

User guidelines for running **TSE** tools (**T**ime-**S**eries cultivar coefficient **E**stimator for DSSAT models)

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In case of urgent questions/Bugs contact author of the program.

This cultivar coefficients optimisation program was developed for estimation of the cultivar coefficient of all available crop models in the current DSSAT Version 4.7 shell. It has been tested with DSSAT4.7 **CROPGRO-Soybean** model and partially with **CERES-Maize** and **CERES-Wheat** models.

Contents

1. The TSE concept overview	2
2. General TSE program settings overview.....	3
3. Running TSE program.....	9
1. Do NOT modify!	11
2. Select desired model and Initialize selected!	12
3. Select cultivar from model corresponding list.....	13
4. Select File/s-X from list containing selected cultivar.....	14
5. Select corresponding Treatment/s based on the File/s-X containing selected cultivar.....	15
6. Execute (Check the DSSAT file setup) selected treatment/s with DSSAT model to check if core DSSAT files are runnable, and select Default/Advanced.....	16
7. Select optimisation of Phenology/Growth -related coefficients and corresponding methods.....	17
8. Selecting desired coefficients and coefficient ranges and increment steps.	22
9. Check if optimisation software setup is correct.....	26
10. Run the model!	27
11. Additional options	28
I. [Reset coefficient ranges] or estimate	28
II. [Multi TRT comb]	29
III. Execute [Gbuild]	29
IV. [Exit] the program and all running threads.....	29
APPENDIX	30
1 The nRMSE error minimisation method	30
2 The nRMSE multiple treatment based goodness of fit criteria.....	31
3 The RW-nRMSE	32

1. The TSE concept overview

The cultivar coefficients estimation program was developed to work with DSSAT crop growth models (CROPGRO and CERES). It will work only if fully functional DSSAT files are available such as experiment file (FileX), weather file, soil profile, functional species, ecotype and cultivar files, time-series file containing in-season observations (FileT) and summary file (FileA - optional) are available.

Overall program run can be separated in three steps:

1. Selection of the FileX and corresponding treatments defined in FileX. Based on the selected experiment corresponding in-season observations (as time-series data) are read in as temporal inputs (all available time-series observations can be used), and cultivar coefficients designated for optimisation (phenology- and/or growth-related) are selected with desired coefficient ranges (Figure 1, step 1).
2. For each cultivar coefficient combination defined in first step crop model is executed with simulated outputs being coupled with in-season observations and saved for later analysis (Figure 1, step 2).
3. After all cultivar coefficient combinations were used and simulated outputs coupled with in-season observations statistical analysis is conducted based on the target variables used in the cultivar coefficient estimation process and the combination with the best statistical agreement between simulated and observed is selected as “optimum”.

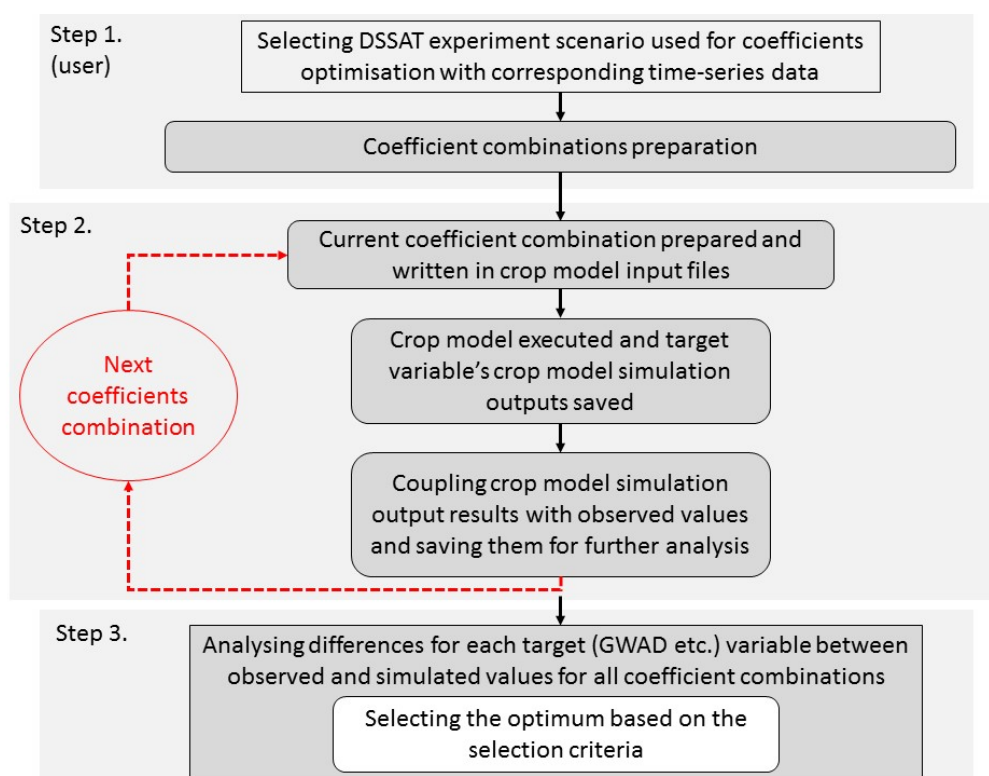


Figure 1: Flow chart showing overall program run in three steps (GWAD – grain weight) (Memic et al. 2020)

The program can be used for optimising cultivar coefficients based on single or multiple experiment data sets. User should first optimise phenology-related cultivar coefficients. After phenological events are correctly optimised, growth-related cultivar coefficients are optimised. Phenology-related cultivar coefficient optimisation is not conducted based on the time-series data (FileT), but by using FileA observations and simply minimising the difference between simulated and observed phenological event as day after planting. Growth-related cultivar coefficients are optimised by using FileT in-season observations by means of normalised RMSE throughout season. The combination providing lowest difference between simulated and observed values based on nRMSE is selected as optimum. Cultivar coefficient ranges initial values are predefined (by existing minimum and maximum values in cultivar files) but can be modified according to user's needs.

2. General TSE program settings overview

The program was developed (in Windows environment, for use on Windows) as standalone and has no specific installation requirements. In addition to the required DSSAT files all required files for running the program are shared with gitHub_TSE.zip file.

The “gitHub_TSE_[date_stamp].zip” file has to be unzipped as “gitHub_TSE_[date_stamp]” working directory. From “gitHub_TSE_[date_stamp]” directory “TSE” folder copied to the Tools directory: “C:\DSSAT47\Tools” (Figure 2).

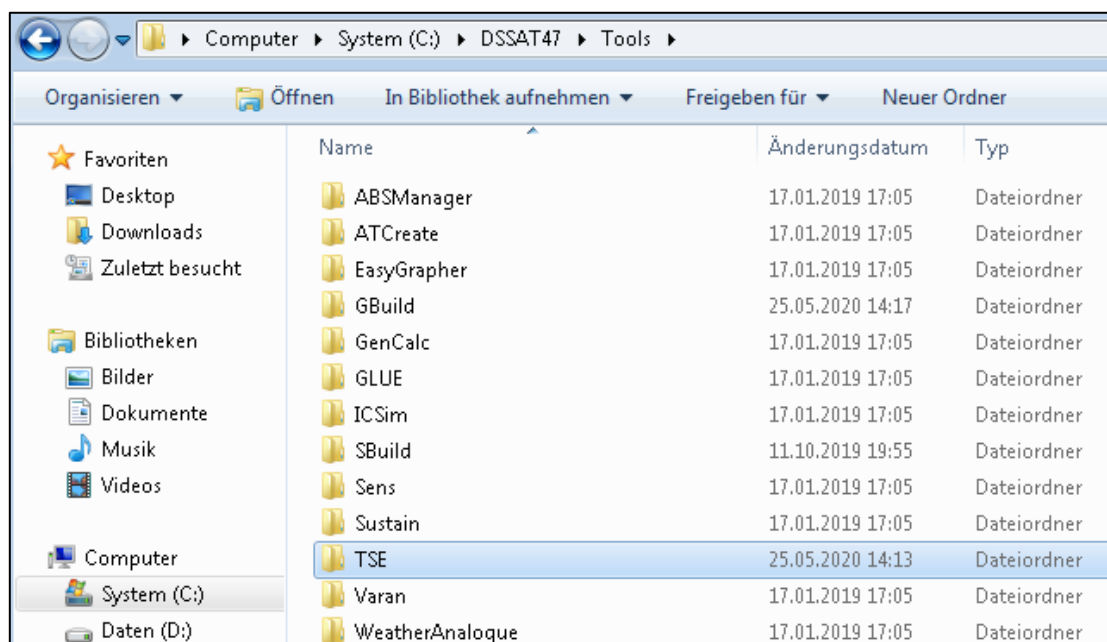


Figure 2 “C:\DSSAT47\Tools\TSE”

In folder “TSE” “C:\DSSAT47\Tools\TSE” (Figure 3) TSE_calibrator_DSSAT.exe windows runnable has to be **executed as “Administrator”** (Figure 4).

