User guidelines for running TSE 4.1 version of software
(Time-Series cultivar coefficient Estimator for DSSAT crop models)
Standalone external DSSAT plug-in

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TSE **T**ime-**S**eries cultivar coefficient **E**stimator

For writing this 4.1 user guidelines DSSAT 4.8.5 version was used.

- PC scale layout:
  - The computer screen scale layout must be set to 100% for fully operable TSE!
  - The scale layout set at 125% is displayed properly to a certain degree (TSE partially operable).
  - Windows scale layout 150% will not display TSE options properly! (TSE inoperable!)

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I - The TSE concept overview (Memic et al. 2021)

The cultivar/ecotype coefficients estimation program will work only if fully functional DSSAT files are available such as experiment file (File-X), weather file, soil profile, functional species, ecotype and cultivar files, time-series file containing in-season observations (File-T) and summary file (File-A - optional) are available.

The overall program run can be separated into three steps as shown in Figure 1.

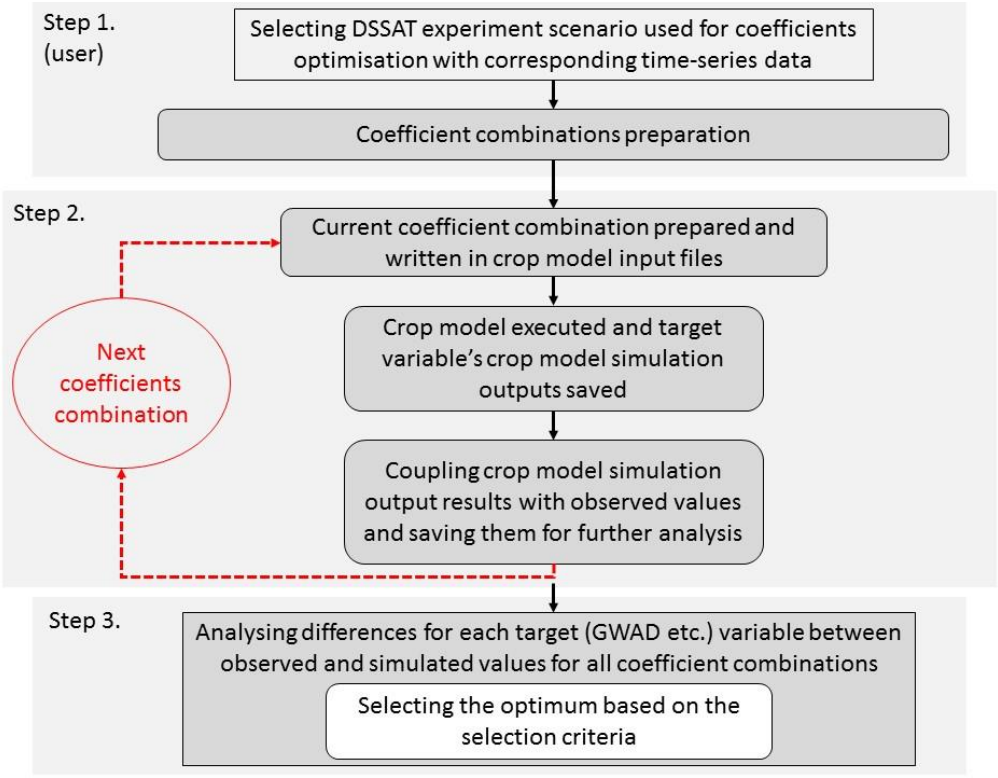

Figure 1. Flow chart showing overall program run in three steps (GWAD – grain weight) (Memic et al. 2021)

The program can be used for optimizing cultivar coefficients based on single or multiple experiment data sets. User should first optimize phenology-related cultivar coefficients. After phenological events are correctly optimized, growth-related cultivar coefficients are optimized. Phenology-related cultivar coefficient optimization is not conducted based on the time-series data (File-T), but by using File-A observations and by simply minimizing the difference between simulated and observed phenological event as day after planting. Growth-related cultivar coefficients are optimized by using File-T in-season observations by means of normalized RMSE (among others) 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.

II - General TSE program settings overview

The program was developed (in Windows environment, for use on Windows) as standalone external DSSAT plug-in and has no specific installation requirements. All required files for running the program are shared in DSSAT installation or on GitHub via zipped file.

VERY IMPORTANT:

I. **PlantGro.Out** (or other time-series) crop model outputs are coupled to those in **File-T** (phenology- or growth-related) time-series in-season observations.

II. **Evaluate.Out** crop model outputs are used for optimizing Phenological events which are passed into the model through **File-A**.

III. If sub-model (e.g. WHAPS) is initialized in the File-X, the calibrator might NOT work! (in File-X in *SIMULATION CONTROLS in GENERAL line, column SMODEL **do NOT initialize sub-models such as WHAPS, IXIM etc.!**). This does TSE program.

IV. For multi-TRT optimizations only target variables simultaneously available in all **File-T**/s (for corresponding **File-X**/s Treatment/s) are accessible for optimization.

V. **File-T** observations: **All in-season observations available including 0 are used!** *Only "-99" values are ignored by TSE*.

VI. The program matches DOY from **File-T** with those in PlantGro.OUT. If the user setup in File-X reporting frequency for example every fifth day and exact observation DOY is not present in the PlantGro.OUT as it is written in the File-T, the program will NOT be able to match them for comparing simulated with observed.

VII. PlantGro.OUT default DSSAT time-series output file used! Additionally other DSSAT time-series output files can be used such as: PlantGr2.OUT etc.

The TSE program is creating additional directory "**TSE_workspace**" ("**C:\DSSAT48\TSE_workspace"**) (Figure 2) and modifying the cultivar file in that directory, which is then executed by main DSSAT model executable.

