SPO v.2-User guidelines

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IMPORTANT!

This program is still not fully user friendly. Some of the SPO interface features are not fully robust and additional statistical criteria (d-stat, d1-stat – based on Yang et al. 2014) are not fully tested. The program was developed on specific data set and tested on multiple other. It's a generic external python plug-in that is expected to work with all crop models available in DSSAT shell. Some of the features are still a work in progress and will be improved.

More detailed description of the SPO program can be found in following publication:

Generic optimization approach of soil hydraulic parameters for site-specific model applications

Jonas Trenz, Emir Memic, William D. Batchlor, Simone Graeff-Hönninger
Precision Agriculture journal - Springer (October 2023, accepted)

For any additional questions contact the author of the SPO tool!

Contents

1. Conceptual framework of SPO

1.1 Soil profile optimization – field scale to site-specific scale - overview

Soil Profile Optimization tool (SPO) can be used for optimizing soil profile-related coefficients available in standard DSSAT soil profiles. In total seven coefficients can be optimized with SPO: entire profile coefficients (SLDR, SLRO, SLPF) and soil-layer coefficients (SLLL, SDUL, SRGF, SSKS). The SPO was designed in a way to use already existing field-specific soil profile setup. Simplified conceptual framework of SPO used for site-specific soil profile analysis is shown in Figure 1. In this example in Figure 1 three phases of optimization are shown: a) field specific soil profile (n=1) with field specific yield (n=3, referring to three seasons), b) field specific soil profile (n=1) and site-specific yield over three years (n=60) where for each season 20 site-specific yield measurements are available, and c) site-specific soil profile (n=20) and 60 site-specific yield measurements. For site-specific soil profiling three parameters were selected: soil water lower limit, root growth factor and runoff curve, under the assumption that indeed these parameters can be derived based on measured site-specific yield variability and are shown in Figure 2 (Memic et al. 2023).

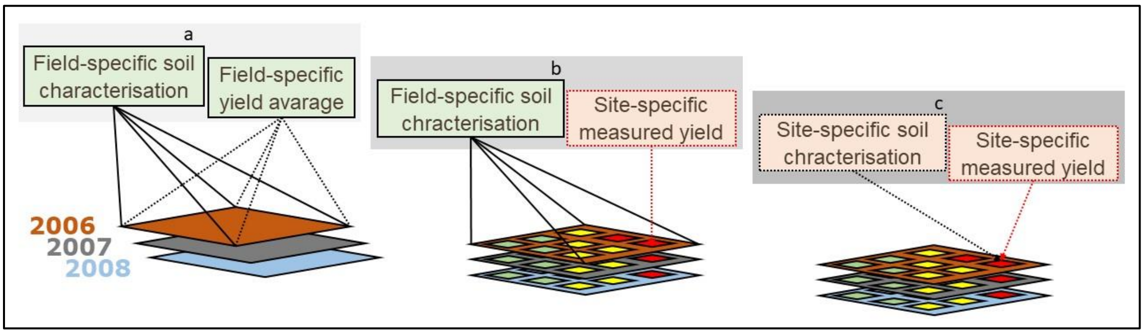

Figure 1 a) field-specific soil profile characterization (n=1) and field-specific simulated and measured yield over three years (n=3) (Figure 2, left), b) field-specific soil profile characterization (n=1) and site-specific simulated and measured yield over three years (n=60) (Figure 2, middle) and c) site-specific soil profiles (n=20) and site-specific simulated and measured yield over three years (n=60) after soil profile optimization (Figure 2, right) .

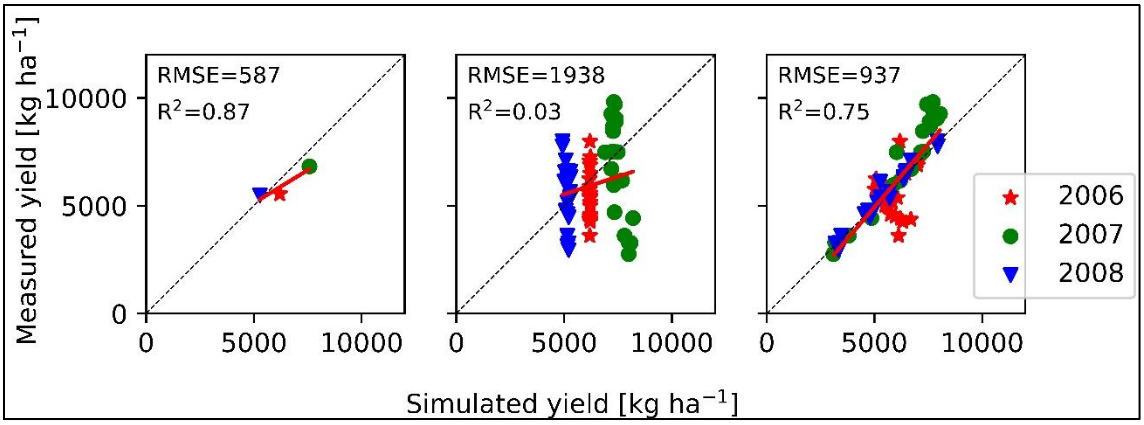

Figure 2 Simulated and measured yield shown in 1:1 graphs for: field-specific soil characterisation and field-specific measured yield (left), field-specific soil characterisation with site-specific measured yield (middle) and site-specific soil characterisation (inverse modelling) with site-specific measured yield (right). (Memic et al. 2023).

1.2 Error minimisation method – time-series measurements over multiple target variables

SPO was based on already published Time-Series cultivar coefficient Estimator (TSE) software tool for DSSAT (Memic et al. 2021). Error minimization method used in TSE was implemented in similar way in SPO. Same error minimisation method was implemented because multiple in-season observations (time-series data) for multiple target variables (grain yield, tops weight, leaf area index, soil water content etc.) can be used in optimisation process simultaneously. This method creates potential of using sensor-based measurements for site-specific soil profile generation in future, by replacing sample cuts with sensor-based measurements. Maximum four target variables simultaneously can be initialized in SPO. Simple example of error minimisation method can be seen in Table 1 for one site-specific unit (one soil profile) with only one target variable grain yield (GWAD). Optimization was conducted with only one soil coefficient in soil profile (SLLL) for this example. The SLLL values 0.7 to 1.2 (min=0.7 and max=1.2) with increment step 0.1 correspond to 30% reduction of the soil layer SLLL value in soil profile (Baseline) as minimum and 1.2 to 20% increase of Baseline as maximum with in between increments 10% (Table 1). This method of creating different soil profile scenarios used in sensitivity analysis was implemented as mathematical multiplier because of programming simplicity (Table 1). In Figure 3a boxplot shows to what degree target variable is sensitive to variation of selected coefficient. The setup shown in Table 1 corresponds to establishment of seven different SLLL scenarios shown as point lines in Figure 3b. The percentual reduction of Baseline SLLL (where SLLL=1.0) is conducted through entire soil profile (all soil layers) with nRMSE being calculated based on available in-season observations. In this simple example nRMSE-GWAD is equal to AVG-nRMSE because only one target variable (GWAD) was analysed and the scenario with the lowest AVG-nRMSE is considered "optimum" (lowest difference between simulated and observed grain yield based on nRMSE). Example of multiple target variable analysis is shown in Table 2 with corresponding target variable boxplots shown in Figure 4a and same SLLL scenario sensitivity analysis shown in Figure 4b. Based on the sensitivity analysis and error minimization it can be seen that target variable selection affects the optimum. For this example grain yield (GWAD), tops weight (CWAD) and harvest index (HIAD) was selected.

