APEXSENSUN Uncertainty and Sensitivity Analysis Software

Mansour Talebizadeh and Daniel Moriasi

A Software package of the USDA ARS Grazinglands Research Laboratory

El Reno, OK

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SECTION 1 Introduction

The Agricultural Policy/Environmental Extender (APEX) model is a daily time step model for simulating whole farms or small watersheds to evaluate agricultural production and environmental impacts. APEXSENSUN is a package in R for performing uncertainty and sensitivity analysis (SA) for the APEX model. APEXSENSUN reads the required inputs for Monte Carlo simulation and SA from text files provided by user and exports the SA outputs in text files. APEXSENSUN depends on "sensitivity" package, therefore, make sure you have "sensitivity" package loaded in R.

SECTION 1.1 Purpose

The purpose of this document is to provide a step-by-step procedure for using APEXSENSUN software package. This software was developed primarily for USDA-ARS Grazinglands Research Laboratory (GRL) in-house use and for public. This work is funded by USDA Office of Environmental Markets.

USDA ARS GRL and the authors are not responsible for use outside the scope described herein. If you have any comments or suggestions for the improvement of this software, please contact Dr. Daniel Moriasi at daniel.moriasi@ars.usda.gov.

SECTION 1.2 Function help and example project

All functions of APEXSENSUN come with an inbuilt help. In addition, an example folder containing an APEX project and other inputs is available for users to test the package. The rest of this manual provides details of implementing an SA project using the accompanying example folder which can be created through a call to the function in Figure 1.

```
#Loading APEXSENSUN package in R:
  library(APEXSENSUN)

# Creating a copy of tutorial folder
  getExampleFolder()
```

Figure 1 Script for creating example APEXSENUN project

SECTION 2 Steps for using APEXSENSUN

After loading APEXSENSUN and generating a copy of the example folder, the following three steps, described in the next sections should be followed for performing SA (Figure 2).

```
#Steps for performing a sensitivity analysis project using APEXSENSUN

#1) Generating a list object with predefined structure compatible to APEXSENSUN
  global_input <- inputGen()

#2) Performing Monte Carlo simulation using the setting in 'global_input'
  input4SA <- MC4APEX(global_input)

#3) Calculation of sensitivity indices
  SA4APEX(global_input,input4SA)
```

Figure 2 Example script for implementing a SA project

Step1: Input setting

The inputs for a SA project should be set through a list object in R generated through `inputGen` function with no arguments (i.e. step 1 in Figure 2). The generated list object contains general parameters, required by APEXSENSUN for communicating to APEX (Table A1), as well as uncertainty ranges for APEX model parameters (Table A2 and Table A3). The default lower and upper bounds of APEX parameters are set to -1, meaning APEXSENSUN do not consider them as uncertain parameter. Therefore, it is important to replace them with a meaningful lower and upper values to include them in a SA project. Figure 3 illustrates setting of uncertainty bounds for APEX parameters, considered in this tutorial.

```
#Setting lower and upper bounds for uncertain parameters:
  global_input$APEX_PARM$Root_growth_soil[1] = 1.15
  global_input$APEX_PARM$Root_growth_soil[2] = 1.2

  global_input$APEX_PARM$Soil_water_limit[1] = 0
  global_input$APEX_PARM$Soil_water_limit[2] = 1

  global_input$APEX_PARM$Soil_evap_coeff[1] =1.5
  global_input$APEX_PARM$Soil_evap_coeff[2]=2.5

  global_input$APEX_PARM$Soil_evap_plant_cover[1] = 0
  global_input$APEX_PARM$Soil_evap_plant_cover[2] = 0.5

  global_input$APEX_PARM$Runoff_CN_int_abs[1] = 0.05
  global_input$APEX_PARM$Runoff_CN_int_abs[2] = 0.4

  global_input$APEX_PARM$Max_rain_intercept[1] = 0
  global_input$APEX_PARM$Max_rain_intercept[2] = 15

  global_input$APEX_PARM$Rain_intercept_coeff[1] = 0.05
  global_input$APEX_PARM$Rain_intercept_coeff[2] = 0.3

  global_input$APEX_PARM$Microbial_top_soil_coeff[1] = 0.1
  global_input$APEX_PARM$Microbial_top_soil_coeff[2] = 1

  global_input$APEX_PARM$Microbial_decay_coeff[1] = 0.5
  global_input$APEX_PARM$Microbial_decay_coeff[2] = 1.5
```