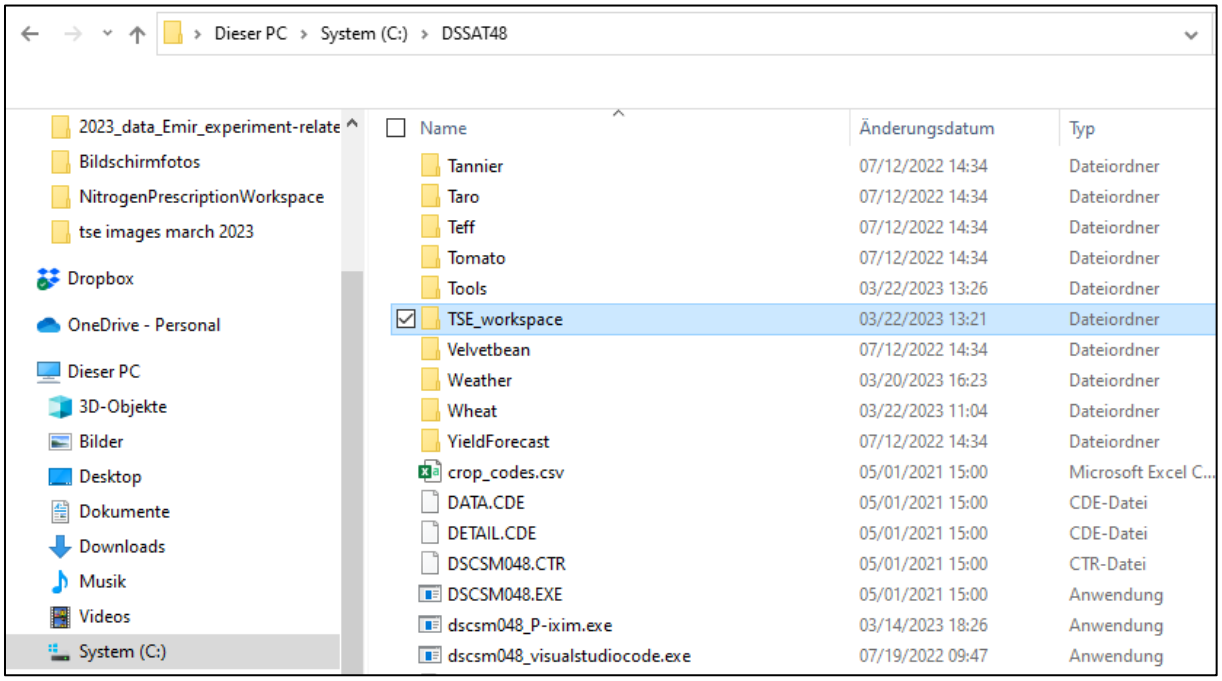

Figure 2. ("**C:\DSSAT48\TSE_workspace"**)

The TSE program does NOT modify core DSSAT files in their original directories!

Program run is considered: From when **"TSE.exe"** is **executed** until "**Exit**" push button is pressed. Any form of optimization done in-between is temporarily saved in the cultivar file in "TSE_workspace" directory as a working version.

After TSE program is started all modifications on Cultivar or Ecotype file are conducted in ("**C:\DSSAT48\TSE_workspace"**). During one program run (until "**Exit**" push button is pressed) different coefficients (or different target variables) can be optimized one after another or simultaneously and cultivar changes will be saved if accepted as "optimums" in cultivar file in **C:\DSSAT48\TSE_workspace**. If user is satisfied with the cultivar coefficient values based on nRMSE (or other) fit, cultivar coefficient combination MUST be copied to "**C:\DSSAT47\Tools\Genotype**" located cultivar or ecotype file **MANUALLY**. If TSE program is started again without saving the combination in **C:\DSSAT47\Tools\Genotype** located cultivar or ecotype file new TSE program start will copy original cultivar or ecotype file located in C:\DSSAT47\Tools\Genotype and overwrite user's working cultivar file in "**C:\DSSAT48\TSE_workspace**".

After model run finished and before the user clicks "**Exit**" push button they can open GBuild from TSE interface and 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 the user opens **PlantGro.OUT** from "**C:\DSSAT48\TSE_workspace**" directory because TSE will create parallel files it requires in this folder, without modifying the original files in DSSAT directory.

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

Example of optimizing cultivar coefficient (*CROPGRO-Soybean, SBGRO048.CUL*):

Every time **TSE.exe** is executed, original cultivar file (SBGRO048.CUL) file from **C:\DSSAT48\Tools\Genotype** will be copied to "**C:\DSSAT48\TSE_workspace** directory (Figure 3) 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\Tools\Genotype** directory into SBGRO048.CUL **Manually**.

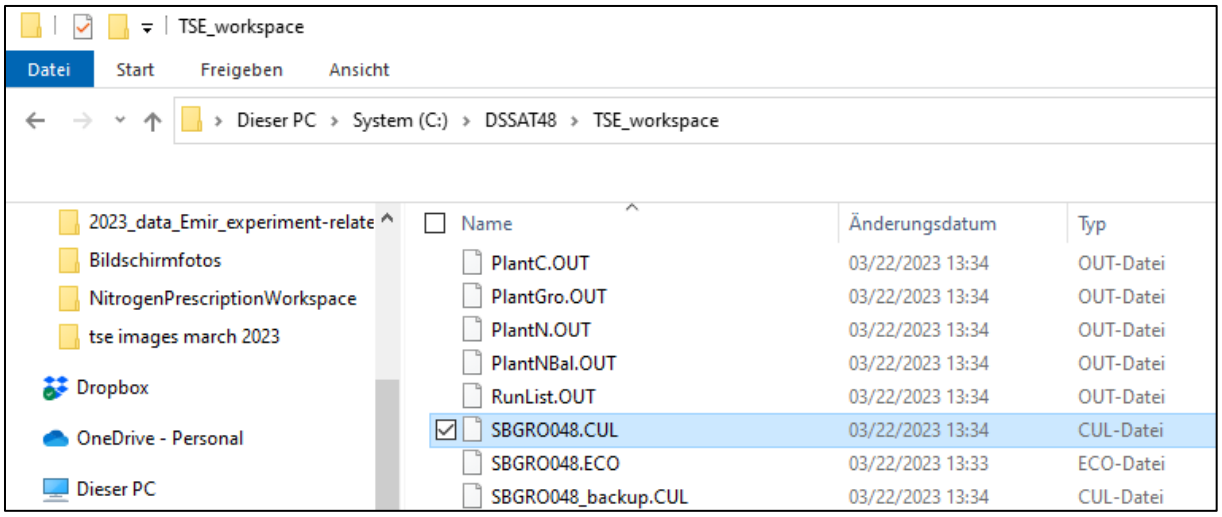

Figure 3. C:\DSSAT48\TSE_workspace\SBGRO047.CUL

The original cultivar coefficients version is saved as **"!Old_timestamp_cultivarID…."** (Figure 4, text editor line 75-76) and the new one (Figure 4, text editor line 73) is saved in that working cultivar file (in **TSE_workspace**) and model is executed.

