Instruction Manual for the Automated AquaCrop-OpenSource (AAOS) tool

17.03.2023

1. Description of user input files

1.1. AquaCrop-OpenSource (AOS) input files

Please refer to the official AOS manuals and associated publications (Foster, T., 2019; Foster et al., 2017).

1.2. AAOS input files

The user needs to specify 2 Matlab functions (".m" format) and several files formatted as comma-separated values (".csv"). Table 1 summarizes every file's storage location, name, and content, and indicates whether it is required or optional. The number of required input files depends on the scope of the analysis and the number of evaluated agricultural lots. The user can modify the available templates from a study of Bruckmaier (2021), which can be found in the respective folders (see Table 1).

For every observation input file (irrigation, canopy cover, and soil water content), the user can decide between two options:

- Option A: All lots are assigned the same values, which are specified within a single file.
- Option B: Every lot is assigned its own values, hence requires its own file.

Table 1 Summary of user input files

<table>
<tr><th rowspan="2">File type</th><th rowspan="2">File location</th><th colspan="2">File Name</th><th rowspan="2">Description</th><th rowspan="2">User input</th></tr>
<tr><th>Option A</th><th>Option B</th></tr>
<tr><td rowspan="11">Comma-separated values (".csv")</td><td rowspan="11">\AAOS\AAOS_Input*User-defined season name*</td><td colspan="2">InputPars_GLUE</td><td>Specifies AOS and AAOS parameter settings, for all lots</td><td>Required</td></tr>
<tr><td rowspan="3">Irrigation_all</td><td>Irrigation_"x1"</td><td rowspan="3">Specifies irrigation schedule for all lots or the lot with the index as indicated in file name</td><td rowspan="3">Optional</td></tr>
<tr><td>…</td></tr>
<tr><td>Irrigation_"xn"</td></tr>
<tr><td rowspan="3">CC_all</td><td>Obs_CC_"x1"</td><td rowspan="3">Specifies canopy cover (CC) observations for respective lot/ all lots</td><td rowspan="7">At least 1 file required</td></tr>
<tr><td>…</td></tr>
<tr><td>Obs_CC_"xn"</td></tr>
<tr><td rowspan="3">SWC_all</td><td>Obs_SWC_"x1"</td><td rowspan="3">Specifies soil water content (SWC) observations for respective lot/ all lots</td></tr>
<tr><td>…</td></tr>
<tr><td>Obs_SWC_"xn"</td></tr>
<tr><td colspan="2">Obs_TargetVar</td><td>Specifies observations for target variable (= either biomass or yield at harvest) for all lots</td></tr>
<tr><td rowspan="2">Matlab function (".m")</td><td rowspan="2">\AAOS\config</td><td colspan="2">default</td><td>Specifies general settings (input file names, type of analysis, output)</td><td rowspan="2">Required</td></tr>
<tr><td colspan="2">Season_*User-defined season name*</td><td>Specifies season-specific settings (output file name, analyzed lots, test variables, phenology parameter conflicts, handling of missing initial water content values, …)</td></tr>
</table>

2. Use instructions

2.1. Specify .csv input files

2.1.1. “InputPars_GLUE.csv”

Starting at Row #2, Column #...

1. AOS parameter name as defined in the Matlab containers created during an AOS simulation (exact matching required)
2. AOS input file name as indicated in the folder “\AOS\AAOS_Input*User-defined season name*”, in which respective parameter is defined (exact matching required)
3. Unit in which parameters values are specified:
    - Phenological parameters: “GDD” (Growing Degree Days) or “CD” (Calendar Days)
    - Rest: “NR” (Not Relevant)
4. Lower value limit in AAOS analysis
5. Upper value limit in AAOS analysis
6. Smallest possible step in AAOS analysis (= rounding of parameter values)

2.1.2. “Irrigation_*... *.csv”

Starting at Row #4, Column #...

1. Day of irrigation event
2. Month of irrigation event
3. Year of irrigation event
4. Applied water during irrigation event [mm]

2.1.3. “CC_*... *.csv”

Starting at row #3, Column #...

1. Simulation day of CC observation
2. Observed CC value [fr]

2.1.4. “SWC_*... *.csv”

Row #2, Column #...

1. Soil depth at observation point #1 [m]

…

n. Soil depth at observation point #n [m]

Starting at Row #3, Column #...

1. Simulation day of SWC observation
    - The first simulation day always needs to be indicated, even when the SWC value is missing
2. SWC value [fr] at observation point #1
    - The SWC content on the first simulation day (“initial SWC”) always needs to be defined, even when it is missing (-> in this case, insert “nan”).

…

n. SWC value [fr] at observation point #n

2.1.5. "TargetVar.csv"

Row #1, Column #...

1. Target variable name: "Biomass" or "Yield"

Starting at Row #2, Column #...

1. Day of harvest
2. Lot index
3. Observed target variable value of [t/ha]

2.1.6. Example files

Cells that should be manipulated by the user are highlighted in light red:

	A	B	C	D	E	F
1	ParametersGLUE	AOS_File	Unit	LowerLimit	UpperLimit	MinStep
2	CDC	Crop	GDD	0.004	0.004	0.0001
3	CGC	Crop	GDD	0.005	0.007	0.0001
4	Emergence	Crop	CD	8	17	1
5	CCx	Crop	NR	0.8	0.99	0.01
6	Senescence	Crop	CD	60	100	1
7	HIstart	Crop	CD	63	84	1
8	Flowering	Crop	CD	11	19	1
9	PlantPop	Crop	NR	2000000	7000000	1
10	SeedSize	Crop	CD	1	2.75	0.01
11	AppEff	IrrigationManagement	NR	40	70	1
12	REW	Soil	NR	9	12	1
13	Ksat	SoilHydrology	NR	14.4	5040	1
14	Zmin	Crop	NR	0.2	0.3	0.01
15	Zmax	Crop	NR	1	1.8	0.01
16	MaxRooting	Crop	CD	5	90	1
17	th_wp	SoilHydrology	NR	0.007	0.336	0.001
18	th_fc	SoilHydrology	NR	0.018	0.466	0.001
19	th_s	SoilHydrology	NR	0.374	0.582	0.001
20	HI0	Crop	NR	0.45	0.5	0.01

