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Documentation and Instruction Manual of the Eddy-Covariance Software Package TK3 (update)

Matthias Mauder

Thomas Foken

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Dr. Matthias Mauder
Atmospheric Environmental Research
Karlsruhe Institute of Technology (KIT) Institute of Meteorology and Climate Research (IMK-IFU)
Kreuzeckbahnstr. 19
82467 Garmisch-Partenkirchen, Germany
Phone: +49 8821 183 119
Email: matthias.mauder@kit.edu
www: http://www.imk-ifu.kit.edu/

Prof. Dr. Thomas Foken
University of Bayreuth
Bayreuther Zentrum für Ökologie und Umweltforschung
Privat: Am Herrgottsbaum 28, 96120 Bischberg
Phone: +49 951 1809655
Email: thomas.foken@uni-bayreuth.de
www: http://www.micrometeorology.de

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Universität Bayreuth, Abteilung Mikrometeorologie
D-95440 Bayreuth

Content

1 Introduction

With the software package TK3 for the calculation of eddy-covariance data a programme version was developed, which is based on more than 25 years experiences. 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, at the University of Bayreuth the comprehensive software package TK2 (Mauder and Foken 2004) was developed, which was updated with the version TK3 (Mauder and Foken 2011). The present documentation includes some more features but was not changed in all basic calculations.

The software package TK2 was based on the 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 et al. 1993), 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 was 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 (Foken et al. 2004).

Within the CarboEurope community the TK2 software was used as a standard of the QA/QC network. It was used for footprint dependent data analysis (Göckede et al. 2008) and for the comparison with other software products on the basis of reference data files for the most typical instrumentations and for tall and low vegetation (Mauder et al. 2008). A good agreement was found with the other software packages, e.g. with EdiRE from Edinburgh and EddySoft from Jena.

The TK2 is listed in the VDI/DIN 3786 (VDI 2008) as a recommended software package.

Since 2007 a free online access on the software is available. Up to June 18, 2015, 614 downloads of the software package are registered, originating from 53 countries, most of them from P.R. China (114), Germany (107), except users of the University of Bayreuth and Karlsruhe Institute of technology IFU Garmisch-Partenkirchen, and USA (74). The countries with equal or more than five users are illustrated in Figure 1.

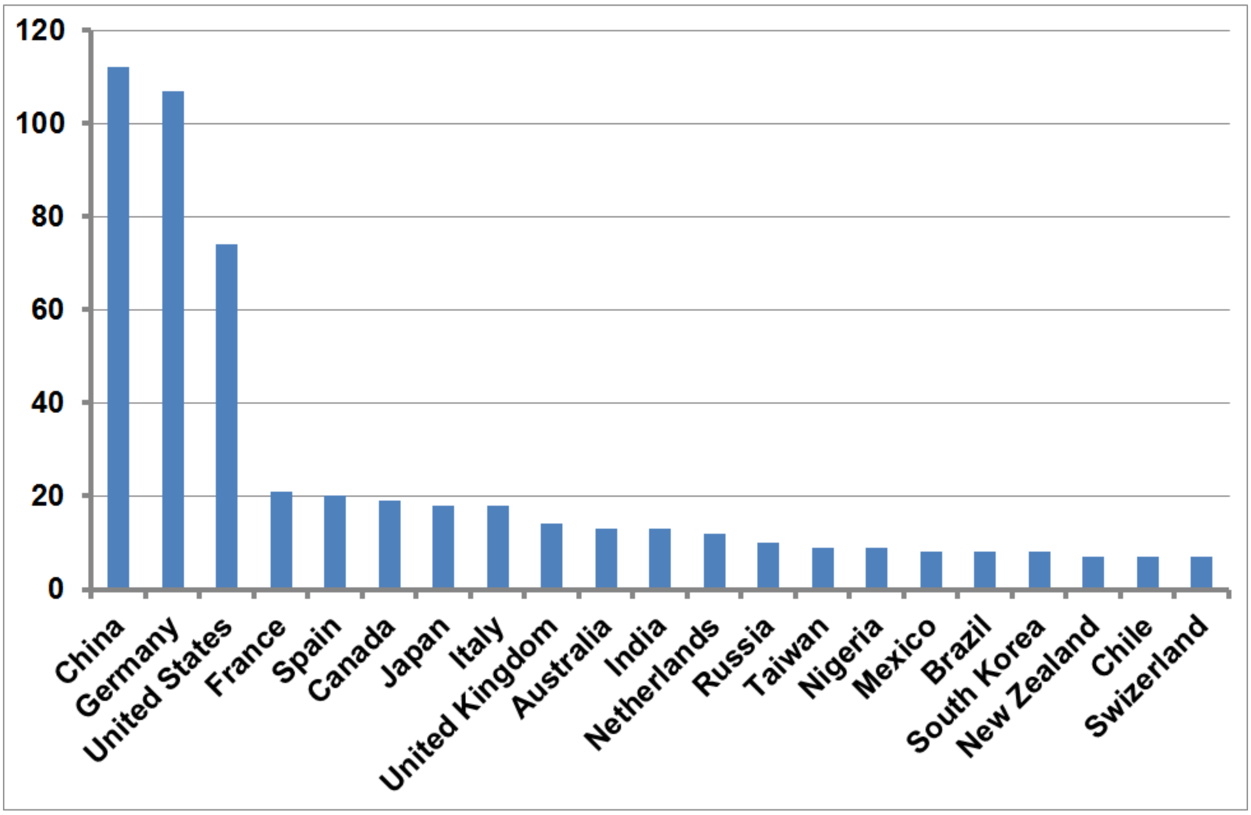


Figure 1: Downloads of the software package TK2 within about nine years up to July 08, 2015. Countries with five or more downloads are shown.

The TK3 version from 2011was is an updated version of TK2. All calculations and correction are compatible to the former version. The update includes a higher flexibility of the input files and new devices and tools ware added. Available statistics files of TK2 (see Section 2.2) could also be used in TK3. The software was successfully tested and compared with other software products (Mauder et al. 2013; Fratini and Mauder 2014) and is also free online available. The statistics of the 416 downloads is shown in Figure 2.

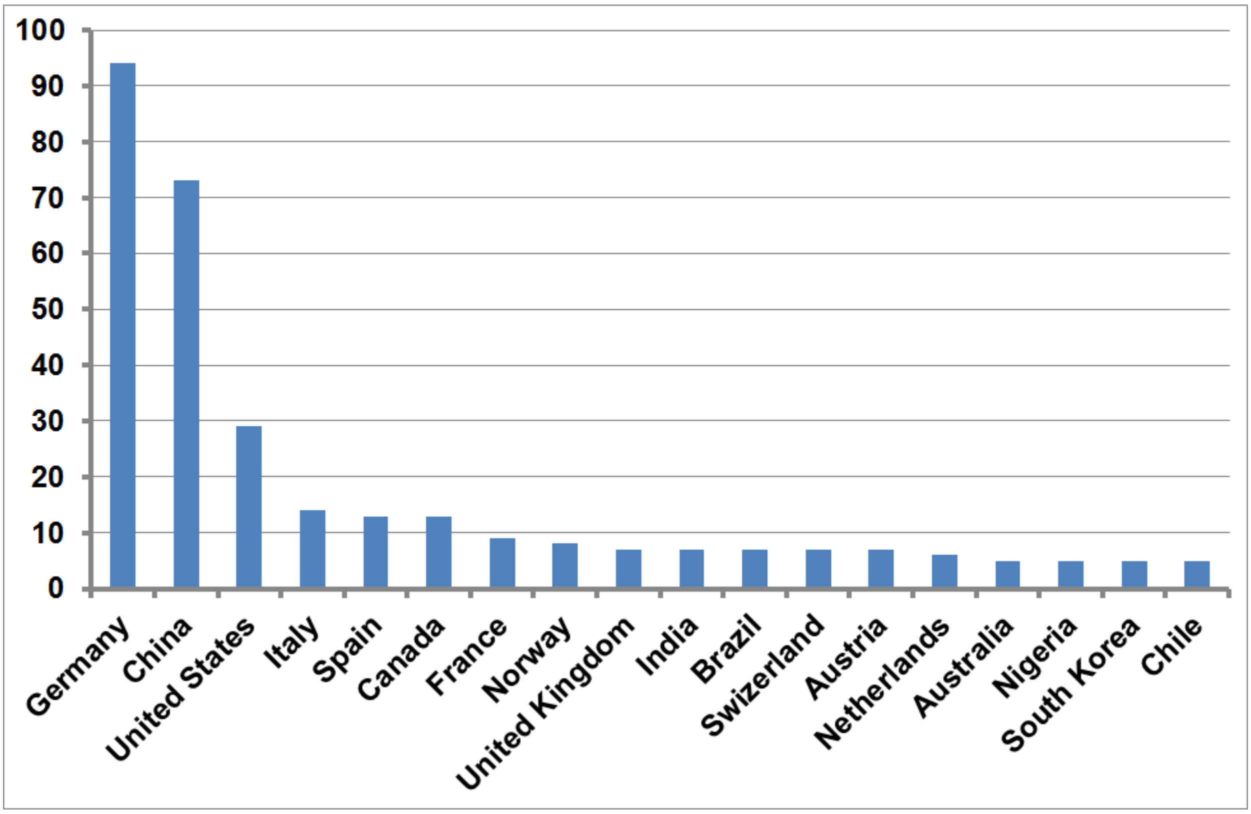


Figure 2: Downloads of the software package TK3 within about four years up to July 08, 2015. Countries with five or more downloads are shown.

The updated version of TK3 is now available on the Zenodo-Server (https://zenodo.org/) under the Creative Commons Attribution-NonCommercial 4.0 International Public License (CC). The software package is free but non-commercially usable with a reference to:

M. Mauder, T. Foken

Eddy-covariance software TK3 (2015)

doi: 10.5281/zenodo.20349

2 General structure of the software package

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.

There are several papers and books available, where the principles of the use of the eddy-covariance method are discussed (Kaimal and Finnigan 1994; Aubinet et al. 2000; Aubinet et al. 2003; Lee et al. 2004; Foken 2008a; Aubinet et al. 2012; Foken et al. 2012b). An overview of the recently used correction methods and its application in different software packages is given by Mauder et al. (2008; 2013). All corrections used in TK3 are in agreement with Foken et al. (2012c).

The TK3 is a research programme and allows different possibilities of the calculations. Therefore, the user needs certain knowledge about micrometeorology and the eddy-covariance method. For users without this background the default settings provide some guidance for an accurate run of the programme. Researchers can switch on and off different tools and can investigate the effects of correction methods and additional parts of the programme. Unfortunately, this makes the programme not user friendly but gives the researcher many advantages.

The programme is written in FORTRAN and runs on a WINDOWS (XP, 7, 8) and LINUX platform. The programme code is not open, to guaranty that the internationally well compared software package cannot be changed in their main parts.

Brake points in the programme make interim results available for the user for individual calculations (see Section 2.2).

Before using the software package, the knowledge about the structure of the software package is important. The software works off-line. For raw data storage specifically designed programmes should be used or commercially available logger-software, data-acquisition tools or eddy-covariance software packages can be applied.

2.1 The “parameter.vbp” file

For running the programme a special file with all necessary information must be generated on the basis of a default file “parameter.vbp”, see Section 7. The file can be adapted on the specific project with a text editor. First the default file should be changed to generate a personal or project default file (Figure 3), which is the basis for the individual files. Every time a parameter-file is read by TK3 a copy of that same file is generated with a timestamp in the file name. This copied file can be used to reanalyse data in the identical way if this file is renamed parameter.vbp.