Table 1 SPO SLLL multiplier translation to percentual reduction and resulting nRMSE and AVG-nRMSE for one target variable GWAD (grain yield)

SLLL multiplier	Translates to percent reduction in SPO	nRMSE-GWAD	AVG-nRMSE
0.7	-30%	0.533	0.533
0.8	-20%	0.462	0.462
0.9	-10%	0.349	0.349
1.0	Baseline	0.242	0.242
1.1	+10%	0.095	0.095
1.2	**+20%**	**0.036**	**0.036**

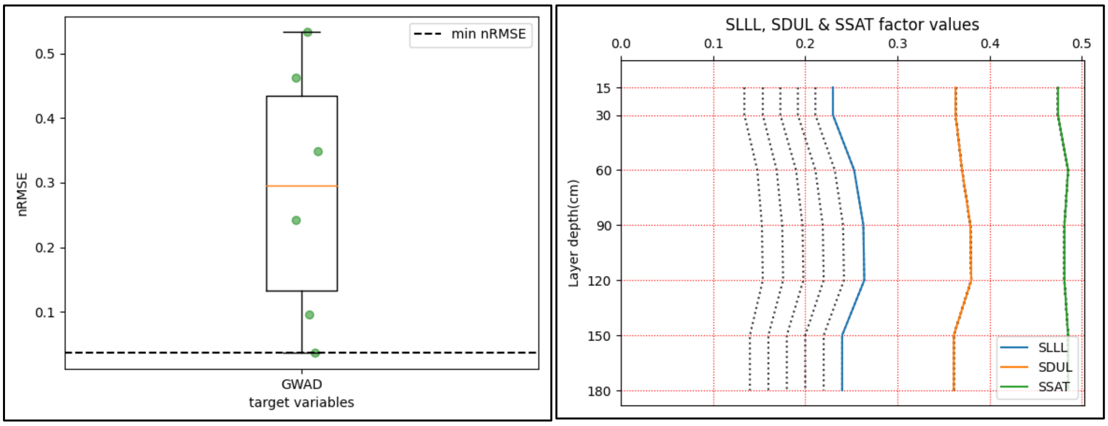

Figure 3 Boxplot (left) and soil-layer based sensitivity analysis of SLLL (right)

Table 2 SPO SLLL sensitivity analysis based on multiple target variables and corresponding multi-target variable AVG-nRMSE

SLLL multiplier	nRMSE-GWAD	nRMSE-CWAD	nRMSE-HIAD	AVG-nRMSE
0.7	0.533	0.204	0.297	0.309
0.8	0.462	0.089	0.367	0.252
0.9	**0.349**	**0.104**	**0.437**	**0.249**
1.0	0.242	0.257	0.52	0.319
1.1	0.095	0.399	0.553	0.362
1.2	0.036	0.54	0.623	0.435

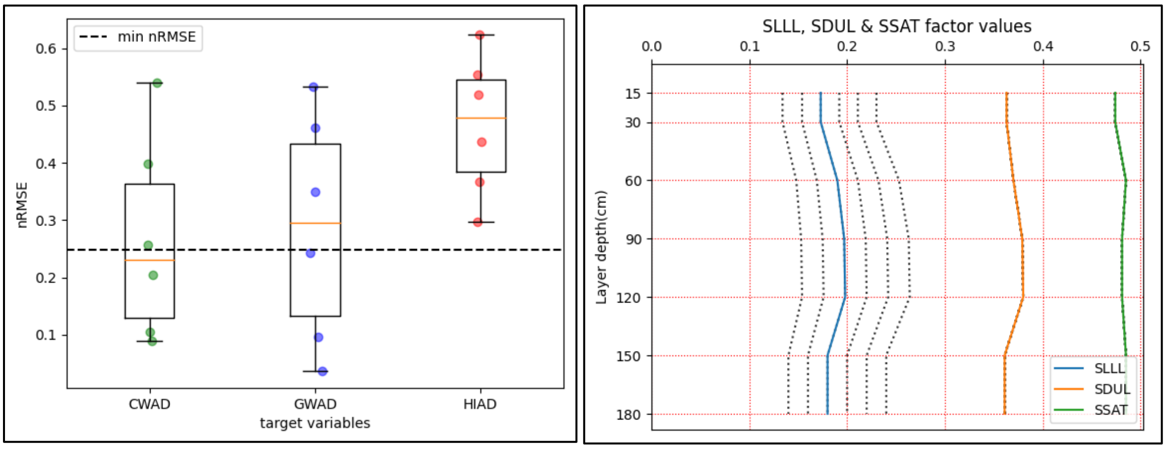

Figure 4 Boxplot (left) and soil profile SLLL over multiple depths (right)

In Figure 5a normalised RMSE of target variable GWAD can be seen during the SLLL coefficient modification. SLLL coefficient optimisation based on multiple target variables (CWAD, GWAD, HIAD) can be seen in Figure 5b. The dotted line indicates lowest AVG-nRMSE in these two different sensitivity analyses. The more target variables are available the more difficult it gets to select "optimum" based on certain statistical or mathematical criteria. For this reason already tested nRMSE method was implemented in SPO.

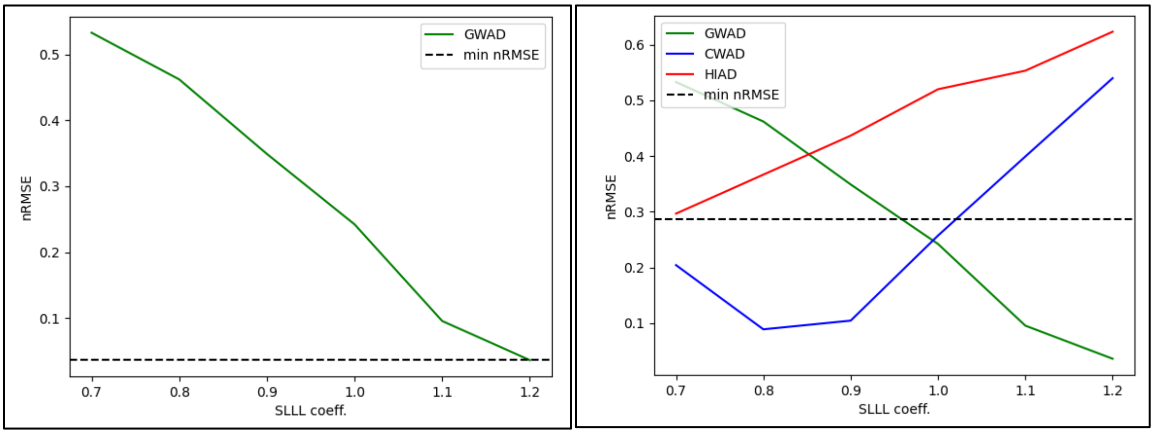

Figure 5 Error minimisation with single target variable (left) and multiple target variables (right)

1.3 General SPO program settings overview

The "**SPO_v.2.7zip**" must be unzipped and copied to the Tools directory: "**C:\DSSAT48\Tools**" (depending on the DSSAT version "C:\DSSAT**\Tools".