Figure 1 InputPars_GLUE.csv

	A	B	C	D
1	Irrigation	2018	All Plots	
2	Day	Month	Year	Depth [mm]
3	29	1	2018	27.4
4	18	2	2018	43
5	4	3	2018	52.4
6	19	3	2018	74.8
7	20	3	2018	150
8	21	3	2018	112.5
9				

Figure 2 Irrigation_all.csv

	A	B
1	CC Observations Lot 8	
2	SimDay	CC
3	36	0.26
4	44	0.48
5	55	0.8
6	59	0.83
7	68	0.83
8	83	0.79
9	90	0.78

Figure 3 Obs_CC_8.csv

	A	B
1	SWC Observations Lot 8	
2	SimDay	0.1
3	1	nan
4	15	0.131867
5	16	0.123344
6	17	0.144896
7	18	0.128299
8	19	0.125466
9	20	0.338497

Figure 4 Obs_SWC_8.csv

	A	B	C
1	HarvestDAS	PlotNo	Biomass
17	100	16	7
18	100	17	7.8
19	100	18	11.4
20	100	19	4.6
21	100	20	13.2
22	100	21	nan
23	100	22	9.6
24	100	23	11

Figure 5 TargetVar.csv

2.2.Specify .m input files

Please follow the instructions provided in the subsequent MATLAB code snippets.

```
%% General/ study-independent specifications, to be determined by the user

%% 1) Define general input and output settings:
% 1.1) Choose season (default: "template"):
Config.season = "Template";
% 1.2) Select type of analysis
% ... available:
% - Generalized Likelihood Uncertainty Estimation ("GLUE")
% - Elementary Effects method ("EE"):
Config.RUN_type = "GLUE";
% 1.3) Add additional text to output filename (-> inserted at the end):
Config.filename_xtra = "";
% 1.4) Determine type of graphical output to be created
% (Config.PlotGraphs = ["x", "y", ...])
%
%% - CURRENTLY UNavailable for EE:
% -- Sensitivity analysis of parameters ("EE")
%
% - available for GLUE (model error analysis for variables & parameters):
%% -- Time-series analysis ("TS")
%% -- Time-series analysis/ Predicton limits ("PL")
%% -- Culminated distribution function for variables ("CDF")
%% -- Distribution of simulations according to model error for 2 variables,
%% classified in quadrants ("Q")
% -- Distribution of behavioural parameter values through boxcharts
%% ---> 1 boxchart = 1 variable combination for all lots & 1 parameter
("BC_Combi")
%% ---> 1 boxchart = 1 lot for 1 variable combination & 1 parameter ("BC_Lots")
% -- Distribution of all parameter values with respect to GLF values classified
% within heatmap, differentiated between lots & variable combinations:
%% ---> differentiated between lots and variable combinations ("HM_Lots")
%% ---> differentiated between variable combinations only ("HM_All")
%% ---> Additional option: all lots & variable combinations stacked within 1
figure
%% or distributed over separate figures ("Config.StackHeatmaps")

Config.PlotGraphs =...
    ["TS","PL","CDF","Q","BC_Combi","BC_Lots","HM_Lots","HM_All"];
% 1.5) Parameter visualization options can result in a high number of graphical
% plots - specify a reduced number of parameters to plot in the following
% array ["x", "y", ...] (when left empty, all parameters will be plotted):
Config.ParametersToPlot = ["Ksat", "th_fc", "th_wp", "Senescence"];
% 1.6) Stack heatmaps for different lots or variable combinations ("Y") or
% plot them in separate figures ("N"):
Config.StackHeatmaps = "Y";
% 1.7) Decide which output to save in Excel sheet: "Y" or "N", respectively
% (only available for Excel file format ".xlsx")
Config.WriteFig = "N"; % Write figures
Config.WriteNum = "N"; % Write numerical output
```