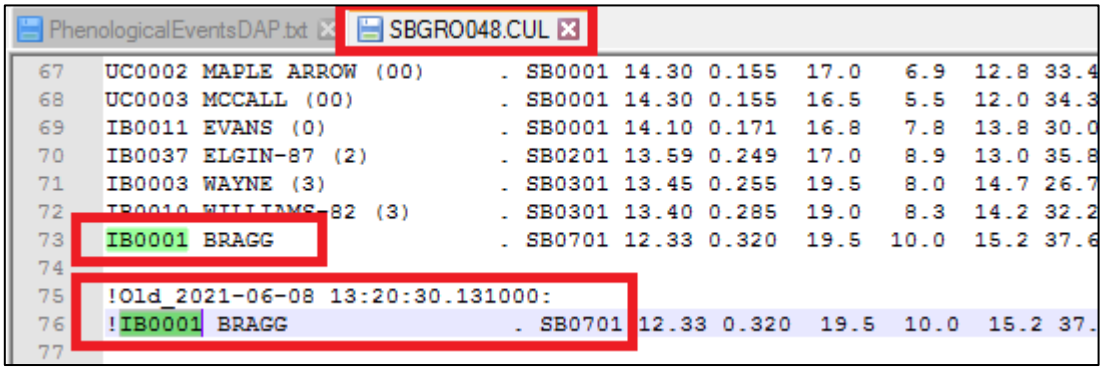

Figure 4. Old and new cultivar

III - Running TSE program

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

1. Crop and Model Selection

2. Cultivar and Experiment Files Selection

3. Phenology and Growth Variables Selection

4. Coefficients Selection and Initialization

5. Running TSE and Results Visualization

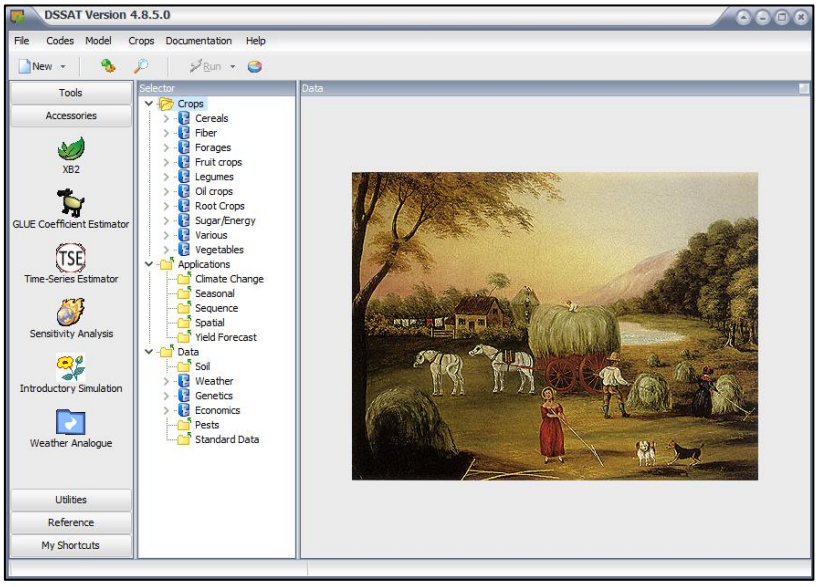

Figure 5. DSSAT Interface – Accessories Section

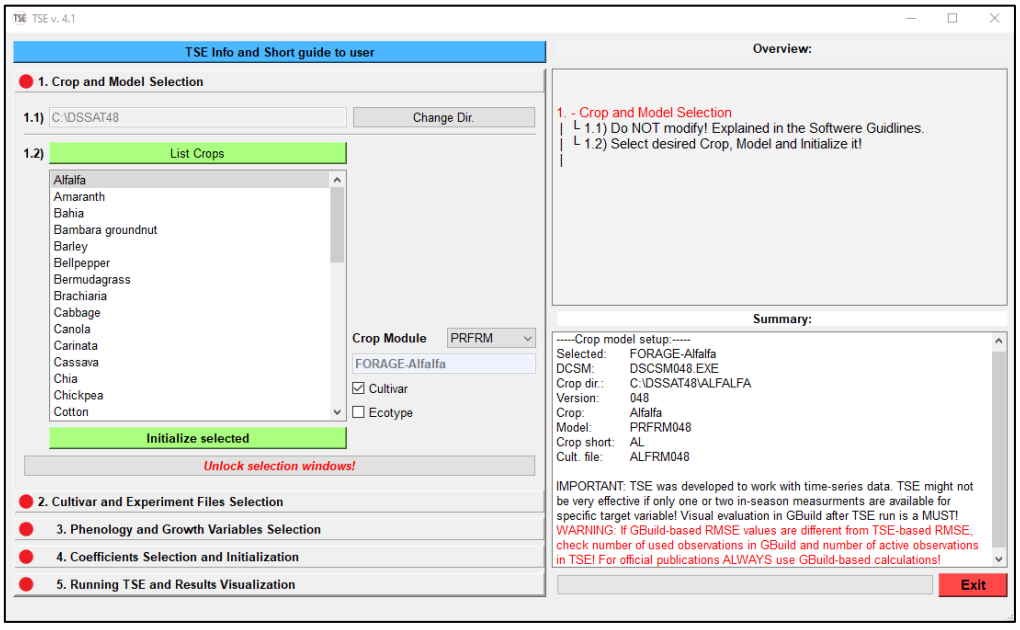

Figure 6. TSE Interface

1. Crop and Model Selection

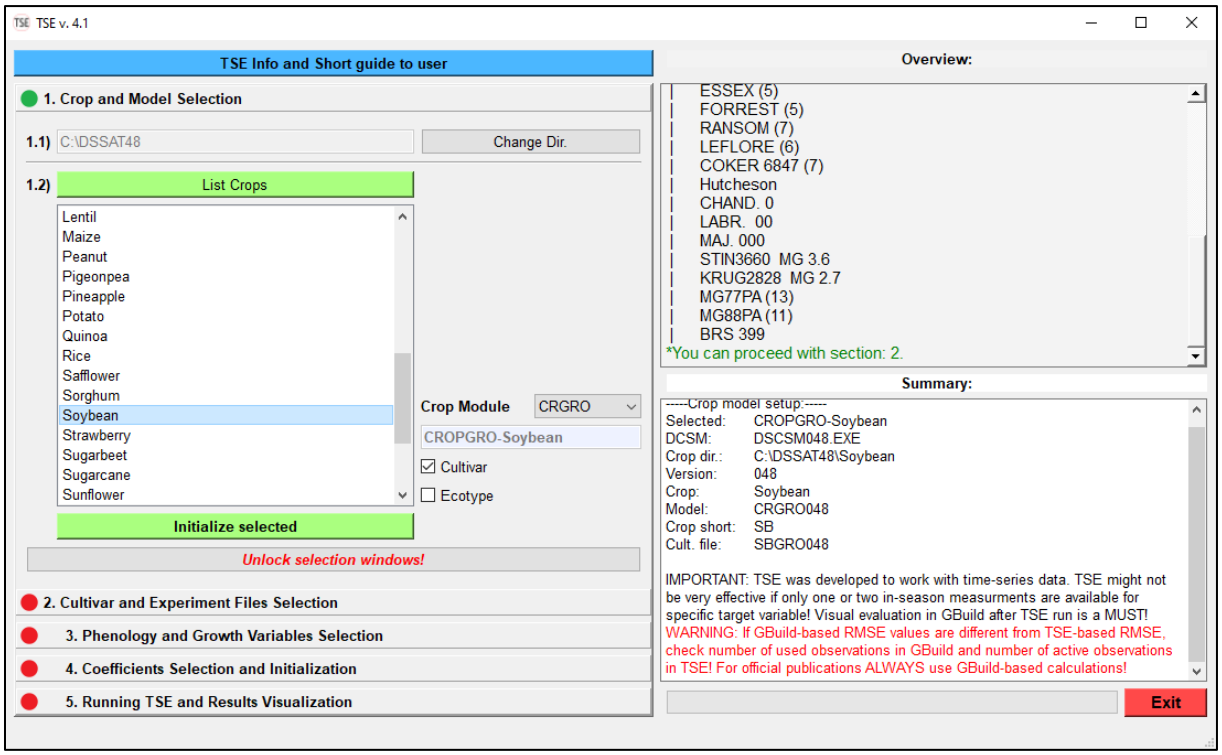

Figure 7. Crop and Model Selection

Figure 7. Section 1.1)