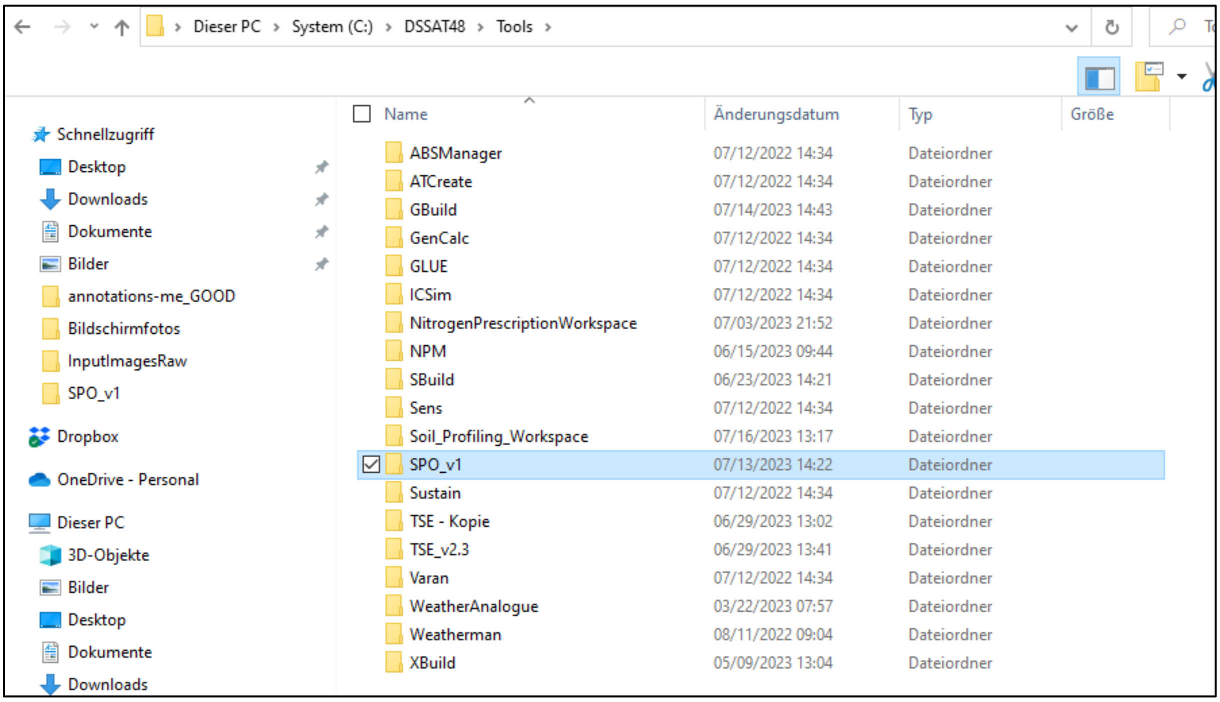

Figure 6 SPO_v1 directory path

In the folder "SPO_v2" "**C:\DSSAT48\Tools\SPO_v2**" (Figure 6) "**SPO_v2.exe**" <u>windows runnable must be executed as</u> "**Administrator**" (Figure 7).

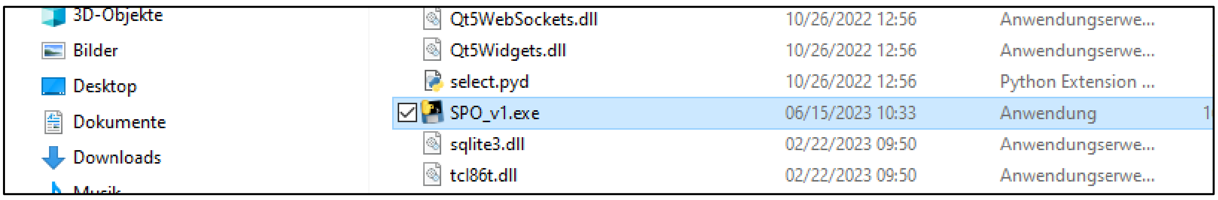

Figure 7 Path to SPO_v2.exe windows runnable

VERY IMPORTANT:

I. In order to use SPO a user has to have their soil profiles in **SOIL.SOL** input **file in native DSSAT Soil directory**.

II.

III. **PlantGro.OUT** (or other time-series) crop model outputs are coupled to those in **File-T** time-series in-season observations.

IV. If sub-model (e.g. WHAPS) is initialized in the File-X, the optimizer 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 SPO program.

V. 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.

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

VII. The program is matching DOY from **File-T** with those in the **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.

The SPO program is creating additional directory "Soil_Profiling_Workspace" (C:\DSSAT48\Tools\Soil_Profiling_Workspace) Figure 8 and modifying the SOIL.SOL in that directory after which is DSSAT crop model executed.