Figure 6 „default.csv" (1/2)

```
%% 2) Define SAFE settings ("Sensitivity Analysis For Everybody" toolbox):
% 2.1) Select error thresholds for determining the model's goodness of fit
(GoF):
% ... here: GoF criteria = fixed:
% - TargetVar -> Absolute Relative Error (ARE) [%]
% - TargetVar -> Normalized Root Mean Square Error (NRMSE) [%]
Config.thresh_TargetVar = 15; % ... for target variable simulations
Config.thresh_TestVar = 15; % ... for test variable simulations
% 2.2) Select sampling strategy & design of sampling space exploration:
Config.SampStrategy = 'lhs' ; % Latin Hypercube Sampling (LHS)
Config.DesignType = 'radial'; % 'radial' or 'trajectory'
% 2.3) Define parameters to be sampled in log scale ["x", "y"]
Config.LogScalePars = ["Ksat"];

%% 3) Define output specifications:
% 3.2) Graphical output:
% 3.2.1) Spreadsheet dimensions (-> Position & size of graphs)
Config.OutputSheet.CellWidth = 2.1; % Cell width
Config.OutputSheet.CellHeight = 0.45; % Cell height
% 3.2.2) Graph characteristics:
Config.GraphFontSizeNormal = 16; % Font size of normal text
Config.GraphFontSizeTitle = 18; % Font size of titles
Config.GraphFontSizeSubtitle = 16; % Font size of subtitles
Config.GraphLineWidth = 4; % Line width
Config.GraphMarkerSizeDotPlot = 50; % Marker size in dot plots
Config.GraphMarkerSize = 14; % Marker size in mixed plots
Config.GraphColors = [[0 0.4470 0.7410]; [0.8500 0.3250 0.0980];...
    [0.9290 0.6940 0.1250]; [0.4940 0.1840 0.5560]; [0.4660 0.6740 0.1880];...
    [0.3010 0.7450 0.9330];[0.6350 0.0780 0.1840]]; % Graph colors
% ... = blue/orange/yellow/purple/green/cyan/red; see...:
% https://www.mathworks.com/help/matlab/creating_plots/specify-plot-colors.html
```
Figure 7 „default.csv" (2/2)

```
%% Study-specific settings to be determined by the user

% Select the lots to be analysed from the available set:
% Options: x; [x y..];
Config.SimulationLots = [8 9 13 14 18 19]; % Available: [8 9 13 14 18 19]
Config.CalibrationLots = Config.SimulationLots;

% Define number of simulation runs = parameter combinations:
Config.N_SimTarget = 100;
Config.TargetVarEE = "Biomass"; % Yield or Biomass
% Determine the number of parameter combinations to be simulated and tested
% against phenological conflicts ("Config.r_test"), as a multitude of the
% number of valid samples that should be created in the end
("Config.r_target").
% Their relationship depends on the specified conflicts and crop/weather
% input data (the fewer the possible valid options for phenology parameters,
% the higher the factor should be):
Config.N_SimTest = Config.N_SimTarget;

% Either load existing samples ("0") or create new samples ("1"):
Config.CreateNewSamples = 0;

% Define file name prefix for samples to be created/loaded:
Config.Samples_FileNamePrefix = "Samples10070_";

% "GLUE" / "EE" / "DEF"/ "CAL"/ "VAL": Choose test variable(s):
% CC (1) and/ or SWC (2) and/ or HI (3):
% Possible combinations: [] (only for option "EE") / [1] / [2] / [1 2] /
% [1 2 3] (automatically resetting to [1 2] when using option "EE");
Config.TestVarIds = [1 2];

% Determine SWC depth idx to be analyzed:
Config.SWC_depth = 1;

% Define type of observation input for irrigation data and all analyzed test
% variables: "1" = 1 file per plot; "0" = 1 file for all plots
% - dim.= ["Irrigation file" "Test variable #1 file" "Test variable #2 file"]
% - test variable no. as defined in "Config.TestVarIds" (see above)
Config.N_FilesObsInput = [0 1 1];

% Define soil depths (centerpoints [m]) to be assigned an initial SWC value
Config.SimulatedSWCdepths = [0.01 0.03 0.1 0.165 2.15];

% Define a substitute for EACH of the above-defined simulation depth,
% catering for the case of % missing soil water content observations:
% Available: a) numerical value [frac], e.g. 0.2; b) value of one of the 3
% hydrological parameters that have been specified for the resp. lot, i.e.
% "th_wp" = wilting point, "th_fc" = field capacity, or "th_sat" = saturation.
%% dimension(Config.SWC_substitute) == dimension(Config.SimulatedSWCdepths)
Config.SWC_substitute(1:4) = "th_fc";
Config.SWC_substitute(5) = "th_wp";

% Define phenological conflicts for the analyzed crop, based on following
% relations (which are stored as follows: Config.PhenoConflicts = X(1:6)):
% Var.Senescence < Var.Emergence + X(1)
% Var.Maturity < Var.Emergence + X(2)
% Var.HIstart < Var.Emergence + X(3)
% Var.Senescence > Var.Emergence + X(4)
% Var.Maturity > Var.Emergence + X(5)
% Var.HIstart > Var.Emergence + X(6)
% -> Determine every x with appropriate values in Growing Degree Days [GDD];
% -> Indicate "-9999" if a conflict shall be ignored during the analysis.
Config.PhenoConflicts =  [1000, 1500, 1000, 2000, 2900, 1300];
% Example values based on:
% Raes, D., Steduto, P., Hsiao, T. C. and Fereres, E. (2018),
% AquaCrop Version 6.0 – 6.1, Reference Manual, FAO.
```

Figure 8 „Season_*User-defined season name*.csv" – here: "season_Template.csv"

2.3.Generate results and visualization

Open and run the file “RUN_AAOS.m” (folder: “\AAOS”).

Depending on the specifications made in the the two Matlab files, “Season/input-independent settings.m”, following output will be generated:

- One or more charts displaying the graphical output
  - … as indicated in “default.csv”/ point “1.4”
- A “.xlsx” file containing numerical and graphical output
  - … if indicated in “default.csv”/ point “1.5”
- A “.mat” file containing the generated samples
  - … if indicated in “Season/input-independent settings.m”/ point “2.1”

The output files are stored in the folder “\AAOS\AAOS_Output”