Figure 3 Setting of uncertainty bounds in APEXSENSUN

Sample size (or length of the discretization of parameters) and type of SA method can be set as in Figure 4.

```
#Setting of sample size and SA type
  global_input$sample_size <- 1000

  global_input$GSA_Type <- "FAST99"
```

Figure 4 Setting of sample size and SA type in APEXSENSUN

Step 2: Monte Carlo simulations using the settings in Step 1

"MC4APEX" function (see 2 in Figure 2) performs Monte Carlo simulations using the settings in "global_input" object. The APEX output files for each Monte Carlo simulation are saved in designated folders (using the setting in "global_input"). In addition, "MC4APEX" function produces a new object (i.e. "input4SA" in Figure 2) that would be used as an input for the SA phase.

Step 3: SA using the settings in Step 1 and Step 2

"SA4APEX" function (see 3 in Figure 2) performs SA using "global_input" and "input4SA" objects and exports the final results to the folder designated for storing SA results (i.e. "GSA_Outputs" in this tutorial).

APENDIX

Table A1 General inputs

Variable name in APEXSENSUN	Description
sample_size	Sample size or length of the discretization of parameter space.
caption_var_sim	Simulated variable name as it appears inside .DWS APEX file.
caption_var_obs	Observed variable names as appears inside observed file.
start_date	Start date for analysis with format: "YYYY MM DD" e.g., "2002 01 01".
end_date	End date for analysis with format: "YYYY MM DD" e.g., "2003 01 01".
label_APEX_exe	APEX executable file name excluding file's extension.
label_watershed_param	APEX PARM file name excluding file's extension.
label_control_param	APEXCONT file name excluding file's extension.
label_output_variable_AWP	APEX .AWP file name excluding file's extension.
label_output_variable_ACY	APEX .ACY file name excluding file's extension.
label_output_variable_DWS	APEX .DWS file name excluding file's extension.
label_observed_var.txt	Observed file name containing observed time series.
folder_path_project	Path to folder containing APEX model.
Back_Up_PARM0806.dat	Path to original APEX file containing PARM parameters.
Back_Up_APEXCONT.dat	Path to original APEX file containing APEXCONT parameters.
folder_path_observed	Path to folder containing observed data file.
folder_path_GSA_Outputs	Path to folder storing SA results.
store_folder_path_watershed	Path to folder storing generated PARM files for Monte Carlo runs.
store_folder_path_control	Path to folder storing generated APEXCONT file for Monte Carlo runs.
Calculated_output_folder_AWP	Path to folder storing calculated .AWP files for Monte Carlo runs.
Calculated_output_folder_ACY	Path to folder storing calculated .ACY files for Monte Carlo runs.
Calculated_output_folder_DWS	Path to folder storing calculated .DWS files for Monte Carlo runs.

GSA_Type	Type of SA method which can be one of the following options: "MORRIS", "SRC", "SRRC", "SOBOL", "SOBOL2002", "SOBOL2007", "SOBOLEFF", "SOBOLJANSEN", "SOBOLMARA", "SOBOLMARTINEZ", "FAST99", "KSTEST".
SA_Parms	A list containing following SA-specific parameters: morris_r: an integer representing design repetition number (i.e. the number of elementary effect computed per factor). morris_levels: an integer specifying the number of levels of the design in OAT (Once At a Time) design. sobolOrder: an integer representing maximum order in the ANOVA decomposition in Sobol method. KS_TEST_PF: A performance function type for "KSTEST" method. Available options are: "NASH", "RMSE", "PBIAS" KS_TEST_Threshold: Threshold value for performance function for determining behavioral from non-behavioral simulations. KS_TEST_sig_level: Significance level used in "KSTEST"

