Documentation and Instruction Manual
of the Eddy Covariance Software Package
TK2

Matthias Mauder
Thomas Foken

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1 Introduction

The fact that micrometeorological measurements of energy exchange processes at the surface are often not able to close the energy balance (Foken and Oncley, 1995) motivated us to address the issue of quality assurance of these surface energy flux measurements. The methodology of determining turbulent heat fluxes with their corrections and quality tests is one key issue in this context. Therefore, in order to obtain quality assured turbulent fluxes, we at the University of Bayreuth developed the comprehensive software package TK2.

The software package TK2 is based on 15 years of experiences with the program ‘Turbulenzknecht’ which was developed to calculate turbulent fluxes automatically for several micrometeorological experiments since 1989. The first run time version of the program was used for the processing of the data from the boundary layer experiment ‘Bohunice 1989’ (Zelený and Foken, 1991) on a home computer of type KC87. The first PC version, called ‘UNIMESS’, was developed for the experiment ‘TARTEX-90’ (Foken, 1991), which made an online output for quality control purposes possible for the first time. In the following years the QA/QC functionality of the program was extended step by step. Until 1993 a program named ‘Turbulenzknecht’ was developed for processing of the eddy-covariance data, including a QA/QC concept which provides an output of quality flags for every calculated value of turbulent fluxes (Foken and Wichura, 1996). Further improvements regarding the input and output formats were realised until 1999 (Foken, 1999). At that time the program was designed to calculate quality controlled turbulent fluxes. No corrections were implemented in the program in that version. Additional programs were necessary, to perform any desired corrections.

To utilize the incredibly fast increasing possibilities of computer power and to cope with new scientific developments regarding the methodology of calculating turbulent fluxes, a new program was created. It is called TK2, which is an abbreviation of Turbulence Knight 2, which symbolizes the advancement from the German ‘Knecht’ to the English ‘Knight’. The version number 2 indicates the continuation of the first version of the Turbulenzknecht. TK2 is based on the experiences of the ‘Turbulenzknecht’ and uses the same QA/QC concept, but the source code of TK2 was totally redeveloped from scratch.

TK2 is capable of performing all of the post processing of turbulence measurements producing quality assured turbulent fluxes for a station automatically in one single run no matter, how many days or files have to be processed. It includes all corrections and tests, which are state of science (Lee et al., 2004). This report will give an instruction for the handling of the software package TK2. But before that an overview of the theoretical background to the post processing of turbulence measurements and the eddy covariance method will be given.
2 Calculation of turbulent fluxes obtained by the eddy covariance method

The only way to measure turbulent heat fluxes directly is the eddy covariance method. In general, turbulent fluxes are calculated as the covariance between the two high frequency time series of vertical wind velocity and a scalar, which can be temperature, humidity or any other trace gas, measured at the same point in space and time.

2.1 Plausibility tests of time series

2.1.1 Consistency limits

Physically or electronically not possible values can be excluded for the calculation of averages, variances and covariances. Values, which exceed certain thresholds, will not be used for later calculations. Recommended default settings for the consistency limits are listed in the following table (Table 1).

Table 1: Default settings for the consistency limits

<table>
<thead>
<tr>
<th>Measured variable</th>
<th>Lower limit</th>
<th>Upper limit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Day of year</td>
<td>0</td>
<td>366</td>
</tr>
<tr>
<td>Daily time</td>
<td>0</td>
<td>2400</td>
</tr>
<tr>
<td>Seconds</td>
<td>0</td>
<td>60</td>
</tr>
<tr>
<td>u-Wind</td>
<td>-50 m/s</td>
<td>+50 m/s</td>
</tr>
<tr>
<td>v-Wind</td>
<td>-50 m/s</td>
<td>+50 m/s</td>
</tr>
<tr>
<td>w-Wind</td>
<td>-10 m/s</td>
<td>+10 m/s</td>
</tr>
<tr>
<td>Sonic temperature</td>
<td>-20° C</td>
<td>50° C</td>
</tr>
<tr>
<td>Running number (CSAT code)</td>
<td>0</td>
<td>63</td>
</tr>
<tr>
<td>Platinum temperature</td>
<td>-20° C</td>
<td>50° C</td>
</tr>
<tr>
<td>CO₂ (e.g. LiCor 7500)</td>
<td>0 mV</td>
<td>5000 mV</td>
</tr>
<tr>
<td>H₂O (e.g. LiCor 7500)</td>
<td>0 mV</td>
<td>5000 mV</td>
</tr>
</tbody>
</table>

2.1.2 Spike detection

A spike detection algorithm is used. The algorithm follows the paper by Vickers and Mahrt (1997) based upon the paper by Højstrup (1993). We recommend that any values, which exceed 5.5 times standard deviations in a window of 10 values, are labelled as spikes. But if this spike criterion is
fulfilled by 4 or more values in a row, they will not be labelled as those. They are supposed to be ‘real’ in this case. Values, which are detected as spikes, can be excluded for later calculations or linearly interpolated.

2.2 Calculation of averages, variances and covariances

2.2.1 Maximization of covariances by cross correlation

There is the possibility that a time delay occurs between two time series, if two different instruments, e.g. a sonic anemometer for wind components and a gas analyser for water vapour. The time delay between the two sensors can be determined automatically by cross correlation analysis for each averaging interval. This method is able to find the maximum value of the covariance, which is supposed to be the ‘real’ value. At the same as we correct for the time delay between two time series we correct for the time, which it takes for an eddy to get from one sensor to the other, i.e. sensor separation in longitudinal wind direction (Moore, 1986). Note that for the remaining correction of the lateral separation the angle between the separated sensor and the wind direction has to be known.

2.2.2 Treatment of missing values

Although it is desirable to avoid missing values in a time series of turbulence measurements, it will always happen that due to malfunction of the instruments or errors in the data collections system a few measurements are missing from time to time. Additionally values of a time series are excluded because of the given consistency limits or the spike detection criteria. There are basically two options how to treat these missing values. They can be marked as missing values (NaN) and are excluded for later calculations. The time series will be shorter by the number of missing values in this case. This can be a good method for calculating statistical parameters like variances and covariances. But for spectral analysis data gaps are not allowed. In this case missing values have to be interpolated, e.g. by taking the last measured value or linear interpolation. TK2 two allows both methods according to requirements. In any case it is important, that the proportion of real measurements in the time series is big enough to be representative. We recommend at least 90 % real measurements. This threshold also can be user-defined.

2.2.3 Combination of short statistical moments to longer averaging intervals

Some data acquisition systems are not capable to collect high frequency raw data of turbulence measurements. Instead they store online averages, variance and covariances of a certain averaging interval. As the calculation of variances and covariances is a nonlinear process, they must not be arithmetically averaged to longer intervals. TK2 allows combining shorter averaging intervals of maybe 5 or 10 minutes to longer intervals of 30 minutes or even longer if desired. It is of course also possible to use a dataset of 30 minute intervals as input. But this is not recommended, because the 5 minute intervals are required for the steady state test (see 3.1).