- DSSAT directory

Figure 7. Section 1.2) List of Crops available in the DSSAT are listed in list widget for selection

- Select Crop in the list
- Select Crop Module in combo box
- Select Cultivar or Ecotype for optimization by checking corresponding check box

2. Cultivar and Experiment Files Selection

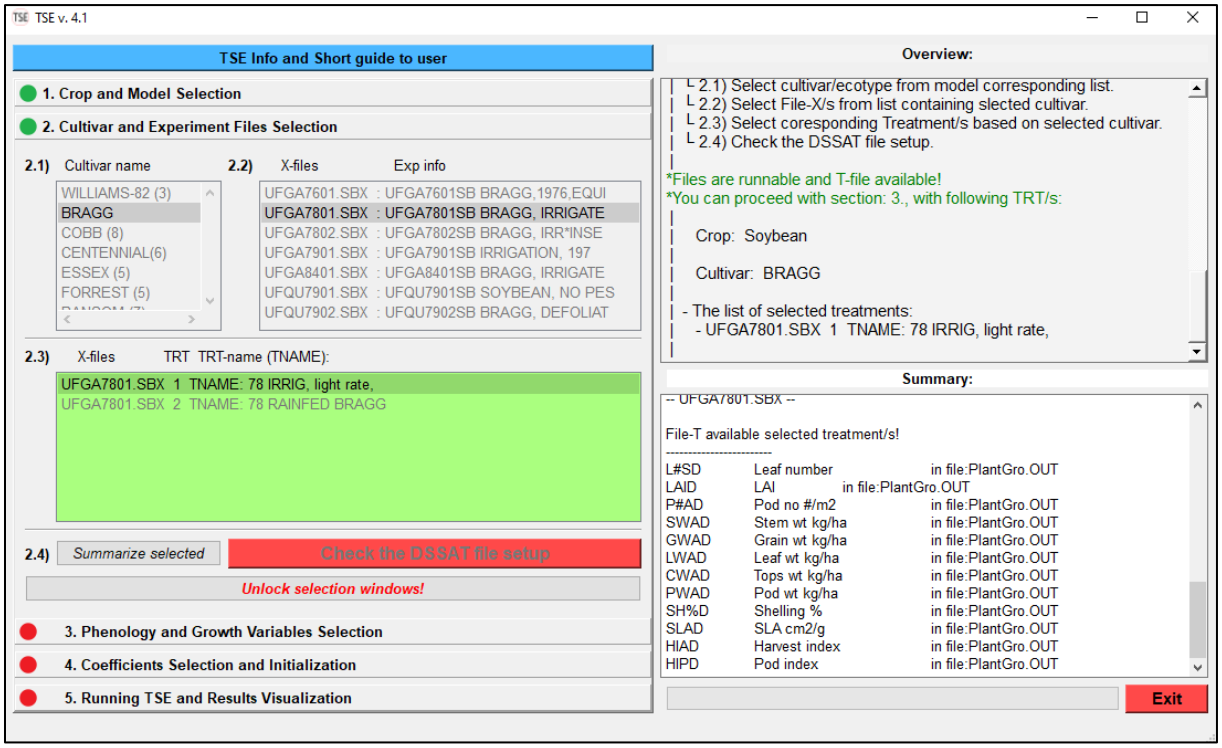

Figure 8. Cultivar and Experiment Files Selection (Multiple treatment (experiment) selection is done by: ***Ctrl+ mouse left button click***).

Figure 8. Section 2.1) Select cultivar from list of cultivars available for corresponding Crop

Figure 8. Section 2.2) Select experiment file (X-file) from the list

Figure 8. Section 2.3) Select specific treatments that are going to be used for optimization

Figure 8. Section 2.4) Click on Check the DSSAT file setup – checking if files are runnable

3. *Phenology and Growth Variables Selection*

Growth Variables

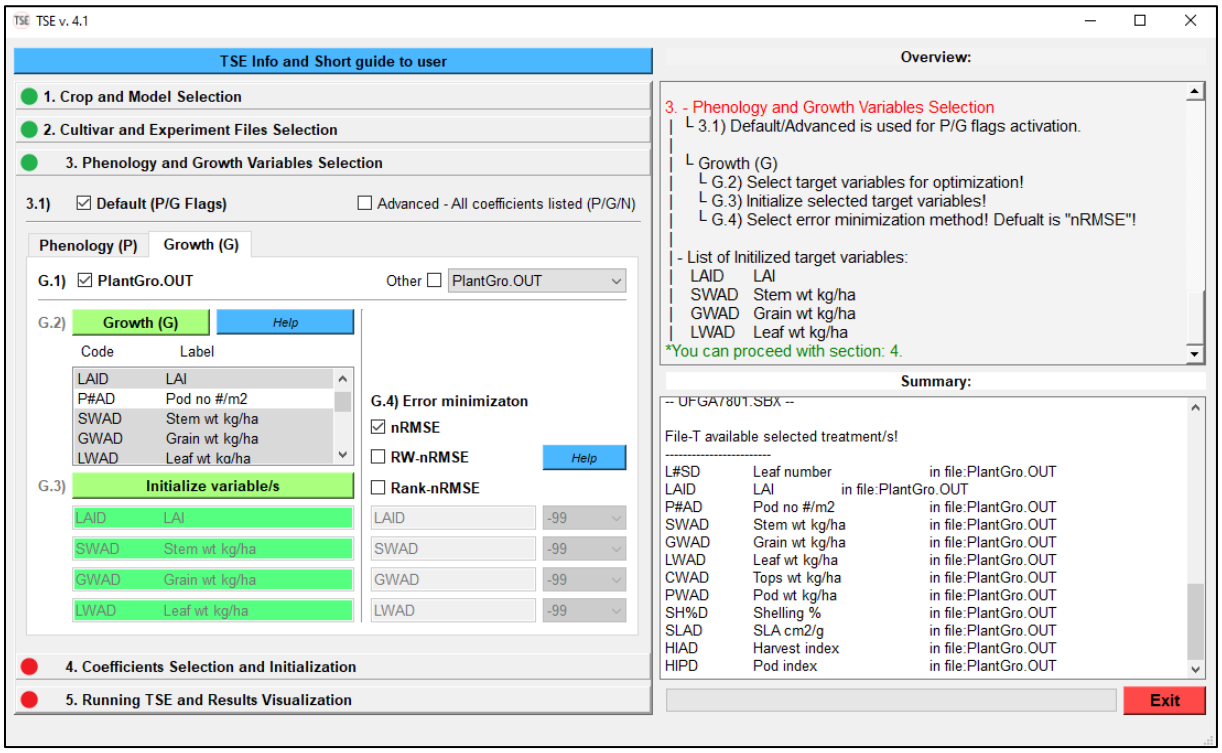

Figure 9. Phenology and Growth Variables Selection (Multiple Growth-target variable is done by: ***Ctrl+ mouse left button click***)

TSE directly opens the window for setting up Growth-related optimization. For Phenology click on Phenology (P) tab widget.