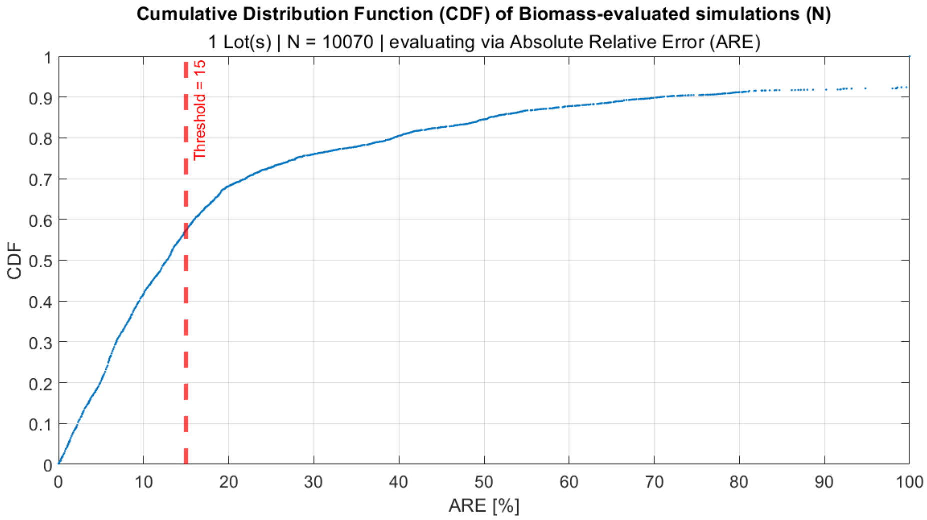

Figure 9 Culminated distribution function (CDF) of Biomass-evaluated simulations of all lots

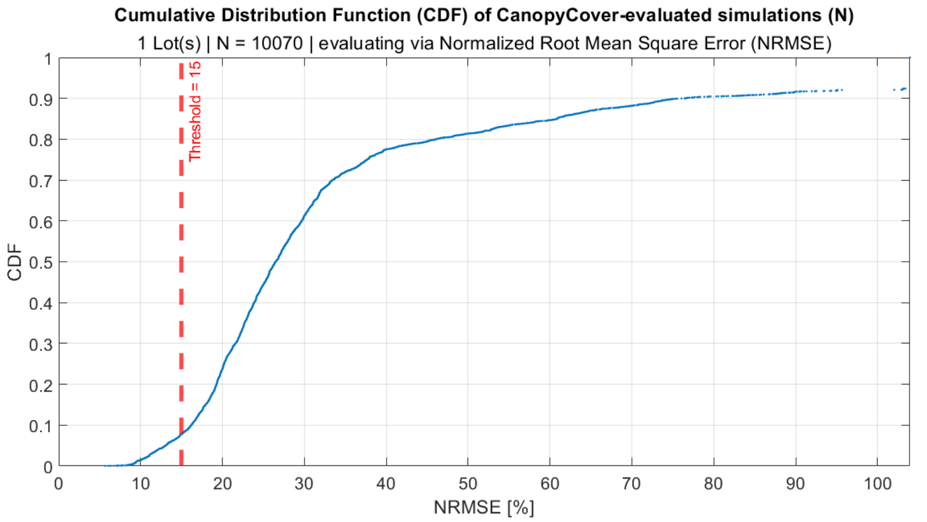

Figure 10 Culminated distribution function (CDF) of Canopy-cover-evaluated simulations of all lots

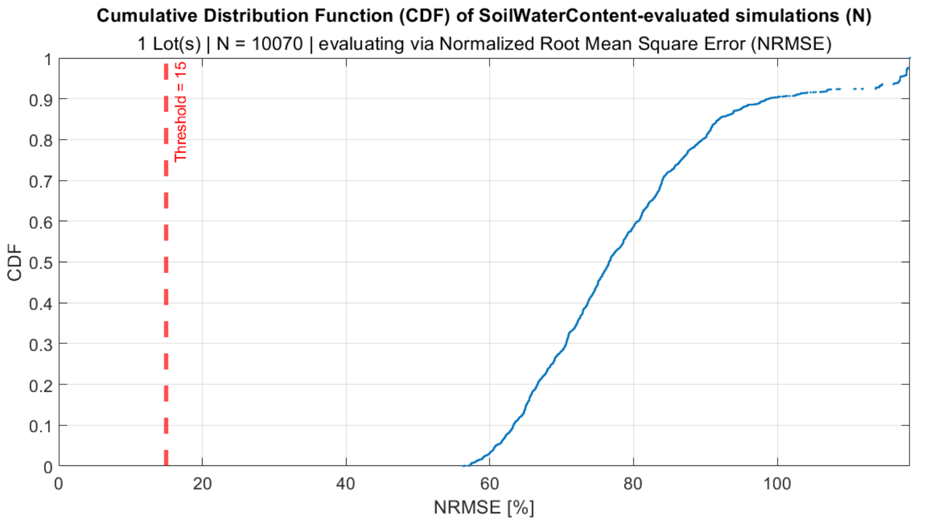

Figure 11 Culminated distribution function (CDF) of Soil-water-content-evaluated simulations of all lots