Formerly calculated (co)variances \( \left( \langle w'x' \rangle \right)_j \) and means values for short-term intervals \( j \) with \( U \) measurements can be combined in order to calculate the (co)variance for the long-term interval \( I \).
comprising $M = N \cdot U$ values \cite{Foken, 1999 #35}:

$$
\bar{w} = \frac{1}{M-1} \left[ (U-1) \sum_{j=1}^{N} (\bar{w} x_j) + U \sum_{j=1}^{N} \bar{w} \cdot \bar{x}_j - \frac{U^2}{M} \sum_{j=1}^{N} \bar{w} \sum_{j=1}^{N} \bar{x}_j \right]
$$  \hspace{1cm} (1)

The right hand side of equation (2) can be rewritten as follows:

$$
\frac{1}{M-1} \left[ (U-1) \sum_{j=1}^{N} (\bar{w} x_j) + U \sum_{j=1}^{N} \bar{w} \cdot \bar{x}_j - \frac{U^2}{M} \sum_{j=1}^{N} \bar{w} \sum_{j=1}^{N} \bar{x}_j \right] = 
$$

$$
= \frac{1}{M-1} \left[ (U-1) \sum_{j=1}^{N} (\bar{w} x_j) + U \sum_{j=1}^{N} \bar{w} \cdot \bar{x}_j - \frac{U}{M} \sum_{j=1}^{N} \bar{w} \sum_{j=1}^{N} \bar{x}_j \right] = 
$$

$$
= \frac{1}{M-1} \left[ (U-1) \sum_{j=1}^{N} (\bar{w} x_j) + U \sum_{j=1}^{N} \bar{w} \cdot \bar{x}_j - \frac{1}{N} \sum_{j=1}^{N} \bar{w} \sum_{j=1}^{N} \bar{x}_j \right]
$$  \hspace{1cm} (2)

The second addend on the third line in equation (3) can be replaced in an analogous manner as in equation (1) yielding (4):

$$
\bar{w} = \frac{1}{M-1} \left\{ (U-1) \sum_{j=1}^{N} (\bar{w} x_j) + U \sum_{j=1}^{N} \left[ (\bar{w}_j - \bar{w}) \cdot (\bar{x}_j - \bar{x}) \right] \right\},
$$  \hspace{1cm} (3)

where

$\bar{w}, \bar{x}$ mean values for long-term interval $I$.

If $U$ varies with interval $j$ equation (4) must be written as (5):

$$
\bar{w} = \frac{1}{M-1} \left\{ \sum_{j=1}^{N} \left( \bar{w}_j U_j - 1 \right) \left( \bar{w} x_j \right) + \sum_{j=1}^{N} \bar{w}_j \cdot \left( \bar{w}_j - \bar{w} \right) \cdot \left( \bar{x}_j - \bar{x} \right) \right\},
$$  \hspace{1cm} (4)

where

$$
M = \sum_{j=1}^{N} \bar{w}_j U_j
$$

$\bar{w}_j U_j$ number of valid data contributing to $\left( \bar{w} x_j \right)$.

### 2.3 Corrections of the fluxes

Inherent to these atmospheric measurements are deficiencies which cause more or less important violations of assumptions to the underlying theory. So, a set of corrections to the calculated covariances is necessary.

#### 2.3.1 Cross wind correction of the sonic temperature

The cross wind correction follows Kaimal and Finnigan \cite{1994} with the specification for different sonic types by Liu et al. \cite{2001}. This correction is related to sonic anemometer coordinate system
and should therefore be applied before any other correction of the measured data. In this paper it is not mentioned that for some types of sonic anemometers a cross wind correction is already done internally. Therefore it would be redundant for these to apply a cross wind correction during the data post processing.

A cross wind correction is implemented for the following sensors:
- Campbell CSAT3
- Gill Solent HS and R3
- NCAR’s NUW Sonic
- Young 81000
- and METEK USA-1 if use of the flux “hf”

A cross wind correction must be applied during post processing for:
- Gill Solent R2
- ATI K-Probe
- METEK USA-1 if covariance calculated from high frequency raw data or use of the covariance “zTcov”

Equations after by Liu et al. (2001)

\[
\sigma_{r_c}^2 = \sigma_{r_n}^2 - \frac{4T^2}{(c^2)} \left( u^2 A^2 + v^2 B^2 + 2u'v'uvAB \right) + \frac{4T}{c^2} \left( u'T'uuA + v'T'vB \right) + \frac{2.04T}{c^2} \left( u'q'uA + v'q'vB \right) \tag{5}
\]

\[
\frac{w'T_c}{w'T} = \frac{w'T}{w'T} + \frac{2T}{c^2} \left( w'u'uA + w'v'vB \right) \tag{6}
\]

Table 2: Coefficients for cross wind correction after Liu et al. (2001)

<table>
<thead>
<tr>
<th>Factors</th>
<th>CSAT3</th>
<th>USA-1</th>
<th>Solent R3,R3A,HS</th>
<th>Solent R2</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>7/8</td>
<td>¾</td>
<td>1 – 2 cos² ( \varphi )</td>
<td>½</td>
</tr>
<tr>
<td>B</td>
<td>7/8</td>
<td>¾</td>
<td>1 – 2 cos² ( \varphi )</td>
<td>½</td>
</tr>
</tbody>
</table>

2.3.2 Coordinate rotation

A wind vector can be transformed from the sonic anemometer coordinate system (index \( m \)) into any other desired coordinate system by matrix multiplication with a rotation matrix \( A \).

\[
\begin{bmatrix}
  u_m \\
  v_m \\
  w_m
\end{bmatrix} = A \begin{bmatrix}
  u \\
  v \\
  w
\end{bmatrix}
\tag{7}
\]

In a 3-dimensional coordinate system the full coordinate transformation can be divided into three rotations around the three axes of the coordinate system \( x, y, z \) (Figure 1). These rotations can be described by three rotation matrices \( B, C, D \) and three angles \( \gamma, \beta, \alpha \).
\[ A = BCD, \]  

where

\[
B = \begin{bmatrix}
\cos \gamma & -\sin \gamma & 0 \\
\sin \gamma & \cos \gamma & 0 \\
0 & 0 & 1 \\
\end{bmatrix},
\]

\[
C = \begin{bmatrix}
1 & 0 & 0 \\
0 & \cos \beta & -\sin \beta \\
0 & \sin \beta & \cos \beta \\
\end{bmatrix},
\]

\[
D = \begin{bmatrix}
\cos \alpha & 0 & \sin \alpha \\
0 & 1 & 0 \\
-\sin \alpha & 0 & \cos \alpha \\
\end{bmatrix}.
\]

Figure 1: Definition of rotation angles after Wilczak et al. (2001)

There are basically two different methods to determine the rotation angles. Both methods intend to nullify the vertical wind velocity \( w \), but on a different time scale.

**Planar Fit Method**

The Planar Fit method after Wilczak et al. (2001) results in \( w \)-value of zero averaged over the whole
data set. This can be of different length. On the one hand it has to be guaranteed that the position of
the sonic anemometer is not moved in this period to have constant conditions for the determination
of the regression plane. On the other hand it is of advantage to cover a wide range of wind
directions, to have a large diversity of points to fit the plane. According to experience a set of five
days of turbulence data is long enough in many cases. Under certain topographical circumstances it
is also possible to split the data set for different wind sectors, to determine different planes for
different wind sectors. As we want to obtain a regression plane, which is representative for the usual
local wind field, we recommend excluding measurements of extreme wind situations for the
regression, e.g. all measurements with wind velocities higher than a certain threshold can be
excluded. This threshold should be defined specifically for each site. For agricultural low land sites
in Central Europe this threshold can be $5 \text{ m s}^{-1}$ for example.