Default (check box) will upload only coefficients with predefined P/G flags (according to selection of the Phenology or Growth). ***Advanced*** (check box) will upload all available cultivar coefficients from cultivar file for potential optimization.

Figure 9. Section G.1) Default optimization is conducted with PlantGro.OUT. For other *.OUT file optimization click on Other check box and select file from combo box list. It is possible to use other DSSAT time-series output files for coefficient optimization in case observations are simultaneously available in corresponding output file (e.g., PlantGr2.OUT) and File-T.

Figure 9. Section G.2) After selecting target variables in the list (maximum four) click on Initialize variables/s push button.

Figure 9. Section G.3) Error minimization method can be selected. Default is nRMSE. Detailed methods description can be found in appendix.

Phenology Variables

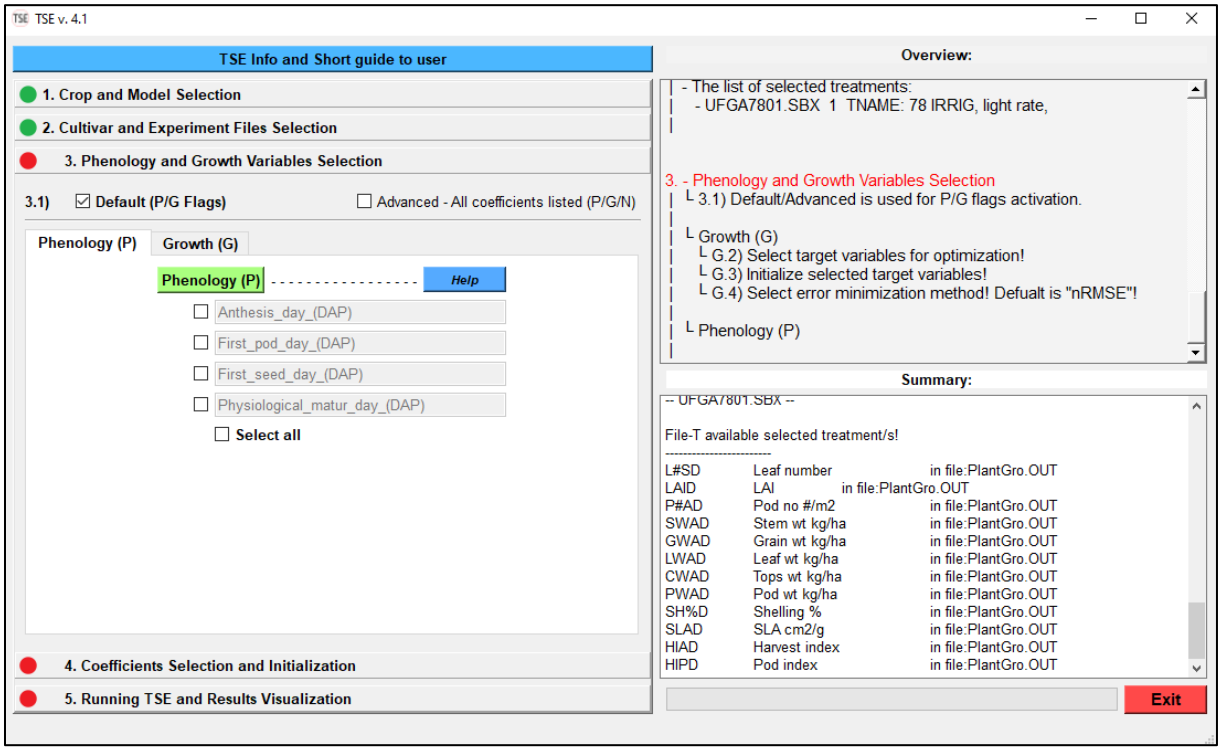

Figure 10. There are four phenological events parameters described in Memic et al. (2021) which are hardcoded in the TSE algorithm, specifically for CROPGRO-Soybean.

This hard coded solution can be over-written with manually customizable text file located in "C:\DSSAT48\Tools\TSE" named: "PhenologicalEventsDAP.txt" (Figure 11). The file setup is explained in the file as shown in following figure and has to be located in "C:\DSSAT48\Tools\TSE" directory and format rules have to be followed!

PhenologicalEventsDAP.txt

```
1  ! Phenological events as Days after planting (DAP)
2  !
3  !  Only four can be read in and the rest should be outcomented with "!"
4  !
5  !  Phenological events can be added to this list!
6  !  In order to work Phenological event - code (etc. ADAP) has to be outputed
7  !  by DSSAT in the Evaluate.OUT and this format has to be followed:
8  !  Example:
9  !  Code      Code_Name
10 !  ADAP      Anthesis_day
11 !
12 !----------------------------------------!
13 ADAP         Anthesis_day_(DAP)
14 PD1P         First_pod_day_(DAP)
15 PDFP         First_seed_day_(DAP)
16 MDAP         Physiological_matur_day_(DAP)
17 !PD1T        First_pod_date_(DAP)(YrDoy)_?
18 !EDAP        Emergence_date_(DAP)
19 !B1DAP       Branch_1_date_(DAP)
20 !B2DAP       Branch_2_date_(DAP)
21 !B3DAP       Branch_3_date_(DAP)
22 !B4DAP       Branch_4_date_(DAP)
23 !FDAP        Forcing_Date_(DAP)
24 !TDAP        Begin_tuber_growth_(DAP)
25 !----------------------------------------!
```