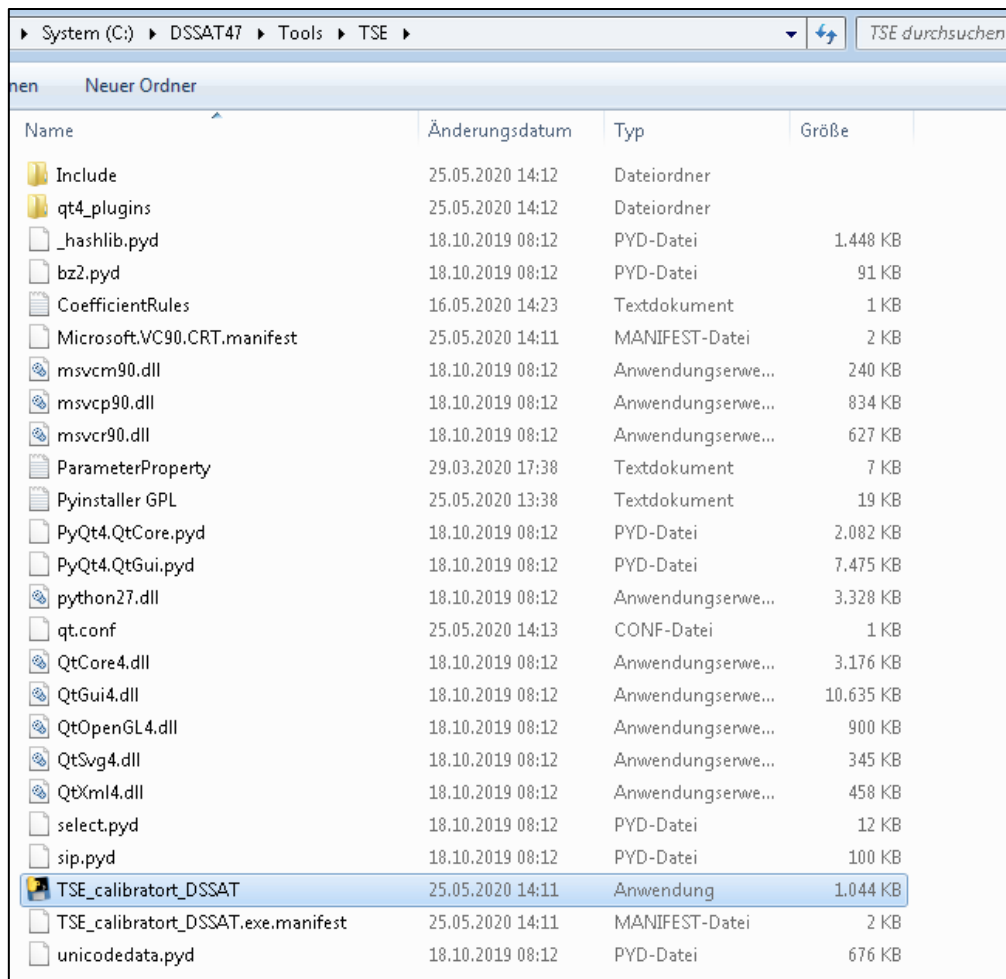


Figure 3 TSE_calibrator_DSSAT.exe windows runnable

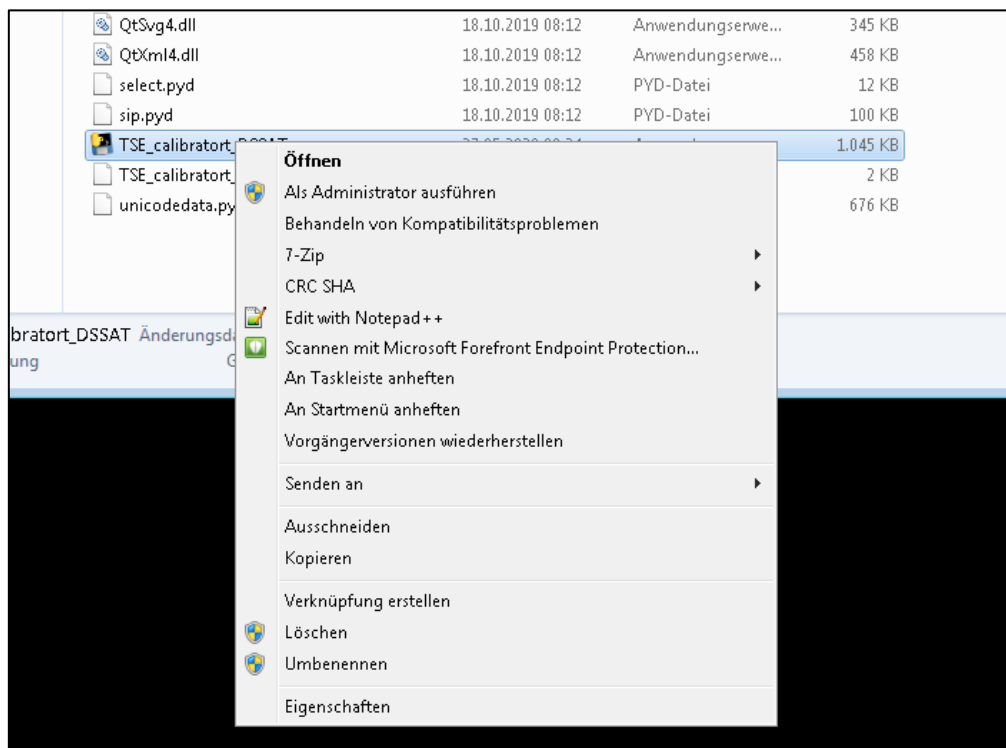


Figure 4 Execute as “Administrator”

VERY IMPORTANT:

- I. PlantGro.Out crop model outputs are coupled to those in FileT (growth-related) time-series in-season observations
- II. Evaluate.Out crop model outputs are coupled to those in FileA (phenology-related) as DAY observations
- III. If sub-model (eg. WHAPS) is initialised in the FileX, the calibrator will not work! (in FileX in *SIMULATION CONTROLS in GENERAL line, column SMODEL **do NOT initialise sub-models!**)
- IV. Only variables such as LAID, CWAD, GWAD etc. initialised in first time occurring “@TRN....” line in FileT is actively used by TSE
- V. For multi TRT optimisations only target variables simultaneously available in all File-T/s (for corresponding File-X/s Treatments) are accessible for optimisation
- VI. If ParameterProperty.txt is NOT in the C:\DSSAT47\Tools\TSE folder, P/G (Phenology/Growth-related flags) are not available in the interface!
- VII. FileT observations (all in-season observations available including 0 are used, only -99 values are ignored by the program) used for estimating the optimum genetic coefficient (phenology- and growth-related)
- VIII. The program is matching DOY from FileT with those in the PlantGro.OUT. If you setup in the FileX reporting frequency for example every fifth day and exact observation DOY is not present in the PlantGro.OUT as it is written in the FileT, the program will not be able to match them for comparing simulated and observed.

The optimiser program is creating additional directory “TSE_workspace” (C:\DSSAT47\TSE_workspace) (Figure 5) and modifying the cultivar file in that directory, which is then used by main DSSAT model executable.

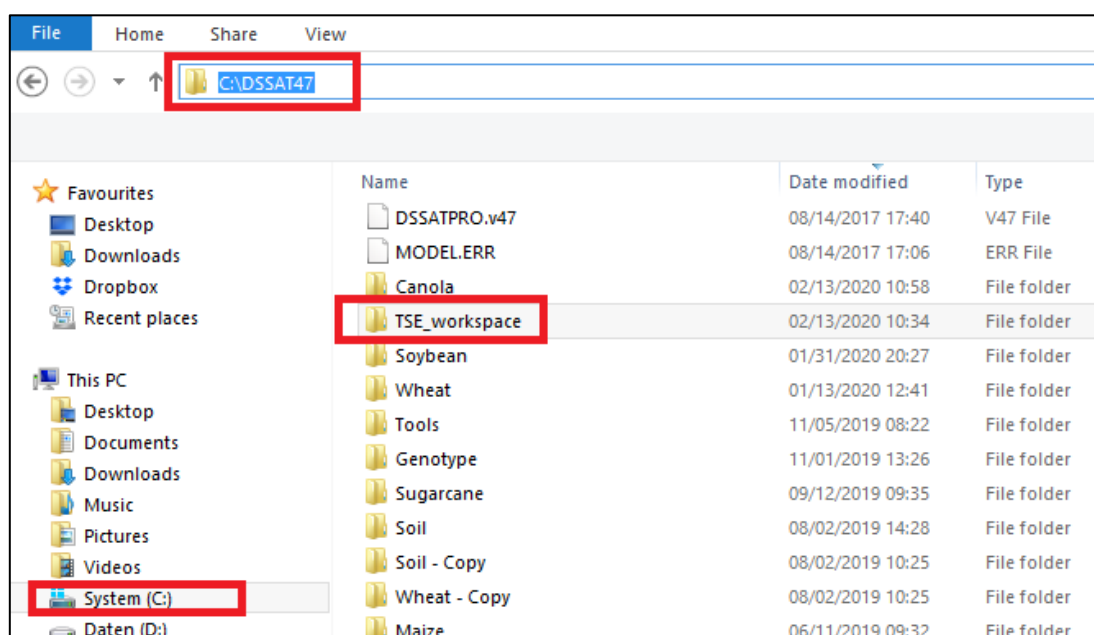


Figure 5 C:\DSSAT47\TSE_workspace

The optimiser program is NOT modifying core DSSAT files in their original directories!

Program run is considered: **Start-** “TSE_calibrator_DSSAT.exe” executed until “Exit” push button is pressed. Any form of optimisation done in-between is temporary saved in the temporary cultivar file in TSE_workspace directory.

After TSE program is started (TSE_calibrator_DSSAT.exe executed) all modifications on Cultivar file are conducted in C:\DSSAT47\TSE_workspace. During one program run (until “Exit” push button is pressed) different coefficients or different target variables can be optimised one after another or simultaneously and cultivar changes will be saved if accepted as “optimums” in cultivar file in C:\DSSAT47\TSE_workspace. If user is satisfied with the cultivar coefficient values based on nRMSE fit cultivar coefficient combination should be copied to C:\DSSAT47\Tools\Genotype located cultivar file, **MANUALLY**. If TSE program is started again without saving the combination in C:\DSSAT47\Tools\Genotype located cultivar file new TSE program start will copy original C:\DSSAT47\Tools\Genotype located cultivar file and overwrite your working cultivar file in C:\DSSAT47\TSE_workspace.

After model run finished and before “Exit” push button is clicked GBuild can be started to check visual and statistical fit (RMSE, d-statistics within GBuild) of the experiment file executed with the “optimum” genetic coefficient combination found in the last model run. With GBuild PlantGro.OUT from C:\DSSAT47\TSE_workspace directory has to be open, because TSE will create parallel files it requires in this folder, without modifying the original files in original DSSAT directories.