On the basis of this individual default file for each programme run (different calibration constants, time intervals etc.) individual parameter files should be generated (Figure 4). It is important to document and save all these files. A copy of the parameter file is saved automatically with a time stamp in the file name for each run of TK3.

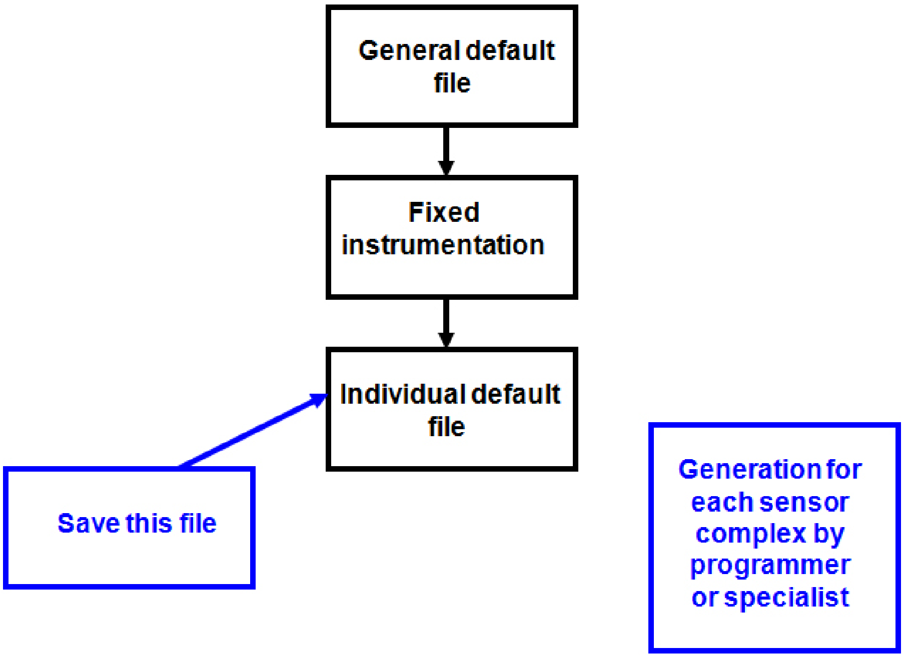


Figure 3: Generation of individual default parameter files based on the general default parameter file "parameter.vbp"

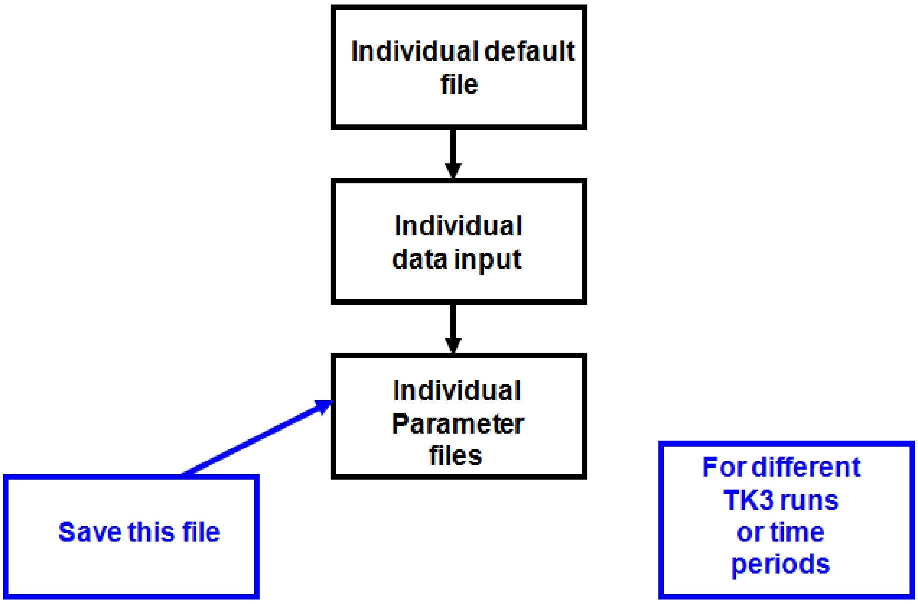


Figure 4: Generation of individual parameter files on the basis of the individual default parameter file.

2.2 The main structure of the programme

The programme has three parts. For each part the results are saved in specific files. This allows the user to use the results of each part for special purposes, but the programme can also run without interruption. The first part is the generation of physically correct data. The output data of this part are binary data (Figure 5) stored in files for 30 minutes with a time stamp in the file name.

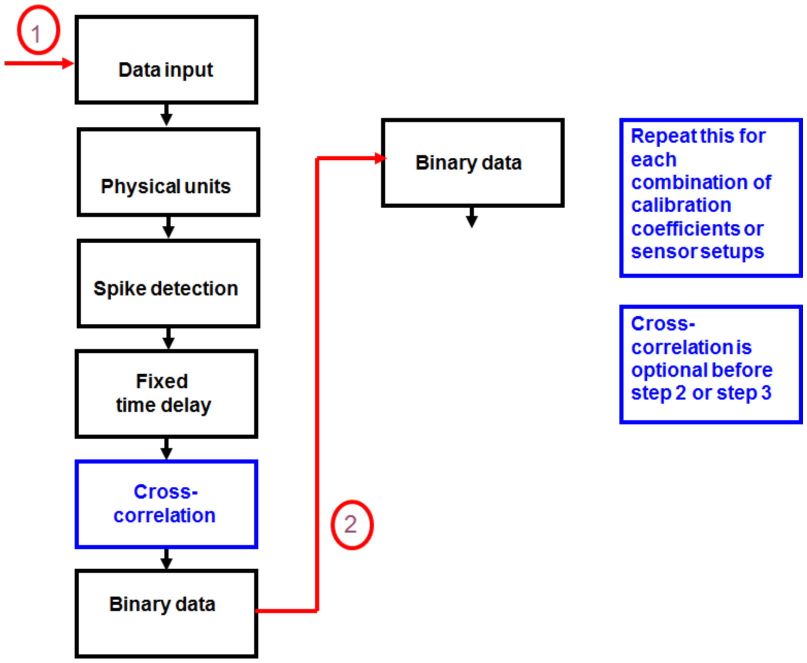


Figure 5: Structure of the programme package TK3, part 1, generation of the physical parameters.

The benefit of the TK3 software is that the input files need no special structure. The individual structure of the ASCII input file can be described in the parameter file. Furthermore a file with slow response reference input data (pressure temperature, humidity) for the calculation of density and other temperature and pressure dependent variables can be included (for more details see Section 6.2)

On the one hand the eddy-covariance measurements should be calculated for longer time series to use an adequate rotation technique and on the other hand instrumentation and calibration settings may change within shorter time series. Therefore the first part of the programme should run for each instrumentation and calibration setting. The set of binary data can be used for further calculation.

The calculations in the first part are the generation of physical correct data using the calibration settings. Then a plausibility of the data is checked on the basis of default or individual given values. Next spikes will be detected and replaced by the last value or interpolated and the time series will be shifted according to given fixed delay times, which can occur for closed path sensor with longer tubes or open path sensors with a certain processing time delay. The details of these steps are described in Section 3.1. Before this calculation the time series will be shifted with a cross correlation up to ±20 time steps, e.g. 1 second at 20 Hz sampling. This step is necessary to correct changing time shifts in the LiCor 7500 sensor, the influence of the drift of turbulent eddies with the wind through anemometers and additional sensors, and also to adjust for a slightly changing tube delay of closed-path sensors. Note, that a longer delay time must be corrected with fixed delay time in part 1 of the programme. The cross correlation can be done before the generation of the physical correct binary files (Figure 4) or in the second part of the programme.

The second part of the programme calculates the raw covariances without any correction (Figure 6) on the basis of the binary files. If the cross correlation was not done in the first part of the programme it will be made before the calculation of the raw covariances.

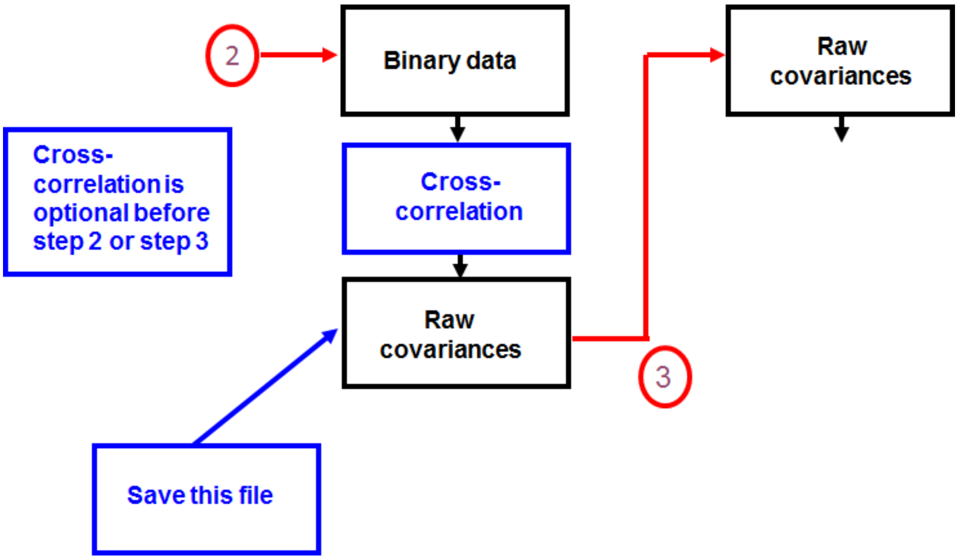


Figure 6: Structure of the programme package TK3, part 2, generation of raw covariances.

If data acquisition systems cannot sample raw data with 10 or 20 Hz and have only about 5 minute covariances and standard deviations available, the TK3 can generate covariances for longer averaging periods. Details of part 2 are given in Section 3.2.

As a result of the second part of the programme *.csv files for 5 minute and 30 minute covariances, standard deviations and mean values are available. The 5 minute series are necessary for the quality checks. These files are automatically saved for each run of TK3 with a time stamp in the file name, which are for documentation purposes only. The calculation is done based on the files ending on M001.csv and 5M001.csv without a time stamp. **For the further calculations no continuously running time of the lines in the covariance file is necessary.** Therefore the lines can be sorted according to some criteria of the user. Typical are selected time periods or wind sectors for the planar fit rotation.

The third part of the programme is the final calculation of the corrections. The first step is the coordinate rotation. While the planar-fit rotation (Wilczak et al. 2001) is recommended, also the double rotation for 30 minute intervals (Kaimal and Finnigan 1994; Aubinet et al. 2000) can be used. The latter should be made, if some disturbed periods (free convection, moving sensor fixing, etc.) does not allow a rotation over a longer time period. Often only the coefficients for the planar fit rotation should be calculated first and with this coefficients part three can be calculated several time, e.g. after change of the sensor, the canopy height etc (Figure 7). For more details see Section 3.3.

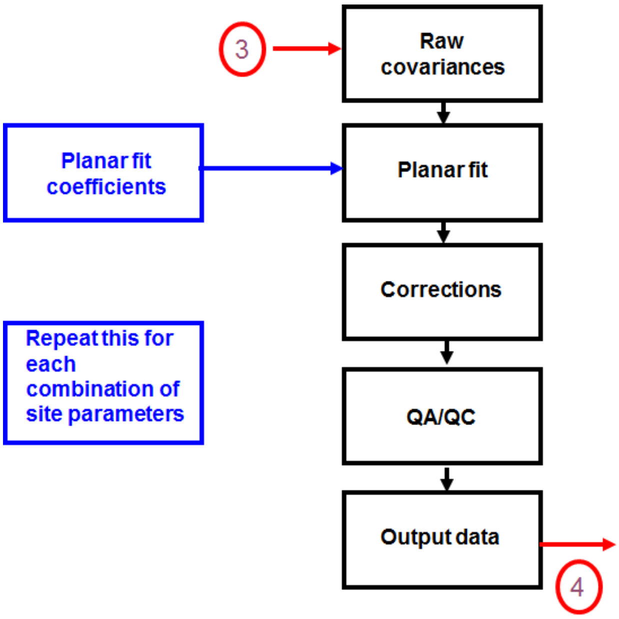


Figure 7: Structure of the programme package TK3, part 3, generation final results.