Figure 11. PhenologicalEventsDAP.txt

4. Coefficients Selection and Initialization

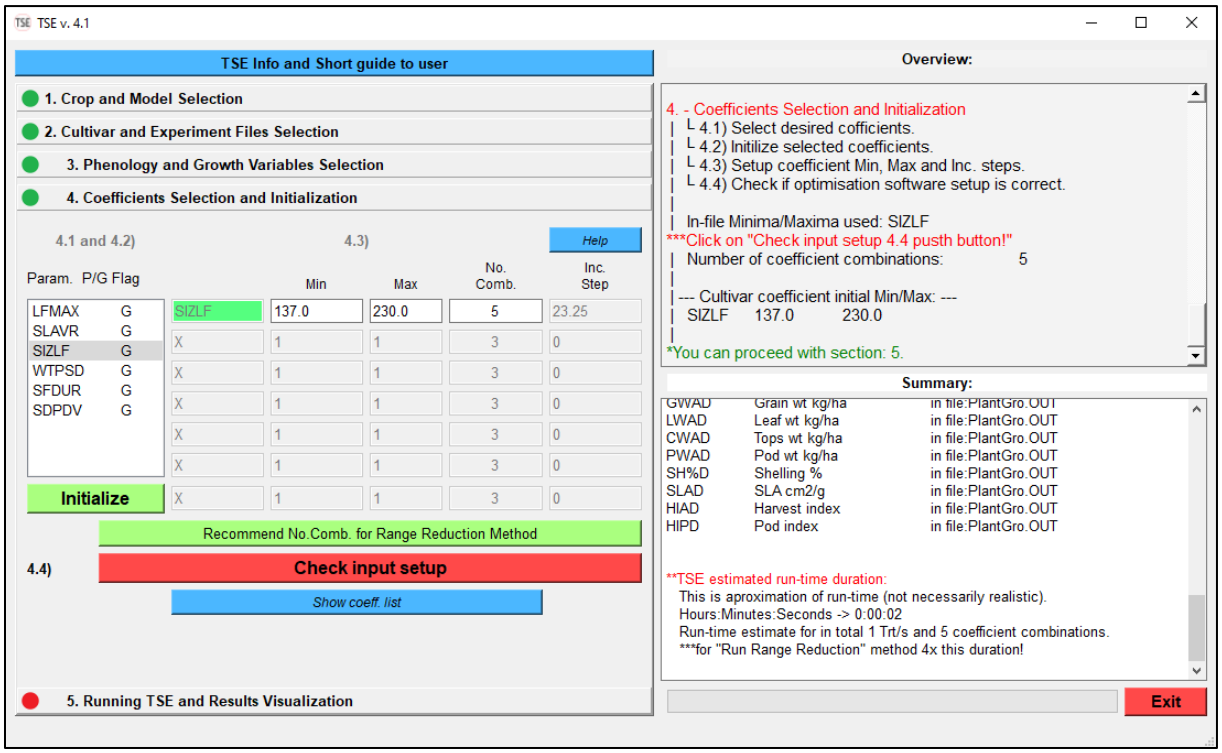

Figure 12. Coefficients Selection (Multiple coefficients selection is done by: ***Ctrl+ mouse left button click***) and Initialization

Figure 12. Section 4.1) and 4.2) In the list of coefficients select coefficients and Initilize

Initialize push button will initialize coefficient Labels in edit boxes and populate Min/Max coefficient ranges with min/max value available in corresponding cultivar file for selected cultivar coefficient (Section 4.3) (Figure 12). Automatically this will create a simple range of Min/Max values with three coefficient combinations that are going to be passed into the cultivar file, and after each model is executed (Figure 12). If the user wants more combinations in between given Min/Max range number of desired coefficient combinations between Min/Max can be given in "No. Comb." edit boxes (Figure 12). After giving the desired number of combinations between Min/Max increment steps are automatically calculated (Figure 12). New option Recommend No. Comb for Range Reduction Method will automatically suggest increment step with No. Comb. If too many recommended that might result in too long optimization session, the user can reduce them.

If a user would like to modify Min/Max values, it can be done directly (manually) in edit boxes below Min/Max labels in step 2 (Figure 12). If Min/Max are modified based on the number of combinations values are automatically calculated and populated in corresponding edit boxes.

If the user wants to fix the value of some coefficient, then they set Min and Max to equal value (same value in the Min edit box as in the Max value edit box).

Starting with the DSSAT4.8.0 version additional MINIMA/MAXIMA coefficient values are included in cultivar files with more details. Since MINIMA/MAXIMA are recommendations made by crop model developers a new code addition was done to the TSE algorithm. The TSE

program will check for these values and populate Min Max edit boxes with those values (Figure 12).

Figure 12. Section 4.3) The push button Check Input setup will check if Min Max and Inc Step setup is runnable with TSE.

The push button Show coeff. list will pop up window with coefficient combinations (Figure 13).