The wind vector in the planar fit coordinate system (index $p$) can be obtained by matrix
multiplication of the measured wind vector (index $m$) with the rotation matrix $P$. The Planar Fit
method can not only be used to correct for a misalignment of the sonic anemometer but also to
subtract an offset $c$ of the sonic anemometer measurements.

\[
\overline{u_p} = P(\overline{u_m} - \overline{c}), \quad (12)
\]

\[
\overline{u_p} = p_{11}(\overline{u_m} - c_1) + p_{12}(\overline{v_m} - c_2) + p_{13}(\overline{w_m} - c_3),
\overline{v_p} = p_{21}(\overline{u_m} - c_1) + p_{22}(\overline{v_m} - c_2) + p_{23}(\overline{w_m} - c_3),
\overline{w_p} = p_{31}(\overline{u_m} - c_1) + p_{32}(\overline{v_m} - c_2) + p_{33}(\overline{w_m} - c_3).
\quad (13)
\]

c_1$ and $c_2$ are considered to be negligible.

A multiple linear regression analysis is used to fit a plane into the 3-dimensional data of the three
wind components. The regression coefficients are called $b_i$.

\[
\overline{w_m} = c_3 - \frac{p_{31}}{p_{33}} \overline{u_m} - \frac{p_{32}}{p_{33}} \overline{v_m} = b_0 - b_1 \overline{u_m} - b_2 \overline{v_m} \quad (14)
\]

The elements of the rotation matrix $P$ are calculated from the regression coefficients $b_i$.

\[
p_{31} = \frac{-b_1}{\sqrt{b_1^2 + b_2^2 + 1}}
p_{32} = \frac{-b_2}{\sqrt{b_1^2 + b_2^2 + 1}}
p_{33} = \frac{-b_3}{\sqrt{b_1^2 + b_2^2 + 1}} \quad (15)
\]

To determine the other elements of the matrix $P$ you can use the equations

\[
P = D^T C^T \quad (16)
\]
and

\[ p_{31} = \sin \alpha, \]
\[ p_{32} = -\cos \alpha \sin \beta, \]
\[ p_{33} = \cos \alpha \sin \beta. \]  

Therefore

\[ \tan \beta = -\frac{p_{32}}{p_{33}}, \]
\[ \sin \beta = -\frac{p_{32}}{\sqrt{p_{32}^2 + p_{33}^2}}, \]
\[ \cos \beta = \frac{p_{33}}{\sqrt{p_{32}^2 + p_{33}^2}}, \]
\[ \sin \alpha = p_{31}, \]
\[ \cos \alpha = \sqrt{p_{32}^2 + p_{33}^2}. \]  

Constant conditions of the system are assumed when applying the multiple linear regression method. So the anemometer must not be moved during the analyzed time series, as already mentioned above. It is also necessary to exclude outliers for the determination of the plane. Therefore all wind velocities above 5 m/s are sorted out. Depending on the geographic conditions of the measuring site it can be very advisable to determine different regression planes for different wind direction sectors.

If the Planar Fit coefficients are required for an online correction during the measurement, e. g. for the Relaxed Eddy Accumulation method, it is possible to determine these coefficients with a test data set of a few days before the actual experiment.

**Double Rotation**

The Double Rotation method (Kaimal and Finnigan, 1994) nullifies the vertical wind velocity for each half our value. Two rotation angles \( \gamma \) and \( \alpha \) are determined for that purpose.

First rotation:

\[ \bar{v} = 0; \quad \tan \gamma = \frac{\nu_m}{u_m}. \]

Second rotation:

\[ \bar{w} = 0; \quad \tan \alpha = \frac{\nu_m}{u_m}. \]

Some authors perform an additional third rotation (Aubinet et al., 2000; Kaimal and Finnigan, 1994). As it can create very unrealistic values, we don’t recommend this third rotation. It is not implemented in TK2.

### 2.3.3 Correction of oxygen cross sensitivity for Krypton hygrometers

Krypton hygrometers are used to measure the water vapour content of the air by absorption of \( \text{H}_2\text{O} \)}
molecules in the ultraviolet spectrum. Due to the used wave length there is a cross sensitivity to O₂ molecules, which has to be corrected for as recommended by Tanner (1993). Recent developments are published in the paper by van Dijk et al. (2003), simplified by Horst (2003).

\[ w'H_2O' = w'KH20' + C_{ko} \left( \frac{\rho_d}{T} \right) w'T' \]  

(21)

where

\[ C_{ko} = \frac{ko}{kw} \cdot \frac{CoMo}{Ma} = 0.23 \cdot \frac{ko}{kw} \]  

(22)

ko and kw are the KH2O extinction coefficients for oxygen and water vapor, Co=0.21 is the percent concentration of oxygen in the atmosphere, Mo=32 and Ma=28.97 are the molecular weights of oxygen and dry air, and rho_d is the density of dry air. The coefficients kw and ko are specific for each single instrument. The extinction coefficient for water kw is given in the calibration certificate by the manufacturer. The extinction coefficient for oxygen ko can be determined experimentally. Tanner et al. (1993) recommend to use a value of ko = -0.0045 (take care of the sign(+) convention), if the instrument specific coefficient is not known.

2.3.4 Correction of spectral loss

The correction algorithm follows basically the idea proposed in paper by Moore (1986). The error \[ \Delta F/F \] of a turbulent flux, which is caused by spectral loss, can be expressed

\[ \frac{\Delta F}{F} = 1 - \int_{0}^{\infty} T_{s(y)}(f) \cdot S_{s(y)}(f) df \]  

(23)

The theoretical form of the (co-)spectrum S has to be known as well as the specific transfer function T for the correction.

High frequency loss due to path length averaging of vectors

Transfer function for line averaging of the vertical wind velocity w (Moore, 1986):

\[ T_w(n) = \frac{2}{mn} \left( 1 + \frac{e^{-2m}}{2} - \frac{3(1-e^{-2m})}{4mn} \right) \]  

(24)

\[ n = \frac{f \cdot p}{u} \]  

(25)

In TK 2 the same transfer function is used for the horizontal wind velocity u.

High frequency loss due to path length averaging of scalars

Transfer function for line averaging of the scalars T, H₂O and CO₂ (Moore, 1986):
\[ T_p(n) = \frac{1}{2\pi n} \left( 3 + e^{-2zn} - 4 \cdot \frac{1 - e^{-2zn}}{2\pi n} \right) \]  
(26)

\[ n = \frac{f \cdot p}{u} \]  
(27)

**High frequency loss due to spatial separation of sensors**

Lateral separation (Moore, 1986):

\[ T_s(n) = e^{-9.9n^{1.5}} \]  
(28)

\[ n = \frac{f \cdot s}{u} \]  
(29)

This equation can only be used in the unstable case, if the sensor separation is less than 10% of the aerodynamic measuring height. Under stable stratification the distance between the sensors should not be greater than 0.7% of the Obukhov length (Moore, 1986). The separation length lateral to the wind direction between two sensors is calculated after formula (30).

\[ s_{lateral} = s_{total} \sin(dir) \]  
(30)

A correction of the longitudinal sensor separation is only necessary, if the covariance was not maximized by cross correlation analysis before (see 2.2.1). After Moore (1986) the transfer function for lateral separation can also be used for the correction of longitudinal separation, since in both cases the 3 dB-point is the same in both transfer functions.