The output of part 3 are files with the mean values, standard deviations and covariances and for carbon dioxide measurements also of the net Ecosystem Exchange (NEE) including the storage term if selected. A summarized quality flag number is given. Furthermore a file with detailed quality flags is available. For quality flagging see Section 4.

As a fourth part special outputs like spectra, triple correlation are available, see Section 5.

Three different directories can be accesses by TK3 to read and write files, input, work and output (all three can also be the same). In the input directory the high-frequency raw data files and the reference data have to be placed. In the working directory the binary and statistics files (both 5- and 30-min) will be written; also, the output of special calculations, such as (co-)spectra and triple covariances, are stored there. The results of the flux-calculation (incl. corrections and conversions) and the QA/QC tests are stored in the output directory. A separate output file is created there for N_2O- and CH_4-fluxes if available. In calculation of ogives is selected, the output will also be written in that directory, and the protocol file containing the selected parameters and status reports about the progress of the calculations can be found there as well

3 Calculation of turbulent fluxes obtained by the eddy-covariance method

3.1 Plausibility tests of time series

3.1.1 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). If a measured variable does not exist in the data file then set the limits to 0, 0. All limits are applied on the unconverted and uncalibrated raw-data, i.e. they are depending on the units in the input file.

Table 1: Default settings for the consistency limits

Measured variable	Lower limit	Upper limit
Day of year	0	366
Daily time	0	2400
Seconds	0	60
u-Wind	-50 m/s	+50 m/s
v-Wind	-50 m/s	+50 m/s
w-Wind	-10 m/s	+10 m/s
Sonic temperature	-20° C	50° C
CSAT diagnostic code (running number)	0	63
Platinum temperature	-20° C	50° C
CO_2	0 mV	5000 mV
H_2O	0 mV	5000 mV
LI-7500 diagnostic	240	252
Licor pressure	80 kPa	110 kPa
O_3 (not fully implemented yet)	0	0
Inclinometer x (not fully implemented yet)	0	0
Inclinometer y (not fully implemented yet)	0	0
CH_4	0 nmol/mol	5000 nmol/mol
N_2O	0 nmol/mol	2000 nmol/mol
HMP reference temperature	-20° C	50° C
HMP reference relative humidity	0%	100%

3.1.2 Spike detection

In TK2/TK3 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 4.5 times standard deviations in a window of 15 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. After the first round of spike elimination is over, four more rounds of spike elimination will be conducted; each time the multiplication factor for the standard deviation threshold will be increased by 0.1 (0.5 for temperature). The window size, the starting multiplication factor for the standard deviation threshold and the number of spikes in a row, which will not be considered as those, can be determined in the parameter-file.

In the updated version a similar algorithm following Mauder et al. (2013) with the median absolute deviation (MAD, Hoaglin et al. 2000), $MAD = median_i\left(\left|x_i - median_j(x_j)\right|\right)$ was implemented, which is more robust. Spikes are values, which are above or below a multiple of MAD:

$$median(x) - \frac{q\,MAD}{0.6745} \leq x_i \leq \frac{q\,MAD}{0.6745} + median(x), \tag{1}$$

where 0.6745 corresponds to the Gaussian normal distribution and the factor q=7 found tob e a useful limit (Mauder et al. 2013).

3.2 Calculation of averages, variances and covariances

3.2.1 Maximisation 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. As we correct also 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.

3.2.2 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. TK3 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. If the number of used data is < 90 % the output file is filled with -9999.9.

3.2.3 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. TK3 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 Section 4.1). In this case you start the application of TK3 at the brake point (3) with raw covariances.

Formerly calculated (co)variances $\left(\overline{w'x'}\right)_j$ 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 (Foken et al. 1997):

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

The right hand side of equation (1) can be rewritten as follows:

$$\begin{aligned}
&\frac{1}{M-1}\left[(U-1)\sum_{j=1}^{N}\left(\overline{w'x'}\right)_j + U\sum_{j=1}^{N}\overline{w}_j \cdot \overline{x}_j - \frac{U^2}{M}\sum_{j=1}^{N}\overline{w}_j\sum_{j=1}^{N}\overline{x}_j\right] = \\
&= \frac{1}{M-1}\left\{(U-1)\sum_{j=1}^{N}\left(\overline{w'x'}\right)_j + U\left[\sum_{j=1}^{N}\overline{w}_j \cdot \overline{x}_j - \frac{U}{M}\sum_{j=1}^{N}\overline{w}_j\sum_{j=1}^{N}\overline{x}_j\right]\right\} = \\
&= \frac{1}{M-1}\left\{(U-1)\sum_{j=1}^{N}\left(\overline{w'x'}\right)_j + U\left[\sum_{j=1}^{N}\overline{w}_j \cdot \overline{x}_j - \frac{1}{N}\sum_{j=1}^{N}\overline{w}_j\sum_{j=1}^{N}\overline{x}_j\right]\right\}
\end{aligned} \tag{3}$$

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

$${}^{I}\overline{w'x'} = \frac{1}{M-1}\left\{(U-1)\sum_{j=1}^{N}\left(\overline{w'x'}\right)_j + U\sum_{j=1}^{N}\left[\left(\overline{w}_j - {}^{I}\overline{w}\right)\cdot\left(\overline{x}_j - {}^{I}\overline{x}\right)\right]\right\}, \tag{4}$$

where

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

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

$$ {}^{I}\overline{w'x'} = \frac{1}{M-1}\left\{ \sum_{j=1}^{N} \left({}^{\overline{w'x'}}U_j - 1\right)\left(\overline{w'x'}\right)_j + \sum_{j=1}^{N} {}^{\overline{w'x'}}U_j \cdot \left(\overline{w}_j - {}^{I}\overline{w}\right)\cdot\left(\overline{x}_j - {}^{I}\overline{x}\right)\right\}, \qquad (5) $$

where

$$ M = \sum_{j=1}^{N} {}^{\overline{w'x'}}U_j , $$

${}^{\overline{w'x'}}U_j$ number of valid data contributing to $\left(\overline{w'x'}\right)_j$.

3.3 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. All corrections can be turned on or off by the user. However, some corrections are only partly required for some sensors or not required at all. TK3 makes some automatic decisions about the corrections if they are turned on depending on the sensor type selected as listed in Tables 2 and 3.

A spectral correction for path-length-averaging is not meaningful for closed-path analyzers. However for those, the path-length is not set to zero for numerical reasons but to 10 mm instead, which is negligibly small to have no significant effect on the resulting fluxes.

Table 2: Supported sonic anemometers and corrections applied by TK3

	CSAT3	Solent-HS/R3	NCAR NUW	Young 81000	METEK USA-1	Solent R2	ATI K-Probe
Cross-wind correction (3.3.1)	-	-	-	-	X see 3.3.1	X	X
Conversion of buoyancy flux into sensible heat flux (3.3.5)	X	X	X	X	X	X	X
Path-length for Moore correction (3.3.4)	120 mm	150 mm	200 mm	150 mm	175 mm	150 mm	200 mm
Separation between u and w for Moore correction (3.3.4)	0	0	0	0	0	0	100 mm

Table 3: Supported H2O/CO2 gas analysers and corrections applied by TK3

	LI-6262	LI-7000	LI-7200	LI-7500	KH20	EC150	EC155	LGR	Aero-dyne
Path-length for Moore correction (3.3.4)	10 mm	10 mm	10 mm	125 mm	12 mm	154 mm	120 mm	10 mm	10 mm
WPL-correction for temperature fluctuations (3.3.6)	-	-	-	X	X	X	-	-	-
WPL-correction for humidity fluctuations (3.3.6)	X	X	-	X	X	X	-	-	-
Tanner correction (3.3.3)	-	-	-	-	X	-	-	-	-
Conversion of high-frequency data to mixing ratio	-	-	-	-	-	-	-	X	-

The LI-7200, the EC155 and the Aerodyne QCL output mixing ratio/dry mole fraction directly. Therefore, no additional conversion nor WPL-correction is required. The LGR FGGA analyzer requires a spectroscopic correction (Hiller et al. 2012; Peltola et al. 2014), which is performed directly in TK3's input routine. Similarly, the spectroscopic corrections for the methane measurements of the LGR FGGA are applied on the high frequency data, which are directly converted to mixing ratios. This conversion to mixing ratios makes an explicit dilution correction redundant (Ibrom et al. 2007). The methane measurements of the LI-7700 are corrected as part of TK3's WPL-module for dilution and spectroscopic effects in a combined procedure as described in the instruments manual.

Table 4: Supported CH4/N2O gas analyzers and corrections applied by TK3

	LI-7700	TGA100	LGR	Aerodyne
Path-length for Moore correction (3.3.4)	500 mm	12 mm	10 mm	10 mm
WPL-correction for temperature fluctuations (3.3.6)	X	-	-	-
WPL-correction for humidity fluctuations (3.3.6)	X	X	-	-
WPL-correction for spectroscopic effects	X	-	-	-
Conversion of high-frequency data to mixing ratio	-	-	X	-

3.3.1 Cross wind correction of the sonic temperature

The cross wind correction follows Kaimal and Finnigan (1994) with the specification for different sonic types by Liu et al. (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) with coefficients given in Table 4.

$$\sigma_{T_c}^2 = \sigma_{Ts}^2 - \frac{4\overline{T}^2}{(c^2)^2}\left(\overline{u'^2}\,\overline{u}^2 A^2 + \overline{v'^2}\,\overline{v}^2 B^2 + 2\overline{u'v'}\,\overline{u}\,\overline{v}AB\right) + \frac{4\overline{T}}{c^2}\left(\overline{u'T'}\,\overline{u}A + \overline{v'T'}\,\overline{v}B\right) + \frac{2.04\overline{T}}{c^2}\left(\overline{u'q'}\,\overline{u}A + \overline{v'q'}\,\overline{v}B\right) \quad \textbf{(6)}$$

$$\overline{w'T'}_c = \overline{w'T'_s} + \frac{2\overline{T}}{c^2}\left(\overline{w'u'}\,\overline{u}A + \overline{w'v'}\,\overline{v}B\right) \quad \textbf{(7)}$$

Table 4: Coefficients for cross wind correction after Liu et al. (2001)

Factors	CSAT3	USA-1	Solent R3,R3A,HS	Solent R2
A	7/8	¾	$1 - 2\cos^2\varphi$	½
B	7/8	¾	$1 - 2\cos^2\varphi$	½

3.3.2 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**.

$$\begin{bmatrix} u_m \\ v_m \\ w_m \end{bmatrix} = \mathbf{A}\begin{bmatrix} u \\ v \\ w \end{bmatrix} \quad \textbf{(8)}$$

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 8). These rotations can be described by three rotation matrices **B**, **C**, **D** and three angles γ, β, α.

$$\mathbf{A} = \mathbf{BCD}, \quad \textbf{(9)}$$

where

$$\mathbf{B} = \begin{bmatrix} \cos\gamma & -\sin\gamma & 0 \\ \sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \textbf{(10)}$$

$$\mathbf{C} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\beta & -\sin\beta \\ 0 & \sin\beta & \cos\beta \end{bmatrix}, \quad \textbf{(11)}$$

$$\mathbf{D} = \begin{bmatrix} \cos\alpha & 0 & \sin\alpha \\ 0 & 1 & 0 \\ -\sin\alpha & 0 & \cos\alpha \end{bmatrix}. \tag{12}$$

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.