The more coefficients are “activated” (used in estimation process) the longer will optimisation last. **For each new coefficient and additional increment step (Inc) number of model runs will increase exponentially.**

For example:

Every time **TSE_calibrator_DSSAT.exe** is executed, original cultivar (**SBGRO047.CUL**) file from **C:\DSSAT47\Genotype** will be copied to **C:\DSSAT47\TSE_workspace** directory (Figure 6), and overwrite cultivar file in that directory (if exist, if not then just copied). If user wants to keep the genetic coefficient combination, it has to be copied to the original cultivar file in **C:\DSSAT47\Genotype** directory into **SBGRO047.CUL** manually.

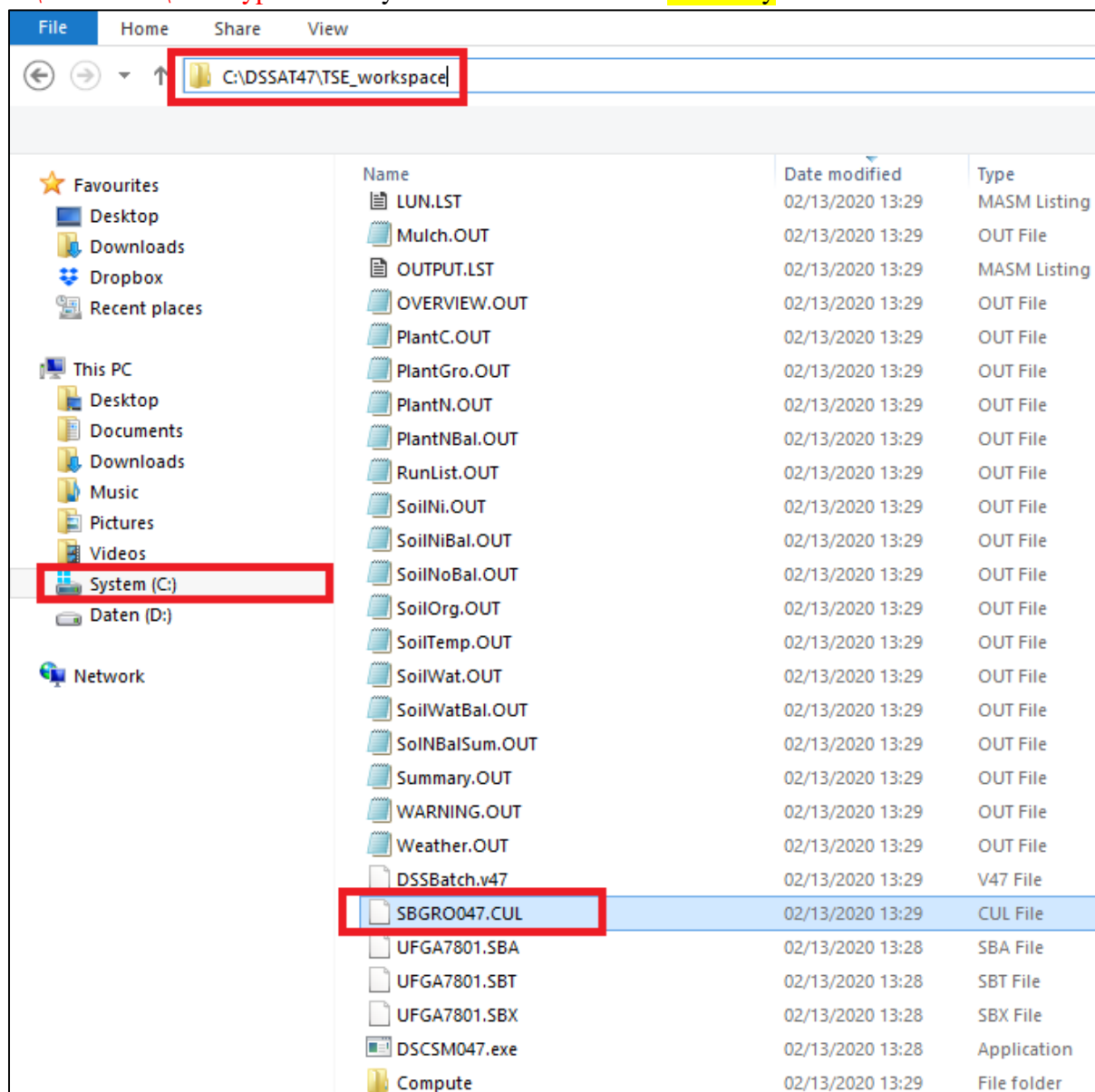


Figure 6 **C:\DSSAT47\TSE_workspace\SBGRO047.CUL**

The original cultivar is saved as “!Old_timestamp_cultivarID...” (Figure 7, text editor line 71) and the new one (Figure 7, text editor line 74) is saved in that working cultivar file (in **TSE_workspace**) and model is executed.

```

64 IB0011 EVANS (0) . SB0001 14.10 0.171 16.8 7.8 13.8 30.00 26
65 IB0037 ELGIN-87 (2) . SB0201 13.59 0.249 17.0 8.9 13.0 35.80 30
66 IB0003 WAYNE (3) . SB0301 13.45 0.255 19.5 8.0 14.7 26.70 28
67 IB0010 WILLIAMS-82 (3) . SB0301 13.40 0.285 19.0 8.3 14.2 32.20 28
68 IB0079 TSC WILLIAMS-82 (3) . SB0301 13.40 0.24 20.0 8.3 13.4 34.20 28
69 IB0090 TSC WILLIAMS-82 (3) . SB0301 13.50 0.38 20.0 8.3 13.0 31.20 28
70
71 !Old 2020-02-13 13:28:50.373000 IB0001 BRAGG . SB0701 12.33
72
73
74 IB0001 BRAGG . SB0701 12.33 0.32 19.5 10.0 15.2 37.6 19
75

```

Figure 7 Old and new cultivar

3. Running TSE program

(The steps of preparing the estimator for run are enumerated in the interface)

1. If directory path shown is “**C:\DSSAT47**”, do NOT modify! If the path is not “**C:\DSSAT47**” (This means that TSE folder was not copied to the “**C:\DSSAT47\Tools**”), then navigate to TSE folder and select it. It will be explained later in more details.
2. Select desired model and Initialize it!
3. Select cultivar from model corresponding list.
4. Select File/s-X from list containing selected cultivar.
5. Select corresponding Treatment/s based on the File/s-X containing selected cultivar.
6. Execute selected treatment/s with DSSAT model to check if core DSSAT files are runnable, and select Default/Advanced.
7. Select optimisation of Phenology/Growth -related coefficients and corresponding methods.
8. Selecting desired coefficients and coefficient ranges and increment steps.
9. Check if optimisation software setup is correct.
10. Run the model!
11. Reset coefficient ranges or estimate Multi treatment based cultivar coefficient combination!

Interface

TSE

User Guide

1.

2.

List Crop Models

Selected:

DCSM:

Crop dir:

v.:

Crop:

Model:

Crp short:

Cult. file:

Initialize selected

3. Cultivar name:

4. Xfiles: Exp info:

5. X-files TRT TRT name

6. ☒ Default ☐ Advanced

7.

Phenology (P)

☐ All

☐ Onset of flower ☐ First pod day
☐ First seed ☐ Phys-maturity

(P)

Growth (G)

Universal code Label Target variables

Initialize target variables

Min-nRMSE

☐ nRMSE

RW-nRMSE(1-4)

☐ RW-nRMSE

Help! Methods...

(G)

Coefficient Rules Help

8. VAR-Name P/G Flag Genetic coefficients setup

Initialize	Min	Max	<input type="checkbox"/>	Inc. Calc.
X	1	1	2	1
X	1	1	2	1
X	1	1	2	1
X	1	1	2	1
X	1	1	2	1
X	1	1	2	1
X	1	1	2	1

9.

10.

Run the Model

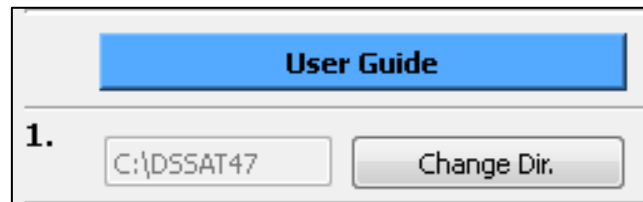
Outputs:

11.

1. Do NOT modify!

If directory path shown is “C:\DSSAT47”, do NOT modify! If the path is not “C:\DSSAT47” then copy TSE folder (not entire gitHub_[date_satemp] extracted folder!, only **TSE** folder from it into the “C:\DSSAT47\Tools”. After re-executing

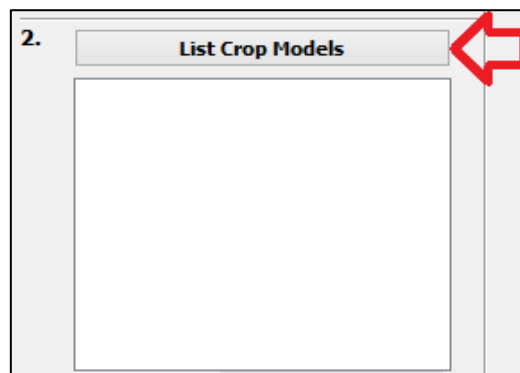
TSE_calibrator_DSSAT.exe from **TSE** -> “C:\DSSAT47\Tools\TSE” the correct path should be red in.