**High frequency loss due to frequency dynamic response**

Transfer function for dynamic frequency response of an additional fast temperature sensor, e.g. PT150 or fine wire thermocouple (Moore, 1986).

\[ G(f) = \left[ 1 + (2\pi f\tau)^2 \right]^{-1/2} \]  
(31)

**Spectral models for stable stratification**

After Moore (1986) normalised spectra are parameterised according to

\[ \left[ f \cdot S_z(f) \right]_{norm} = \frac{n}{A_z + 3.124 \cdot (A_z)^{-2/3} \cdot n^{5/3}} \]  
(32)

Parameter \( A \) for vertical wind velocity \( w \):

\[ A_w = 0.838 + 1.172 \cdot \frac{z}{L} \]  
(33)
Parameter $A$ for scalars $T$, $H_2O$ and $CO_2$:

$$A_r = 0.0961 + 0.644 \cdot \left( \frac{z}{L} \right)^{0.6}$$  

(35)

Note that there is an error in the parameterisations of stable cospectra in Moore (1986). These should not be used but the parameterisations after Kaimal et al. (1972) instead (Bruckmeier, 2001).

In TK2 the cospectra under stable stratification are parameterised after Kaimal et al. (1972) for the covariances $<u'w'>$ and $<w'T'>$ in the following way.

$$f \cdot S_{xy}(f) = \frac{0.88 \cdot \frac{n}{n_0}}{1 + 1.5 \cdot \left( \frac{n}{n_0} \right)^{2.1}}$$  

(36)

$$n_{0,uw} = 0.10 \cdot \left( 1 + 7.9 \frac{z}{L} \right)^{0.75}$$  

(37)

$$n_{0,wt} = 0.23 \cdot \left( 1 + 6.4 \frac{z}{L} \right)^{0.75}$$  

(38)

For the covariances of the scalars $H_2O$ and $CO_2$ the same cospectral model can be used like for $<w'T'>$.  

**Spectral Models for unstable stratification**

Model for spectra of vertical wind velocity $w$ under unstable conditions after Højstrup (1981)

$$f \cdot S_w(f) = \frac{2n}{1 + 5.3n^{5/3}} + \frac{32n \zeta}{(1 + 17n)^{5/3}}$$  

(39)

Model for spectra of horizontal wind velocity $u$ under unstable conditions Højstrup (1981)

$$f \cdot S_u(f) = \frac{105n}{1 + 33n^{5/3}} + \frac{0.5n_i}{(1 + 2.2n_i)^{5/3}} \left( \frac{z_i}{L} \right)^{2/3}$$  

(40)

where

$$n = \frac{f \cdot z}{u}, n_i = \frac{f \cdot z_i}{u}$$  

(41)

Model for spectra of scalars $T$, $H_2O$ and $CO_2$ under unstable conditions after Kaimal et al. (1972)
\[
\frac{f \cdot S_u(f)}{T_s^2} = \left\{ \begin{array}{ll}
\frac{53.4n}{(1 + 24n)^{3/3}} & n < 0.15 \\
\frac{24.4n}{(1 + 12.5n)^{3/3}} & n \geq 0.15
\end{array} \right.
\tag{42}
\]

Cospectra for horizontal wind velocity \(u\) and vertical wind velocity \(w\) (Kaimal et al., 1972)

\[
\frac{f \cdot S_{uu}(f)}{u_s^2} = \frac{14n}{(1 + 9.6n)^{3/4}}
\tag{43}
\]

Cospectra for vertical wind velocity \(w\) and temperature \(T\) (Kaimal et al., 1972)

\[
\frac{f \cdot S_{wT}(f)}{w \cdot T} = \left\{ \begin{array}{ll}
\frac{11n}{(1 + 13.3n)^{1/3}} & n < 1 \\
\frac{4.4n}{(1 + 3.8n)^{2/4}} & n \geq 1
\end{array} \right.
\tag{44}
\]

For the covariances of the scalars \(H_2O\) and \(CO_2\) the same cospectral model can be used like for \(\langle w' \cdot T' \rangle\).

### 2.3.5 Conversion of fluctuations of sonic temperature into actual temperature

Sonic anemometers do not really measure temperature but the speed of sound. The speed of sound depends on the air temperature and also to a minor part on the water vapour content of the air. To obtain the fluctuations of the actual temperature instead of the fluctuations of sonic temperature the humidity effect has to be corrected according to the paper by Schotanus et al. (1983).

\[
\sigma_{T_s}^2 = \sigma_{T_s}^2 - 1.02\overline{T'q'} - 0.51^2 \overline{q'^2} \overline{T'}^2 
\tag{45}
\]

\[
\overline{w' \cdot T'} = \overline{w'T'} - 0.51 \cdot \overline{T} \cdot \overline{w'q'}
\tag{46}
\]

If no fast response measurement of water vapour is available to determine the turbulent latent heat flux equation (45) can not be resolved. In this case the Bowen ratio \(Bo\) derived from profile measurements can be used to convert the sonic temperature fluctuations into fluctuations of the actual temperature (Foken, 2003).

\[
\overline{w' \cdot T'} = \frac{\overline{w'T'}}{1 + \frac{0.51 \cdot \overline{T} \cdot c_p}{\lambda \cdot Bo}}
\tag{47}
\]
2.3.6 Correction for density fluctuations (WPL-correction)

To determine turbulent fluxes of air constituents like $\text{H}_2\text{O}$ and $\text{CO}_2$ the correction after Webb et al. (1980) is necessary. It corrects for two aspects. The first is the conversion of the volume related measurement of the content of a scalar quantity, e.g. absolute humidity [g m$^{-3}$] into a mass related parameter like specific humidity or mixing ratio. The second aspect is the correction of a positive vertical mass flow, which results from the mass balance equation, because vertical velocities of ascending parcels have to be different from descending ones due to density differences (Fuehrer and Frieh, 2002; Liebethal and Foken, 2003; Liebethal and Foken, 2004; Webb et al., 1980) 

In general the correct flux of a scalar quantity is calculated after

$$F_c = w \overline{\rho_c} + \mu \cdot \frac{\rho_c}{\rho_a} \cdot w \overline{\rho_c} + (1 + \mu \sigma) \cdot \overline{\rho_c} \cdot \frac{w^T}{T} \quad (48)$$

$F_c$: correct flux of scalar quantity

$\rho_c$: density of scalar quantity

$\rho_a$: density of dry air

$\rho_v$: density of water vapour

$$\mu = \frac{m_a}{m_v} = 1.6$$

$$\sigma = \frac{\rho_v}{\rho_a}$$

Simplified version of formula (48) for the flux of water vapour

$$F_v = (1 + \mu \sigma) \cdot \left( w \overline{\rho_v} + \rho_v \cdot \frac{w^T}{T} \right) \quad (49)$$