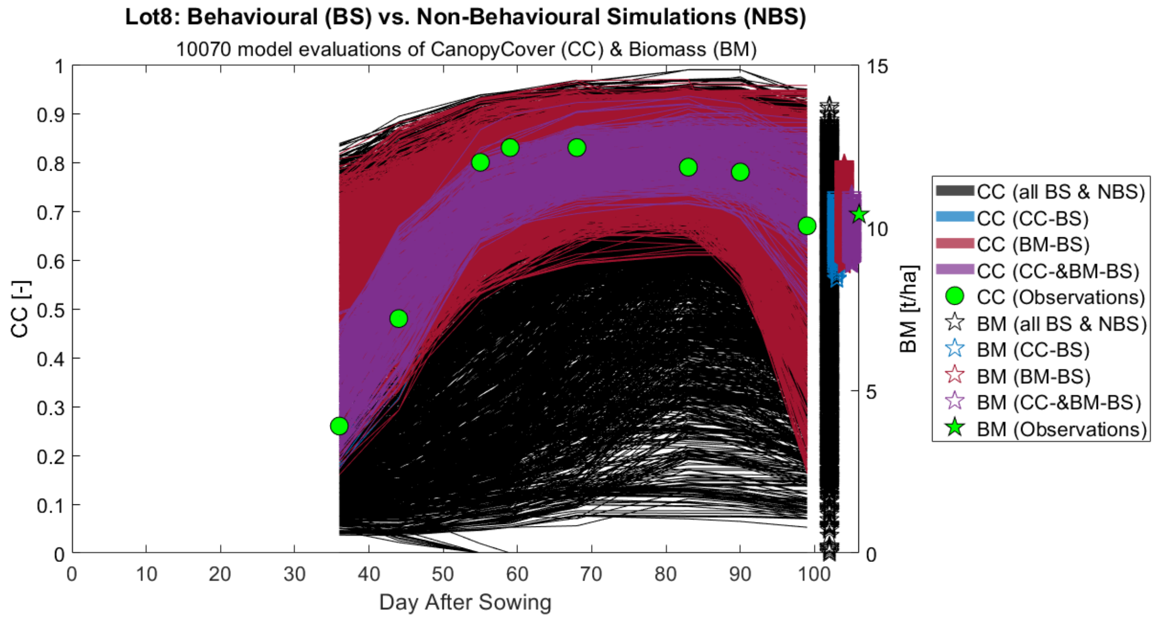

Figure 12 Time-series graph of canopy-cover- and biomass-evaluated simulations of 1 lot

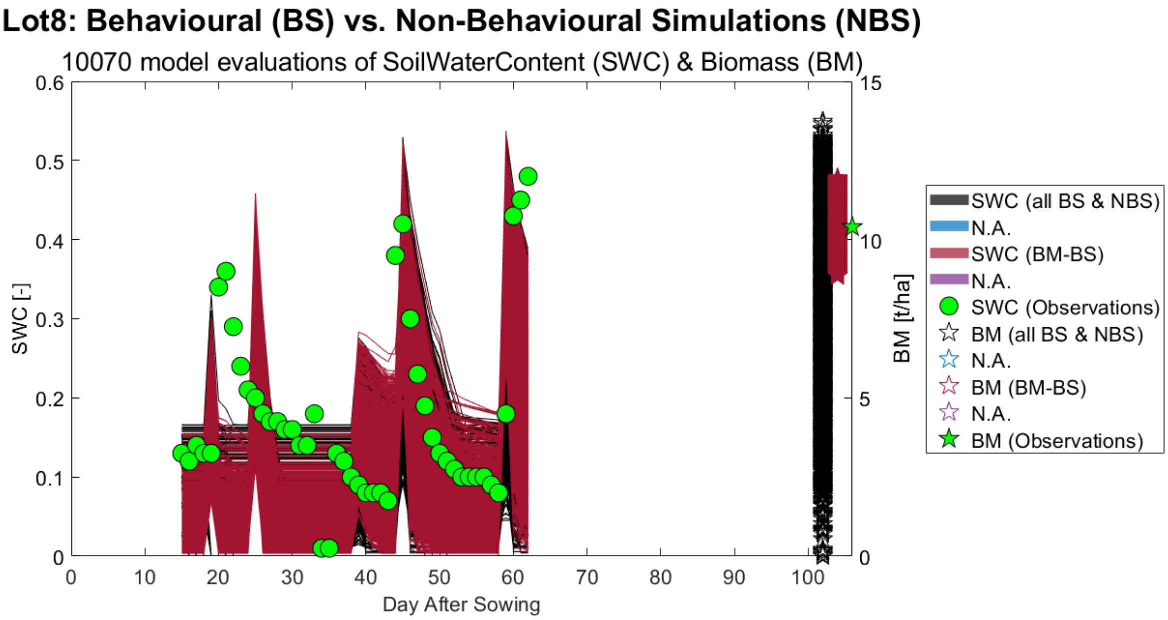

Figure 13 Time-series graph of soil-water-content- and biomass-evaluated simulations of 1 lot

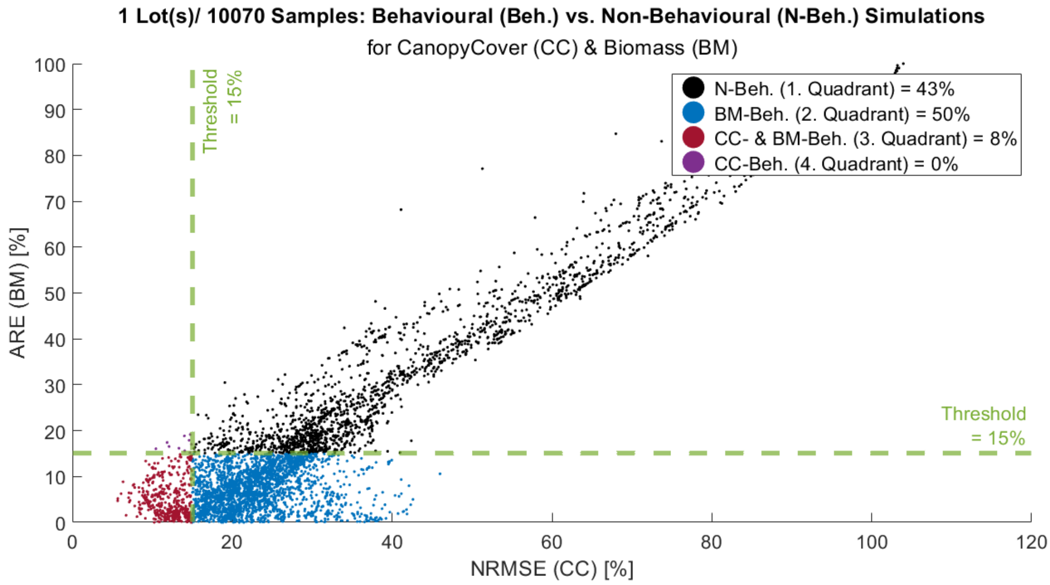

Figure 14 Quadrant-based analysis of canopy-cover- and biomass-evaluated simulations of all lots