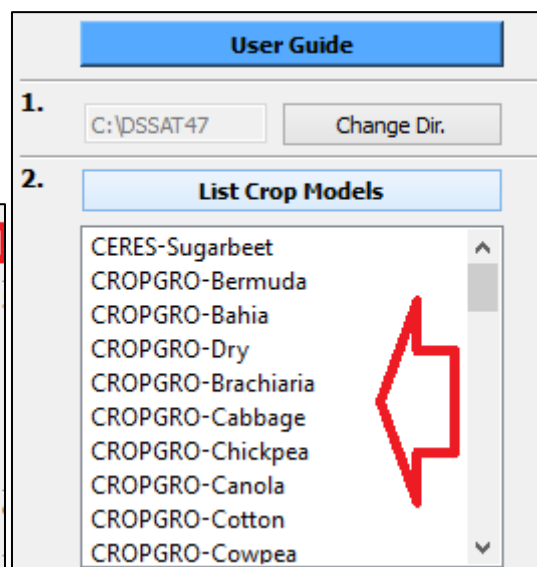
1.1 Interface

2. Select desired model and Initialize selected!

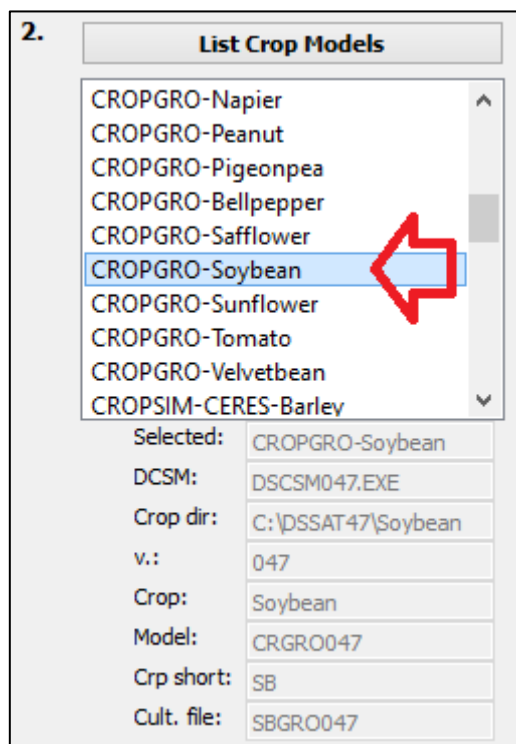
The model list is uploaded from “C:\DSSAT47” SIMULATION.CDE file.



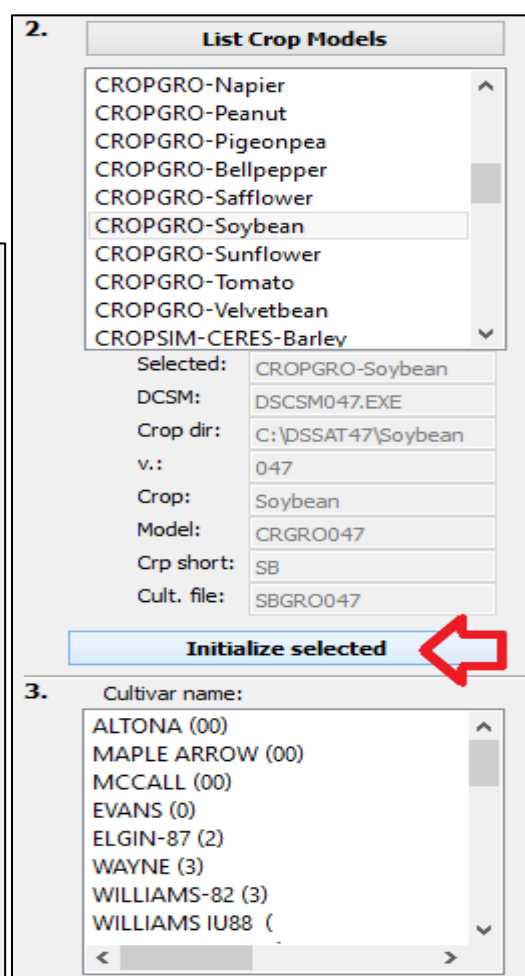
2.1 Interface



2.2 Interface



2.3 Interface



2.4 Interface

3. Select cultivar from model corresponding list.

User Guide

1. C:\DSSAT47 Change Dir.

2. List Crop Models

CROPGRO-Napier
CROPGRO-Peanut
CROPGRO-Pigeonpea
CROPGRO-Bellpepper
CROPGRO-Safflower
CROPGRO-Soybean
CROPGRO-Sunflower
CROPGRO-Tomato
CROPGRO-Velvetbean
CROPSIM-CERES-Barley

Selected: CROPGRO-Soybean
DCSM: DSCSM047.EXE
Crop dir: C:\DSSAT47\Soybean
v.: 047
Crop: Soybean
Model: CRGRO047
Crp short: SB
Cult. file: SBGRO047

Initialize selected

3. Cultivar name:

WAYNE (3)
WILLIAMS-82 (3)
WILLIAMS IU88 (3)
WILLIAMS OH88 (3)
WILLIAMS OH90 (3)
TSC WILLIAMS-82
BRAGG
BRAGG TSC 1978

4. Xfiles: Exp info:

UFGA7601.SBX : UFGA7601SB BRAGG, 1976, EQUI
UFGA7801.SBX : UFGA7801SB BRAGG, IRRIGATE
UFGA7802.SBX : UFGA7802SB BRAGG, IRR*INSE
UFGA7901.SBX : UFGA7901SB IRRIGATION, 197
UFGA8401.SBX : UFGA8401SB BRAGG, IRRIGATE

5. X-files TRT TRT name

6. Check the DSSAT file setup ☒ Default ☐ Advanced

7. Phenology (P)

☐ All ☐ Onset of flower ☐ First pod day
☐ First seed ☐ Phys-maturity

Growth (G)

Universal code Label Target variables

Initialize target variables

Min-nRMSE RW-nRMSE(1-4)

☐ nRMSE ☐ RW-nRMSE

Help! Methods...

3.1 Interface

4. Select File/s-X from list containing selected cultivar.

User Guide

1. C:\DSSAT47 Change Dir.

2. List Crop Models

CROPGRO-Napier
CROPGRO-Peanut
CROPGRO-Pigeonpea
CROPGRO-Bellpepper
CROPGRO-Safflower
CROPGRO-Soybean
CROPGRO-Sunflower
CROPGRO-Tomato
CROPGRO-Velvetbean
CROPSIM-CERES-Barley

Selected: CROPGRO-Soybean
DCSM: DSCSM047.EXE
Crop dir: C:\DSSAT47\Soybean
v.: 047
Crop: Soybean
Model: CRGRO047
Crp short: SB
Cult. file: SBGRO047

Initialize selected

3. Cultivar name:

WAYNE (3)
WILLIAMS-82 (3)
WILLIAMS IU88 (3)
WILLIAMS OH88 (3)
WILLIAMS OH90 (3)
TSC WILLIAMS-82
BRAGG
BRAGG TSC 1978

4. Xfiles: Exp info:

UFGA7601.SBX : UFGA7601SB BRAGG,1976,EQUI
UFGA7801.SBX : UFGA7801SB BRAGG, IRRIGATE
UFGA7802.SBX : UFGA7802SB BRAGG, IRR*INSE
UFGA7901.SBX : UFGA7901SB IRRIGATION, 197
UFGA8401.SBX : UFGA8401SB BRAGG, IRRIGATE

5. X-files TRT TRT name

UFGA7801.SBX 1 TNAME: 78 IRRIG, light rate,
UFGA7801.SBX 2 TNAME: 78 RAINFED BRAGG

6. Check the DSSAT file setup ☒ Default ☐ Advanced

7. Phenology (P)

☐ All ☐ Onset of flower ☐ First pod day
☐ First seed ☐ Phys-maturity

Growth (G)

Universal code Label Target variables

Initialize target variables

Min-nRMSE RW-nRMSE(1-4)

☐ nRMSE ☐ RW-nRMSE

Help! Methods...

4.1 Interface

5. **Select** corresponding **Treatment/s** based on the File/s-X containing selected cultivar.

The green box (green list widget box in the interface) is where the experiment file and treatments for optimising cultivar coefficients are **selected**. Multiple treatments can be selected (multiple treatment/experiment selection is done by: **Ctrl+ mouse left button click**).

The screenshot displays the DSSAT software interface with several numbered steps:

- 1.** Directory path: C:\DSSAT47. A "Change Dir." button is available.
- 2.** **List Crop Models**: A scrollable list of crop models including CROPGRO-Napier, CROPGRO-Peanut, CROPGRO-Pigeonpea, CROPGRO-Bellpepper, CROPGRO-Safflower, CROPGRO-Soybean (selected), CROPGRO-Sunflower, CROPGRO-Tomato, CROPGRO-Velvetbean, and CROPSIM-CERES-Barley. Below the list, fields for "Selected:", "DCSM:", "Crop dir:", "v.:", "Crop:", "Model:", "Crp short:", and "Cult. file:" are populated with values like "CROPGRO-Soybean", "DSCSM047.EXE", "C:\DSSAT47\Soybean", "047", "Soybean", "CRGRO047", "SB", and "SBGRO047". An "Initialize selected" button is at the bottom.
- 3.** **Cultivar name:** A list of cultivars including WAYNE (3), WILLIAMS-82 (3), WILLIAMS IU88 (3), WILLIAMS OH88 (3), WILLIAMS OH90 (3), TSC WILLIAMS-82, BRAGG (selected), and BRAGG TSC 1978.
- 4.** **Xfiles:** A list of experiment files with their corresponding crop models and treatments, such as "UFGA7601.SBX : UFGA7601SB BRAGG, 1976, EQUI".
- 5.** **X-files TRT TRT name**: A green box containing a list of treatments. The first two are "UFGA7801.SBX 1 TNAME: 78 IRRIG, light rate," and "UFGA7801.SBX 2 TNAME: 78 RAINFED BRAGG". A red arrow points to the first treatment.
- 6.** **Check the DSSAT file setup**: A checkbox for "Default" (checked) and "Advanced".
- 7.** **Phenology (P)**: A section with checkboxes for "All", "Onset of flower", "First pod day", "First seed", and "Phys-maturity".
- Growth (G)**: A section with a table of target variables. The table has columns for "Universal code", "Label", and "Target variables". The variables listed are L#SD (Leaf number), LAID (LAI), P#AD (Pod no #/m2), SWAD (Stem wt kg/ha), GWAD (Grain wt kg/ha), and LWAD (Leaf wt kg/ha). Below the table, there are fields for "Min-nRMSE" and "RW-nRMSE(1-4)", and a "Help! Methods..." button.