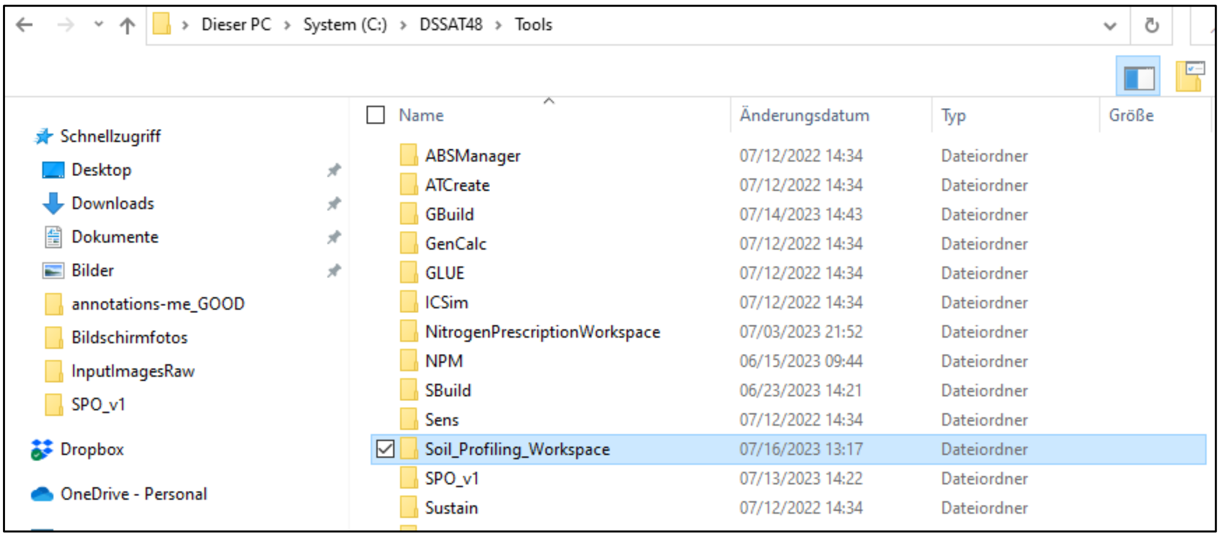

Figure 8 "Soil_Profiling_Workspace" is located in **"Tools"** directory

1.4 SPO program run

The **SPO** program **does NOT modify original DSSAT files in their native directories**. The program creates copies in "Soil_Profiling_Workspace" and do the sensitivity analysis by modifying targeted files in that directory.

After selecting desired files for optimization and setting up sensitivity analysis scenarios all modifications on soil profile are conducted in "Soil_Profiling_Workspace" in SOIL.SOL. Every time Run the Model push button is clicked the SPO will copy SOIL.SOL from "C:\DSSAT48\Soil" directory to Soil_Profiling_Workspace" and start optimization from beginning even if user did not exit SPO interface in the meantime.
After the model is executed the SPO algorithm creates backup of original SOIL.SOL soil profiles and modifies targeted soil profile isolated in SOIL.SOL in Soil_Profiling_Workspace. After soil profile optimization is conducted and before exiting SPO interface a user can open SOIL.SOL from Soil_Profiling_Workspace in text editor and MANUALLY copy soil profile to the "C:\DSSAT48\Soil" SOIL.SOL.

If user is using a target variable for optimizing specific parameters in soil profile that is insensitive to the variations of the coefficient, they will not result in different values of nRMSE, and it will result in having multiple soil profiles in SOIL.SOL (repetitive profiles) in Soil_Profiling_Workspace. This can be used as an indicator to check if it makes any sense to use such target variable for optimizing soil profile coefficient. In Soil_Profile_Workspace more systemic overview of target variable sensitivity to coefficient/s variations can be checked in BoxPlot figures.

SPO program running through section flow:

1. **List and select crop model**
2. **Load File-X list to the list widget in interface**
3. **File-X selection**
4. **File-X treatment (TRT) selection**
5. **Original DSSAT files setup test run**
6. **Target variable selection and initialization (default error minimization method is nRMSE)**
7. **Soil profile coefficient selection and coefficient min/max/increment range setup**
8. **Checking the setup of SPO and potentially initialization of Figure generators**

