Measurement data analysis - Data processing and test of goodness of fit with 4C

Basic principle

After simulation, data processing can be started. Therefore, a file with measurements (in compliance with certain requirements, see below) is read in after prompting. Comparison and test of goodness of fit apply to the generated (or existing) 4C-output files.
A descriptive statistic is calculated for each measurement type and each run, containing simulation value, measurement, residuum and various error measures (see Table 3).
After each run, the norm of the vector is formed over all measurement types for selected metrics.

Start of Program

The program can be started directly from 4C subsequent to the simulation or as a stand-alone program with already existing 4C-output files.

Start with 4C

Set flag_stat > 0 in the simulation control. Calculation is deactivated with flag_stat = 0. With this flag, analysis of goodness of fit as well as the output can be controlled.

Table 1 Allocation of flag flag_stat

Value of flag_stat	Meaning
0	No data processing
1	Processing of measurements with output of results in file xxx_stat.res
2	In addition to **1**, output of residua etc. in file xxx_resid.res
3	In addition to **2**, output of filled measurements in file xxx_mess.mes

For activation of measurement processing, specification of **one** file of measurements is necessary after configuring is finished for the first simulation run (example).

Separate start without 4C
All necessary information about the 4C files and the measurement file are queried via dialogue.

Structure of measurement files

There are two different categories of files:

- data as daily values
- data as annual values

Any number of comment lines is permissible at the beginning of the file (marked with **!**). The first column correlates the measurements with date or year, the next columns can contain any number of measurements identified via their name in the header.
The data has a header row, with first **Datum** (or **date**) or **Jahr** (or **year**) describing the temporal resolution and names of any measurements after that. Missing values in the time series are indicated by **-9999.99**. Admissible measurement names and their assignment to simulated values can be found in Table 2.
Any necessary conversions are carried out internally while processing.
Names in the header as well as the data have to be separated with spaces or tabulators.
The date has to be in the form of **TT.MM.JJJJ**, with the year as **four-digit** number.

Table 2 Names of admissible measurements, their meaning and assignment

Name des Messwerts	Name und Zuordung im Output-File	Output-File des Simula-tionswerts	Bedeutung
AET	AET	day	Actual evapotranspiration [mm/d]
	AET	soil	Actual evapotranspiration [mm/y]
BIOM	analog **STVOL**		
DG	Meddiam	veg	Medium diameter of stand (quadratic mean) [cm]
DG_bi	Meddiam	veg_bi	Medium diameter of birch (quadratic mean) [cm]
DG_pi	Meddiam	veg_pi	Medium diameter of pine (quadratic mean) [cm]
DG_sp	Meddiam	veg_sp	Medium diameter of spruce (quadratic mean) [cm]
DBH	mean_diam	veg	Mean diameter of stand (arithmetic mean) [cm]
DBH_bi	mean_diam	veg_bi	Mean diameter of birch (arithmetic mean) [cm]
DBH_pi	mean_diam	veg_pi	Mean diameter of pine (arithmetic mean) [cm]
DBH_sp	mean_diam	veg_sp	Mean diameter of spruce (arithmetic mean) [cm]
Fol	Fol_Bio	veg	Foliage biomass of stand [kg DW/ha]

Name des Messwerts	**Name und Zuordung im Output-File**	**Output-File des Simula-tionswerts**	**Bedeutung**
Fol_bi	Fol_Bio	veg_bi	Foliage biomass of birch [kg DW/ha]
Fol_pi	Fol_Bio	veg_pi	Foliage biomass of pine [kg DW/ha]
Fol_sp	Fol_Bio	veg_sp	Foliage biomass of spruce [kg DW/ha]
GPP	GPP	sum (daily)[1]	Gross production [g C/m^2/d]
	GPP	c_bal	Gross production [kg C/ha/y]
HO	Domhei / 100	veg	Medium height of dominant trees [m]
HO_bi	Domhei / 100	veg_bi	Medium height of dominant birch trees [m]
HO_pi	Domhei / 100	veg_pi	Medium height of dominant pine trees [m]
HO_sp	Domhei / 100	veg_sp	Medium height of dominant spruce trees [m]
LAI	LAI	veg	Leaf Area Index of whole crown [m^2/m^2]
LAI_bi	LAI	veg_bi	Leaf Area Index of birch [m^2/m^2]
LAI_pi	LAI	veg_pi	Leaf Area Index of pine [m^2/m^2]
LAI_sp	LAI	veg_sp	Leaf Area Index of spruce [m^2/m^2]
Litter	Dry mass - fol_litter	litter	Foliage litter – dry mass [kg/ha/y]
MH	mean_height / 100	veg	Mean height of all trees [m]
MH_bi	mean_height / 100	veg_bi	Mean height of all birches [m]
MH_pi	mean_height / 100	veg_pi	Mean height of all pines [m]
MH_sp	mean_height / 100	veg_sp	Mean height of all spruces [m]
NEE	NEE	sum (daily)[1]	Net ecosystem exchange [g C/m^2/d]
NEP	NEP	c_bal	Net ecosystem production [kg C/ha/y]
NTREE	Tree	veg	Number of trees
NTREE_bi	Tree	veg_bi	Number of birch trees
NTREE_pi	Tree	veg_pi	Number of pine trees