5.1 Interface

6. Execute (**Check the DSSAT file setup**) selected treatment/s with DSSAT model to check if core DSSAT files are runnable, and select Default/Advanced.

6. ☒ **Default** ☐ **Advanced**

6.1 Interface

4. Xfiles: Exp info:
 UFGA7601.SBX : UFGA7601SB BRAGG,1976,EQUI
 UFGA7801.SBX : UFGA7801SB BRAGG, IRRIGATE
 UFGA7802.SBX : UFGA7802SB BRAGG, IRR*INSE
 UFGA7901.SBX : UFGA7901SB IRRIGATION, 197
 UFGA8401.SBX : UFGA8401SB BRAGG, IRRIGATE

5. X-files TRT TRT name
 UFGA7801.SBX 1 TNAME: 78 IRRIG, light rate,
 UFGA7801.SBX 2 TNAME: 78 RAINFED BRAGG

6. ☒ **Default** ☐ **Advanced**

7. **Phenology (P)**
☐ All ☐ Onset of flower ☐ First pod day
☐ First seed ☐ Phys-maturity

Growth (G)

Universal code	Label	Target variables
L#SD	Leaf number	
LAID	LAI	
P#AD	Pod no #/m2	
SWAD	Stem wt kg/ha	
GWAD	Grain wt kg/ha	
I WAD	Leaf wt kg/ha	

Initialize target variables

Min-nRMSE RW-nRMSE(1-4)
☐ nRMSE ☐ RW-nRMSE

Help! Methods...

6.2 Interface

Cultivar specific coefficient flags (Phenology and Growth – P/G) are listed in the “C:\DSSAT47\Tools\TSE” in a file “**ParameterProperty.txt**”. **Default** (check box) will upload only coefficients with predefined P/G flags (according to selection of the Phenology or Growth). **Advanced** will upload all available cultivar coefficients from cultivar file for potential optimisation.

7. Select optimisation of Phenology/Growth-related coefficients and corresponding methods.

In this step error minimisation method (nRMSE or RW-nRMSE, explained in the APPENDIX) is selected. Maximum four different target variables (e.g. LWAD, CWAD, PWAD and SHAD) can be selected. If four are not available, one or two can be selected as well. Optimal is four, the rest should be used with precaution. In first round of optimisation four can be selected and in second next four, or with some other combinations.

Phenology (P): Option “All” is only available when all four phenological events observations are available. For the crop models that don’t have these four events, phenological events have to be optimised one-by-one. (In the next version more flexible options will be introduced).

4. Xfiles: Exp info:
 UFGA7601.SBX : UFGA7601SB BRAGG,1976,EQUI
 UFGA7801.SBX : UFGA7801SB BRAGG, IRRIGATE
 UFGA7802.SBX : UFGA7802SB BRAGG, IRR*INSE
 UFGA7901.SBX : UFGA7901SB IRRIGATION, 197
 UFGA8401.SBX : UFGA8401SB BRAGG, IRRIGATE

5. X-files TRT TRT name
 UFGA7801.SBX 1 TNAME: 78 IRRIG, light rate,
 UFGA7801.SBX 2 TNAME: 78 RAINFED BRAGG

6. Check the DSSAT file setup ☒ Default ☐ Advanced

7. Phenology (P)
☐ All ☐ Onset of flower ☐ First pod day
☐ First seed ☐ Phys-maturity

Growth (G)

Universal code	Label	Target variables
L#SD	Leaf number	
LAID	LAI	
P#AD	Pod no #/m2	
SWAD	Stem wt kg/ha	
GWAD	Grain wt kg/ha	
LWAD	Leaf wt kg/ha	

Initialize target variables

Min-nRMSE ☐ nRMSE RW-nRMSE(1-4) ☐ RW-nRMSE

Help! Methods...

7.1 Interface

Growth (G): Push button will initialize growth-related section.

4. Xfiles: Exp info:

UFGA7601.SBX	: UFGA7601SB BRAGG,1976,EQUI
UFGA7801.SBX	: UFGA7801SB BRAGG, IRRIGATE
UFGA7802.SBX	: UFGA7802SB BRAGG, IRR*INSE
UFGA7901.SBX	: UFGA7901SB IRRIGATION, 197
UFGA8401.SBX	: UFGA8401SB BRAGG, IRRIGATE

5. X-files TRT TRT name

UFGA7801.SBX	1	TNAME: 78 IRRIG, light rate,
UFGA7801.SBX	2	TNAME: 78 RAINFED BRAGG

6. Check the DSSAT file setup ☒ Default ☐ Advanced

7. Phenology (P)

☐ All
(P)

☐ Onset of flower
☐ First seed
☐ First pod day
☐ Phys-maturity
(P)

Growth (G)

Universal code	Label	Target variables
L#SD	Leaf number	
LAID	LAI	
P#AD	Pod no #/m2	
SWAD	Stem wt kg/ha	
GWAD	Grain wt kg/ha	
I WAD	Leaf wt kg/ha	

Initialize target variables

Min-nRMSE

☐ nRMSE

RW-nRMSE(1-4)

☐ RW-nRMSE

Help! Methods...

8.

VAR-Name	P/G Flag
LFMAX	G
SLAVR	G
SIZLF	G
WTPSD	G
SFDUR	G
SDPDV	G

9. Inputs setup check

Show comb-s

10. Run the Model

11. Reset coeff ranges

7.2 Interface

“Ctrl + mouse left click”- for selecting multiple target variables simultaneously!
 First: 1, 2 or 4 target variables are selected as shown in Interface 7.3 (red arrows).

4.

Xfiles:

Exp info:

UFGA7601.SBX : UFGA7601SB BRAGG,1976,EQUI
UFGA7801.SBX : UFGA7801SB BRAGG, IRRIGATE
UFGA7802.SBX : UFGA7802SB BRAGG, IRR*INSE
UFGA7901.SBX : UFGA7901SB IRRIGATION, 197
UFGA8401.SBX : UFGA8401SB BRAGG, IRRIGATE

5.

X-files

TRT

TRT name

UFGA7801.SBX 1 TNAME: 78 IRRIG, light rate,
UFGA7801.SBX 2 TNAME: 78 RAINFED BRAGG

6.

Check the DSSAT file setup

☒ Default
☐ Advanced

7.

Phenology (P)

☐ All
☐ Onset of flower
☐ First pod day
☐ First seed
☐ Phys-maturity

Growth (G)

Universal code

Label

Target variables

LAI
LAI
P#AD
Pod no #/m2
SWAD
Stem wt kg/ha
GWAD
Grain wt kg/ha
LWAD
Leaf wt kg/ha
CWAD
Tons wt kg/ha

Initialize target variables

Min-nRMSE

RW-nRMSE(1-4)

☐ nRMSE
☐ RW-nRMSE

Help!

Methods...

8.

VAR-Name

P/G Flag

LFMAX
SLAVR
SIZLF
WTPSD
SFDUR
SDPDV

9.

Inputs setup check

Show comb-s

10.

Run the Model

11.

Reset coeff ranges

7.3 Interface

The selected variables are initialized only after “Initialize target variables” push button is clicked (Interface 7.4) (red arrow).

4.

Xfiles:

Exp info:

UFGA7601.SBX : UFGA7601SB BRAGG,1976,EQUI
UFGA7801.SBX : UFGA7801SB BRAGG, IRRIGATE
UFGA7802.SBX : UFGA7802SB BRAGG, IRR*INSE
UFGA7901.SBX : UFGA7901SB IRRIGATION, 197
UFGA8401.SBX : UFGA8401SB BRAGG, IRRIGATE

5.

X-files

TRT

TRT name

UFGA7801.SBX 1 TNAME: 78 IRRIG, light rate,
UFGA7801.SBX 2 TNAME: 78 RAINFED BRAGG

6.

Check the DSSAT file setup

☒ Default
☐ Advanced

7.

Phenology (P)

☐ All
☐ Onset of flower
☐ First pod day
☐ First seed
☐ Phys-maturity

Growth (G)

Universal code

Label

Target variables

LAI
Pod no #/m2
Stem wt kg/ha
Grain wt kg/ha
Leaf wt kg/ha
Tons wt kg/ha

Initialize target variables

LAI
Grain wt kg/ha
Tops wt kg/ha
Leaf wt kg/ha

Min-nRMSE

RW-nRMSE(1-4)

☐ nRMSE
☐ RW-nRMSE

Help!

Methods...

8.

VAR-Name

P/G Flag

LFMAX
SLAVR
SIZLF
WTPSD
SFDUR
SDPDV

9.

Inputs setup check

Show comb-s

10.

Run the Model

11.

Reset coeff ranges

7.4 Interface

20

After initializing desired target variables error minimisation method has to be selected (Interface 7.5) e.g. nRMSE (Appendix 1) (red arrow).

4.

Xfiles:

Exp info:

UFGA7601.SBX : UFGA7601SB BRAGG,1976,EQUI
UFGA7801.SBX : UFGA7801SB BRAGG, IRRIGATE
UFGA7802.SBX : UFGA7802SB BRAGG, IRR*INSE
UFGA7901.SBX : UFGA7901SB IRRIGATION, 197
UFGA8401.SBX : UFGA8401SB BRAGG, IRRIGATE

5.

X-files

TRT

TRT name

UFGA7801.SBX 1 TNAME: 78 IRRIG, light rate,
UFGA7801.SBX 2 TNAME: 78 RAINFED BRAGG

6.

Check the DSSAT file setup

☒ Default
☐ Advanced

7.