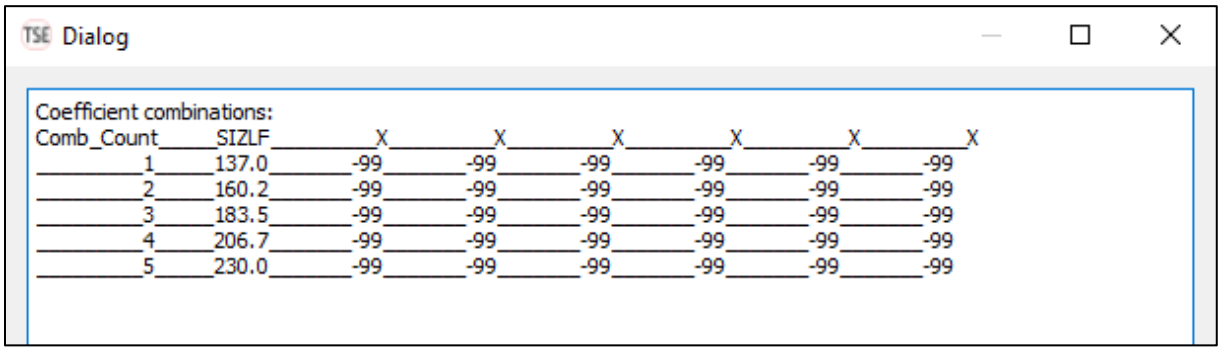

Figure 13. List of coefficient/s combinations

5. Running TSE and Results Visualization

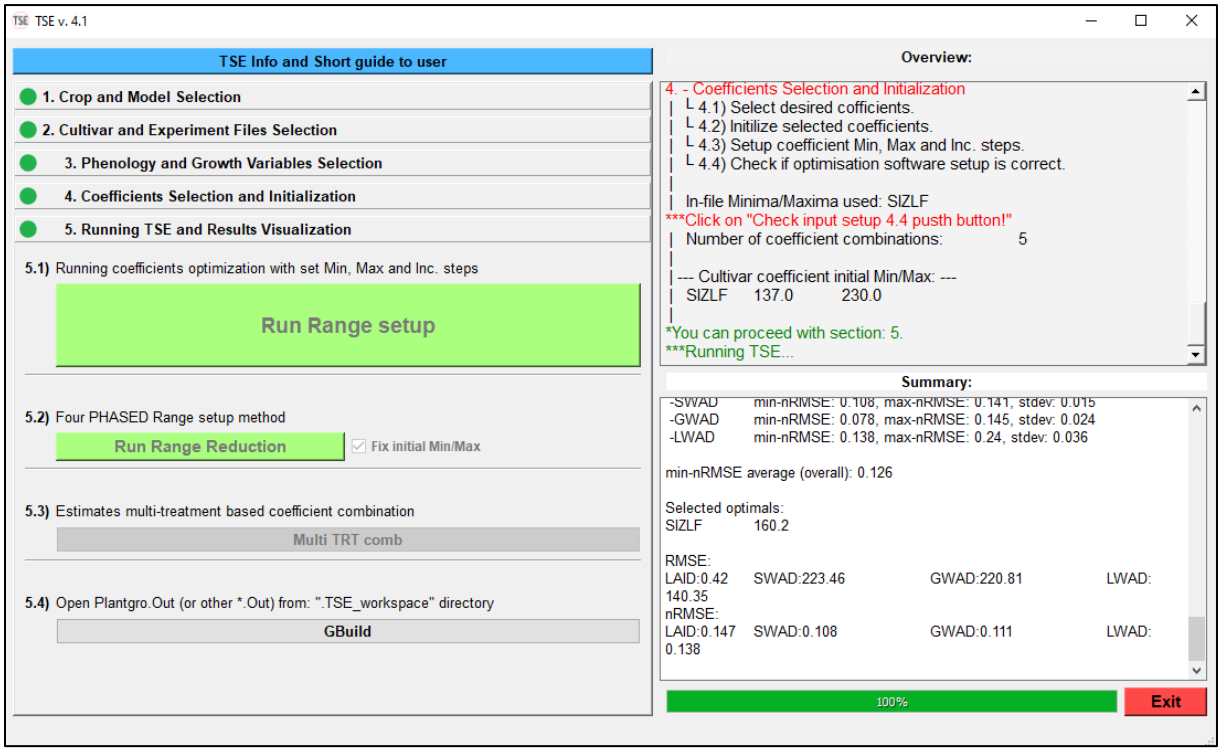

Figure 14. Running TSE and GBuild

Run Range setup – For example if coefficient **Min/Max/No Comb**. (of TSE interface section 4) is set to **130/230/5** this will pass to the cultivar/ecotype file only these five coefficients as shown in Figure 15.

Coefficient combinations:

Comb_Count	SIZLF	X	X	X	X	X	X
1	130.0	-99	-99	-99	-99	-99	-99
2	155.0	-99	-99	-99	-99	-99	-99
3	180.0	-99	-99	-99	-99	-99	-99
4	205.0	-99	-99	-99	-99	-99	-99
5	230.0	-99	-99	-99	-99	-99	-99

Figure 15: **Run-Range setup**

Run Range Reduction – will use initial **Min/Max/NoComb (130/230/5)** and increment step as a starting point and through four run cycles try to localize (find local optimum) the best coefficient value based on the error minimization method for coefficient values that are not tested at all in simple
"Run-Range Reduction", as shown in following figure 16.

```
Range reduction phase:  1
130.0   1.0 1.0 1.0 1.0 1.0 1.0
155.0   1.0 1.0 1.0 1.0 1.0 1.0
180.0   1.0 1.0 1.0 1.0 1.0 1.0
205.0   1.0 1.0 1.0 1.0 1.0 1.0
230.0   1.0 1.0 1.0 1.0 1.0 1.0
"optmal comb:   155.0   1.0 1.0 1.0 1.0 1.0 1.0

Range reduction phase:  2
146.0   1.0 1.0 1.0 1.0 1.0 1.0
150.5   1.0 1.0 1.0 1.0 1.0 1.0
155.0   1.0 1.0 1.0 1.0 1.0 1.0
159.5   1.0 1.0 1.0 1.0 1.0 1.0
164.0   1.0 1.0 1.0 1.0 1.0 1.0
"optmal comb:   164.0   1.0 1.0 1.0 1.0 1.0 1.0

Range reduction phase:  3
162.3   1.0 1.0 1.0 1.0 1.0 1.0
163.1   1.0 1.0 1.0 1.0 1.0 1.0
163.9   1.0 1.0 1.0 1.0 1.0 1.0
164.7   1.0 1.0 1.0 1.0 1.0 1.0
165.6   1.0 1.0 1.0 1.0 1.0 1.0
"optmal comb:   165.6   1.0 1.0 1.0 1.0 1.0 1.0

Range reduction phase:  4
165.3   1.0 1.0 1.0 1.0 1.0 1.0
165.4   1.0 1.0 1.0 1.0 1.0 1.0
165.5   1.0 1.0 1.0 1.0 1.0 1.0
165.6   1.0 1.0 1.0 1.0 1.0 1.0
165.8   1.0 1.0 1.0 1.0 1.0 1.0
"optmal comb:   165.8   1.0 1.0 1.0 1.0 1.0 1.0
```

Figure 16. **Run-Range reduction**

Multi TRT comb

If this push button clicked multi treatment-based cultivar coefficient combination will be estimated, as described in appendix A.2 (Figure 14).

Gbuild

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

If the **PlantGro.Out** in "**C:\DSSAT48\TSE_workspace**" is open with GBuild visual and statistical fit across all used experiments of coefficient optimization can be seen in GBuild (Figure 14).

The "**Reset**" button will unlock the access to the selection of the crop model, cultivar/ecotype and File-Xs.

Exit the program and all running threads.

APPENDIX

A.1 The nRMSE error minimisation method (nRMSE) (Memic et al. 2021)

For quantifying the variation between simulated (Si) and observed (Oi) values the statistical method of nRMSE (Eq. 2) is used. The nRMSE, is RMSE (Eq. 1) normalized by mean ($\overline{O}$) for each observed crop variable.

$$RMSE = \left[\frac{1}{n}\sum_{i=1}^{n}(S_i - O_i)^2\right]^{0.5} \quad (1)$$

$$nRMSE = \frac{RMSE}{\bar{O}} \quad (2)$$

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. 3).

$$AVG_{nRMSE(n)} = (GWAD_{nRMSE(n)} + LAID_{nRMSE(n)} + CWAD_{nRMSE(n)} + LWAD_{nRMSE(n)})/4 \quad (3)$$

The selection of the coefficient combination with the lowest nRMSEs average across all target variables proves to be a good solution (Table 1, AVG-nRMSE=0.12).

Table *1* 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 nRMSEs for multiple target variables (each) and optimum selection based on the average nRMSE (AVG-nRMSE) over multiple target variables (Memic et al.2021).

LFMAX	**nRMSE**				**AVG**	
(G -Growth**)**	**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

A.2 The nRMSE multiple treatment-based goodness of fit criteria (nRMSE) *(Memic et al. 2021)*

Cultivar coefficients can be optimized 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 optimization 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 seasons and locations. In Table 2 are shown single treatment "optimums" and multiple treatment "optimum".

For demonstrating single treatment and multiple treatment-based cultivar coefficient optimization 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 localizing "optimums". First single treatment "optimums" are localized based on the lowest average nRMSE (AVG-nRMSE, Table 2, section a, grey fields).