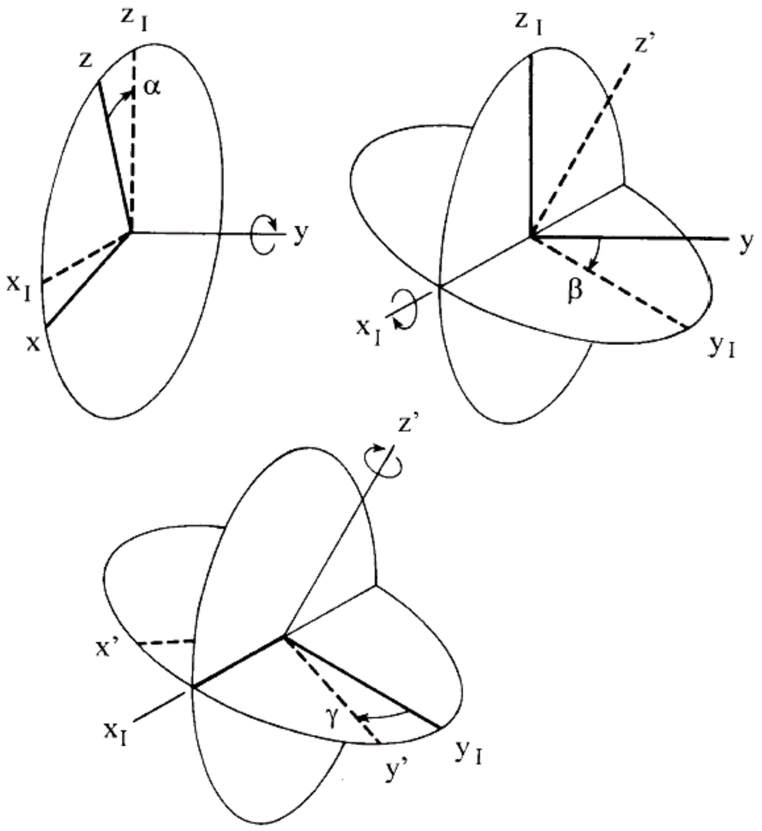


Figure 8: Definition of rotation angles after Wilczak et al. (2001)

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 (Paw U et al. 2000; Siebicke et al. 2012), 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 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.

$$\overline{\vec{u}_p} = \mathbf{P}\left(\overline{\vec{u}_m} - \vec{c}\right), \tag{13}$$

$$\begin{aligned} \overline{u_p} &= p_{11}(\overline{u_m} - c_1) + p_{12}(\overline{v_m} - c_2) + p_{13}(\overline{w_m} - c_3), \\ \overline{v_p} &= p_{21}(\overline{u_m} - c_1) + p_{22}(\overline{v_m} - c_2) + p_{23}(\overline{w_m} - c_3), \\ \overline{w_p} &= p_{31}(\overline{u_m} - c_1) + p_{32}(\overline{v_m} - c_2) + p_{33}(\overline{w_m} - c_3). \end{aligned} \tag{14}$$

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.

$$\overline{w_m} = c_3 - \frac{p_{31}}{p_{33}}\overline{u_m} - \frac{p_{32}}{p_{33}}\overline{v_m} = b_0 - b_1\overline{u_m} - b_2\overline{v_m} \tag{15}$$

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

$$\begin{aligned} p_{31} &= \frac{-b_1}{\sqrt{b_1^2 + b_2^2 + 1}} \\ p_{32} &= \frac{-b_2}{\sqrt{b_1^2 + b_2^2 + 1}} \\ p_{33} &= \frac{1}{\sqrt{b_1^2 + b_2^2 + 1}} \end{aligned} \tag{16}$$

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

$$\mathbf{P} = \mathbf{D}^{\mathbf{T}}\mathbf{C}^{\mathbf{T}} \tag{17}$$

and

$$\begin{aligned} p_{31} &= \sin\alpha, \\ p_{32} &= -\cos\alpha\sin\beta, \\ p_{33} &= \cos\alpha\sin\beta. \end{aligned} \tag{18}$$

Therefore

$$
\begin{aligned}
&\tan\beta = -p_{32} / p_{33}, \\
&\sin\beta = -p_{32} / \sqrt{p_{32}^2 + p_{33}^2}, \\
&\cos\beta = p_{33} / \sqrt{p_{32}^2 + p_{33}^2}, \\
&\sin\alpha = p_{31}, \\
&\cos\alpha = \sqrt{p_{32}^2 + p_{33}^2}.
\end{aligned}
\tag{19}
$$

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.

In TK3, the coordinate transformation is not applied on the high-frequency data but on the already calculated averages, variances and covariances, which is much more time-efficient and leads to the same results.

Coordinate rotation of scalar covariances:

$$
\begin{bmatrix} \overline{u_m'T'} \\ \overline{v_m'T'} \\ \overline{w_m'T'} \end{bmatrix} = \mathbf{A} \begin{bmatrix} \overline{u'T'} \\ \overline{v'T'} \\ \overline{w'T'} \end{bmatrix}
\tag{20}
$$

Coordinate rotation of the stress tensor:

$$
\begin{bmatrix} \overline{u_m'u_m'} & \overline{u_m'v_m'} & \overline{u_m'w_m'} \\ \overline{v_m'u_m'} & \overline{v_m'v_m'} & \overline{v_m'w_m'} \\ \overline{w_m'u_m'} & \overline{w_m'v_m'} & \overline{w_m'w_m'} \end{bmatrix} = \mathbf{A} \begin{bmatrix} \overline{u'u'} & \overline{u'v'} & \overline{u'w'} \\ \overline{v'u'} & \overline{v'v'} & \overline{v'w'} \\ \overline{w'u'} & \overline{w'v'} & \overline{w'w'} \end{bmatrix} \mathbf{A}^{\mathbf{T}}
\tag{21}
$$

Double Rotation

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

First rotation:

$$
\bar{v} = 0\,; \;\; \tan\gamma = \left(\frac{\overline{v_m}}{\overline{u_m}} \right).
\tag{22}
$$

Second rotation:

$$\overline{w} = 0\,;\;\; \tan\alpha = \left(\frac{\overline{w_m}}{\overline{\overline{u_m}}}\right). \tag{23}$$

Some authors perform an additional third rotation (Kaimal and Finnigan 1994; Aubinet et al. 2000). As it can create very unrealistic values, we don't recommend this third rotation (Aubinet et al. 2003). It is not implemented in TK3. For permanent running measuring programmes, the double rotation is often easier to handle than the planar fit method (Rebmann et al. 2012), because critical data at night and with low winds are excluded with the u_*-criterion.

3.3.3 Correction of spectral loss

The correction algorithm follows basically the idea proposed in paper by Moore (1986), not considering the phase shift of a low pass-filter as proposed by Horst (2000). The error *ΔF/F* of a turbulent flux, which is caused by spectral loss, can be expressed

$$\frac{\Delta F}{F} = 1 - \frac{\int_0^\infty T_{x(y)}(f)\cdot S_{x(y)}(f)\,df}{\int_0^\infty S_{x(y)}(f)\,df} \tag{24}$$

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

Other used methods (Eugster and Senn 1995; Moncrieff et al. 1997; Massman 2000) are not implemented. For comparison of the methods see Fratini and Mauder (2014).

High frequency loss due to path length averaging of vectors

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

$$T_w(n) = \frac{2}{\pi n}\cdot\left(1 + \frac{e^{-2\pi n}}{2} - \frac{3\left(1 - e^{-2\pi n}\right)}{4\pi n}\right) \tag{25}$$

$$n = \frac{f\cdot p}{\overline{u}} \tag{26}$$

In TK3 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, H_2O and CO_2 (Moore 1986):

$$T_p(n) = \frac{1}{2\pi n}\left(3 + e^{-2\pi n} - 4\cdot\frac{1 - e^{-2\pi n}}{2\pi n}\right) \tag{27}$$

$$n = \frac{f\cdot p}{\overline{u}} \tag{28}$$

High frequency loss due to spatial separation of sensors

Lateral separation (Moore 1986):

$$T_s(n) = e^{-9.9n^{1.5}} \tag{29}$$

$$n = \frac{f \cdot s}{\bar{u}} \tag{30}$$

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).

$$s_{lateral} = s_{total} \left|\sin(dir)\right| \tag{31}$$

A correction of the longitudinal sensor separation is only necessary, if the covariance was not maximized by cross correlation analysis before (see 3.2.1). 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).

$$G(f) = 1/[1 + (2\pi f \tau)^2] \tag{32}$$

Note that Moore (1986) incorrectly uses the square root of (32) in his analysis (Horst 1997).

High frequency loss due to electronic filtering

Some gas analysers apply an electronic or digital low-pass filter in order to reduce high frequency noise and aliasing. The corresponding high frequency loss of the actual signal can be corrected for by using this transfer function if the cut-off frequency n_0 is known (Moore 1986).

$$G(f) = 1/[1 + \left(\frac{n}{n_0}\right)^4] \tag{33}$$

This same transfer function can also be used for correcting **tube dampening effects** of closed-path sensors, if the corresponding cut-off frequency has been determined from analysis of the measured spectra. Note that again Moore (1986) incorrectly uses the square root of (33) in his analysis.

Spectral models for stable stratification

After Moore (1986) normalised spectra are parameterised according to

$$[f \cdot S_x(f)]_{norm} = \frac{n}{A_x + 3.124 \cdot (A_x)^{-2/3} \cdot n^{5/3}} \tag{34}$$

Parameter *A* for vertical wind velocity w:

$$A_w = 0.838 + 1.172 \cdot \frac{z}{L} \tag{35}$$

Parameter *A* for horizontal wind velocity u:

$$A_u = 0.2 \cdot A_w \tag{36}$$

Parameter *A* for scalars T, H_2O and CO_2:

$$A_T = 0.0961 + 0.644 \cdot \left(\frac{z}{L}\right)^{0.6} \tag{37}$$

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 (Foken 2008a). In TK3 the cospectra under stable stratification are parameterised after Kaimal et al. (1972) for the covariances $\overline{w'u'}$ and $\overline{w'T'}$ in the following way.

$$\frac{f \cdot S_{xy}(f)}{u_* \cdot y_*} = \frac{0.88 \frac{n}{n_0}}{1 + 1.5 \cdot \left(\frac{n}{n_0}\right)^{2.1}} \tag{38}$$

$$n_{0,uw} = 0.10 \cdot \left(1 + 7.9 \frac{z}{L}\right)^{0.75} \tag{39}$$

$$n_{0,wT} = 0.23 \cdot \left(1 + 6.4 \frac{z}{L}\right)^{0.75} \tag{40}$$

For the covariances of the scalars H_2O and CO_2 the same cospectral model can be used as for $\overline{w'T'}$.

Spectral models for unstable stratification

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

$$\frac{f \cdot S_w(f)}{u_*^2} = \frac{2n}{1 + 5.3n^{5/3}} + \frac{32n\zeta}{(1 + 17n)^{5/3}} \tag{41}$$

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

$$\frac{f \cdot S_u(f)}{u_*^2} = \frac{105n}{1 + 33n^{5/3}} + \frac{0.5n_i}{(1 + 2.2n_i)^{5/3}} \left(\frac{z_i}{-L}\right)^{2/3} \tag{42}$$

where

$$n = \frac{f \cdot z}{\overline{u}}, n_i = \frac{f \cdot z_i}{\overline{u}} \tag{43}$$

and z_i is the boundary-layer height. For simplicity, TK3 sets z_i = 1000 m.