Phenology (P)

☐ All
☐ Onset of flower
☐ First pod day
☐ First seed
☐ Phys-maturity

Growth (G)

Universal code

Label

Target variables

LAI
Pod no #/m2
Stem wt kg/ha
Grain wt kg/ha
Leaf wt kg/ha
Tops wt kg/ha

Initialize target variables

LAI LAI
Grain wt kg/ha
Tops wt kg/ha
Leaf wt kg/ha

Min-nRMSE

☒ nRMSE
☐ RW-nRMSE

Help!

Methods...

8.

VAR-Name

P/G Flag

LFMAX G
SLAVR G
SIZLF G
WTPSD G
SFDUR G
SDPDV G

9.

Inputs setup check

Show comb-s

10.

Run the Model

11.

Reset coeff ranges

7.5 Interface

21

8. Selecting desired coefficients and coefficient ranges and increment steps.

First coefficient/s are selected from the list (for selecting multiple coefficients **Ctrl + left mouse click**) (Interface 8.1, red arrow).

8.

VAR-Name	P/G Flag
LFMAX	G
SLAVR	G
SIZLF	G
WTPSD	G
SFDUR	G
SDPDV	G

Genetic coefficients setup

Initialize	Min	Max	<input type="checkbox"/>	Inc. Calc.
X	1	1	2	1
X	1	1	2	1
X	1	1	2	1
X	1	1	2	1
X	1	1	2	1
X	1	1	2	1
X	1	1	2	1

9.

Inputs setup check

Show comb-s

2020-07-10 09:43:25.741000
2020-07-10 09:43:27.116000
DSSAT run time elapsed:0:00:01.375000
File-T available selected treatment/s!

10.

Run the Model

8.1 Interface

After selecting desired coefficients in step 8. from list widget window Initialize push button will initialize coefficient Labels (names) in edit boxes and populate Min/Max coefficient ranges with min/max value available in corresponding cultivar file for selected cultivar coefficient (Interface 8.2). Automatically this will create simple range of Min/Max value with two coefficient combinations that are going to be passed into the cultivar file, where after each model is executed. If the user wants more combinations in between given Min/Max range **Check Box** next to the **Inc. Calc.** has to be **Checked** (Interface 8.3) and number of desired coefficient combinations between Min/Max can be given (Interface 8.4). After giving the desired number of combinations between Min/Max increment step is calculated by **Inc. Calc.** push button [(Max-Min)/number of combinations] (Interface 8.5). If user would like to modify Min/Max values it can be done directly (manually) in edit boxes below Min/Max labels in step 8. If Min/Max are modified based on the number of combinations after Inc. Calc. push button is clicked new Min/Max and Increment values are calculated and populated in corresponding edit boxes in step 8.

After selecting coefficient/s “Initialize” push button is clicked! (Interface 8.2)

8.

VAR-Name	P/G Flag	Genetic coefficients setup				
LFMAX	G	Initialize	Min	Max	<input type="checkbox"/>	Inc. Calc.
SLAVR	G	LFMAX	0.869	1.25	2	0.381
SIZLF	G	X	1	1	2	1
WTPSD	G	X	1	1	2	1
SFDUR	G	X	1	1	2	1
SDPDV	G	X	1	1	2	1
		X	1	1	2	1
		X	1	1	2	1
		X	1	1	2	1
		X	1	1	2	1

8.2 Interface

8.

VAR-Name	P/G Flag	Genetic coefficients setup				
LFMAX	G	Initialize	Min	Max	<input checked="" type="checkbox"/>	Inc. Calc.
SLAVR	G	LFMAX	0.869	1.25	2	0.381
SIZLF	G	X	1	1	2	1
WTPSD	G	X	1	1	2	1
SFDUR	G	X	1	1	2	1
SDPDV	G	X	1	1	2	1
		X	1	1	2	1
		X	1	1	2	1
		X	1	1	2	1

8.3 Interface



8.

VAR-Name	P/G Flag	Genetic coefficients setup				
LFMAX	G	Initialize	Min	Max	<input checked="" type="checkbox"/>	Inc. Calc.
SLAVR	G	LFMAX	0.869	1.25	5	0.381
SIZLF	G	X	1	1	2	1
WTPSD	G	X	1	1	2	1
SFDUR	G	X	1	1	2	1
SDPDV	G	X	1	1	2	1
		X	1	1	2	1
		X	1	1	2	1
		X	1	1	2	1

8.4 Interface

8. **Genetic coefficients setup**


VAR-Name	P/G Flag	Initialize	Min	Max	<input checked="" type="checkbox"/>	Inc. Calc.
LFMAX	G	LFMAX	0.869	1.25	5	0.0952
SLAVR	G	X	1	1	2	1
SIZLF	G	X	1	1	2	1
WTPSD	G	X	1	1	2	1
SFDUR	G	X	1	1	2	1
SDPDV	G	X	1	1	2	1

8.5 Interface

8. **Genetic coefficients setup**

VAR-Name	P/G Flag	Initialize	Min	Max	<input checked="" type="checkbox"/>	Inc. Calc.
LFMAX	G	LFMAX	0.869	1.25	5	0.0952
SLAVR	G	X	1	1	2	0
SIZLF	G	X	1	1	2	0
WTPSD	G	X	1	1	2	0
SFDUR	G	X	1	1	2	0
SDPDV	G	X	1	1	2	0



8.6 Interface

Example 1. With one coefficient (range and increment)

Genetic coefficients setup

VAR-Name	P/G Flag	Initialize	Min	Max	<input checked="" type="checkbox"/>	Inc. Calc.
LFMAX	G	LFMAX	0.99	1.25	5	0.065
SLAVR	G	X	1	1	2	0
SIZLF	G	X	1	1	2	0
WTPSD	G	X	1	1	2	0

Coefficient combinations

Comb_Count	LFMAX	X	X	X	X	X	X
1	0.99	-99	-99	-99	-99	-99	-99
2	1.055	-99	-99	-99	-99	-99	-99
3	1.12	-99	-99	-99	-99	-99	-99
4	1.185	-99	-99	-99	-99	-99	-99
5	1.25	-99	-99	-99	-99	-99	-99

Example 2. With two coefficients (ranges and increments)

4. Xfiles: Exp info:

UFGA7601.SBX : UFGA7601SB BRAGG,1976,EQUI
 UFGA7801.SBX : UFGA7801SB BRAGG, IRRIGATE
 UFGA7802.SBX : UFGA7802SB BRAGG, IRR*INSE
 UFGA7901.SBX : UFGA7901SB IRRIGATION, 197

8. VAR-Name P/G Flag

LFMAX G
 SLAVR G
 SIZLF G
 WTPSD G

Genetic coefficients setup

Initialize LFMAX SIZLF

Min	Max		Inc. Calc.
0.99	1.25	3	0.13
137.0	230.0	3	46.5
1	1	2	0
1	1	2	0
1	1	2	0
1	1	2	0
1	1	2	0

Estimated time:
 Estimated duration:
 minutes:seconds,milliseconds

Coefficient combinations

Coefficient combinations:

Comb_Count	LFMAX	SIZLF	X	X	X	X	X
1	0.99	137.0	-99	-99	-99	-99	-99
2	0.99	183.5	-99	-99	-99	-99	-99
3	0.99	230.0	-99	-99	-99	-99	-99
4	1.12	137.0	-99	-99	-99	-99	-99
5	1.12	183.5	-99	-99	-99	-99	-99
6	1.12	230.0	-99	-99	-99	-99	-99
7	1.25	137.0	-99	-99	-99	-99	-99
8	1.25	183.5	-99	-99	-99	-99	-99
9	1.25	230.0	-99	-99	-99	-99	-99

If you want to fix the value of some coefficient, in other words not to vary it during the program run, then you set Min and Max to equal value (same value in the Min edit box as in the Max value edit box).

9. Check if optimisation software setup is correct.

“Inputs setup check” push button when clicked will check if some of the necessary steps were skipped or if there is a problem with coefficient ranges etc. and warn user accordingly with popup Warning! message (Interface 9.1).

8. Genetic coefficients setup

VAR-Name	P/G Flag	Initialize	Min	Max	<input checked="" type="checkbox"/>	Inc. Calc.
LFMAX	G	LFMAX	0.869	1.25	5	0.0952
SLAVR	G	X	1	1	2	0
SIZLF	G	X	1	1	2	0
WTPSD	G	X	1	1	2	0
SFDUR	G	X	1	1	2	0
SDPDV	G	X	1	1	2	0

9. Inputs setup check

Show comb-s

10. Run the Model

Aproximated time:
TSE estimated duration:
hours:minutes:seconds,miliseconds
0:00:06.875000

9.1 Interface

The push button “Show comb-s” will directly display coefficient combinations predefined to be passed into the crop model cultivar file (Interface 9.2).