In second step multiple treatment cultivar coefficient "optimum" is localized 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 2, section b, grey fields) with lowest treatment based average nRMSE (Table 2, section b, blue field).

Table 2 '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 et al. 2021)

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)

A.3 The Relative Weight –nRMSE (RW-nRMSE)

A *Relative Weight -nRMSE* (*RW-nRMSE*) complementary method was developed with relative weights assigned to the selected target variables (1 to 5). A relative weight can be assigned to each target variable separately, where 5 is the most accurate and 1 the least accurate, in relative terms. Each accuracy weight has weight coefficient assigned to it in the TSE code. With relative weights each target variable's accuracy can be selected, giving users more flexibility in terms of target variable prioritization in the cultivar coefficients estimation process. The relative weights multiplier (rw) in Eq. 4 is used to artificially inflate nRMSE of specific target variables. By doing so the size of specific target variable is artificially increased in the overall AVG-nRMSE that results at the end in cultivar coefficient combination prioritizing those variables over others.

$$AVG_{nRMSE(n)} = (rw_1 * GWAD_{nRMSE(n)} + rw_2 * LAID_{nRMSE(n)} + rw_3 * CWAD_{nRMSE(n)})/3 \quad (4)$$

It will be additionally explained!

A.4 The Rank Weighting –nRMSE (Rank-nRMSE)

A *Relative Weight -nRMSE* (*RW-nRMSE*) complementary method was developed with priority ranks (1 to 5). A rank can be assigned to each target variable separately, where 1 is the most accurate and 5 the least accurate, in relative terms. Each accuracy rank has weight coefficient assigned to it in the TSE code (Table 4), 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 prioritization in the cultivar coefficients estimation process (Table 4), as shown in the following example with GWAD having rank 1 and the other target variables rank 4.

Table 4 RW-nRMSE method target variable ranking with weight coefficients.

RW-nRMSE		
	Rank	**Coefficient weight**
LAID	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 A.1a). The initial selection criteria were set to 0.0 (Figure A.1a). With the initial selection criteria, the *while* loop (flow controlling statement executed repeatedly until specified conditions are meet in the programming language) is initialized (Figure A.1b). Within the *while* loop, the *if* condition is set for finding an overall statistically acceptable solution (Figure A.1c). 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 4) 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 laid, 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-laid-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-laid-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-laid-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.

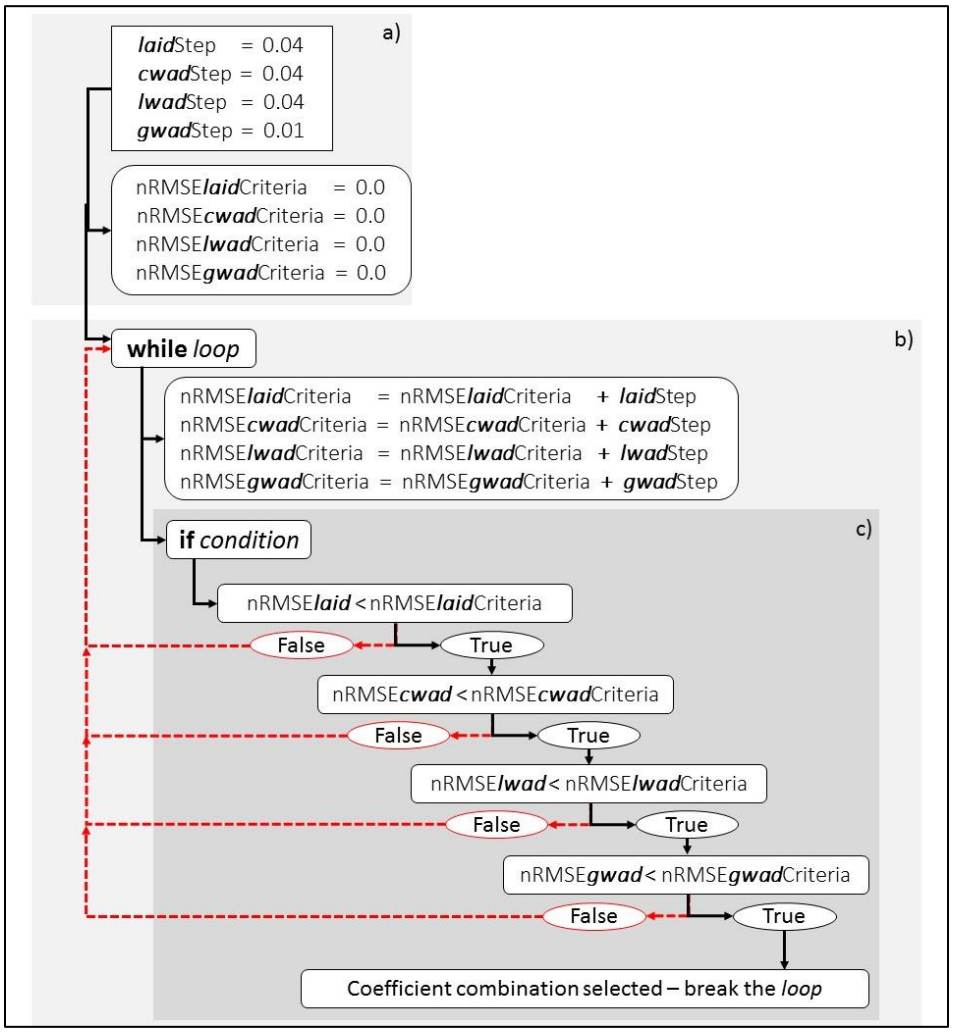

Figure A.1 The RW-nRMSE cultivar coefficient combination selection method (Röll et al. 2020)

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 1.

Table *5* 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 et al.2021).

	nRMSE				
LFMAX (G)	**gwad**	**laid**	**cwad**	**lwad**	**AVG-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**
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*

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Memic, E (2022): Combining crop growth models with the Precision Agriculture concept of yield gap analysis to evaluate yield limiting and reducing factors. Uni Kassel, Germany. *Dissertation.*

Röll, G., Memic, E., Graeff-Hönninger, S. (2020): Implementation of an automatic time-series calibration method for the DSSAT wheat models to enhance multi-model approaches. Agronomy Journal 112(5), 3891-3912. https://doi.org/10.1002/agj2.20328

Interface:
The TSE_v4.1 user interface was created in Qt Designer 5
(https://doc.qt.io/qtcreator/index.html)

Programming language:
The TSE_v4.1 algorithm was written in python 3.7
Python Software Foundation. Python Language Reference, version 3.7. Available at http://www.python.org

Windows runnable:
TSE_v4.1 was compiled into windows runnable with Pyinstaller
(https://www.pyinstaller.org/)

TSE_v4.1 algorithm and interface development/setup by Emir Memic.