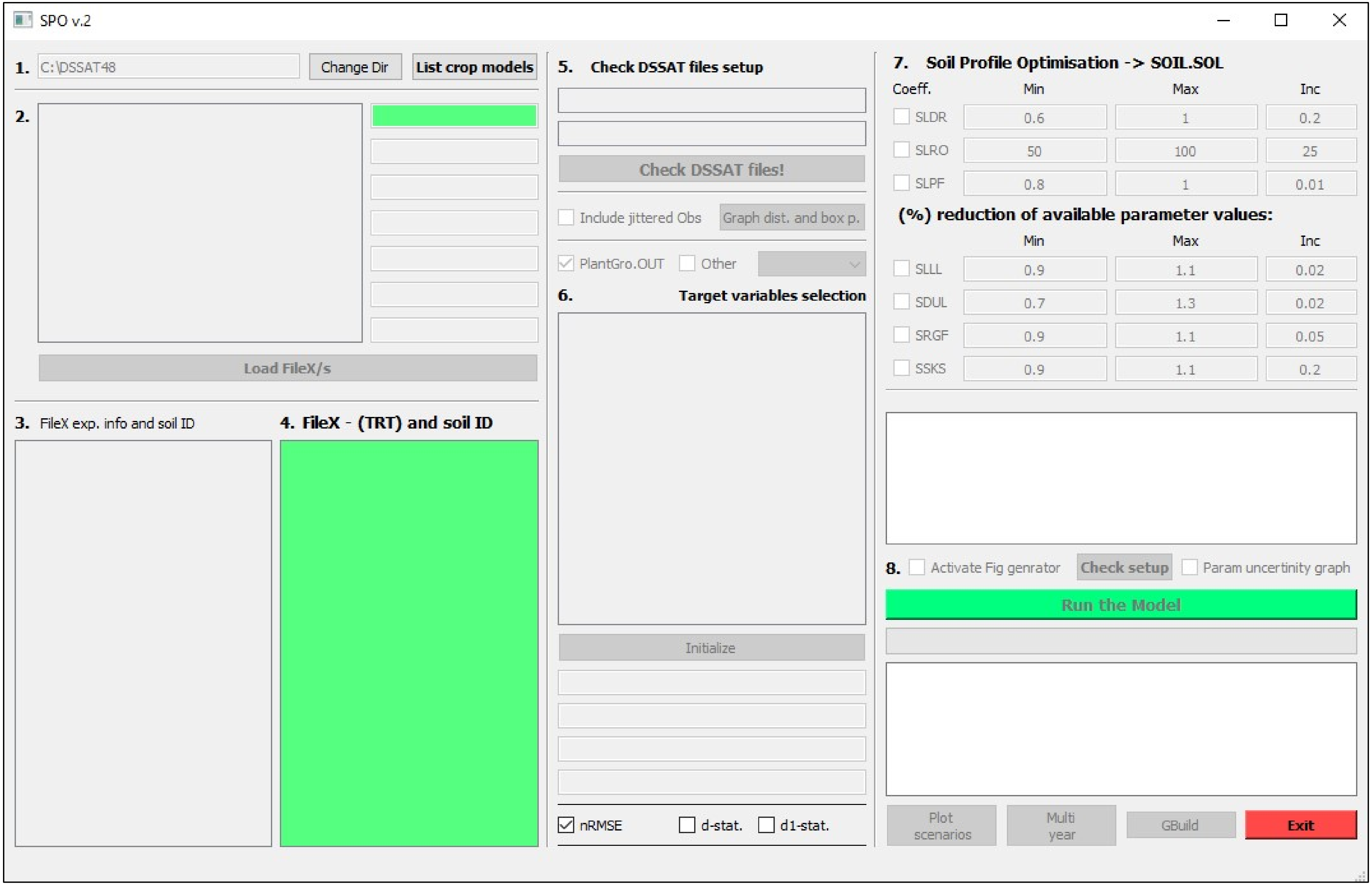

Figure 3 Interface

2. Crop model selection and initialization

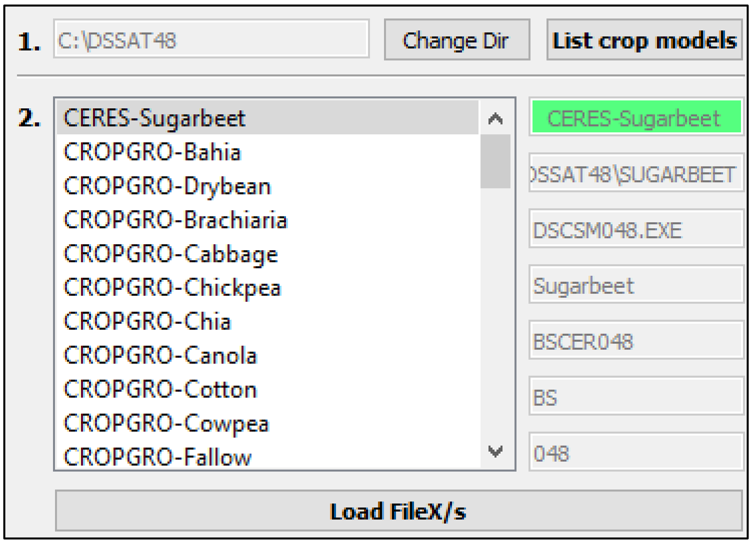

Figure 4 After SPO windows runnable is executed and "List crop models" button pressed all crop models available in DSSAT shell are offered for selection in section 2.

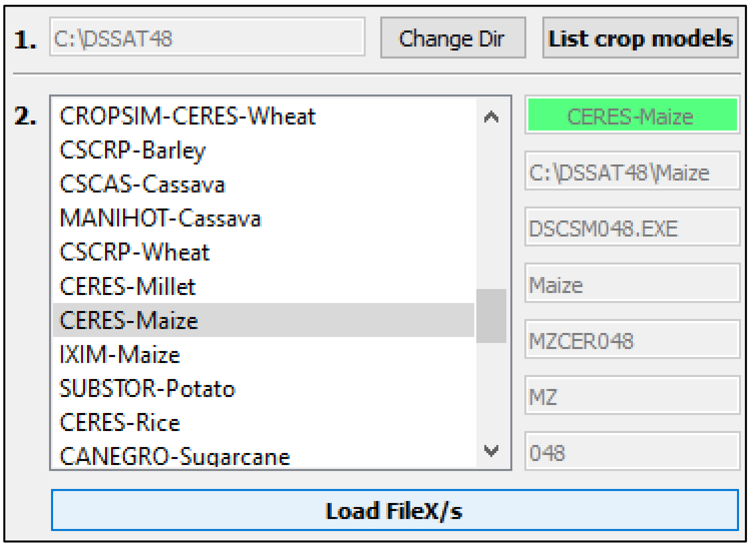

Figure 5 After desired crop growth model is selected in section 2 and "Load FileX/s" button pressed all available experiment files are loaded into list widget window in Section 3.

3. Experiment files initialization

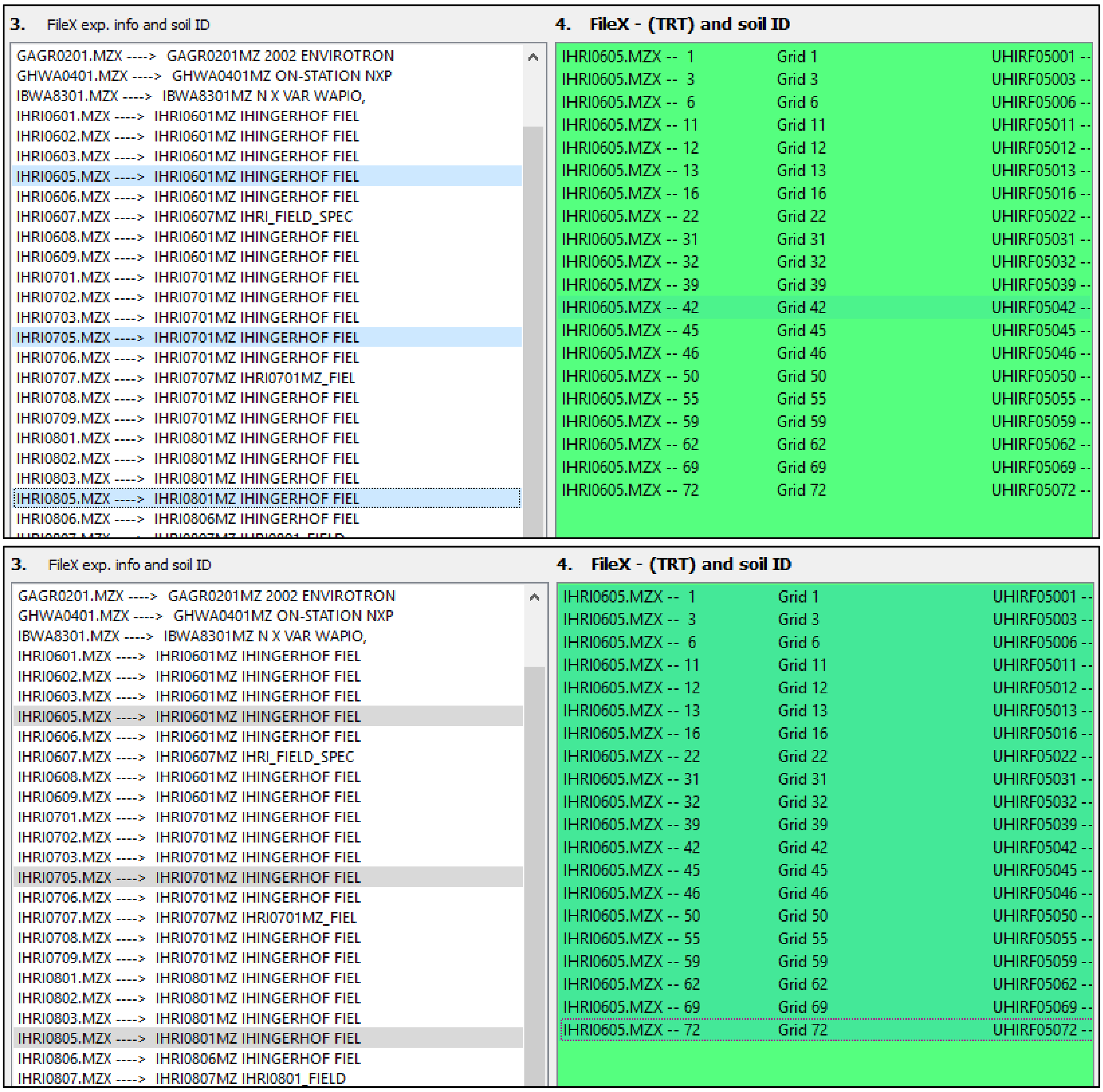

Figure 6 In this figure we can see two different list widgets shown as section 3 and 4. Section 4 shows experiment files (File X/s). When FileX is clicked on in section 3 and available treatments (TRT/s) in FileX/s are shown in section 4, for selection. FileX treatments correspond to the site-specific units analyzed with DSSAT crop growth models. Selected active treatments from section 4 are shown in text browser windows in section 7 (Figure 7)