Coefficient combinations

Coefficient combinations:							
Comb_Count	LFMAX	X	X	X	X	X	X
1	0.869	-99	-99	-99	-99	-99	-99
2	0.964	-99	-99	-99	-99	-99	-99
3	1.059	-99	-99	-99	-99	-99	-99
4	1.154	-99	-99	-99	-99	-99	-99
5	1.249	-99	-99	-99	-99	-99	-99
6	1.344	-99	-99	-99	-99	-99	-99

9. Inputs setup check

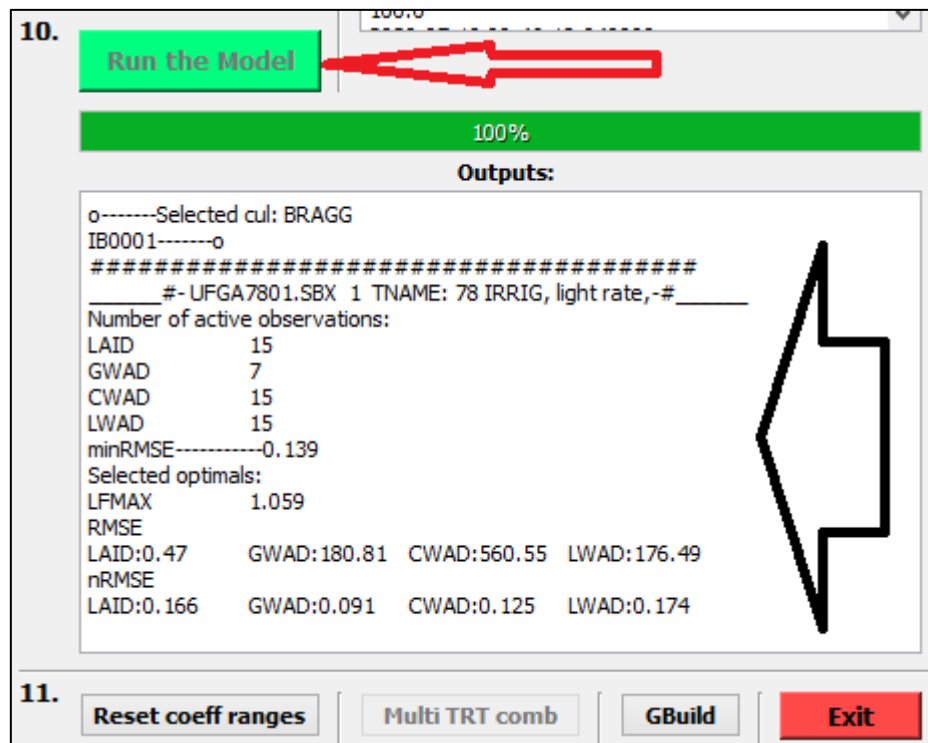
Show comb-s

10. Run the Model

9.2 Interface

10. Run the model!

“Run the model” push button will start coefficient estimation and at the end results can be seen in browser window in the interface (Interface 10.2).



10.2 Interface

11. Additional options

I. [Reset coefficient ranges] or estimate

If “optimal” coefficient combination is found based on wide ranges and big increment steps this button will take those “optimums” and set new Min/Max range based on “optimum’s” values (“optimum” coefficient value * 0.25 and new Min=“optimum” – (“optimum”*0.25), Max=“optimum” + (“optimum”*0.25). Increment steps are calculated based on the desired number of combinations in between. (More details about this approach and Range reduction method can be found in *Memic et al. 2020* and *Röll et al. 2020*).

The image displays two side-by-side screenshots of a software interface, likely for genetic coefficient estimation. Both screenshots show the same layout, but the right one has a red arrow pointing to the 'Reset coeff ranges' button, indicating it has been clicked.

8. Genetic coefficients setup

VAR-Name	P/G Flag	Initialize	Min	Max	Inc. Calc.
LFMAX	G	1	0.869	1.25	5
SLAVR	G	1	1	1	0.0952
SIZLF	G	1	1	1	0
WTPSD	G	1	1	1	0
SFDUR	G	1	1	1	0
SDPDV	G	1	1	1	0

9. Inputs setup check

Number of coefficient combinations: 5

10. Run the Model

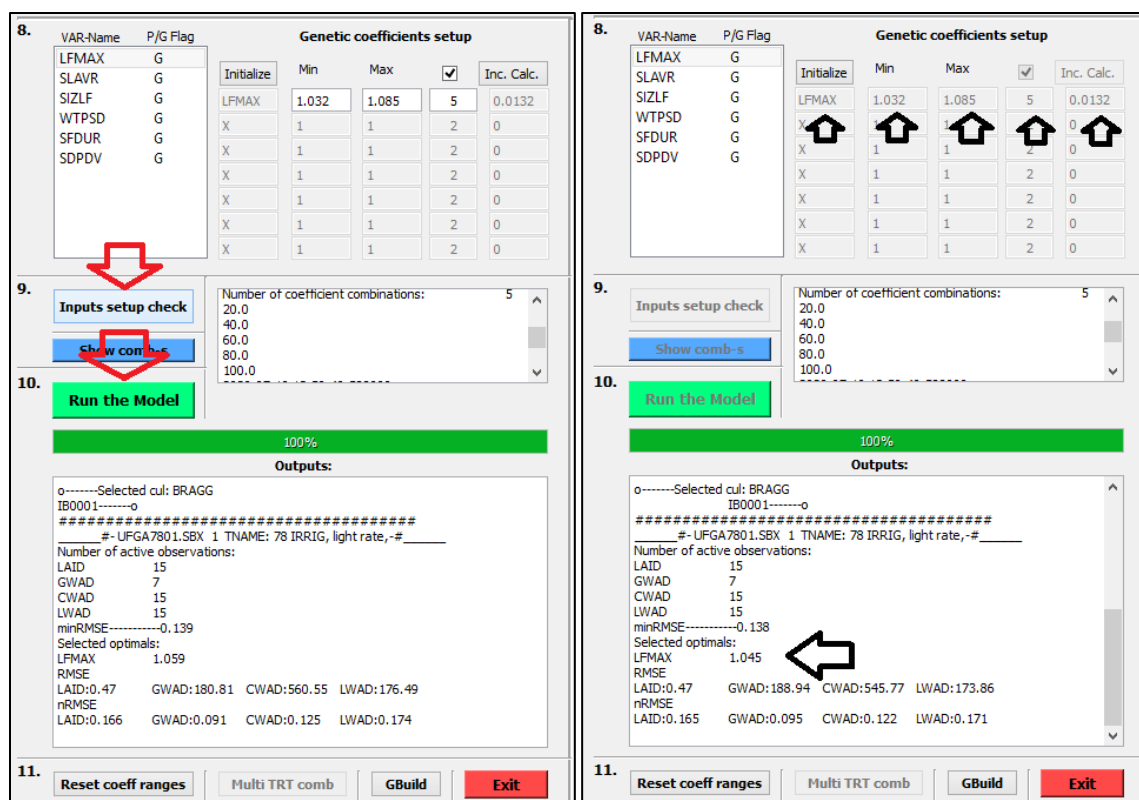
100%

Outputs:

```

o-----Selected cul: BRAGG
IB0001-----o
#####
#- UFGA7801.SBX 1 TNAME: 78 IRRIG, light rate,-#
Number of active observations:
LAID      15
GWAD      7
CWAD      15
LWAD      15
minRMSE-----0.139
Selected optimals:
LFMAX      1.059
RMSE
LAID:0.47  GWAD:180.81  CWAD:560.55  LWAD:176.49
nRMSE
LAID:0.166  GWAD:0.091  CWAD:0.125  LWAD:0.174
  
```

11. Reset coeff ranges Multi TRT comb GBuild Exit



II. [Multi TRT comb]

If this push button clicked multi treatment based cultivar coefficient combination will be estimated (as described in the publication *Memic et al. 2020*).

III. Execute [Gbuild]

With **GBuild** PlantGro.Out can be opened in **TSE_workspace** directory to see how good new combination is. If more than one experiments were used (if Multi-TRT) combination was found, all used treatments can be seen in Gbuild simultaneously...

Again if the PlantGro.Out in TSE_workspace is open with GBuild visual and statistical fit across all used experiments of coefficient optimisation can be seen in GBuild.

IV. [Exit] the program and all running threads

Intermediate computation files can be found in: "C:\DSSAT47\TSE_workspace\Compute"

For example:

C:\DSSAT47\TSE_workspace\Compute\RMSE-Outputs.txt

APPENDIX

1 The *nRMSE* error minimisation method

The *nRMSE* is a simplified selection criterion that is applicable across multiple target variables with different scales. The coefficients are estimated across multiple target variables, with specific objective of locating coefficients combination with lowest *nRMSE* over all targeted variables (Eq. 1).

$$AVG_{nRMSE(n)} = (GWAD_{nRMSE(n)} + LAID_{nRMSE(n)} + CWAD_{nRMSE(n)} + LWAD_{nRMSE(n)})/4 \quad (1)$$

The selection of the coefficient combination with the lowest *nRMSE*s average across all target variables proves to be a good solution (Table 4, AVG-*nRMSE*=0.12).

Table 4 The *nRMSE* - simplified example of varying one of the cultivar parameters affecting growth (G) related target variables (GWAD, LAID, CWAD, and LWAD) of Gainesville 1978 treatment with calculated *nRMSE*s for multiple target variables (each) and optimum selection based on the average *nRMSE* (AVG-*nRMSE*) over multiple target variables (Memic et al.2020).

LFMAX (G -Growth)	nRMSE				AVG	
	GWAD	LAID	CWAD	LWAD	nRMSE	
0.8	0.208	0.22	0.185	0.203	0.204	
0.912	0.131	0.153	0.119	0.146	0.137	
1.024	0.082	0.145	0.109	0.144	0.12	0.12
1.136	0.078	0.171	0.137	0.173	0.14	
1.248	0.109	0.209	0.178	0.211	0.177	

LFMAX – CROPGRO coeff., GWAD - grain weight, LAID - leaf area index, CWAD - tops weight, LWAD - leaf weight

2 The nRMSE multiple treatment based goodness of fit criteria

Cultivar coefficients can be optimised based on the in-season observation of one experiment (single treatment/experiment) or multiple experiment data sets (multiple season and/or locations). Using only one experimental data set for optimisation will lead to better statistical agreement between simulated and observed, but potentially result in over-fitting of simulation outputs with observations. Cultivar coefficients should perform well across multiple seasons and locations and as such should be derived based on multiple season and locations. In **Table 5** are shown single treatment “optimums” and multiple treatment “optimum”.

For demonstrating single treatment and multiple treatment based cultivar coefficient optimisation one cultivar coefficient (LFMAX) and three treatments have been selected (Gainesville 1978, Gainesville 1979 and Gainesville 1984). Cultivar coefficient value minimum (0.85), maximum (1.25) and increment step (0.1) were written in the corresponding cultivar file and crop model was executed. For each cultivar coefficient simulated and observed GWAD, LAID, CWAD and LWAD average nRMSE was calculated for localising “optimums”. First single treatment “optimums” are localised based on the lowest average nRMSE (AVG-nRMSE, **Table 5**, section a, grey fields). In second step multiple treatment cultivar coefficient “optimum” is localised based on the single treatment based AVG-nRMSEs with formula:

$$[(TRT_1+TRT_2+TRT_3)/3]$$

Based on the averaging of the single treatment based AVG-nRMSEs multiple treatment based optimum is selected (**Table 5**, section b, grey fields) with lowest treatment based average nRMSE (**Table 5**, section b, blue field).