2.3.7 Iterative determination of the sensible and latent heat flux

In the correction equations above can be seen that there is interdependence between the sensible and latent heat flux. As it is not possible to calculate these turbulent heat fluxes simultaneously without unwanted simplifications, the sensible and the latent heat flux have to be determined iteratively. TK2 iterates the corrections until the results for the heat fluxes don’t change more than 0.01 % from one step to the next one.
3 Quality control

3.1 Steady state test

The steady state test according to Foken and Wichura (1996) is based on developments of Russian scientists (Gurjanov et al., 1984) and compares the statistical parameters determined for the averaging period and for short intervals within this period. For instance the time series for the determination of the covariance of the measured signals w (vertical wind) and x (horizontal wind component or scalar) of about 30 minutes duration will be divided into \( M=6 \) intervals of about 5 minutes. \( N \) is the number of measuring points of the short interval (\( N=6,000 \) for 20 Hz scanning frequency and a 5 minutes interval):

\[
\begin{align*}
\sum_i \sum_j (x_i w_j) = \frac{1}{M} \sum_i \left( \sum_j x_j \cdot w_j \right) - \frac{1}{M} \left( \sum_j x_j \cdot \sum_i w_j \right) \\
\bar{x}^i w^j = \frac{1}{M} \sum_i \left( x^i w^j \right)
\end{align*}
\]

This value will be compared with the covariance determined for the whole interval:

\[
\bar{x'} w' = \frac{1}{M-N} \left[ \sum_i \left( \sum_j x_j \cdot w_j \right) \right] - \frac{1}{MN} \sum_i \left( \sum_j x_j \cdot \sum_i w_j \right)
\]

A time series is considered to be steady state if the difference between both covariances \( R_{N_{Cov}} \) is lower 30%.

\[
R_{N_{Cov}} = \left| \frac{(x' w')_{eq(50)} - (x' w')_{eq(51)}}{(x' w')_{eq(51)}} \right|
\]

This value is found by long experiences but is in a good agreement with other test parameters also of other authors (Foken and Wichura, 1996).
Table 3: Classification scheme for the steady state test after Foken et al. [1999 #35]

<table>
<thead>
<tr>
<th>Class</th>
<th>range</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0–15 %</td>
</tr>
<tr>
<td>2</td>
<td>16–30 %</td>
</tr>
<tr>
<td>3</td>
<td>31–50 %</td>
</tr>
<tr>
<td>4</td>
<td>51–75 %</td>
</tr>
<tr>
<td>5</td>
<td>76–100 %</td>
</tr>
<tr>
<td>6</td>
<td>101–250 %</td>
</tr>
<tr>
<td>7</td>
<td>251–500 %</td>
</tr>
<tr>
<td>8</td>
<td>501–1000 %</td>
</tr>
<tr>
<td>9</td>
<td>&gt; 1000 %</td>
</tr>
</tbody>
</table>

3.2 Integral Turbulence Characteristics test

To test the development of turbulent conditions the so-called flux-variance similarity is a good measure. This similarity means that the ratio of the standard deviation of a turbulent parameter and its turbulent flux is nearly constant or a function, e.g. of the stability. These so-called integral turbulence characteristics are basic similarity characteristics of the atmospheric turbulence (Foken and Wichura, 1996; Kaimal and Finnigan, 1994) and can be found in all textbooks (Kaimal and Finnigan, 1994; Stull, 1988). Foken and Wichura (1996) used for their test such functions determined by Foken et al. (1991). These functions depend on stability and have the general form for standard deviations of wind components

\[
\frac{\sigma_{u,v,w}}{u_*} = c_1 \left( \frac{z}{L} \right)^{c_2}
\]

where \( u \) is the horizontal or longitudinal wind component, \( v \) the lateral wind component, \( u_* \) the friction velocity and \( L \) the Obukhov length. For scalar fluxes the standard deviations are normalized by their dynamical parameters (e.g., the dynamical temperature \( T_* \))

\[
\frac{\sigma_{X_*}}{X_*} = c_1 \left( \frac{z}{L} \right)^{c_2}
\]
Table 4: Constant values for $c_1$ und $c_2$ after Foken and Wichura (1996)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$z/L$</th>
<th>$c_1$</th>
<th>$c_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_u$</td>
<td>$0 &gt; z/L &gt; -0.032$</td>
<td>2.7</td>
<td>0</td>
</tr>
<tr>
<td>$u_*$</td>
<td>$-0.032 &gt; z/L$</td>
<td>4.15</td>
<td>1/8</td>
</tr>
<tr>
<td>$\sigma_w$</td>
<td>$0 &gt; z/L &gt; -0.032$</td>
<td>1.3</td>
<td>0</td>
</tr>
<tr>
<td>$u_*$</td>
<td>$-0.032 &gt; z/L$</td>
<td>2.0</td>
<td>1/8</td>
</tr>
<tr>
<td>$\sigma_T$</td>
<td>$0.02 &lt; z/L &lt; 1$</td>
<td>1.4</td>
<td>-1/4</td>
</tr>
<tr>
<td>$T_*$</td>
<td>$0.02 &gt; z/L &gt; -0.062$</td>
<td>0.5</td>
<td>-1/2</td>
</tr>
<tr>
<td></td>
<td>$-0.062 &gt; z/L &gt; -1$</td>
<td>1.0</td>
<td>-1/4</td>
</tr>
<tr>
<td></td>
<td>$-1 &gt; z/L$</td>
<td>1.0</td>
<td>-1/3</td>
</tr>
</tbody>
</table>

As there are no parameterisations for stable stratifications available, we used the same parameterisations as in the unstable case.

For the neutral range the external forcing assumed by Johansson et al. (2001) and analysed for the integral turbulence characteristics by Thomas and Foken (2002) was considered with the Coriolis parameter $f$. This model has priority compared to the model after Foken and Wichura (1996) in the stability range, which it is defined for.

Table 5: Model for integral turbulence characteristics for near neutral stratifications after Thomas and Foken (2002)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$-0.2 &lt; z/L &lt; 0.4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_u$</td>
<td>$u_*$</td>
</tr>
<tr>
<td>$\sigma_w$</td>
<td>$u_*$</td>
</tr>
</tbody>
</table>

The test can be done for the integral turbulence characteristics of both parameters used to determine the covariance. The measured and the modelled parameter will be compared according to

$$ ITC_\sigma = \left| \frac{\sigma_{x}/X_x}_{\text{model}} - \left( \frac{\sigma_{x}/X_x}_{\text{measurement}} \right) \right| $$

If the test parameter $ITC_\sigma$ is $< 30\%$ a well developed turbulence can be assumed.