[1] Set flag_sum=1 in the simulation control file.

Name des Messwerts	Name und Zuordung im Output-File	Output-File des Simulationswerts	Bedeutung
NTREE_sp	Tree	veg_sp	Number of spruce trees
prec_stand	Prec - Interc	soil	Throughfall [mm/y]
Snow	snow	day	Water equivalent of snow [mm]
STBIOM	Sap_Bio + Hrt_Bio	veg	Stem biomass of whole stand [kg DW/ha]
STBIOM_bi	Sap_Bio + Hrt_Bio	veg_bi	Stem biomass of birch [kg DW/ha]
STBIOM_pi	Sap_Bio + Hrt_Bio	veg_pi	Stem biomass of pine [kg DW/ha]
STBIOM_sp	Sap_Bio + Hrt_Bio	veg_sp	Stem biomass of spruce [kg DW/ha]
STVOL	Stemvol	veg	Stem volume of whole stand [m^3/ha]
STVOL_bi	Stemvol	veg_bi	Stem volume of birch [m^3/ha]
STVOL_pi	Stemvol	veg_pi	Stem volume of pine [m^3/ha]
STVOL_pi	Stemvol	veg_sp	Stem volume of spruce [m^3/ha]
Stem_inc	Stem_inc	veg	Stem increment [kg DW/ha/y]
Stem_inc_bi	Stem_inc	veg_bi	Stem increment of birch [kg DW/ha/y]
Stem_inc_pi	Stem_inc	veg_pi	Stem increment of pine [kg DW/ha/y]
Stem_inc_sp	Stem_inc	veg_sp	Stem increment of spruce [kg DW/ha/y]
TER	TER	sum (daily)[1]	Total ecosystem respiration [g C/m^2/d]
	TER	c_bal	Total ecosystem respiration [kg C/ha/y]
transtree	trans_tree	day	Transpiration demand of trees [mm/d]
TS_002	temps(1)	temp	Soil temperature, +2 cm depth (humus layer) [°C]
TS_xx	temps(i); Bestimmung von i intern aus File ..._soil.ini	temp	Soil temperature, xx cm depth (mineral soil) [°C]
WC_002	watvol(1)	water	Soil water, +2cm (humus layer) [Vol%]
WC_xx	watvol(i);); Bestimmung von i intern aus File ..._soil.ini	water	Soil waterin xx cm depth (mineral soil) [Vol%]

Instruction for programmers:

New measurements have to be incorporated in the CASE statement via the subroutine read_simout. This does not include new variations of TS and WC, as their assignment to the simulation values for the depths is carried out automatically.

Calculations and Output

File stat with statistical values

The name of the output file containing statistical calculations is put together as follows:

< Site name of the first run >_stat.res

Calculated values are output corresponding to the header rows characterising the columns. They are identified as

ipnr - Number of run
site_id - Site name
kind - Kind of measurement.

For residua, simulation values and measurements descriptive statistics contain the mean, minimum, maximum, standard deviation, variance and variation coefficient are output. Further values for evaluating the margin of errors can be found in Table 3.
Variables for which calculations do not make sense are indicated as missing values (-9999).
After each run, the norm of the vector is calculated over all measurement types for selected metrics.

File resid with residua, simulated and observed values

The name of the output file containing residua is put together as follows:

< Site name of the Runs >_resid.res

For each kind of observed values output of residua, simulated and observed values take place in blocks. The header contains the kind of observed value and the number of observed values. Each triple is characterised by the day of the year (day) and the four-digit year (year). In case of annual values, day = 0.