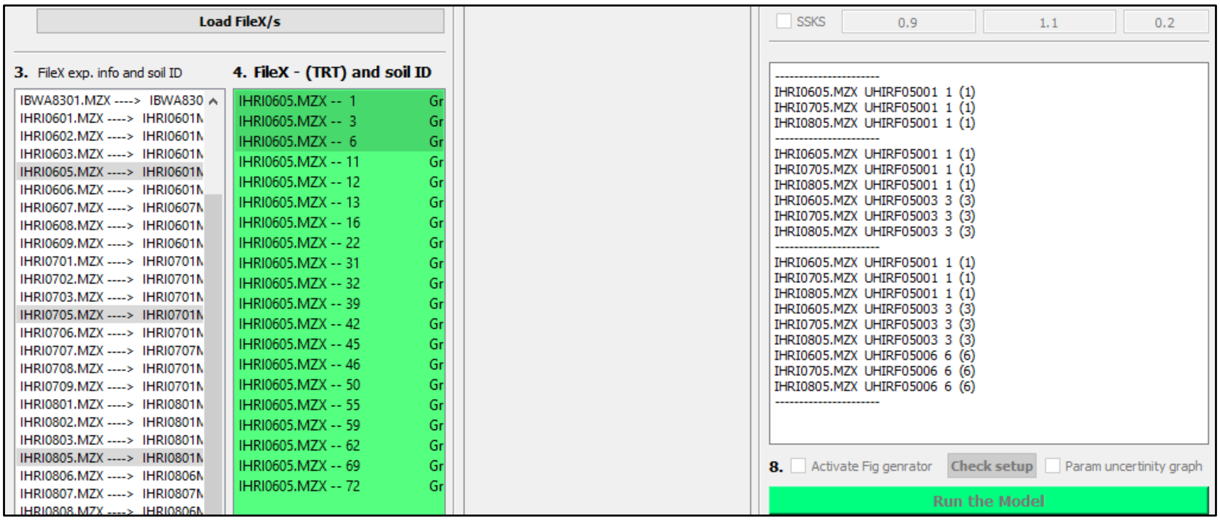

Figure 7 Functionally usable selected treatments are shown in text browser window

4. Experiment file and soil profile setup

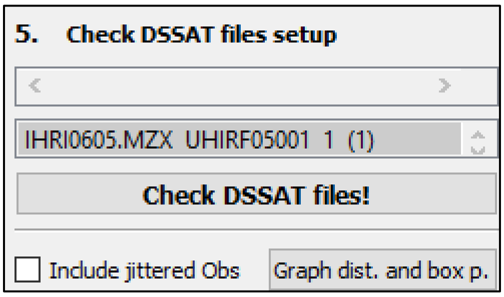

Figure 8 After site-specific units (TRT/s) are selected in section 4 it is shown in section 7 text browser window for multiple years that have same soil profiling. The UHIRF05001 is soil identifier used for labeling soil profile in SOIL.SOL file. Since it is the same for all three years in this case, this soil profile can be optimized based on three years of crop model maize parametrization and weather data (to investigate seasonality factor with respect to specific soil profile characterization).

Once Check DSSAT files! push button is pressed the DSSAT crop model is executed in order to check if all files are runnable. If the files are runnable and usable for soil profile optimization, they are shown in text browser windows in section 8 (Figure 9).

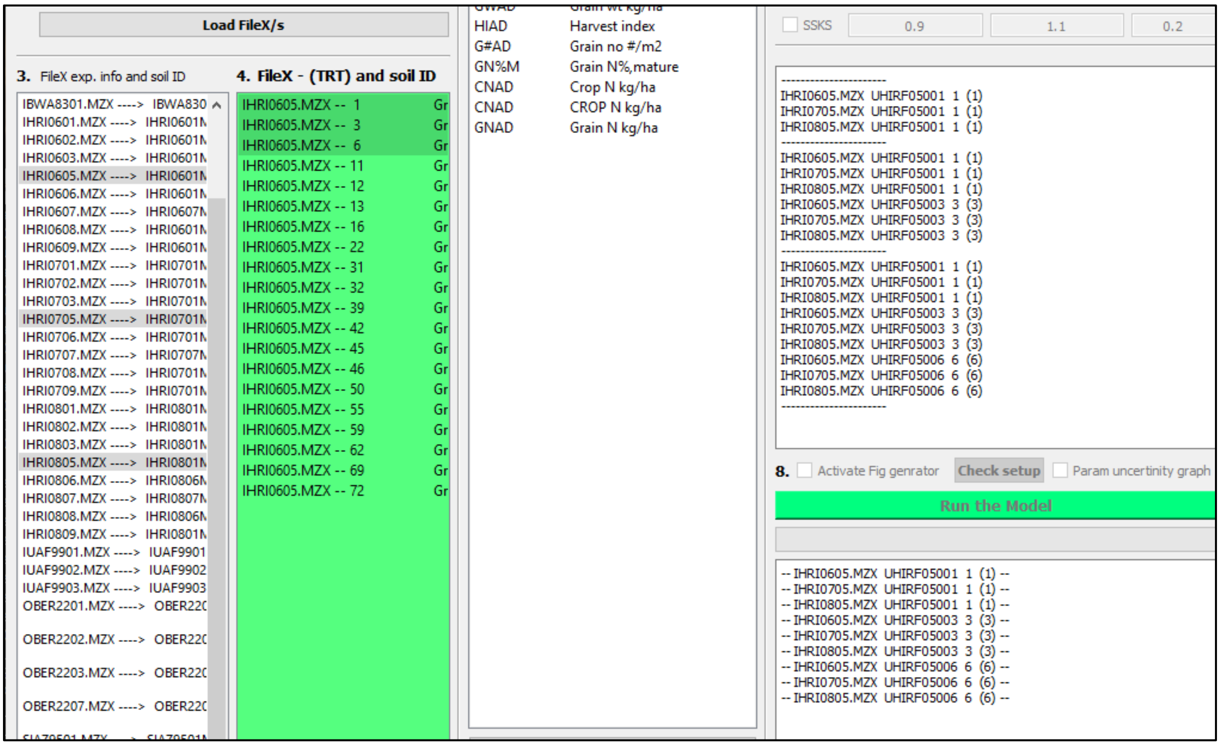

Figure 9 Functionally usable selected treatments are shown in text browser window after DSSAT files setup is checked by SPO