Table A2 APEX model parameters located inside PARM****.dat file

Variable name in APEXSENSUN	Parameter description in APEX
Crop_canopy_PET	Crop canopy-PET
Root_growth_soil	Root growth-soil strength
Water_stress_harvest	Water stress-harvest index
Water_storage_N	Water storage N leaching
Soil_water_limit	Soil water lower limit
Winter_dormancy	Winter dormancy
N_fixation	N fixation
Soluble_P_runoff	Soluble phosphorus runoff coefficient
Pest_damage_moisture	Pest damage moisture threshold
Pest_damage_cover	Pest damage cover threshold,
Moisture_req_seed_germ	Moisture required for seed germination
Soil_evap_coeff	Soil evaporation coefficient
Wind_erod_coeff	Wind erodibility coefficient
Nitrate_leac_ratio	Nitrate leaching ratio
Runoff_CN_Adj_parm	Runoff CN Residue Adjustment Parameter
Expand_CN_ret_parm	Expands CN retention parameter
Soil_evap_plant_cover	Soil evaporation – plant cover factor
Sedim_rout_exponent	Sediment routing exponent
Sedim_rout_coeff	Sediment routing coefficient
Runoff_CN_int_abs	Runoff curve number initial abstraction
Soluble_C_adsorp_coeff	Soluble Carbon adsorption Coefficient
CN_retention_frozen_soil	Reduces NRCS Runoff CN Retention Parameter for Frozen Soil
Harg_equation_parm	Hargreaves PET equation coefficient
Pest_leach_ratio	Pesticide leaching ratio
Expo_coeff_rainfall	Exponential coefficient used to account for rainfall intensity on curve number
Matur_frac_spring	Fraction of maturity at spring growth initiation
CEC_effect_nitrification	CEC effect on nitrification & volatilization
N_fixation_limit	Upper Nitrogen Fixation limit
Biological_mix_efficiency	Biological mixing efficiency
Soluble_P_exponent	Soluble phosphorus runoff exponent
Max_depth_bio_mixing	Maximum depth for biological mixing
OrgP_loss_exponent	Organic P loss exponent
MUST_coeff	Coefficient in MUST EQ
Harg_PET_exponent	Hargreaves PET equation exponent
Denit_soil_threshold	Denitrification soil-water threshold
Daily_denit_limit	Upper Limit of Daily Denitrification rate
SWAT_delivery_ratio_exponent	Exponent in Delivery Ratio for SWAT Output
Water_stress_coeff	Water stress weighting coefficient
Puddling_sat_conduct	Puddling Saturated Conductivity
Groundwater_stor_threshold	Groundwater storage threshold

Root_temp_stress_exponent	Plant root temperature stress exponent
SCS_index_coeff	SCS curve number index coefficient
Plow_depth	Plow layer depth
CN_retention_param	Upper Limit of Curve Number Retention Parameter
sediment_rout_travel_coeff	Sediment routing travel time coefficient,
RUSLE_c_factor_res	RUSLE C-factor coefficient
RUSLE_c_factor_height	RUSLE C-factor coefficient
Climate_stress_factor	Adjusts climatic stress factor
Max_rain_intercept	Maximum rainfall interception by plant canopy
Rain_intercept_coeff	Rainfall interception coefficient
Water_stor_residue_coeff	Water stored in litter (residue) coefficient
Tillage_residue_decay_rate_coeff	Exponential coefficient in EQUATION expressing tillage effect on residue decay rate
Microbial_soil_depth_coeff	Coefficient in oxygen EQUATION used in modifying microbial activity with soil depth
N_enrich_coeff	N enrichment ratio coefficient for routing
N_enrich_rout_exponent	N enrichment ratio exponent for routing
Fraction_destroyed_burn	Fraction destroyed by burn operation
P_enrich_rout_coeff	P enrichment ratio coefficient for routing
P_enrich_rout_exponent	P enrichment ratio exponent for routing
P_move_evap_coeff	P upward movement by evaporation coefficient
Max_days_grazed_rotation	Maximum number of days a pasture is grazed before rotation
Soil_water_up_flow_limit	Soil water Upward Flow Limit
Manure_erosion_equation_coeff	Manure erosion equation coefficient
N_enrich_ratio_delivery	N Enrichment Ratio for Delivery to SWAT
Dust_distribution_coeff	Dust distribution coefficient
RUSLE2_trans_capacity	RUSLE2 transport capacity parameter
RUSLE2_trans_capacity_threshold	RUSLE2 threshold transport capacity coefficient
Dust_distribution_exponent	Dust distribution dispersion exponent
Manure_erosion_exponent	Manure erosion exponent
Microbial_top_soil_coeff	Coefficient adjusts microbial activity function in the top soil layer
Microbial_decay_coeff	Microbial decay rate coefficient
Manure_erosion_coeff	Manure erosion coefficient
Volt_nitrification_partition_coeff	Volatilization/nitrification partitioning coefficient
Hydrograph_dev_param	Hydrograph development parameter
Partition_N_flow_groundwater	Partitions Nitrogen flow from groundwater
P_enrich_ratio_deliver_SWAT	P Enrichment Ratio for Delivery to SWAT
Stand_dead_fall_rate_coeff	Standing Dead fall rate coefficient
Runoff_2_delay_pest	Runoff amount to delay pest application
Soil_water_2_delay_tillage	Soil water value to delay tillage
Auto_mov_lower_limit	Auto mow lower limit
Nitrification_vol_upper_limit	Upper Limit of Nitrification-Volatilization