File mess with observed values

The name of the output file containing residua is put together as follows:

< Site name of the Runs >_mess.mes

All imported measurements are output for the complete simulation time. The header shows the kind of measurement. The first two columns contain continuous day of the year (day) and the four-digit year (year). Missing values are allocated **-9999.0**.

Table 3 **Name and meaning of the calculated values in the output file stat**

Output Code	Term		Formula
	German	English	
Analysis of simulated (P_i predicted values) and observed values (O_i observed values)			
variance	Streuung, Varianz	variance	$\sigma^2 = \frac{1}{N-1}\sum_{i=1}^{N}\left(X_i - \bar{X}\right)^2$
stand_dev	Standard-abweichung	Standard deviation	σ
var_coeff	Variations-koeffizient	Coefficient of variation	$\frac{\sigma}{\bar{X}}$
mean	Mittelwert	Mean, average	$\bar{X} = \frac{1}{N}\sum_{i=1}^{N} X_i$
cor_coeff	Korrelations-koeffizient	Correlation coefficient	$\rho = \frac{\sum_{i=1}^{N}\left(X_i - \bar{X}\right)\left(Y_i - \bar{Y}\right)}{\sqrt{\sum_{i=1}^{N}\left(X_i - \bar{X}\right)^2 \sum_{i=1}^{N}\left(Y_i - \bar{Y}\right)^2}}$
rsquare	Bestimmtheitsmaß	Coefficient of determination	$B = \rho^2$
Analysis of residua $R_i = P_i - O_i$			
mean (residual)	Mittlerer Fehler (Mittelwert)	Average error Mean error	$\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i) = \frac{1}{N}\sum_{i=1}^{N} R_i = \bar{P} - \bar{O}$
NME	Normalisierter mittlerer Fehler	Normalised mean error	$\frac{\bar{P} - \bar{O}}{\bar{O}}$
MAE	Mittlerer absoluter Fehler	Mean absolute error	$\frac{1}{N}\sum_{i=1}^{N}\lvert P_i - O_i\rvert = \frac{1}{N}\sum_{i=1}^{N}\lvert R_i\rvert$
NMAE	Normalisierter mittlerer absoluter Fehler	Normalised mean absolute error	$\frac{\frac{1}{N}\sum_{i=1}^{N}\lvert P_i - O_i\rvert}{\lvert\bar{O}\rvert} = \frac{\frac{1}{N}\sum_{i=1}^{N}\lvert R_i\rvert}{\lvert\bar{O}\rvert}$
SSE	Fehlerquadrat-summe	Sum of square error	$\sum_{i=1}^{N}(P_i - O_i)^2 = \sum_{i=1}^{N} R_i^2$

Output Code	Term		Formula
	German	English	
RMSE	Mittlerer quadratischer Fehler	Root mean square error	$\sqrt{\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)^2} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}R_i^2}$
NRMSE	Normalisierter mittlerer quadratischer Fehler	Normalised root mean square error	$\frac{1}{\lvert\bar{O}\rvert}\sqrt{\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)^2} = \frac{1}{\lvert\bar{O}\rvert}\sqrt{\frac{1}{N}\sum_{i=1}^{N}(R_i)^2}$
PME	Mittlerer prozentualer Fehler	Percentage mean error	$\frac{1}{N}\sum_{i=1}^{N}\frac{\lvert P_i - O_i\rvert}{\lvert O_i\rvert} = \frac{1}{N}\sum_{i=1}^{N}\frac{\lvert R_i\rvert}{\lvert O_i\rvert}$
PRMSE	Mittlerer quadratischer prozentualer Fehler	Percentage root mean square error	$\sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\frac{P_i - O_i}{O_i}\right)^2} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\frac{R_i}{O_i}\right)^2}$
TIC	Theilscher Ungleichheits-koeffizient	Theil's inequality coefficient	$\frac{\sqrt{\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)^2}}{\sqrt{\frac{1}{N}\sum_{i=1}^{N}P_i^2} + \sqrt{\frac{1}{N}\sum_{i=1}^{N}O_i^2}} = \frac{\sqrt{\frac{1}{N}\sum_{i=1}^{N}(R_i)^2}}{\sqrt{\frac{1}{N}\sum_{i=1}^{N}P_i^2} + \sqrt{\frac{1}{N}\sum_{i=1}^{N}O_i^2}}$
MEFF	Modellgüte	Nash–Sutcliffe model efficiency coefficient	$1 - \frac{\sum_{i=1}^{N}(O_i - P_i)^2}{\sum_{i=1}^{N}(O_i - \bar{O})^2} = 1 - \frac{\sum_{i=1}^{N}R_i^2}{\sum_{i=1}^{N}(O_i - \bar{O})^2} = 1 - \frac{\sum_{i=1}^{N}R_i^2}{(N-1)\,\sigma^2}$
average	Mittelwert über alle Größen	Average of all n characteristics M_1, …., M_n *)	$\frac{1}{N}\sum_{i=1}^{N}M_i$
tot_match1	Gesamtanpassung aus Mittelwerten von TIC und MEFF	Total performance from averages of TIC and MEFF	$\frac{1}{2}\left(TIC + \left(1 - MEFF\right)\right)$
tot_match2	Gesamtanpassung aus Mittelwerten von TIC, MEFF und rsquare	Total performance from averages of TIC, MEFF, and rsquare	$\frac{1}{3}\left(TIC + \left(1 - MEFF\right) + \left(1 - rsquare\right)\right)$
tot_match3	Gesamtanpassung aus Mittelwerten von TIC, MEFF, rsquare und NRMSE	Total performance from averages of TIC, MEFF, rsquare, and NRMSE	$\frac{1}{4}\left(TIC + \left(1 - MEFF\right) + \left(1 - rsquare\right) + NRMSE\right)$