The ITC-test is not applied for the sensible heat flux ($H_{Ts}$ or $H_{Tp}$) under direct neutral conditions, when the absolute value sensible heat flux is smaller than $10\text{Wm}^{-2}$, because $\sigma_T/T_*$ is not well defined in this case.
Table 6: Classification scheme for the integral turbulence characteristics test after Foken et al. {, 1999 #35}

<table>
<thead>
<tr>
<th>Class</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0–15 %</td>
</tr>
<tr>
<td>2</td>
<td>16–30 %</td>
</tr>
<tr>
<td>3</td>
<td>31–50 %</td>
</tr>
<tr>
<td>4</td>
<td>51–75 %</td>
</tr>
<tr>
<td>5</td>
<td>76–100 %</td>
</tr>
<tr>
<td>6</td>
<td>101–250 %</td>
</tr>
<tr>
<td>7</td>
<td>251–500 %</td>
</tr>
<tr>
<td>8</td>
<td>501–1000 %</td>
</tr>
<tr>
<td>9</td>
<td>&gt; 1000 %</td>
</tr>
</tbody>
</table>

3.3 Overall flag systems

An overall quality flag is created by the TK2 software for the test parameters friction velocity \( u_{\text{star}} \), sensible heat flux determined by sonic temperature measurement \( H_{Ts} \), sensible heat flux determined by platinum temperature measurement \( H_{Tp} \), latent heat flux \( L_{E} \), and the CO\(_2\)-flux \( w^{'}CO_{2}^{'} \). Table 7 shows which test is applied for which test parameter.

Table 7: Overview of the applied tests for each test parameter

<table>
<thead>
<tr>
<th>Test parameter</th>
<th>Steady state test</th>
<th>ITC ( \sigma_{u} / u_{\text{star}} ) test</th>
<th>ITC ( \sigma_{\text{w}} / u_{\text{star}} ) test</th>
<th>ITC ( \sigma_{Ts} / Ts_{\text{star}} ) test</th>
<th>ITC ( \sigma_{Tp} / Tp_{\text{star}} ) test</th>
</tr>
</thead>
<tbody>
<tr>
<td>( u_{\text{star}} )</td>
<td>( u^{'}w^{'} ), ( v^{'}w^{'} )</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>( H_{Ts} )</td>
<td>( w^{'}T_{s}^{'} )</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>( H_{Tp} )</td>
<td>( w^{'}T_{p}^{'} )</td>
<td>x</td>
<td>x</td>
<td></td>
<td>x</td>
</tr>
<tr>
<td>( L_{E} )</td>
<td>( w^{'}a^{'} )</td>
<td></td>
<td>x</td>
<td></td>
<td>x</td>
</tr>
<tr>
<td>( w^{'}CO_{2}^{'} )</td>
<td>( w^{'}CO_{2}^{'} )</td>
<td></td>
<td>x</td>
<td></td>
<td>x</td>
</tr>
</tbody>
</table>

The combined result of the applied tests can be summarized after three different classification schemes.

3.3.1 Scheme after Foken et al. {, 1999 #35}

Integral turbulence characteristics are calculated for \( w, u, T \). The quality flag for one flux is composed of its result of the steady state test and the results of the ITC-test of the two time series, of which the covariance is calculated. If the results of the two ITC-tests do not agree, the higher flag or bigger deviation is used for the overall classification.
Table 8: Overall flag system after Foken et al. [, 1999 #35]

<table>
<thead>
<tr>
<th>steady state</th>
<th>integral turbulence characteristic</th>
<th>Final flag</th>
</tr>
</thead>
<tbody>
<tr>
<td>(flag)</td>
<td>(flag)</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>1 – 2</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>1 – 2</td>
<td>2</td>
</tr>
<tr>
<td>1 – 2</td>
<td>3 – 4</td>
<td>3</td>
</tr>
<tr>
<td>3 – 4</td>
<td>1 – 2</td>
<td>4</td>
</tr>
<tr>
<td>1 – 4</td>
<td>3 – 5</td>
<td>5</td>
</tr>
<tr>
<td>5</td>
<td>≤ 5</td>
<td>6</td>
</tr>
<tr>
<td>≤ 6</td>
<td>≤ 6</td>
<td>7</td>
</tr>
<tr>
<td>≤ 8</td>
<td>≤ 8</td>
<td>8</td>
</tr>
<tr>
<td>9</td>
<td>9</td>
<td>9</td>
</tr>
</tbody>
</table>

Table 9: Overall flag system after Foken et al. [, 1999 #35]; deviations in %

<table>
<thead>
<tr>
<th>steady state</th>
<th>integral turbulence characteristic</th>
<th>Final flag</th>
</tr>
</thead>
<tbody>
<tr>
<td>(deviation in %)</td>
<td>(deviation in %)</td>
<td></td>
</tr>
<tr>
<td>0 – 15</td>
<td>0 – 30</td>
<td>1</td>
</tr>
<tr>
<td>16 – 30</td>
<td>0 – 30</td>
<td>2</td>
</tr>
<tr>
<td>0 – 30</td>
<td>31 – 75</td>
<td>3</td>
</tr>
<tr>
<td>31 – 75</td>
<td>0 – 30</td>
<td>4</td>
</tr>
<tr>
<td>0 – 75</td>
<td>31 – 100</td>
<td>5</td>
</tr>
<tr>
<td>76 – 100</td>
<td>0 – 100</td>
<td>6</td>
</tr>
<tr>
<td>0 – 250</td>
<td>0 – 250</td>
<td>7</td>
</tr>
<tr>
<td>0 – 1000</td>
<td>0 – 1000</td>
<td>8</td>
</tr>
<tr>
<td>&gt; 1000</td>
<td>&gt; 1000</td>
<td>9</td>
</tr>
</tbody>
</table>

The uses of such a scheme must know the appropriate use of the flagged data. The presented scheme was classified (by micrometeorological experience) so classes 1 to 3 can be used for fundamental research, such as the development of parameterizations. The classes 4-6 are available for general use like for continuously running systems of the FLUXNET program. Classes 7 and 8 are only for orientation. Sometimes it is better to use such data instead of a gap filling procedure, but these data should not differ significantly from the data before and after these data in the time series. Data of class 9 should be excluded under all circumstances.
3.3.2 Scheme after Rebmann et al. {, 2005 #134}

Integral turbulence characteristics are calculated for u, w, T.

Table 10: Overall flag system after Rebmann et al. {, 2005 #134}

<table>
<thead>
<tr>
<th>steady state (flag)</th>
<th>integral turbulence characteristic (flag)</th>
<th>Final flag</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 – 2</td>
<td>1 – 2</td>
<td>1</td>
</tr>
<tr>
<td>1 – 2</td>
<td>3 – 4</td>
<td>2</td>
</tr>
<tr>
<td>3 – 4</td>
<td>3 – 4</td>
<td>3</td>
</tr>
<tr>
<td>3 – 4</td>
<td>5 – 6</td>
<td>4</td>
</tr>
<tr>
<td>5 – 9</td>
<td>7 – 9</td>
<td>5</td>
</tr>
</tbody>
</table>

Table 11: Overall flag system after Rebmann et al. {, 2005 #134}; deviations in %

<table>
<thead>
<tr>
<th>steady state (deviation in %)</th>
<th>integral turbulence characteristic (deviation in %)</th>
<th>Final flag</th>
</tr>
</thead>
<tbody>
<tr>
<td>0-30</td>
<td>0-30</td>
<td>1</td>
</tr>
<tr>
<td>0-30</td>
<td>31-75</td>
<td>2</td>
</tr>
<tr>
<td>31-75</td>
<td>31-75</td>
<td>3</td>
</tr>
<tr>
<td>31-75</td>
<td>76-250</td>
<td>4</td>
</tr>
<tr>
<td>&gt;75</td>
<td>&gt;250</td>
<td>5</td>
</tr>
</tbody>
</table>

The scheme after Rebmann et al. {, 2005 #134} is a simplified version of the scheme after Foken et al. {, 1999 #35}. Classes 1 and 2 are suitable for fundamental research. Classes 3 and 4 still can be used for continuously running measurement programs to obtain monthly or annual sums of fluxes. Data of quality flag 5 should be excluded for any further analysis.
3.3.3 Scheme after the Spoleto agreement, 2004 for CarboEurope-IP

Integral turbulence characteristics are calculated for \( w \) only, not for \( T \).