Tech_coeff	Technology Coefficient
Drainage_lateral_conduct	Estimates drainage system lateral hydraulic conductivity
P_flux_labile_active_coeff	Coefficient regulating P flux between labile and active pool
P_flux_active_stable_coeff	Coefficient regulating P flux between active and stable pool
N_salt_evap_coeff	Nitrogen and Salt Upward movement by evaporation coefficient
Water_table_recession_coeff	Water table recession coefficient
Water_table_move_limit	Limits daily water table movement
Water_table_recession_exponent	Water table recession
Subsurface_flow_factor	Subsurface flow factor
Flood_evap_limit	Flood Evaporation Limit
Runoff_adj_link	Runoff Volume Adjustment for Direct Link
Water_erosion_threshold	Water Erosion Threshold
Wind_erosion_threshold	Wind Erosion Threshold
Crop_stress_temp_exponent	Exponent of Crop Stress Temperature function
Soluble_P_leach_KD	Soluble Phosphorus Leaching KD value
Irrigation_cost	Cost of Irrigation Water
Lime_cost	Cost of Lime
Fuel_cost	Cost of Fuel
Labor_cost	Cost of Labor

Table A3 APEX control parameters located inside APEXCONT.dat file

Variable name in APEXSENSUN	Parameter description in APEX
RFN	Average concentration of nitrogen in rainfall
CO2	Carbon dioxide concentration in atmosphere
CQN	Concentration of NO3-N in irrigation water in ppm
PSTX	Pest damage scaling factor
YWI	Number years of maximum monthly 0.5 hour rainfall available
BTA	COEF (0-1) governing wet-dry probabilities given days of rain
EXPK	Parameter used to modify exponential rainfall amount distribution
QG	Channel Capacity Flow Rate
QCF	Exponent in watershed area flow rate equation
CHSO	Average upland slope (m/m) in watershed
BWD	Channel bottom width/depth in m/m; Channel flow rate (QG) > 0
FCW	Floodplain width/channel width in m/m
FPSC	Floodplain saturated hydraulic conductivity in mm/h
GWSO	Maximum ground water storage in mm
RFTO	Ground water residence time in days
RFPO	Return Flow / (Return Flow + Deep Percolation)
SATO	Saturated Conductivity adjustment factor
FL	Field length (if wind erosion is to be considered) in kilometers
FW	Field width (if wind erosion is to be considered) in kilometers
ANG	Clockwise angle of field length from north (if wind erosion is to be considered)
UXP	Power Parameter of Modified Exponential Distribution of Wind Speed (if wind erosion is to be considered)
DIAM	Soil Particle Diameter(if wind erosion is to be considered)
ACW	Wind Erosion Adjustment Factor
GZL0	Grazing limit
RTN0	Number of years of cultivation at start of simulation
BXCT	Linear coefficient of change in rainfall from east to west (PI/PO/KM)
BYCT	Linear coefficient of change in rainfall from south to north (PI/PO/KM)
DTHY	Time interval for flood routing (hours)
QTH	Routing Threshold (mm) – VSC routing used when QVOL>QTH
STND	VSC Routing used when reach storage > STND
DRV	Equation for Water Erosion

PCO0	Fraction of subareas controlled by ponds
RCC0	USLE Crop Management Channel Factor
CSLT	Salt Concentration in Irrigation Water
BUS1	Exponents of MUSI equation
BUS2	
BUS3	