*) M_i see Table 2

Interpretation

rsquare

- The coefficient of determination alone should not be used for model quantification, because it can produce high values for very bad model results, because it is based on correlation only.
- It is very sensitive to peaks.

(Krause et al. 2005)

NRMSE

The normalised root mean square error ranges from -∞ to +∞, with zero denoting a match between measured and simulated values.

TIC

Theil's inequality coefficient U

$$0 \leq \mathbf{U} \leq 1$$

A value of 0 for U indicates perfect prediction, while a value of 1 corresponds to perfect inequality or negative proprtionality between the actual and predicted values. (Leuthold 1975)

MEFF

- The maximum value 1 of the model efficiency indicates the best fit; a value of zero indicates that the model predicts the measured values no better than the mean. Values less than zero imply, for instance, that the mean square error exceeds the variance of the measured data and that the model is not consistent to the measured data.
  Model efficiency or Nash–Sutcliffe efficiencies can range from −∞ to 1. An efficiency of 1 (**MEFF = 1**) corresponds to a perfect match of modeled discharge to the observed data. An efficiency of 0 (**MEFF = 0**) indicates that the model predictions are as accurate as the mean of the observed data, whereas an efficiency less than zero (**MEFF < 0**) occurs when the observed mean is a better predictor than the model or, in other words, when the residual variance (described by the nominator in the expression above), is larger than the data variance (described by the denominator).
  Essentially, the closer the model efficiency is to 1, the more accurate the model is.
  (Wikipedia, 9.4.2010), (Nash and Sutcliffe 1970)
- MEFF is primarily focused on the peaks and very sensitive to peaks. (Krause et al. 2005)

totm1, totm2, totm3

The performance is an average of several statistical indicators, each as average over all measurement kinds. The minimum value is zero and indicates the perfect prediction.

It can be stated that none of the efficiency criteria described and tested performed ideally. Each of the criteria has specific pros and cons which have to be taken into account during model calibration and evaluation. (Krause et al. 2005)

Examples

Simulation control file

The following simulation control file starts the simulation at site1 with daily and yearly output and delivers the comparison between simulated and measured values of the elements listed in the measurement file **site1.mes** on daily time scale.
The flag_stat, flag_sum and the additional file with measured data is marked with red.

```
  1  ! Run option 0 = single run, 1 multi run
 1  !
! *** simulation specifications  **************************************
 54  ! number of simulation years
1948  ! start year for simulation
1000. ! patch size [m²]
 50.0 ! thickness of foliage layers [cm]
  7  ! time step photosynthesis calculations [d]
! *** choice of model options ******************************************
  3  ! mortality flag (flag_mort)
  0  ! regeneration flag (flag_reg)
  0  ! use FORSKA environmental factors and regeneration (flag_forska)
  1  ! initialization flag (flag_stand)
  0  ! soil vegetation flag (flag_sveg)    !!! new !!!
  3  ! management flag (flag_mg)
  0  ! disturbance flag (flag_dis)
  4  ! ligth algorithm number (flag_light)
  1  ! foliage-height relationship (flag_folhei)
  1  ! volume function (flag_volfunc)
  0  ! respiration flag (flag_resp)
  3  ! limitation flag (flag_limi)
  1  ! decomposition model (flag_decomp)
  0  ! root activity function flag (flag_sign)
  1  ! soil water uptake flag (flag_wred)
  1  ! root distribution flag (flag_wurz)
  0  ! heat conductance flag (flag_cond)
  0  ! interception flag (flag_int)
  7  ! evapotranspiration flag (flag_eva)
 103  ! CO2 flag (flag_CO2)
  0  ! dummy flag (flag_dum1)
  0  ! dummy flag (flag_dum2)
  1  ! dummy flag (flag_stat)
! *** output specifications *********************************************
  1  ! Yearly output flag
 veg_pi
 veg
 soil
 end
  1 ! Daily output flag
temp
watvol
end
  0  ! cohort output flag
 end
  1  ! summation output flag
! *** input files *********************************************************
input/species_neu.par
test_site1
input/site1.cli
input/site1.sop
input/site1.soi
input/site1.ini
9999
input/site1.man
```