Table 12: Overall flag system after the Spoleto agreement, 2004 for CarboEurope-IP

<table>
<thead>
<tr>
<th>steady state (flag)</th>
<th>integral turbulence characteristic (flag)</th>
<th>Final flag</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 – 2</td>
<td>1 - 2</td>
<td>0</td>
</tr>
<tr>
<td>&lt;= 5</td>
<td>&lt;= 5</td>
<td>1</td>
</tr>
<tr>
<td>&gt;= 6</td>
<td>&gt;= 6</td>
<td>2</td>
</tr>
</tbody>
</table>

Table 13: Overall flag system after the Spoleto agreement, 2004 for CarboEurope-IP, deviations in %

<table>
<thead>
<tr>
<th>steady state (deviation in %)</th>
<th>integral turbulence characteristic (deviation in %)</th>
<th>Final flag</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt; 30</td>
<td>&lt; 30</td>
<td>0</td>
</tr>
<tr>
<td>&lt; 100</td>
<td>&lt; 100</td>
<td>1</td>
</tr>
<tr>
<td>&gt; 100</td>
<td>&gt; 100</td>
<td>2</td>
</tr>
</tbody>
</table>

Description of the classes:

Class 0: high quality data, use in fundamental research possible

Class 1: moderate quality data, no restrictions for use in long term observation programs

Class 2: low data quality, gap filling necessary

The quality flags of the different classification schemes presented contain more or less similar information (Table 14).

Table 14: Comparative overview of the different overall quality flag schemes presented

<table>
<thead>
<tr>
<th>Flags after Foken et al. {, 1999 #35}</th>
<th>Flags after Rebmann et al. {, 2005 #134}</th>
<th>Flags after the Spoleto agreement</th>
</tr>
</thead>
<tbody>
<tr>
<td>high quality data, use in fundamental research possible</td>
<td>1-3</td>
<td>1-2</td>
</tr>
<tr>
<td>moderate quality data, for use in long term observation programs</td>
<td>4-6</td>
<td>3-4</td>
</tr>
<tr>
<td>low data quality, gap filling necessary</td>
<td>7-9</td>
<td>5</td>
</tr>
</tbody>
</table>
4 Data Input Formats

The data formats described in the following section represent a standardised data format of already calibrated values in meteorological units. Besides the capability of reading these standard formats TK2 is also able to read the direct output files of data acquisition systems, e. g. output Campbell Scientific data loggers CR23X and CR10X, SLT-files produced by EDDYMEAS (meteotools, Jena) or file format of the data acquisition software ATEM (Johannes Ruppert, University of Bayreuth). A standard data format was developed for the data exchange in CarboEurope-IP. This is described in the following sections. Example files can be found on the enclosed CD-ROM.

4.1 Format for high frequency raw data

The file format for high frequency raw data requires an ASCII character set. Columns are separated by commas. For the number format decimal places are separated by a dot (1.23456). Missing values are indicated by ‘-9999.9’.

Coordinate system: Wind components u, v, w are defined in a right hand coordinate system.

File header information like this example:

```
High frequency data format
site: DE-Wei
time used: UTC
Name of responsible person: Matthias Mauder
Sonic type: CSAT3 **)
Analyser type: LI-7500 ***)
measuring height above ground (m): 2.70
canopy height (m): 0.50
orientation of the u-component (0-360): 220
Height above sea level (m): 72
Latitude (deg,min,sec): 52,13,55
Year of measurement: 2003
sampling frequency (Hz): 20
orientation of analyser against sonic (0-360): 220
sensor separation sonic - analyser (m): 0.30
sensor separation add. fast temperature sensor (m)*): 0.05
time constant of add. fast temperature sensor (s)*): 0.02
DOY,HHMM,SEC,u(m/s),v(m/s),w(m/s),Ts(C),Tp(C),a(g/m3),CO2(mmol/m3)
121,1200,00.10, 3.455,-0.123, 0.045, 18.18, 17.72, 8.423, 15.371
```

The data producer can decide about the decimal places as well as about the length of the data files.
*) sensor type not available at all sites, line is optional

**) please use only: CSAT3, USA-1, Solent-HS, Solent-R2, Solent-R3, ATI-K, Young

***) please use only LI-7500, LI-6262, LI-7000, KH20

Convention about the file names: **SSSSSS_H####.dat**

SSSSSS: abbreviation code of the station, e.g. DE-Wei for Waldstein/Weidenbrunnen

####: running number of the files (4digits), please number the data files continuously.

4.2 Low frequency reference data

Accurate reference data for temperature, humidity and pressure are necessary for meteorological calculations during the eddy covariance data post processing. These are usually averaged over time periods like 5 or 10 minutes.

File header information like this example:

```
Low frequency reference data format
site: DE-Wei
time used: UTC
Name of responsible person: Matthias Mauder
measuring height above ground (m): 2.70
canopy height (m): 0.50
DOY,HHMM,SEC(begin),DOY,HHMM,SEC(end),T_ref(C),a_ref(g/m3),p_ref(hPa)
121,1200,00,121,1210,00,19.532,10.7992,1013.0
```

Convention about the file names: **SSSSSS_L####.dat**

SSSSSS: abbreviation code of the station, e.g. DE-Wei for Waldstein/Weidenbrunnen

####: running number of the files, number the data files continuously.

4.3 5 min averaged Data

Raw data files are often useful to find reason for eventual errors. But if you consider it to cause too much effort to create the raw data files, it is possible to use averaged data as input data for TK2 alternatively. These files contain averages, variances and covariances for 5 minute intervals. It is necessary to have averages not longer than 5 minutes to make it possible to perform the steady state quality test. If only averages of 30 minutes are available, the steady state test can not be performed.

Coordinate system: wind components u, v, w are defined in a right hand coordinate system.
File header information like this example:

Averaged data format  
site: DE-Wei  
time used: UTC  
Name of responsible person: Matthias Mauder  
Sonic type: CSAT3 **)  
Analyser type: LI-7500 ***)  
measuring height above ground (m): 2.70  
canopy height (m): 0.50  
orientation of the u-component (0-360): 220  
Height above sea level (m): 72  
Latitude (deg,min,sec): 52,13,55  
Year of measurement: 2003  
sampling frequency (Hz): 20  
orientation of analyser against sonic (0-360): 220  
sensor separation sonic - analyser (m): 0.30  
sensor separation add. fast temperature sensor (m)*): 0.05  
time constant of add. fast temperature sensor (s)*): 0.02

see also EXAMPLE_5M001.CSV

Convention about the file names: SSSSSS_5M###.CSV

SSSSSS: abbreviation code of the station, e.g. DE-Wei for Waldstein/Weidenbrunnen
5M: for 5 minute averaging interval
###: running number of the files, number continuously
CSV: file suffix

Header line with identifier for the quantity and its unit
Dot as decimal separator, columns comma separated, -9999.9 as identifier for wrong or missing values.