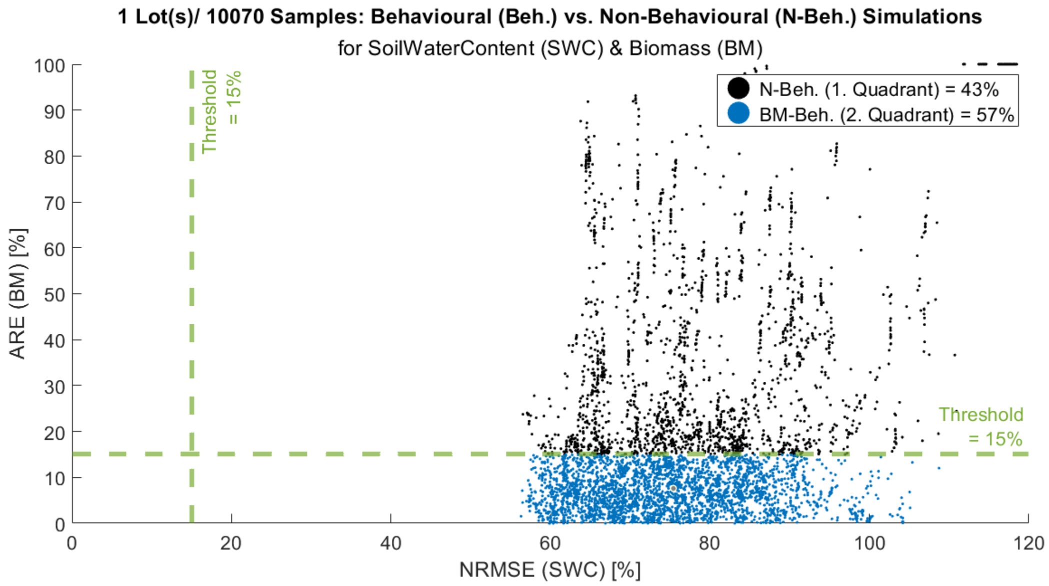

Figure 15 Quadrant-based analysis of soil-water-content- and biomass-evaluated simulations of all lots

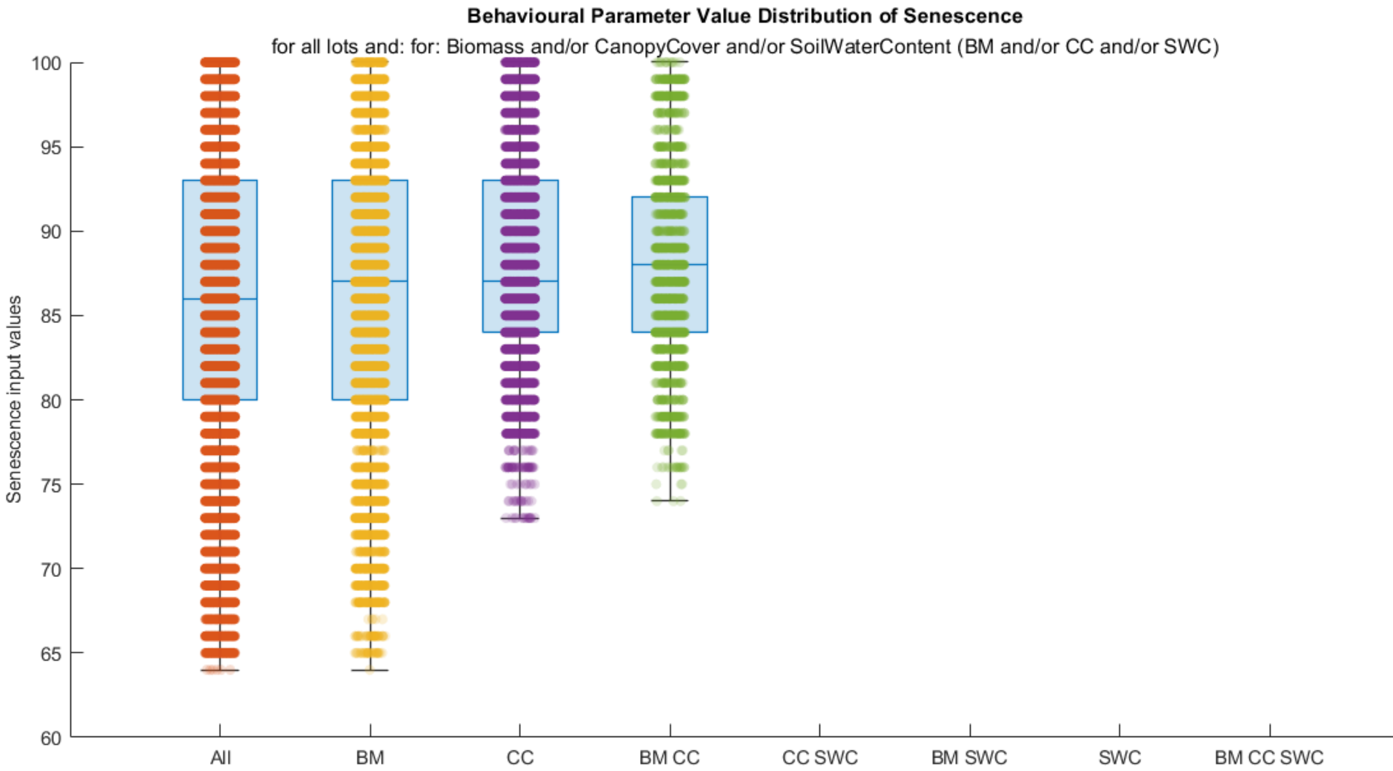

Figure 16 Boxchart analysis of behavioural values of parameter "Senescence" for all lots, differentiating between targeted variable combinations – "All" = all simulations, i.e. including behavioural and non-behavioural parameter values