Model for spectra of scalars T, H_2O and CO_2 under unstable conditions after Kaimal et al. (1972)

$$\frac{f \cdot S_T(f)}{T_*^2} = \begin{cases} \dfrac{53.4n}{(1+24n)^{5/3}} & n < 0.15 \\ \dfrac{24.4n}{(1+12.5n)^{5/3}} & n \geq 0.15 \end{cases} \tag{44}$$

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

$$-\frac{f \cdot S_{uw}(f)}{u_*^2} = \frac{14n}{(1+9.6n)^{2.4}} \tag{45}$$

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

$$\frac{f \cdot S_{wT}(f)}{\overline{w'T'}} = \begin{cases} \dfrac{11n}{(1+13.3n)^{1.75}} & n < 1 \\ \dfrac{4.4n}{(1+3.8n)^{2.4}} & n \geq 1 \end{cases} \tag{46}$$

For the covariances of the scalars H_2O and CO_2 the same cospectral model can be used like for $\overline{w'T'}$.

3.3.4 Conversion of fluctuations of sonic temperature into actual temperature (SND-correction)

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). This Schotanus-correction was recently renamed as SND-correction according to the three authors of the paper (Foken et al. 2012c).

$$\sigma_{T_c}^2 = \sigma_{Ts}^2 - 1.02\overline{Tq'T'} - 0.51^2\,\overline{q'^2}\,\overline{T}^2 \tag{47}$$

$$\overline{w'T'} = \overline{w'T_s'} - 0.51 \cdot \overline{T} \cdot \overline{w'q'} \tag{48}$$

If no fast response measurement of water vapour is available to determine the turbulent latent heat flux equation (48) cannot be resolved. In this case the Bowen ratio *Bo* derived from profile or gradient measurements can be used to convert the sonic temperature fluctuations into fluctuations of the actual temperature (Foken 2008a) using the following equation:

$$\overline{w'T'} = \frac{\overline{w'T_s'}}{1+\frac{0.51\cdot\overline{T}\cdot c_p}{\lambda\cdot Bo}} \qquad (49)$$

However, this calculation is not implemented in TK3 as standard option (only for the Modified Bowen Ratio Method) and has to be applied by the user manually. There two options to do this. (1) Determine Bo from profile measurements and use Eq. 49 to do the correction after running the TK3. (2) Determine Bo from profile measurements and calculate the latent heat flux λE = H/Bo and insert this λE in the TK3 raw statistics file for periods with missing direct latent heat flux measurements. Both options lead to some additional error of the heat flux estimates. For both options, λE is calculated using an uncorrected H. However, this problem can be resolved by doing this calculation in an iterative manner. If option 2 is applied, an additional error can occur since the inserted λE estimates will be treated by TK3 as eddy-covariance fluxes and therefore exposed to further corrections (e.g. planar fit, WPL, Moore) which do not apply for fluxes from profile measurements.

Note: If the output of the buoyancy flux is required, then run programme without SND-correction.

3.3.5 Correction for density fluctuations (WPL-correction)

To determine turbulent fluxes of air constituents like H_2O and 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 (Webb et al. 1980; Fuehrer and Friehe 2002; Liebethal and Foken 2003; Liebethal and Foken 2004; Leuning 2007; Foken et al. 2012c).

In general the correct flux of a scalar quantity, e.g. CO_2 or CH_4, is calculated after

$$F_c = \overline{w^{'}\rho_c^{'}} + \mu\cdot\frac{\overline{\rho_c}}{\overline{\rho_a}}\cdot\overline{w^{'}\rho_v^{'}} + (1+\mu\sigma)\cdot\overline{\rho_c}\cdot\frac{\overline{w^{'}T^{'}}}{\overline{T}} \qquad (50)$$

F_c: correct flux of scalar quantity

ρ_c: density of scalar quantity

ρ_a: density of dry air

ρ_v: density of water vapour

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

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

The general formula (50) can be simplified for the correction of H_2O-fluxes /latent heat fluxes

$$F_v = (1+\mu\sigma)\cdot\left(\overline{w'\rho_v'} + \overline{\rho_v}\cdot\frac{\overline{w'T'}}{\overline{T}}\right) \tag{51}$$

For open-path sensors the above equations should be applied (Eq. for H_2O and Eq. 50 for all other trace gases). For closed-path sensors, the pressure and temperature effect on density fluctuations can be considered negligible, and only the humidity effect should be accounted for, i.e. the term containing the temperature covariance in Eq. 49 is zero and the rest of the equations stays the same. If N_2O is measured by a Campbell TGA-100 normally a scrubber is used to remove H_2O from the sampling air, then also the second term of Eq. 49 becomes zero and no WPL-correction is needed provided the H_2O is completely removed. This correction is implemented depending on the instrument type in TK3 (see Table 3).

An energy balance closure correction for WPL according to (Liu et al. 2006) is not recommended since the lack of energy balance closure is not attributed to turbulent transport at the location of the sonic, which would cause density fluctuations, but rather to very long wavelength flux contributions, spatially stationary circulations or advection (Foken 2008b; Foken et al. 2012b).

3.3.6 Correction of oxygen cross sensitivity for Krypton hygrometers

Krypton hygrometers are used to measure the water vapour content of the air by absorption of H_2O molecules in the ultraviolet spectrum. Due to the used wave length there is a cross sensitivity to O_2 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)

$$\overline{w'H_2O'} = \overline{w'KH20'} + C_{ko}\left(\frac{\rho_d}{T}\right)\overline{w'T'} \tag{52}$$

where

$$C_{ko} = \frac{ko}{kw}\cdot\frac{CoMo}{Ma} = 0.23\cdot\frac{ko}{kw} \tag{53}$$

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 *k*o 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.

3.3.7 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. TK3 iterates the corrections until the results for the heat fluxes and CO_2 fluxes don't change more than 0.01 % from one step to the next one according to Mauder and Foken (Mauder and Foken 2006).

3.3.8 Conversion of units

The covariances are generally calculated in kinematic units, e.g. K m s^{-1} for the sensible heat flux, and are converted to fluxes in energetic units after all corrections described above are carried out. This is done using the following equations in accordance with Foken (2008a) and Stull (1988).

The sensible heat flux is

$$Q_H[Wm^{-2}] = c_p \cdot \rho \cdot \overline{w'T'}[\mathrm{Kms^{-1}}] \tag{54}$$

The latent heat flux is

$$Q_E[Wm^{-2}] = \lambda \cdot \overline{w'a'}[\mathrm{kgm^{-2}s^{-1}}] \tag{55}$$

The specific heat capacitiy of dry air at constant pressure is

$$c_{p,d} = 1004.67\mathrm{JK^{-1}kg^{-1}} \tag{56}$$

The specific heat capacitiy of moist air at constant pressure is

$$c_p = c_{p,d} \cdot (1 + 0.84 \cdot q)\,, \tag{57}$$

where *q* is the specific humidity in kg kg^{-1}

$$q = 0.622\frac{e}{p - 0.378 \cdot e}\,, \tag{58}$$

where *e* is the vapour pressure in hPa

$$e = \frac{a \cdot T}{0.21668} \tag{59}$$

The density of the air is

$$\rho = \frac{p[\text{Pa}]}{R_a \cdot T_v[\text{K}]}, \tag{60}$$

where R_a is the gas constant for dry air

$$R_a = 287.0586 \text{Jkg}^{-1}\text{K}^{-1} \tag{61}$$

and T_v the virtual temperature

$$T_v = T(1 + 0.61q) \tag{62}$$

If humidity measurements are not available the sonic temperature is used, which is nearly equal to the virtual temperature (Kaimal and Gaynor 1991).

The specific heat of evaporation is

$$\lambda[\text{Jkg}^{-1}] = 2501000 - 2370 \cdot t[°\text{C}] \tag{63}$$

4 Quality control

4.1 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):

$$\left(\overline{x'w'}\right)_i = \tfrac{1}{N-1}\left[\sum_j x_j \cdot w_j - \tfrac{1}{N}\left(\sum_j x_j \cdot \sum_j w_j\right)\right] \tag{64}$$

$$\overline{x'w'} = \tfrac{1}{M}\sum_i \left(\overline{x'w'}\right)_i$$

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

$$\left[\overline{x'y'}\right]_{30\,\mathrm{min}} = \frac{1}{M \cdot N - 1}\left\{\sum_i \left(\sum_j x_j \cdot y_j\right)_i - \frac{1}{M \cdot N}\left[\sum_i \left(\sum_j x_j\right)_i \cdot \sum_i \left(\sum_j y_j\right)_i\right]\right\} \tag{65}$$

A time series is considered to be steady state if the difference between both covariances RN_{Cov} is lower 30 %.

$$RN_{Cov} = \left|\frac{\overline{\left(x'w'\right)}_{eq(50)} - \overline{\left(x'w'\right)}_{eq(51)}}{\overline{\left(x'w'\right)}_{eq(51)}}\right| \tag{66}$$

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). The classification is given in Table 5.

Table 5: Classification scheme for the steady state test after Foken (1999)

Class	range
1	0–15 %
2	16–30 %
3	31–50 %
4	51–75 %
5	76–100 %
6	101–250 %
7	251–500 %
8	501–1000 %
9	> 1000 %

4.2 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 (Kaimal and Finnigan 1994; Foken and Wichura 1996) and can be found in all textbooks (Stull 1988; Kaimal and Finnigan 1994; Foken 2008a). 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

$$\frac{\sigma_{u,v,w}}{u_*} = c_1 \cdot \left(\frac{z}{L}\right)^{c_2} \tag{67}$$

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_*)

$$\frac{\sigma_x}{X_*} = c_1 \cdot \left(\frac{z}{L}\right)^{c_2} \tag{68}$$

For coefficients see Table 6.

Table 6: Constant values for c_1 und c_2 after Foken at al. (1991)

Parameter	z/L	c_1	c_2
$\frac{\sigma_u}{u_*}$	0 > z/L > -0,032	2.7	0
	-0,032 > z/L	4.15	1/8
$\frac{\sigma_w}{u_*}$	0 > z/L > -0,032	1.3	0
	-0,032 > z/L	2.0	1/8
$\frac{\sigma_T}{T_*}$	0.02 < z/L <1	1.4	-1/4
	0.02 > z/L >-0.062	0.5	-1/2
	-0.062 > z/L >-1	1.0	-1/4
	-1 > z/L	1.0	-1/3

As there are no parameterisations for stable stratifications available, we used the same parameterisations as in the unstable case for |z/L|. Nevertheless, particularly the parameterisations for normalized temperature are not well defined for stable stratification. Therefore, TK3 offers the option to turn this test off in the parameter file (!use_itc_T). All quality tests are applied after the flux conversions and corrections.

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 Table 6 in the stability range, which it is defined in Table 7.

Table 7: Model for integral turbulence characteristics for near neutral stratifications after Thomas and Foken (2002)

Parameter	-0.2 < z/L < 0.4
$\frac{\sigma_u}{u_*}$	$0.44\ln\left(\frac{z_+ \cdot f}{u_*}\right) + 6.3 \qquad z_+ = 1m$
$\frac{\sigma_w}{u_*}$	$0.21\ln\left(\frac{z_+ \cdot f}{u_*}\right) + 3.1 \qquad z_+ = 1m$

For measurements inside the canopy (z < h_c) a parameterization according to Rannik et al. (2003) should be applied

$$\frac{\sigma_i}{u_*} = a_i\left\{\exp\left[-\alpha_i\left(1-\frac{z}{h_c}\right)^{\beta_i}\right](1-\gamma_i)+\gamma_i\right\} \tag{69}$$

$$i = u, v, w; \quad z < h_c$$

and above the canopy the above given parameterizations are used. The values are given in Table 8. A selection of the coefficients sets is possible.