5. Site-specific yield variability check (optional for site-specific yield optimization)

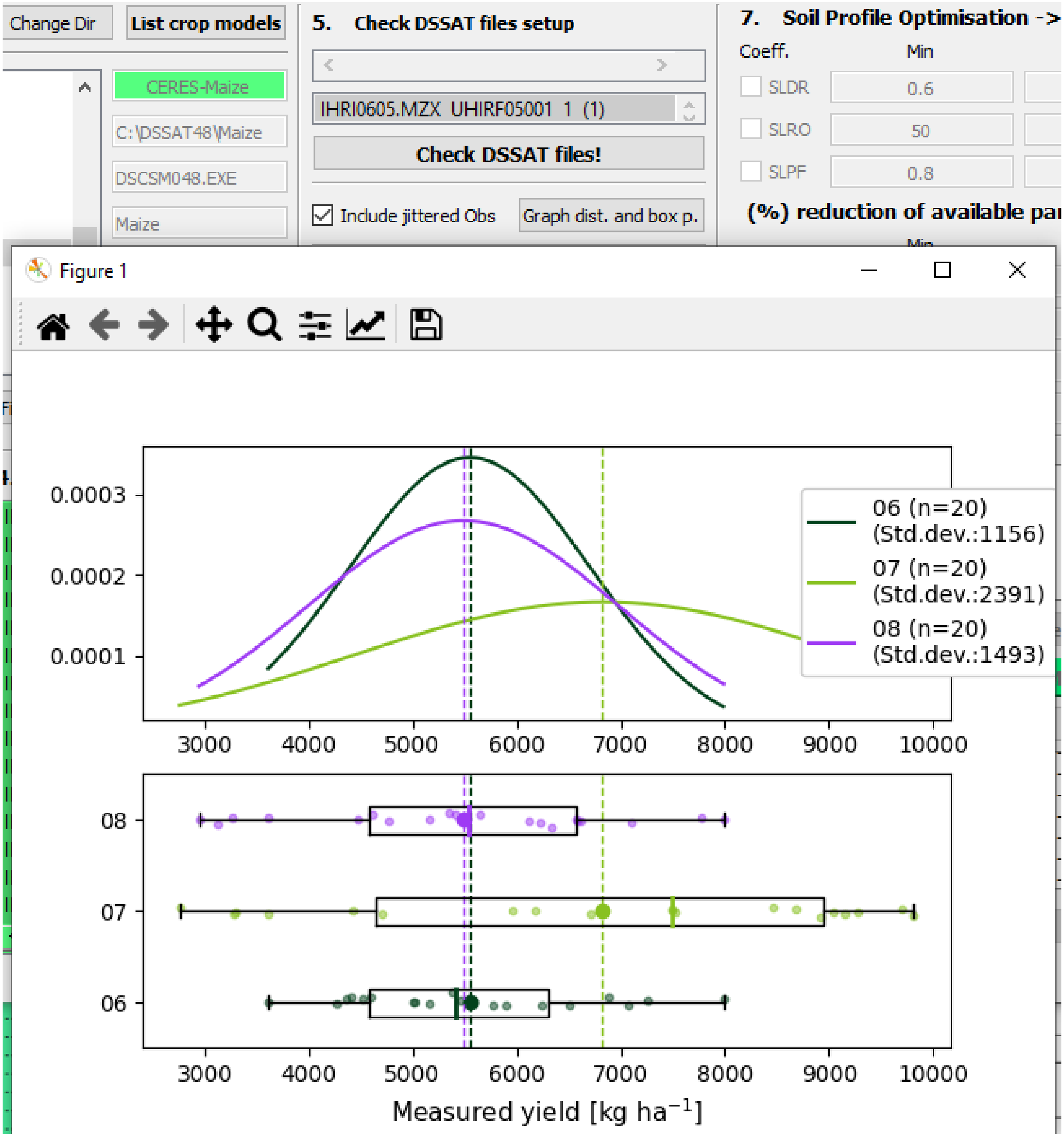

Figure 10 It is possible to investigate distribution of the individual target variables with standard deviation and corresponding boxplots.

6. Target variable selection and initialization

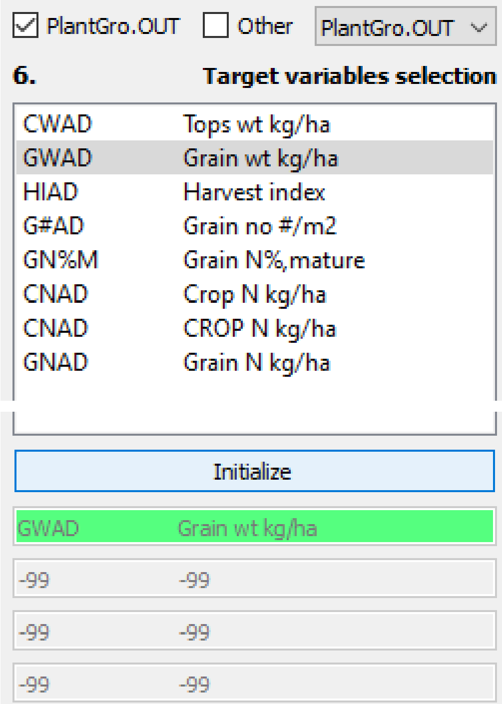

Figure 11 In this section of the SPO a user can select multiple target variables for optimization based on either on DSSAT PlantGro.OUT or some other DSSAT time-series output file (if "other" checkbox is initialized.

7. Soil profile parameters selection and setup

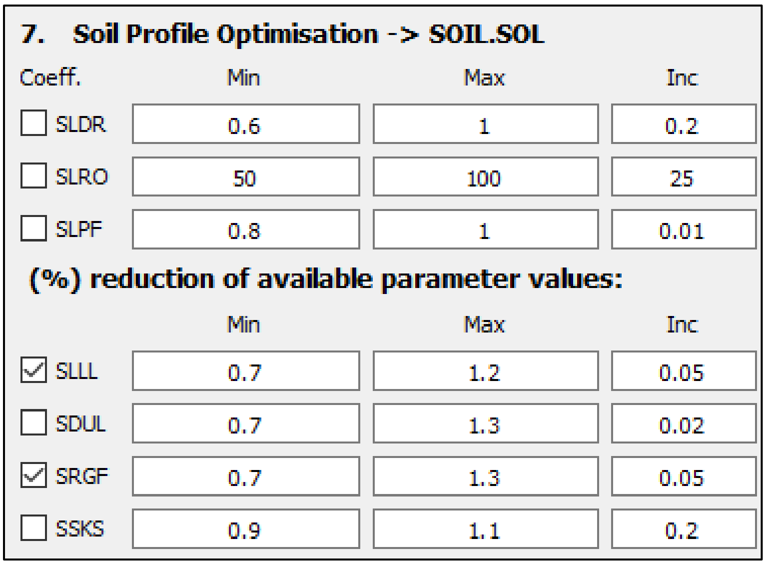

Figure 12 In section 7 ("(%) reduction of available parameter values:") of SPO interface a user can initialize specific soil profile coefficients for conducting sensitivity analysis. At the moment coefficient initialization is conducted based on multiplier approach where each multiplier setup based on coefficient min/max and increment step creates various soil profile scenarios. Every multiplier translates to percentual values as shown in Table 3.