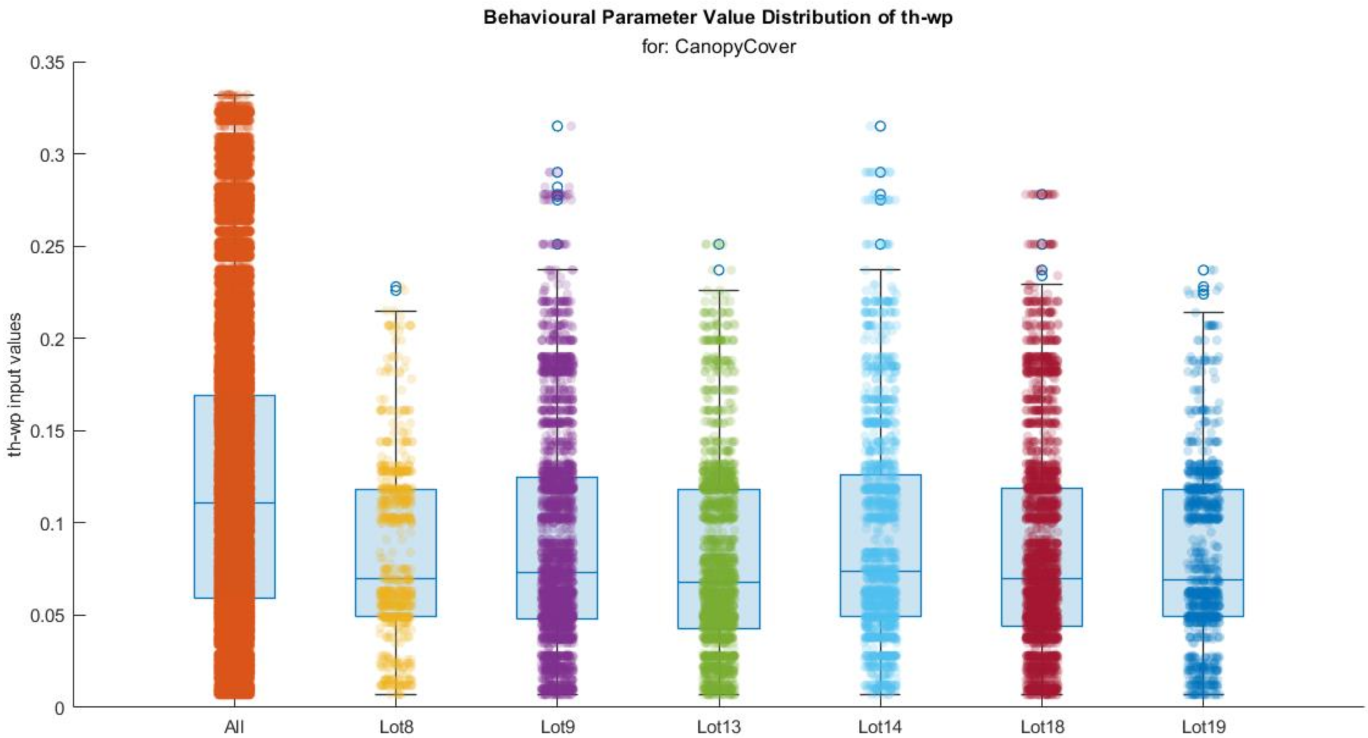

Figure 17 Boxchart analysis of behavioural values of parameter "th_wp" for target variable "Canopy Cover", differentiating between lots – "All" = all simulations, i.e. including behavioural and non-behavioural parameter values

