code in a high-level programming language. Aside from enabling direct feedback from the research community, this also provides community members (e.g. students at graduate level) a straightforward and hands-on toolbox for data processing of micrometeorological measurements.

9 FUTURE PLANS AND MODIFICATIONS

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

10 APPENDIX

10.1 Acronyms

Acronym	**Description**
ATBD	Algorithm theoretical basis document
C^3	Command, control, and configuration document
CI	Cyberinfrastructure (NEON project team)
CO_2	Carbon dioxide
DP	Data product
EC	Eddy covariance
EC-TES	Eddy-covariance turbulent exchange subsystem
FIU	Fundamental instrument unit (NEON project team)
NEON	National Ecological Observatory Network
QA/QC	Quality Assurance/Quality Control
TGUC	Trace gas unit conversion
$\#_{CI}$	Value computed by CI with the algorithms provided in this document

10.2 Parameters

Parameter	**Description**	**Numeric value**	**Units**
c	Constant, coefficient	User-defined	User-defined
e	Euler's number	≈2.71828	Dimensionless

Parameter	**Description**	**Numeric value**	**Units**
ε	Ratio of molar masses	$M_{H2O}\, M_{dry}^{-1} = 0.62198$	Dimensionless (ratio)
M_{dry}	Molar mass of dry air	28.9645	kg $kmol^{-1}$
M_{H2O}	Molar mass of water vapor	18.0753	kg $kmol^{-1}$
M_X	Molar mass of air constituent	E.g., M_{CO2}=44.0095 (Carbon dioxide)	kg $kmol^{-1}$
N	Sample size	User-defined	Dimensionless (count)
R	Universal gas constant	8314.4621	J K^{-1} $kmol^{-1}$ ≡ kg m^2 s^{-2} K^{-1} $kmol^{-1}$
T_{zero}	Absolute zero temperature	−273.15	°C

10.3 Subscripts

Subscript	**Description**
0	Potential quantity, unless otherwise specified (i.e., under NIST (National Institute of Standards and Technology) standard conditions T_0 = 293.15 K, p_0 = 101.325 kPa
1…N	Numeric identifier
air	Air (sum of dry air and water vapor)
CO2	Carbon dioxide
dry	Dry air
eff	Effective
H2O	Water vapor

Subscript	Description
H2Omax	Saturation water vapor
i	Running index
X, Y	Placeholder for atmospheric quantities

10.4 Variables

Variable	Description	Units
DF	Degrees of freedom	Dimensionless (count)
FD_{mass}	Dry mass fraction	$\mathrm{kg\ kg^{-1}}$
FD_{mole}	Dry mole fraction	$\mathrm{kmol\ kmol^{-1}}$
FW_{mass}	Wet mass fraction	$\mathrm{kg\ kg^{-1}}$
FW_{mole}	Wet mole fraction	$\mathrm{kmol\ kmol^{-1}}$
k	Expansion factor	Dimensionless
p	Pressure	$\mathrm{Pa} \equiv \mathrm{kg\ m^{-1}\ s^{-2}}$
ρ_{mass}	Mass density	$\mathrm{kg\ m^{-3}}$
ρ_{mole}	Molar density	$\mathrm{kmol\ m^{-3}}$
T	Absolute temperature	K
T_{H2O}	Dew point temperature	K
U	Standard uncertainty	Depending on unit of atmospheric quantity
U_{c}	Combined standard uncertainty	Depending on unit of atmospheric quantity

Variable	**Description**	**Units**
X, Y	Placeholder for atmospheric quantities	Depending on unit of atmospheric quantity

11 BIBLIOGRAPHY

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12 CHANGELOG

DATE	**CHANGE DESCRIPTION**	**AUTHOR**
05/28/2013	Initial release	S. Metzger