input/con.dep
input/Peitz.red
input/dummy.lit
input/site1.mes

Daily values

File **site1.mes** with some daily measurements of water content (WC_30, WC_50, WC_120, WC_350) in 30, 50, 120 and 350 cm depth, soil temperature (TS_05, TS_30) in 5 and 30 cm depth, actual evapotranspiration (AET) and net ecosystem exchange (NEE). The units are listed in Table 2.

! Site1: Forest
! Daily measurements, fragmentary

!	[Vol%]	[Vol%]	[Vol%]	[Vol%]	[°C]	[°C]	mm/d	g/cm2/D
date	WC_30	WC_50	WC_120	WC_350	TS_05	TS_30	AET	NEE
05.01.2003	18.04	13.87	16.93	-9999.99	-9999.99	-9999.99	-9999.99	-9999.99
06.01.2003	17.77	14.01	16.93	-9999.99	-9999.99	-9999.99	-9999.99	-9999.99
07.01.2003	17.52	14.07	16.87	-9999.99	-9999.99	-9999.99	-9999.99	-9999.99
18.05.2004	10.94	11.37	14.31	16.29	-9999.99	10.9	3.28	-2.754
19.05.2004	10.60	11.26	14.22	16.31	-9999.99	11.1	2.42	-0.583
20.05.2004	10.31	11.12	14.12	16.30	-9999.99	11.1	2.61	-1.575
21.05.2004	10.07	10.99	14.04	16.29	-9999.99	10.9	2.19	-3.040
22.05.2004	9.81	10.84	13.96	16.20	-9999.99	10.6	2.65	-2.596
23.05.2004	9.68	10.71	13.91	16.24	-9999.99	10.2	2.52	-2.879
30.09.2004	12.06	-9999.99	7.02	13.23	11.80	12.7	0.59	2.552
01.10.2004	12.51	6.42	7.02	13.22	11.27	12.3	1.23	-0.390
02.10.2004	12.17	6.40	7.02	13.22	11.27	12.2	0.89	-0.238
03.10.2004	11.79	6.39	7.04	13.21	11.61	12.3	0.45	1.830
04.10.2004	11.21	6.37	7.04	13.17	11.40	12.1	0.30	3.053
05.10.2004	10.57	6.38	7.06	13.19	12.98	12.7	0.94	2.155

Annual values

The following example (filename **site1_y.mes**) contains yearly measurements of total net ecosystem production (NEP), total actual evapotranspiration (AET), leaf area index (LAI), number of trees (NTREE), and the biomass (BIOM). The units are listed in Table 2.

! Site2: Annual measurements

year	NEP	AET	LAI	NTREE	BIOM
1997	-1959.9	337.2	2.98	1835	50.26
1998	-2205.2	246.9	3.01	1837	53.37
1999	-1466.5	256.9	3.05	1837	56.71
2002	-2388	344.0	2.52	1523	54.33
2008	-2441.5	340.0	3.09	1525	72.59
2009	-3563.2	368.0	-9999.00	1525	-9999.00

References

Krause P, Boyle DP, Bäse F (2005) Comparison of different efficiency criteria for hydrological model assessment. Advances in Geosciences 5:89-97

Leuthold RM (1975) On the Use of Theil's Inequality Coefficients. American Journal of Agricultural Economics 57:344-346. doi:10.2307/1238512

Nash JE, Sutcliffe JV (1970) River flow forecasting through conceptual models, Part I - A discussion of principles. J Hydrol 10:282-290. doi:10.1016/0022-1694(70)90255-6