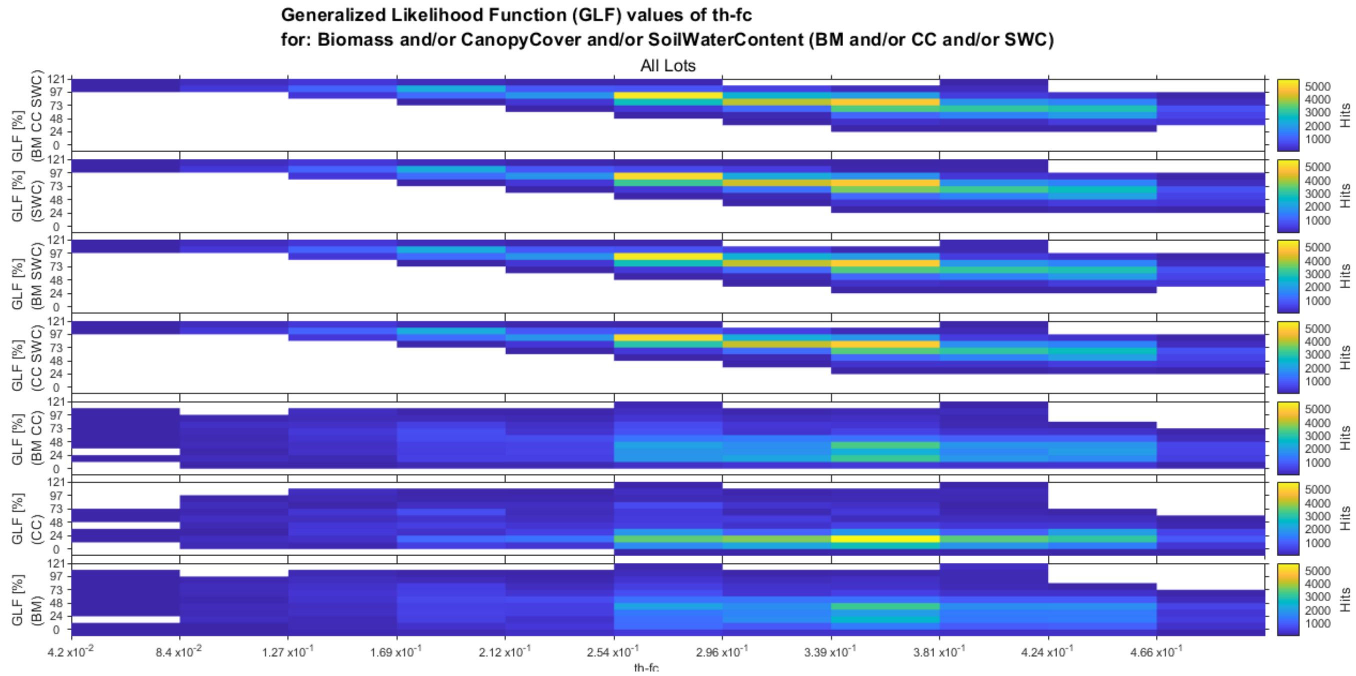

Figure 18 Heatmap analysis of all simulated Generalized Likelihood Function (GLF) values (vertical axis) vs. input values of parameter "th_fc" (horizontal axis), differentiating between target variable combinations (stacked vertically), summing up values for all lots; frequency of GLF/parameter value combinations ("Hits") indicated by the colorbar on the right.

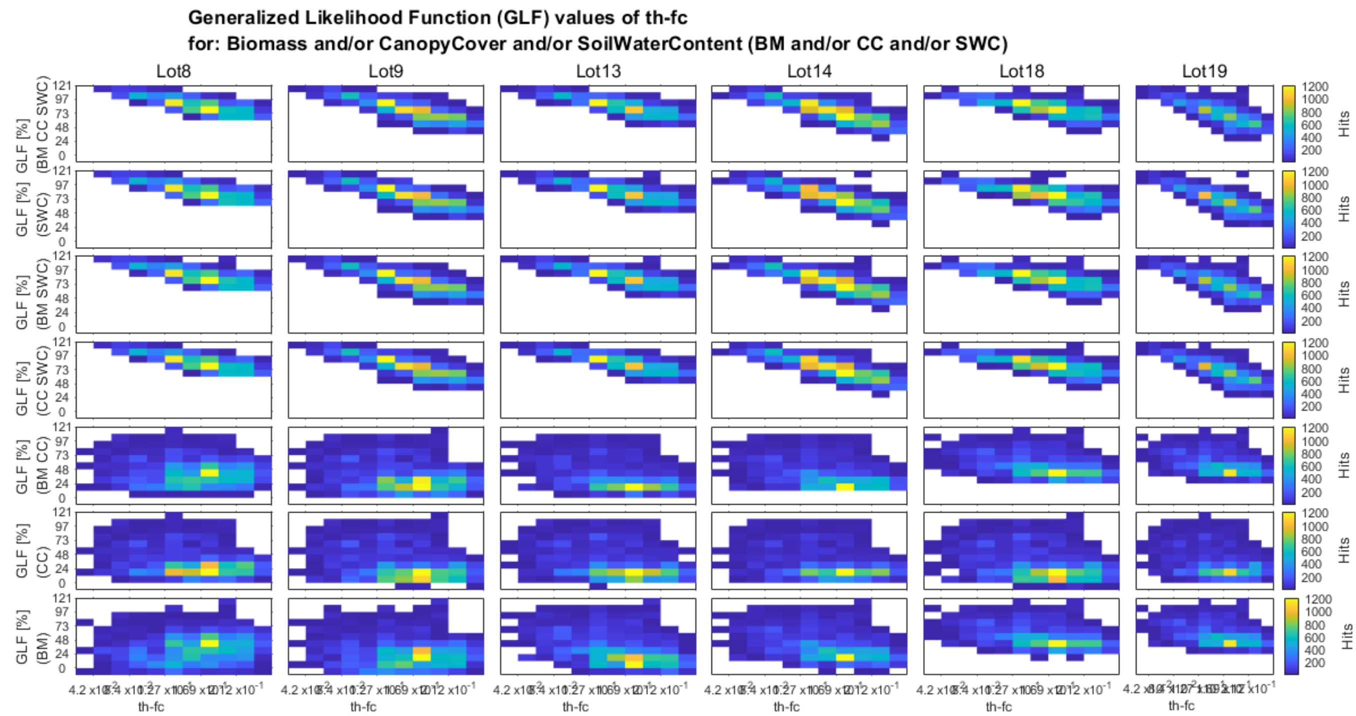

Figure 19 Heatmap analysis of all simulated Generalized Likelihood Function (GLF) values (vertical axis) vs. input values of parameter "th_fc" (horizontal axis) differentiating between target variable combinations (stacked vertically) as well as between lots (stacked horizontally); frequency of GLF/parameter value combinations ("Hits") indicated by the colorbar on the right.

References

Bruckmaier, F. (2021), 'Quantification of yield loss due to water and temperature stress with AquaCrop for wheat in Northern India'. [Unpublished study project]. Chair of Hydrology and River Basin Management, TUM Department of Civil, Geo and Environmental Engineering, Technical University of Munich.

Available at: http://dx.doi.org/10.13140/RG.2.2.15557.93920.

Foster, T. (2019), AquaCrop-OS v6.0a Reference Manual, University of Manchester.

Foster, T., Brozović, N., Butler, A., Neale, C., Raes, D., Steduto, P., Fereres, E. and Hsiao, T. (2017), 'AquaCrop-OS: An open source version of FAO's crop water productivity model', Agricultural Water Management 181, 18–22.

Available at: https://www.sciencedirect.com/science/article/pii/S0378377416304589