The order of the columns must be in the same way like in the example file EXAMPLE_5M001.CSV. If the quantities, which are listed in a column, are not measured, please fill up these columns with -9999.9. For example the columns for low frequency reference measurements can be filled up with -9999.9, if these measurements are not available. These reference data attribute to the confidence of the analysis. But in case they are not available the analysis can be performed without them. In order to be able to calculate averages, variances and
covariances, it is necessary to have information about the specific number of values.

DOY,HHMM,SEC(begin): Beginning of the averaging interval in UTC
DOY,HHMM,SEC(end): Ending of the averaging interval in UTC
u(m/s): horizontal wind component for the direction in which the sonic is oriented
v(m/s): horizontal wind component for the direction rectangular to the orientation of the sonic
w(m/s): vertical wind component
Ts(C): sonic temperature
Tp(C): temperature from an additional fast response sensor, PT150 or Fine Wire Thermocouple
a(g/m3): absolute humidity averaged from turbulence measurement
CO2(mmol/m3): CO2 concentration averaged from turbulence measurement
T_ref(C): temperature measurement from a slow response reference sensor
a_ref(g/m3): absolute humidity from a slow response reference sensor
p_ref(hPa): air pressure
Var(u), Var(v), Var(w): Variance of the wind components
Var(Ts): Variance of sonic temperature
Var(Tp): Variance of Temperature from a additional fast response sensor
Var(a): Variance of absolute humidity
Var(CO2): Variance of CO2 concentration
Cov(u'v'): Covariance between the wind components u and v
Cov(v'w'): Covariance between the wind components v and w
Cov(u'w'): Covariance between the wind components u and w
Cov(u'Ts'), Cov(v'Ts'), Cov(w'Ts'): Covariance between the three wind components and the sonic temperature
Cov(u'Tp'), Cov(v'Tp'), Cov(w'Tp'): Covariance between the three wind components and the temperature from an additional fast response sensor
Cov(u'a'), Cov(v'a'), Cov(w'a'): Covariance between the three wind components and absolute humidity
Cov(u'CO2'), Cov(v'CO2'), Cov(w'CO2'): Covariance between the three wind components and the CO2 concentration
N(u), N(v), N(w), N(Ts), N(Tp), N(a), N(CO2): Number of values for the respective quantity
N(u'v'), N(v'w'), N(u'w'), N(u'Ts'), N(v'Ts'), N(w'Ts'), N(u'Tp'), N(v'Tp'), N(w'Tp'), N(u'a'), N(v'a'), N(w'a'), N(u'CO2'), N(v'CO2'), N(w'CO2'): Number of values going into the calculation of the
The file header information is required as input for the calculations and quality tests in TK2. Changes in the measurement setup can be tracked as they are given in the beginning of each file. TK2 offers also the alternative to give all the information about the measurement setup in a parameter file at once. This option is only suitable, if the configurations don’t change for one run of the program. The graphical user interface, which is described in the following chapter, is designed to enter all the configurations.
5 Graphical User Interface

The executables for TK2 are designed for Microsoft Windows® PCs.

Unzip all files into directory C:\

TK2 consists of two executables, TK2_VBP.exe and TK2.exe.

Execute TK2_VBP.exe to open the graphical user interface of TK2. TK2.exe will be started automatically later.

Frame 1: TK2

- Click Settings to enter all settings.
Frame 2: TK2 – File Names and Paths

- Enter name of executing person.
- Click through directory boxes.
- Enter abbreviation of project name. This will be part of every file name created by TK2 (max. 5 letters).
- Click through.

- Orientation of the sonic coordinate system’s u-component [°]. (e.g. 180° if positive u values stand for wind coming from the south, 270° for wind coming from west etc.)

- Enter the latitude of the measurement site [degree,minutes,seconds as integer numbers or alternatively, degree as a decimal number]

- Enter the year of measurements.

- Enter start time and end time of the required period for calculations of turbulent fluxes.

- TK2 will create binary files of high frequency data, which are calibrated, spike tested, gap filled, and have an equidistant time scale. The user can decide about the length of these files. 30 minutes is recommended for 30 minutes flux calculation interval. These files don’t have to be created again, if they were already created during an earlier run of TK2.
- Click through and enter required information.
- Enter time delay of channels in raw data file if necessary.
- Select if sonic measurements have to be converted from lefthand into righthand coordinate system.
- TK2 can calculate the METEK head correction during the post processing if measurements are operated in mode HC = 0. Select 0 if head correction is not necessary or you use a different sonic type.
- Enter calibration constants if necessary.
Enter consistency limits. TK2 will check if data have a value inside the selected limits.
- TK2 allows using slow response reference measurements of temperature, humidity and pressure for calculations. These measurements can be of any averaging interval. 1 or 5 minutes is recommended. A file/files containing reference measurements have to be in the input directory.

- Take last value as option for the treatment of missing values is very important as well as the fill up NaNs at begin option.

- The data which are written in the binary files can also be written in ASCII files additionally, e.g. for error detection.
TK2 will create comma separated ASCII files (*.csv) containing averages, variances and covariances without any corrections in the work directory. These files don’t have to be created again, if they were already created during an earlier run of TK2. The user can select between three alternative output formats. Format 0 stands for the standard exchange format of the LITFASS-2003 measurement campaign. Format 1 contains additional information about the number of values measured with the sonic anemometer in one averaging interval. Format 2 contains more information about the number of measurement about all parameters in detail (recommended).

TK2 can combine files of shorter averaging intervals to longer averaging intervals, e.g. 5 minutes interval to 30 minutes interval.

30 minutes calculation time interval and 5 minutes short term interval is recommended.
Frame 9: **TK2 – Correction of Fluxes (1)**

- Planar Fit coordinate rotation after Wilczak et al. (2001)
- Correction for oxygen cross sensitivity of krypton hygrometers after Tanner et al. (1993)
Correction of spectral loss after Moore (1986)
- If covariances are maximized by cross correlation analysis it is only necessary to correct for the sensor separation lateral to the wind direction. Therefore the Direction of the additional sensor is required.
- Correction after Schottanus et al. (1983)
- Correction after Webb et al. (Webb et al., 1980)
Frame 11: **TK2 – QA/QC**

- **Last step.....**

  - Perform stationary test?  
    - Yes
    - No

  - Test on developed turbulent conditions with integral turbulence characteristics?  
    - Yes
    - No

  - Quality flags after  
    - Foken et al. 2004 (1-3)
    - Rebsmann et al. 2004 for CARBDEUROPE (1-5)
    - Spoleto agreement, Jan. 2004 (0-2)

- Back
- Exit
- Finish

- Quality tests
- click *Finish*
- Frame 11 closes automatically
- Click *Execute Calculations* to start the FORTRAN core program in a dos box.
- All settings are listed in an ASCII file named *parameter.vbp*.
- TK2 will create the following files in the output directory:
  - *protocol*: containing all important setting for the actual TK2 run
  - *result*: containing corrected values for averages, variances and covariances including quality flags for turbulent fluxes
  - *QA_QC*: containing detailed results of the quality tests
6 References


Bisher erschienene Arbeiten der Reihe ‚Universität Bayreuth, Abt. Mikrometeorologie, Arbeitsergebnisse’

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