Table 3 Conversion of multipliers to percentual values

SLLL	Translates to percent reduction in SPO
0.7	-30%
0.8	-20%
0.9	-10%
1.0	Baseline
1.1	+10%
1.2	+20%

8. SPO run

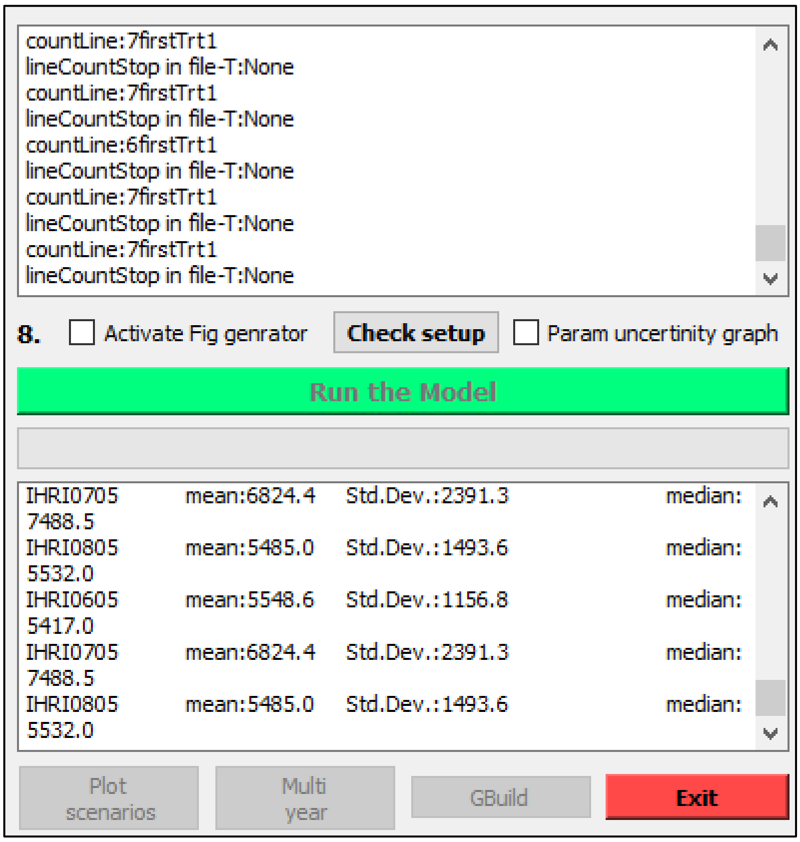

Figure 13 In section 8 a user can activate the figure option of creating figures showing coefficient-based scenarios (Figure 12) or boxplots as a form of parameter sensitivity analysis (Figure 13).

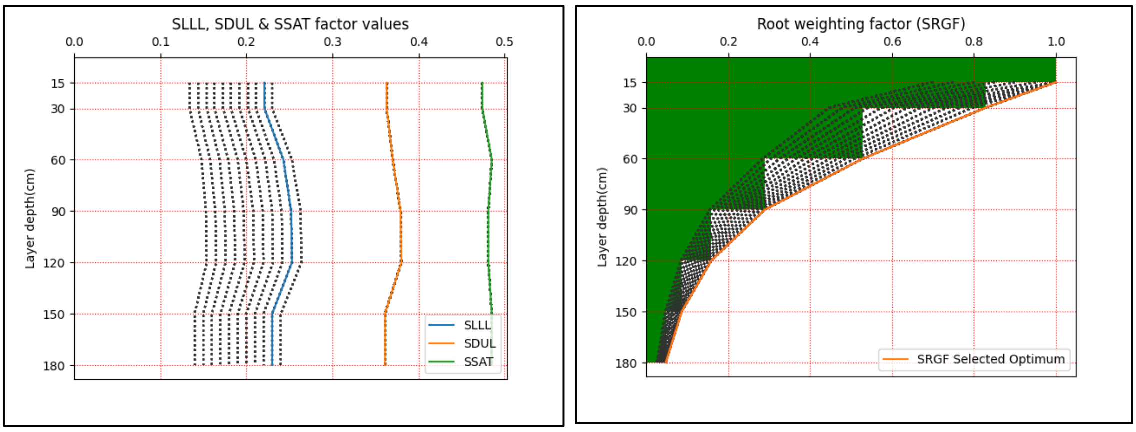

Figure 14 Coefficient based soil profile scenarios: SLLL (left) and SRGF (right)

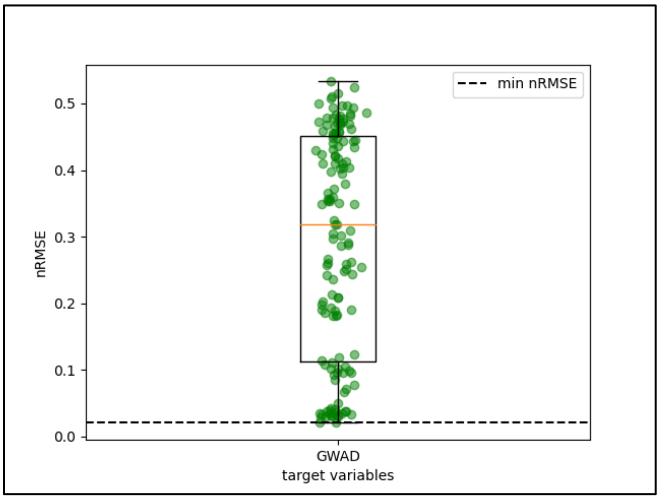

Figure 15 Boxplot sensitivity analysis output

9. Appendix

References

Memic E., Trenz J., Heshmati S., Graeff H. (2023). Evaluation of crop model-based marginal net return maximizing nitrogen application rates on site-specific level in maize. 23 Proceedings of the European Conference on Precision Agriculture, Bologna, Italy, 2 July 2023.

Memic E., Graeff, S., Boote, K. J., Hensel O., Hoogenboom G. (2021). Cultivar coefficient estimator for the cropping system model based on time-series data-a case study for soybean. In Transactions of the ASABE, (Transactions of the ASABE 2021, doi: 10.13031/trans.14432).

Yang, J.Y.M., Yang, J.Y.M., Liu, S., Hoogenboom, G., 2014. An evaluation of the statistical methods for testing the performance of crop models with observed data. Agric. Syst. 127, 81–89. https://doi.org/10.1016/j.agsy.2014.01.008.

Interface:
The SPO_v2 user interface was created in Qt Designer 5
(https://doc.qt.io/qtcreator/index.html)

Programming language:
The SPO_v2 algorithm was written in python 3.7
Python Software Foundation. Python Language Reference, version 3.7. Available at http://www.python.org

Windows runnable:
SPO_v2 was compiled into windows runnable with Pyinstaller
(https://www.pyinstaller.org/)

SPO_v2 algorithm and interface development/setup by Emir Memic.