Table 5 ‘Bragg’ cultivar (*DSSAT Default*) is shown for soybean experiments conducted in Gainesville 1978, Gainesville 1979 and Gainesville 1984, with LFMAX cultivar coefficient variations from 0.85 to 1.25 with increment step 0.1 with 5 coefficient combinations for each treatment (Memic at al. 2020 – in submission process).

a) Single treatment “optimums”				b) Multi treatment based “optimum”					
Year	TRT	LFMAX	AVG nRMSE	Year	TRT	LFMAX	AVG nRMSE	Multiple treatment average	Optimum
1978	1	0.85	0.17	1978	1	0.85	0.17		
1978	1	0.95	0.128	1979	2	0.85	0.119		
1978	1	1.05	0.122	1984	3	0.85	0.408	0.232	
1978	1	1.15	0.142	1978	1	0.95	0.128		
1978	1	1.25	0.175	1979	2	0.95	0.14		
1979	2	0.85	0.119	1984	3	0.95	0.374	0.214	0.214
1979	2	0.95	0.14	1978	1	1.05	0.122		
1979	2	1.05	0.177	1979	2	1.05	0.177		
1979	2	1.15	0.21	1984	3	1.05	0.355	0.218	
1979	2	1.25	0.239	1978	1	1.15	0.142		
1984	3	0.85	0.408	1979	2	1.15	0.21		
1984	3	0.95	0.374	1984	3	1.15	0.346	0.233	
1984	3	1.05	0.355	1978	1	1.25	0.175		
1984	3	1.15	0.346	1979	2	1.25	0.239		
1984	3	1.25	0.345	1984	3	1.25	0.345	0.253	

- LFMAX-defined in Table 3,

- TRT-treatment,

- AVG-nRMSE-average of normalised RMSE over four target variables (grain weight, leaf area index, Tops weight, Leaf weight)

3 The RW-nRMSE

A *Relative Weight -nRMSE (RW-nRMSE)* complementary method was developed with priority ranks (1 to 4). A rank can be assigned to each target variable separately, where 1 is the most accurate and 4 the least accurate, in relative terms. Each accuracy rank has weight coefficient assigned to it in the TSE code (Table 6), rank 1 with weight coefficient of 0.01 and rank 4 with values 0.04 used in selection criteria. With ranks each target variable's accuracy can be selected, giving users more flexibility in terms of target variable prioritisation in the cultivar coefficients estimation process (Table 6), as shown in the following example with gwad having rank 1 and the other target variables rank 4.

Table 6 RW-nRMSE method target variable ranking with weight coefficients

RW-nRMSE		
	Rank	Coefficient weight
LAI	4	0.04
CWAD	4	0.04
LWAD	4	0.04
GWAD	1	0.01

Initially the weight coefficients are defined (by ranking) for creating a mathematical threshold used in the program (Figure 2a). The initial selection criteria was set to 0.0 (Figure 2a). With the initial selection criteria the *while* loop (flow controlling statement executed repeatedly until specified conditions are met in the programming language) is initialised (Figure 2b). Within the *while* loop, the *if* condition is set for finding an overall statistically acceptable solution (Figure 2c). The *while* loop will be stopped only if the calculated nRMSEs for multiple target variables satisfies the RW-nRMSE selection criteria.

If accurate grain yield is the goal (other target variables less accurate) of the optimisation then the relative weight coefficients based on RW-nRMSE criteria (Table 6) gwad rank 1 and the other three variables rank 4 offers more accurate results of gwad target variable. The rank 1 for gwad and rank 4 for lai, cwad and lwad initializes RW-nRMSE mathematical threshold in to code for while loop first run of 0.01 for nRMSE-gwad and 0.04 for nRMSE-lai-cwad-lwad. In practice this means when the first loop run is searching through calculated nRMSEs for all target variables only coefficient combinations that have calculated nRMSE-gwad lower than 0.01 and nRMSE-lai-cwad-lwad lower than 0.04 is selected as optimum. If in first while loop run none of the coefficient combinations have calculated nRMSE as defined with relative weights the while loop is restarted for the second time with new mathematical threshold for nRMSE-gwad lower than 0.02 and nRMSE-lai-cwad-lwad lower than 0.8. If the newly formed mathematical threshold doesn't provide coefficient combination with calculated nRMSEs the while loop will be started again with nRMSE-gwad mathematical threshold of 0.03 etc. until coefficient combination providing calculated nRMSEs for target variables is located.

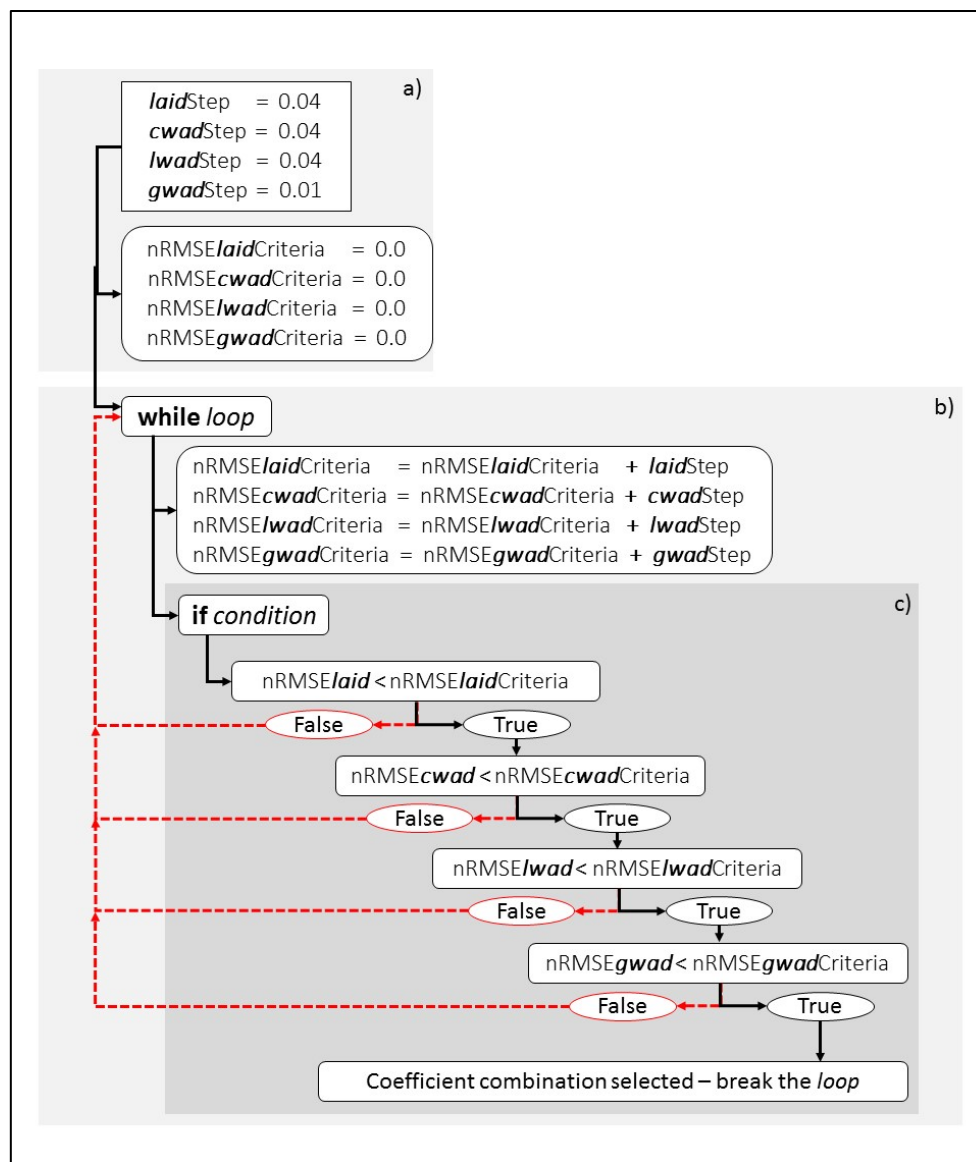


Figure 2 The RW-nRMSE cultivar coefficient combination selection method

With RW-nRMSE-gwad rank 1 and RW-nRMSE-laid-cwad-lwad rank 4 while loop with if conditions is repeated 8 times (Table 7) with desired LFMAX coefficient of 1.136 providing the most accurate simulations for grain weight (gwad). This coefficient values is different from the one selected with simple nRMSE criteria results shown in Table 5.

Table 7 The RW-nRMSE - simplified example of varying one of the cultivar parameters with calculated nRMSEs for multiple target variables demonstrating selected combinations with target variable with relative weights ranking in TSE (Memic at al. 2020 – in submission process).

LFMAX (G)	nRMSE				AVG-nRMSE
	gwad	laid	cwad	lwad	
0.8	0.208	0.22	0.185	0.203	0.204
0.912	0.131	0.153	0.119	0.146	0.137
1.024	0.082	0.145	0.109	0.144	0.12
1.136	0.078	0.171	0.137	0.173	0.14
1.248	0.109	0.209	0.178	0.211	0.177

G – growth, gwad - grain weight, laid - leaf area index, cwad - tops weight, lwad - leaf weight

References

Memic et al. 2020 – in submission process.

Röll G., Memic E. and Graeff-Hönniger (2020) Implementation of an automatic time-series calibration method for the DSSAT Wheat models to enhance multi-model approaches. *Agronomy Journal*.
<https://doi.org/10.1002/agj2.20328>