Table 8: Coefficients for Eq. (66)

Reference	i	a_i	α_i	β_i	γ_i
Rannik et al. (2003), neutral, for Hyytiäla site	u	2.30	1.0	1.0	-0.3
	v	1.75	1.0	0.85	-0.2
	w	1.25	0.9	1.2	-0.63
Foken et al (2012a), near neutral Waldstein Weidenbrunnen site	u	2.01	8.97	1.37	0.29
	v	1.60	5.18	1.11	0.34
	w	1.13	0.9	1.2	-0.63

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

$$ITC_\sigma = \left| \frac{\left(\sigma_x / X_* \right)_{model} - \left(\sigma_x / X_* \right)_{measurement}}{\left(\sigma_x / X_* \right)_{model}} \right| \tag{70}$$

If the test parameter ITC_σ *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 $10 Wm^{-2}$, because σ_T / T_* is not well defined in this case. The classification is given in Table 9.

Table 9: Classification scheme for the integral turbulence characteristics test after Foken (1999)

Class	Range
1	0–15 %
2	16–30 %
3	31–50 %
4	51–75 %
5	76–100 %
6	101–250 %
7	251–500 %
8	501–1000 %
9	> 1000 %

4.3 Overall flag systems

An overall quality flag is created by the TK3 software for the test parameters friction velocity *ustar*, sensible heat flux determined by sonic temperature measurement H_{Ts}, sensible heat flux determined by platinum temperature measurement H_{Tp}, latent heat flux *LvE*, and the CO_2-flux $\overline{w'CO_2'}$. Table 10 shows which test is applied for which test parameter.

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

Table10: Overview of the applied tests for each test parameter

Test parameter	Steady state test	ITC σ_u / u_* test	ITC σ_w / u_* test	ITC σ_{Ts} / Ts_* test	ITC σ_{Tp} / Tp_* test
Ustar	$\overline{u'w'}$, $\overline{v'w'}$	x	x		
H_{Ts}	$\overline{w'T_s'}$		x	x	
H_{Tp}	$\overline{w'T_p'}$		x		x
LvE	$\overline{w'a'}$		x		
$\overline{w'CO_2'}$	$\overline{w'CO_2'}$		x		

4.3.1 Scheme after Foken (1999)

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 11, 12). For details see also Foken et al. (2004; 2012c).

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.

Table 11: Overall flag system after Foken (1999)

steady state (flag)	integral turbulence characteristic (flag)	Final flag
1	1 – 2	**1**
2	1 – 2	**2**
1 – 2	3 – 4	**3**
3 – 4	1 – 2	**4**
1 – 4	3 – 5	**5**
5	≤ 5	**6**
≤ 6	≤ 6	**7**
≤ 8	≤ 8	**8**
9	9	**9**

Table 12: Overall flag system after Foken (1999); deviations in %

steady state (deviation in %)	integral turbulence characteristic (deviation in %)	Final flag
0 – 15	0 – 30	**1**
16 – 30	0 – 30	**2**
0 – 30	31 – 75	**3**
31 – 75	0 – 30	**4**
0 – 75	31 – 100	**5**
76 – 100	0 – 100	**6**
0 – 250	0 – 250	**7**
0 – 1000	0 – 1000	**8**
> 1000	> 1000	**9**

4.3.2 Scheme after Rebmann et al. (2005)

Integral turbulence characteristics are calculated for u, w, T (Table 13 and 14). This system was used for footprint calculations in combination with a data quality analysis (Rebmann et al. 2005; Göckede et al. 2008).

Table 13: Overall flag system after Rebmann et al. (2005)

steady state (flag)	integral turbulence characteristic (flag)	Final flag
1 – 2	1 – 2	**1**
1 – 2	3 – 4	**2**
3 – 4	3 – 4	**3**
3 – 4	5 – 6	**4**
5 – 9	7 – 9	**5**

Table 14: Overall flag system after Rebmann et al. (2005); deviations in %

steady state (deviation in %)	integral turbulence characteristic (deviation in %)	Final flag
0-30	0-30	**1**
0-30	31-75	**2**
31-75	31-75	**3**
31-75	76-250	**4**
>75	>250	**5**

The scheme after Rebmann et al. (2005) is a simplified version of the scheme after Foken (1999). 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.

4.3.3 Scheme after the Spoleto agreement, 2004 for CarboEurope-IP

Integral turbulence characteristics are calculated for w only, not for T (Table 15, 16). For details see also Mauder et al. (Mauder et al. 2013).

Table 15: Overall flag system after the Spoleto agreement, 2004 for CarboEurope-IP

steady state (flag)	integral turbulence characteristic (flag)	Final flag
1 – 2	1 - 2	**0**
<= 5	<= 5	**1**
>= 6	>= 6	**2**

Table 16: Overall flag system after the Spoleto agreement, 2004 for CarboEurope-IP, deviations in %

steady state (deviation in %)	integral turbulence characteristic (deviation in %)	Final flag
< 30	< 30	**0**
< 100	< 100	**1**
> 100	> 100	**2**

4.3.4 Interpretation of the quality classes

For practical application the quality flags can be interpreted in the following way:

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 17).

Table 172: Comparative overview of the different overall quality flag schemes presented

	Flags after Foken (1999), see also Foken et al. (2004; 2012c)	Flags after Rebmann et al. (2005)	Flags after the Spoleto agreement, see also Mauder et al. (2013)
high quality data, use in fundamental research possible	**1-3**	**1-2**	**0**
moderate quality data, for use in long term observation programs	**4-6**	**3-4**	**1**
low data quality, gap filling necessary	**7-9**	**5**	**2**

5 Special calculations

5.1 Spectra

It is possible to calculate spectra and cospectra using TK3. If the option !spectra_on is turned on, the calculation is done after the creation of the binary files. The output is also in the work-directory. The file names are for the same periods as the binary files, just with spe as suffix instead of bin. These files are in comma-separated ASCII-format and have the following columns:

```
f,Su,Sv,Sw,STs,Sa,Sc,Sn2o,SCH4,Co uw,Co wTs,Co wa,Co wc,Co n2o, Co CH4
```

where f is the natural frequency, and S indicates the spectral energy density for a specific variable and Co indicates the cospectral energy density of two variables.

The spectral analysis is based on Stull (1988) including bell tapering and linear detrending. The option !spectra was only programmed for test purposes. If the user decides to turn this option on we recommend careful plausibility tests of the results.

5.2 Triple covariances

TK3 also provides an option to calculate third order statistical moments or so-called triple covariances (!3rd moments). These results are written into a separate output file with a name ending on 3rd001.csv in the work-directory. These files are in comma-separated ASCII-format and have the following columns:

```
T_begin,T_end,<w'u'u'> (m3 s-3),<w'v'v'> (m3 s-3),<w'w'w'> (m3 s-3),<w'Ts'Ts'> (K2 m s-1),<w'a'a'> (g2 m-5 s-1),<w'Ts'a'> (K g m-2 s-1),<Ts'Ts'Ts'> (K3),<a'a'a'> (g3 m-9),<w'w'Ts'> (K m2 s-2) ,<w'w'a'> (g m-1 s-2),<w'w'u'> (m3 s-3)
```

5.3 Ogives

It is possible to calculated fluxes for extending averaging time with TK3 using the option !ogives_on. This calculation is based on the short term averaging interval and these covariances are then put together using Eq. (4) for increasing intervals up to 720 minutes. The output of this function is in the output-directory. This was only programmed for test purposes. If the user decides to turn this option on we recommend careful plausibility tests of the results.

5.4 Storage flux

A simple method for estimating the CO_2 storage flux F_S from one point CO_2 measurements was suggested by Hollinger et al. (1994). It assumes the same mean CO_2 density ρ_C for the entire air column below measurement height (z_m):

$$F_S = \frac{\overline{\rho_{C(i+1)}} - \rho_{C(i-1)}}{t_{(i+1)} - t_{(i-1)}} z_m \qquad (71)$$

where *i* denotes a certain measurement interval and *t* the time reference of a measurement interval. If the option !stor_flux is set true then this calculation is conducted and this storage flux is added to the NEE output in the result file. Otherwise the NEE output corresponds to the corrected covariance between the vertical velocity *w* and CO_2. This simple storage flux calculation is controversial, particularly for measurements above tall vegetation. It is not generally recommended and an analysis of CO_2 profile measurements may be preferable.

5.5 Footprint

In addition to the established quality-control procedures, such as the test of Foken and Wichura (1996) it is also necessary to check whether the measurements at the tower are of the ecosystem flux of the target land cover (Göckede et al. 2008). This problem is usually addressed using footprint models (Schmid 1997). TK3 uses the footprint model of Kormann and Meixner (2001) to determine the fraction of the footprint that lies in the area of interest. Up to two target land covers can be defined in a gridded map indicated by numbers 1 and 2. The rest of the area that is not targeted is indicated by 0. Areas, where no data are available can be indicated by a number as well, e.g. -9999. This map has to be saved as ARC-GIS/ESRI compatible ASCII grid with the suffix .asc (http://en.wikipedia.org/wiki/Esri_grid). This file requires a header like the following example

```
ncols         627

nrows         429

xllcorner     4429831.1322128

yllcorner     5348237.0618119

cellsize      10

NODATA_value  -9999
```

Where ncols stands for the number of columns, nrows for the number of rows, xllcorner for the x-coordinate of the lower left corner of the map and yllcorner for the y-coordinate of the map. As coordinate system, we recommend using UTM, but it is also possible to use any other relative coordinates in units of metres. Of course the position of the tower has to be provided in the same coordinate system; this is done in the parameter for example in the following manner

```
#Sensor location in UTM coordinate system [REAL]

!m_easting

654093

!m_northing

5350514
```

6 Data input/output 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 TK3 is also able to read the direct output files of data acquisition systems, e. g. output Campbell Scientific data loggers CR23X and CR10X, CR3000, CR5000, SLT-files produced by EDDYMEAS (meteotools, Jena) or file format of the data acquisition software ATEM (Ruppert 2005). A standard data format was developed for the data exchange in CarboEurope-IP.

6.1 Format for high frequency raw data

One important improvement of TK3 compared to the previous version is a more flexible and comfortable input routine. It is now possible (when choosing ASCIIcsv as input format) to read in data in comma-separated ASCII-format with up to 18 columns. The number and the order of the columns can be specified in the parameter-file. For the time-stamp the following formats are allowed, which also has to be defined in the parameter-file:

1 = CR23x, e.g. 254,1030,30.44

2 = TOA5, e.g. "2005-09-11 10:30:30.44"

3 = LabView, e.g. 254,10:30:30.44

Moreover, typical different units for specific columns can be selected in the parameter-file.

The old HIRATE input file format is still supported. 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 normally defined in a right hand coordinate system if not differently specified (parameter !lefthand).

A file header information like this example is optional (parameter !header_info):

```
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.

Normally, all the information about the measurement setup is provided in the parameter file. This option is only suitable, if the configurations don’t change for one run of the program. The file header information is an optional input for the calculations and quality tests in TK3. Changes in the measurement setup can be tracked as they are given in the beginning of each file and can be considered for the calculations.

6.2 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.

A file header information like this example is optional (parameter !header_info):

```
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.

6.3 5-min and 30-min averaged data

High-frequency data files are often useful to find the reason for possible errors. However, only averaged data are available sometimes. Then, it is possible to use averaged data as input data for TK3 alternatively. This option can also be useful for reanalyzing data that were previously processed by TK3 with different setting for corrections or quality tests. These averaged input 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 cannot be performed.

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

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.

Different formats for averaged data are available in TK3. These can be selected in the parameter-file (!format_cov). See also EXAMPLE_5M001.CSV. This file corresponds to format_cov == 2.

If the quantities, which are listed in a column, are not measured, please fill up these columns with -9999.9. In order to be able to calculate averages, variances and covariances, it is necessary to have information about the specific number of values.

T_begin: Beginning of the averaging interval

T_end: Ending of the averaging interval

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 respective covariance

Cov[q'Ts']: covariance between specific humidty q and sonic temperature Ts, used for the Schotanus correction of the sonic temperature variance

h2o_lag, co2_lag: lag in time-steps of the automatic delay time determination by maximizing the covariance

If fluxes of the additional scalars N2O and CH4 shall be calculated (!format_cov = 8) then the statistics of these data are appended in subsequent columns:

N2O[nmol/mol], Var[N2O], Cov[u'N2O'], Cov[v'N2O'], Cov[w'N2O'], N(N2O), N(u'N2O'), N(v'N2O'), N(w'N2O'), lag(N2O), CH4[nmol mol], Var[CH4], Cov[u'CH4'], Cov[v'CH4'], Cov[w'CH4'], N(CH4), N(u'CH4'), N(v'CH4'), N(w'CH4'), lag(CH4)

6.4 Output of error estimates

The random error of the flux measurements is output in a separate file in the work directory called XXXXX_E001.csv if desired (!format_cov = 7; errors = T), . All calculations are as describe by Mauder et al. (2013). The random error due to the stochastic nature of turbulence (variance of a covariance, Finkelstein and Sims, 2001) is labeled rerr_ and the random error due to instrumental noise is labeled noise_. The columns are named as follows:

T_begin, T_end, rerr_uw, rerr_vw, rerr_wTs, rerr_wH2O, rerr_wCO2, rerr_wN2O, rerr_wCH4, noise_uw, noise_vw, noise_wTs, noise_wH2O, noise_wCO2, noise_wN2O, noise_wCH4

6.5 Output in result file

The first 34 columns of the result file contain the same quantities as in the 5-min or 30-min statistics file. However the corrections are now applied. Then follow:

Nvalue: Number of values in time interval (for u)

dir [°]: wind direction in degrees

ustar [m/s]: friction velocity

HTs[W/m2]: sensible heat flux from sonic temperature after application of all selected corrections and conversions

HTp[W/m2]: sensible heat flux from additional fine-wire temperature probe

LvE [W/m2]: latent heat flux

z/L: stability parameter, $z = z_m\text{-}d$; L is the Obukhov-length calculated with the actual temperature and the sensible heat flux

z/L-virt: stability parameter, $z = z_m\text{-}d$; L is the Obukhov-length calculated with the virtual temperature and the buoyancy flux (correct but not so common)

Flag(ustar): combined QA/QC-flag for ustar

Flag(HTs): combined QA/QC-flag for HTs

Flag(HTp): combined QA/QC-flag for HTp

Flag(LvE): combined QA/QC-flag for LvE

Flag(wCO2): combined QA/QC-flag for Cov(w'CO2')/NEE

T_mid: middle of time interval

FCstor[mmol/m2s]: storage flux

NEE [mmol/m2 s]: net ecosystem exchange comprising the Cov(w'CO2') and the storage flux if selected

Footprint_trgt_1: proportion of footprint from target area 1

Footprint_trgt_2: proportion of footprint from target area 2

Ftprnt_xmax[m]: x-distance of the maximum of the footprint function

r_err_ustar[%], r_err_HTs[%], r_err_LvE[%], r_err_co2[%], noise_ustar[%], noise_HTs[%], noise_LvE[%], noise_co2[%]

6.6 Output for N_2O

If N_2O concentrations are provided in the input data, the computed statistics, fluxes and results of the QA/QC-test are output in a separate file with in the output-directory with a filename [project]_n2o_[timestamp].csv. This file contains the following columns:

T_begin, T_end, N2O[umol/mol], Var[N2O], Cov[u'N2O'], Cov[v'N2O'], Cov[w'N2O'],

Fn2o (umol/m²s): N_2O-flux converted in units of (µmol/m²s),

Flag(Fn2o): combined flag representing the ITC-test for w and the steady state test for [w’n2o‘],

statflag_N2O: flag of the steady state test for [w’n2o‘]

r_err_N2O[%], noise_N2O[%]: stochastic error and noise error of N_2O-flux in %

6.7 Output for CH_4

If CH_4 concentrations are provided in the input data (!format_cov = 8), the computed statistics, fluxes and results of the QA/QC-test are output in a separate file with in the output-directory with a filename [project]_ch4_[timestamp].csv. This file contains the following columns:

T_begin, T_end, CH4[µmol/mol], Var[CH4], Cov[u'CH4'], Cov[v'CH4'], Cov[w'CH4'],

Fch4 (umol/m²s): CH4-flux converted in units of (µmol/m²s),

Flag(Fch4): combined flag representing the ITC-test for w and the steady state test for [w’ch4‘],

statflag_CH4: flag of the steady state test for [w’ch4‘]

r_err_CH4[%], noise_CH4[%]: stochastic error and noise error of CH_4-flux in %

6.8 Output of footprint maps

TK3 can calculate and output the two-dimensional footprint distribution for every 30-min interval (!footprint_out = T) in the same format as the land-use map that is required as input for this calculation (Sect. 5.5). This map is saved as ARC-GIS/ESRI compatible ASCII grid with the suffix .asc including a time stamp in the file name (http://en.wikipedia.org/wiki/Esri_grid). The header will be similar to the the following example

```
ncols         627
nrows         429
xllcorner     4429831.1322128
yllcorner     5348237.0618119
cellsize      10
NODATA_value  -9999
```

This output can then be used to calculate a cumulative flux footprint for a given site for a specified period of time, which is also called a footprint climatology (Göckede et al. 2008).

7 Commented example of the “parameter.vbp” file

```
# parameter.vbp
#
# The new Turbulence Knight (TK3) reads all input parameters from this file.
# TK3 may also be controlled by editing this file.
#
# Lines beginning with '!' serve as label for parameters to be read in the next line
# Lines beginning with '#' serve as comments and will be ignored
# Blank lines will be ignored as well
# Parameters shall be given with an explanation in the line above for better reading of this Input-File
#
#--------------------------------------------
# Path of input data
!path_in
'I:\Fendt\'
# Path of working directory
!path_work
'I:\Fendt\work\'
# Path of output data
!path_out
'I:\Fendt\out\'

# who did calculations
!author
'Matthias Mauder'

# Project Name
!project
TERENO

!header_info
F
#################### site and device data ####################
# sonic type (CSAT3,USA-1,Solent-HS,Solent-R3,Solent-R2,ATI-K,NUW,YOUNG)
!sonic_type
```

- Specify the paths of your directories.
- Enter name of executing person.
- Enter abbreviation of project name. This will be part of every file name created by TK2 (max. 5 letters).
- If !header_info is TRUE, then the following site and and device parameters will be taken from file header instead of this parameter file, see section 6.3.

```
'CSAT3'


# H20/CO2 instrument type (LI-7500,KH20,LI-6262,LI-7000,LI-7200,EC150,EC155,LGR,NONE)
!h2o_type
'LI-7500'
```

- The Sonic and H_2O/CO_2 instrument type are used for path length information required by the Moore correction and to determine the sonic path geometry required by the Schotanus/Liu correction.

```
# CH4 instrument type (LI-7700,LGR,Aerodyne,NONE)
!ch4_type
'NONE'


# hd: measuring height of the device in m (for each measuring complex), (REAL)
# hc: canopy height below the device in m (for each measuring complex), (REAL)
# wd: wind direction or of  the sonic’s orientation, i.e. what wind direction correspondes to positive u in deg. (REAL)
# height above sea level (REAL)
!dev_data
9.00,2.00,210.,1300.


# latitude(INTEGER)
!latitude
49,6,0
```

- Measurement height and canopy height are required for the calculation of the stability parameter z/L and height-dependent (co-)spectral models for the Moore correction.
- The latitude is required for the integral turbulence statistics test, specifically the parameterization under near-neutral conditions.

```
# Start time (day of year, hour, second) and end-time (integer,integer,real)s
!start
294,1200,0.0
!end
294,1400,0.0
!year
2009
```

Enter start and end time of data processing period.

```
# minutes in binary files (REAL)
!t_interval
 30
```

It is recommended to use the same interval for the binary files as for the flux averaging interval, which is in most cases 30 min.

```
# if binary files exist, type T (LOGICAL)
!load_binary
F
######################## INPUT DATA FILE ###################################
#Input file format ('ASCIIscv','SLT')
!input_file_format
'ASCIIcsv'

#High-frequency data are split into hourly files using the program
HourlySplitData by Danilo Dragoni and HaPe Schmid
!HourlySplitData
F

#number of records, total number of columns in input file, including time stamps
(INTEGER)
!number_of_records
15

#Format of time stamp
#1 = CR23x, e.g. 254,1030,30,44
#2 = TOA5, e.g. "2005-09-11 10:30:30.44"
#3 = LabView, e.g. 254,10:30:30.44
#4 = HaPe Split program, e.g. 254,10,30,33
!time_format
2

#Start column of each channels in input files, if not associated enter '0'
!column
       0,           1, 5, 6, 7,   8,      9, 10 ,   11,   13   , 0 ,   0,       0,
0,    12,    0,    0,    0,    14 , 15
#log_num, time_stamp, u, v, w, Ts,diagCS, co2, h2o,diagLI, Tp, o3, incl_x,
incl_y, LI_p, LI_T, CH4, N2O, HMP_T,HMP_RH

!Aerodyne_file
F
```

```
!data_Aero%file_name
'140821_000000.str'

#Units of channels in input data file, if not associated enter '0'
!unit_wind ('m s-1','cm s-1')
'm s-1'
!unit_Ts ('degC','K')
'degC'
!unit_co2 ('mV','mmol m-3','µmol mol-1','mg m-3')
'mg m-3'
!unit_h2o ('mV','g m-3','mmol mol-1','mmol m-3')
'g m-3'
!unit_Tp ('R R0-1','degC','K')
'0'
!unit_o3 ('µg m-3','ppb')
0
!unit_LI_p('kPa','hPa')
'kPa'
!unit_LI_T
0
!unit_CH4 ('umol mol-1','nmol mol-1','umol m-3')
0
!unit_N2O ('nmol mol-1')
0
!unit_HMP_T
'degC'
!unit_HMP_RH
'%'
```

It is planned to have the possibility to calculate fluxes of O$_3$, but this functionality is not fully implemented yet; so please enter ‘0’ for those scalars. CH$_4$ and N$_2$O are now supported.

```
#consistency limits, in same units as in input file
!input%log_num #Logger program ID number, e.g. for CR23X
0,0
!input%day #Day of year
1,366
!input%hour #Daily time
0,2400
!input%second #Seconds
0.0,60.0
```

Set 0,0 if not associated, IMPORTANT!

```
!input%u #Wind u
-50.0,50.0
!input%v #Wind v
-50.0,50.0
!input%w #Wind w
-10.0,10.0
!input%Ts #Sonic temperature
-20.,50.0
!input%diagCS #CSAT error code, usually counts up from 0 to 63
0,64
!input%co2 #CO2
0,5000
!input%h2o #H2O
0,5000
!input%Tp #Platinum temperature
0.,0.
!input%o3 #Ozone
0,0
!input%diagLI #diagnostic Licor
240,252
!input%incl_x #Inclinometer x-axis
0,0
!input%incl_y #Inclinometer y-axis
0,0
!input%LI_p
80,110
!input%LI_T
0,0
!input%CH4
0,0
!input%N2O
0,0
!input%HMP_T
-20,50
!input%HMP_RH
0,100

#Fixed time delays of channels in input data file [seconds]
```

```
!lag
0.1,0.1,0.1,0.1,0.3,0.3,0.0,0.0,   0.3,   0.0,   0.0,0.3 ,0.0 ,0.0,0.0, 0.0 , 0.0
#u , v , w , Ts,co2,h2o, Tp, o3, diagLI, incl_x, incl_y, LI_p, LI_T, CH4, N2O, HMP_T, HMP_RH

!lag_Aerodyne
4.,4.
#CH4,N2O

#Parameters are required to create an equidistant time scale
#TK3 will search for the data line in input file that matches the given time stamp best
#desired time interval or measure interval in sec (REAL)
#minimal time interval in sonic data file: very important (REAL
!calc_data
0.05,0.049

#What is missing value, what is the code for missing values in input file
!NaN
-99999

#name of first data file (all other files will be found by TK3 according to the given time window)
#lines in datafile must not contain more than 4096 characters, otherwise specification in TK3
#has to be changed
#format of the data file:
#Last 4 letters before the suffix: continuous number of file
#Example: EVAG1_0009.dat
!data%file_name
'CR3000_Eddy01.dat'

#What to do with missing values
#0 = insert NaN
#1 = take last value
#2 = interpolate
!mv_option
 0
```

```
#Missing values at the beginning of blocks will be ignored(F) or replaced(T)
!fill_up_missing_values_at_begin
F

## Calibration data #################
#left hand coordinate system (e.g. USA-1,Solent-R2):
!lefthand
F
#Head Correction for METEK USA-1: (0,1,3)
!HC
0
#Licor CO2: 0V and 5V equal [mmol/m³] if LI-7500 in mV, or [µmmol mol-1] if LI-
7000/LI-6262 in mV
!calib_data%co2
0, 1.

#Licor H2O: 0V and 5V equal [mmol/m³] if LI-7500 in mV, or [mmmol mol-1] if LI-
7000/LI-6262 in mV
!calib_data%h2o
0.,1.

#KH20: V0[mV], x, kw, ko
!calib_data%kh20
0.00, 0.0000,  0.0000, -0.0450
#AIR 150 cold wire thermometer
#offset at t0, reference resistivity, resistivity at t0, tk
!calib_data%pt150
17.5,100.,146.84,0.00366

!apply_spike_test #Apply MAD spike test (Mauder et al., 2013)
T
#values exceeding median+-'7'*std equivalent are spikes
7

#################### REFERENCE FILE ################################
#Reference option?
#0 = no reference measurements for pressure, temperature and humidity
```

```
#1 = reference measurements in same data file as turbulent data (e.g. from HMP45)
#2 = reference measurements in second data file (e.g. A6__M001.csv)
!ref_option
1

#Reference filename (includes reference for pressure, humidity and temperature)
!reference_daten%file_name
LI_A6_L0001.csv

#consistency limits
#Temperatur reference (degC)
!input%temp
0.,50.
#Humidity reference (g/m3)
!input%hum
0.,50.
#Pressure reference (hPa)
!input%pressure
800.,1100.

#------------------------------------------------------------------
```

Reference measurements are required for air, temperature T_ref, humidity a_ref and pressure p_ref to calculate the air density for example and to do unit conversions.

If no reference measurements are available (option 0) then T_ref is taken from the sonic temperature, a_ref is taken from the fast-response h2o-instrument, and p_ref is calculated using the height above sea-level and assuming standard atmospheric conditions.

If reference measurements are available in the high-frequency data file, e.g. from HMP45 and LI-7500 pressure then those can be used (option 1).

If reference measurements are recorded at a lower sampling rate, e.g. 1 min or 10 min, and stored in a separate data file then those can be read using the format described in sect. 6.2 (option 2).

```
############################ OUTPUT ################################
!ascii #ASCII Output of raw data(T/F),with flags (T) or without (F)
T,T
```

TK3 outputs error flags in the binary files and also in the high-frequency ASCII files, if selected (!ascii == T,T), for every high-frequency data point, providing information about the results of the automatic data quality assessment. This flag is encoded in a maximum 5 digit binary number. 0 means the data passed all tests. A binary digit is set from 0 to 1 for the following reasons, from right to left, position 0 being the rightmost digit:

0 = no value

1 = replaced with precursor

2 = out of bounds, exceeding consistency limits

3 = rejected by spike test

4 = interpolated

```
!invalid_data
T
```

- If invalid data is set true then whenever an error occurs during reading the input data then that line will be written into a separate file. This can be used for trouble shooting.

```
################## Calculation parameters ##########################
!load_statistics #files with Covariances already exist?
F
!calc_data%t_interval1 # Calculation time intervals in minutes
30
!calc_data%bad_max # maximum allowed number of missing/bad values in averaging
interval in % (REAL)
10
#format of the covariance output file
#0 = LITFASS-2003 standard exchange format
#1 = Mikrometeo with Sonic Nvalue (incl. wind direction, <w'e'>)
#2 = Mikrometeo and detailed Nmiss
#5 = Mikrometeo with Sonic Nvalue plus MBR psychrometers
```

```
#6 = Mikrometeo and detailed Nmiss, incl. N2O

#7 = like 2 plus random errors (allows for error calculation)

#8 = like 7, plus CH4, and N2O (allows for processing CH4 and N2O data)

!format_cov

7
```

- Option 5 is designated for the Modified Bowen Ratio system, including a sonic and two psychrometers, e.g. as distributed by METEK GmbH. This is not possible with input_format ASCIIcsv. Rather 5 or 10 min averages can serve as input and then be combined to longer time periods.
- Option 8 should be used if N_2O/CH_4 flux shall be evaluated; then separate output files will also be generated containing the results of those additional scalar fluxes. Currently, the only two N_2O-instrumented tested are the TGA-100 by Campbell Sci. and the Aerodyne QCL.

```
!errors
#calculate random errors and instrumental noise (Mauder et al., 2013)

T

!x_max #perform cross correlation to maximise covariances of additional sensors
with w

T
```

If this automatic delay time correction is turned on then the parameter `!lateral #spatial separation only for lateral wind component(T) only or total (F)` should be set T because this correction already compensates for the longitudinal separation between sensors.

```
!combine #combine short-term moments for longer time periods(T/F), only useful
if no high-frequency data are available

F

!calc_data%t_interval2 #short-term averaging interval [min]

5

!calc_data%t_interval3 #Interval between two subsequent averaging intervals,
only applies if combine = T, else enter '0'

0

!checkn # Check if sufficient number of values in short term interval (INTEGER),
only applies if combine = T

F
```

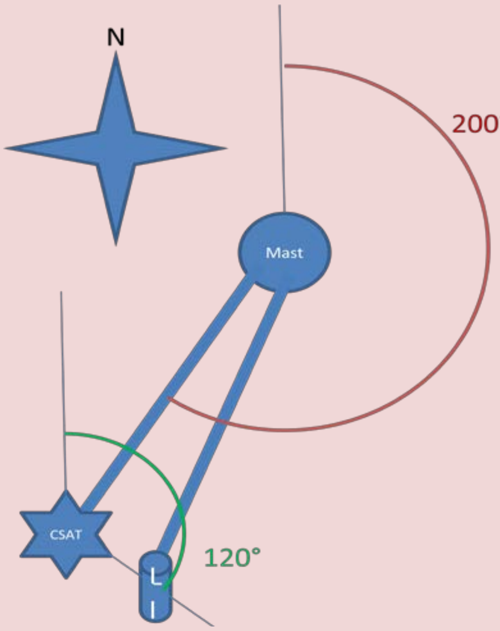
```
!shouldbe # How many values should be short term averaging interval, only
applies if combine = T, else enter '0'
0
#-------------------------------------------------------------------
#################### Correction of Fluxes ################################
!planar_correct #Planar fit method (Wilczak et al.,2001)
T
!read_pf #read(T) or calculate(F) coefficients of multiple regression
T
!bk #b-coefficients, default 0.,0.,0. means no tilt correction, only rotation
into mean wind
0.,0.,0.
!mean_wind #perform rotation into mean wind direction
T
!scalar_fluxes #transformation of scalar fluxes
T
!double_rotation #apply the double rotation method (T/F), should only be applied
if !planar_correct = F
F

!tanner_correct #Tanner oxygen Correction
F
!moore_correct #Moore correction
T
!sa #sensor separation w - a [m]
0.30
!sc #sensor separation w - CO2 [m]
0.30
!n0 #cut-off frequency for CO2, H2O, CH4, N2O [Hz]
20,20,20,20
!sTp #sensor separation w - Tp [m]
0.01
!sn2o  #sensor separation w - N2O [m]
0.01
!sch4  #sensor separation w - CH4 [m]
0.23
!Tptau #time constant of add. fast temperature sensor [s]
0.01
!lateral #spatial separation only for lateral wind component(T) only or total
```

```
(F)
T
!drctn #direction of H2O/CO2 measurement [degree] against N
120.

!drctn_CH4  #direction of CH4 measurement [degree] against N
0
```

Schematic example for !drctn = 120 and !wd = 200, looking from above on the tower/mast:



```
!liu_correct #Schotanus/Liu correction
T

!wpl_correct #WPL correction
T


#------------------------------------------------------------------
############################ QA/QC ##################################
!stat #Perform stationarity test
T
!itc #Test on developed turbulent conditions with integral turbulence characteristics
T
```

```
# coefficients for sigma_u/u* parameterizations according to Rannik et al.
(2003) or Biermann (2008)

!within_canopy_u # a_i, alpha_i, beta_i, gamma_i

2.01,8.97,1.37,0.29

# coefficients for sigma_w/u* parameterizations according to Rannik et al.
(2003) or Biermann (2008)

!within_canopy_w # a_i, alpha_i, beta_i, gamma_i

1.13,0.9,1.2,-0.63


#Check for interdependence of quality flags due to corrections: ustar > LvE and
HTs/HTp > NEE (Mauder et al., 2013)

!chk_interdependence

T


#Check for w-offset (Mauder et al., 2013)

!chk_wind

T


#Quality Flags

#(1)after Foken et al. 2004 (1 - 9) or

#(2)after Rebmann et al. 2004 (2) for CARBOEUROPE (1 - 5)or

#(3)according the scheme found on the 1st CARBOEUROPE IP Meeting in Spoleto
(Mauder et al., 2013) (0 - 2)

!howto_combine

1


#Use ITC of temperature for the sensible heat flux flag, only applies for
!howto_combine = 1 or 2

#if !howto_combine = 3, the ITC of temperature is not used anyways

!use_itc_T

F


#-------------------------------------------------------------------
############################ Footprint #############################

#Perform footprint analysis according to Kormann and Meixner (2001)

!footprint

F

#File name of input file with landuse information, required for footprint
analysis, in ESRI compatible ASCII grid (*.asc)

#The target landuse has to be labelled as '1'; a second target landuse can be
```

```
labelled as '2'
!map_name
'hoeglwaldUTM.asc'
#Sensor location in UTM coordinate system [REAL]
!m_easting
654093
!m_northing
5350514

!footprint_out #output of footprint distribution as ESRI compatible ASCII grid (*.asc)
F
#------------------------------------------------------------------
############################ output #################################
#time information in filename
!timeinfo
T
#append result to existing file
!append
F
!spectra_on
F
!stor_flux
F
!3rd_moments
F
```

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