APEX-CUTE 2.0 USER'S MANUAL

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Overview

The Agricultural Policy Environmental eXtender - auto-Calibration and UncerTainty Estimator (APEX-CUTE) is coded in Python. The current version includes sensitivity analysis (SA) and the dynamically dimensioned search (DDS) algorithm (Tolson and Shoemaker, 2007) for APEX auto-calibration. Three methods are provided in APEX-CUTE for SA: method of Morris (or EE), Sobol', and Fourier amplitude sensitivity testing (FAST). As with any SA and/or auto-calibration tools, users should conduct necessary checks for model input and initial runs before conducting SA and/or auto-calibration to make sure that the basic APEX input and setup are correct.

APEX-CUTE interacts with APEX by modifying APEX input files with candidate solution, running APEX, evaluating model output by calculating performance statistics, perturbing current best solution to generate candidate solution, and iteratively repeating the process until maximum number of objective function evaluations completed.

Calibration Parameters

APEX parameters and input that may be chosen by users to be included in the auto-calibration process (Table 1) were based on previous APEX studies (Wang et al., 2006; Yin et al., 2009) and APEX developers' experience and recommendations, as summarized by Wang et al. (2012). Users can select all the relevant parameters for the calibration components listed in Table 1, or they can conduct a SA first and then decide which parameters to be included for calibration. Because water is a potential force that interacts with or drives almost all environmental processes within a watershed system, the hydrological conditions prevalent in the watershed are critical to the estimations of sediment and nutrient losses. Therefore, if the erosion/sedimentation component is to be calibrated, the hydrology-related parameters must also be selected for calibration. When sediment data are available, it is often the case that flow data are also available for calibration. For nutrient calibration, both hydrology and sediment related parameters should be involved in the calibration (Wang et al., 2014).

In APEX-Cute v2.0 version, the number of available parameters for calibration and SA has increased from 36 to 152. In this update, all PARM parameters in PARM0806.DAT and some coefficients in APEXCONT.DAT potentially available for calibration were added.

Table 1. Choice of APEX parameters available in APEX-CUTE 1.0.

Process impacted directly	Influential input or parameter	Description	Range	Default
Runoff CN method	CN2	Initial condition II curve number (CN2) or landuse number (LUN)	± 5	-
	Parm42 (if NVCN=4)	Curve Number index coefficient	0.5 - 2.5	0.5
	Parm92 (if NVCN=0)	Curve number retention parameter coefficient	0.8 – 1.5	1
	Parm20	Runoff curve number initial abstraction	0.05 – 0.4	0.2
Green & Ampt	SAT0	Saturated conductivity adjustment factor	0.1–10.0	1
Evapotranspiration (PET)	Parm34 (if Hargreaves PET)	Equation exponent	0.5 – 0.6	0.5
	Parm1 (if Penman-Monteith)	Canopy PET factor	1 - 2	2
ET	Parm12	Soil evaporation coefficient	1.5 – 2.5	1.5
	Parm17	Evaporation plant cover factor	0 – 0.5	0.1
Irrigation (if used)	EFI	Irrigation runoff ratio	0 -1	0
Tile/drainage flow	Parm83	Estimates drainage system lateral Hydraulic conductivity	0.1 - 10	4
Base flow	RFP0	Return flow ratio: (Return flow)/(Return flow + Deep percolation)	0.05 - 0.95	0.5
	Parm40	Groundwater storage threshold	0.001 - 1.0	0.25
	RFTO	Groundwater residence day	10 - 50	30
Erosion/ sedimentation	Parm46	RUSLE c factor coefficient in exponential residue function in residue factor	0.5 - 1.5	0.5
	Parm47	RUSLE c factor coefficient in exponential crop height function in biomass factor	0.01 - 3.0	1.0
	PEC (if having conservation practice)	Erosion control factor	0 - 1	1
	APM	Peak rate – EI_{30} adjustment factor	0 - 1.0	1.0
Routing	Parm18	Sediment routing exponent of water velocity function for estimating potential sediment concentration	1 - 1.5	1.5
	Parm19	Potential sediment concentration when flow velocity is 1.0 m/s	0.005 - 0.05	0.05
	RCCO or RCHC	Channel cover factor	0.001 - 1.0	0.7
	RCHK	Soil edibility factor	0.001 - 0.5	0.3
Nitrogen cycling Phosphorus cycling	Parm29	Biological mixing efficiency	0.1 – 0.5	0.1
	Parm8	Soluble P runoff coefficient	10 – 20	15
	Parm59	P upward movement by evaporation coefficient	1 – 30	1
	Parm14	Nitrate leaching ratio	0.1 – 1.0	0.2
	Parm35	Denitrification soil water threshold	0.9 – 1.1	0.99
	Parm7	N fixation coefficient	0 – 1	0.9
	Parm72	Volatilization/nitrification partitioning coefficient	0.05 – 0.5	0.15
Carbon Cycling	Parm70	Microbial decay rate coefficient	0.05 – 1.5	1
	FHP	Fraction of humus in passive pool	0.3 – 0.9	0.3

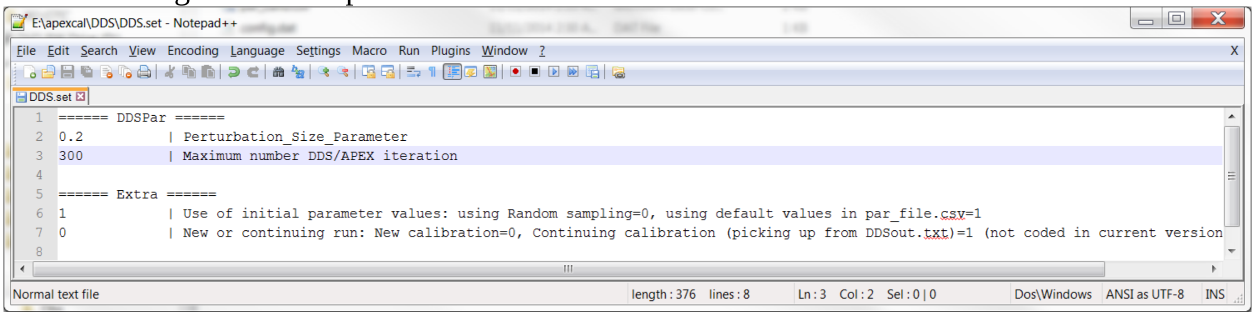
Data Structure

Input

Three default APEX-CUTE setup files are required for APEX-CUTE.

1) DDS.set

Figure 1. Example of the DDS.set file.



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====== DDSPar ======
0.2          | Perturbation_Size_Parameter
300          | Maximum number DDS/APEX iteration

====== Extra ======
1            | Use of initial parameter values: using Random sampling=0, using default values in par_file.csv=1
0            | New or continuing run: New calibration=0, Continuing calibration (picking up from DDSout.txt)=1 (not coded in current version
```

The DDS perturbation size parameter (dds_pertsize) and the user-input maximum number of function evaluations (dds_ndraw) are saved in DDS.set (Fig. 1). The parameter dds_pertsize defines the scalar neighborhood size perturbation which determines the random perturbation size standard deviation as a fraction of the decision variable (to be perturbed APEX parameter) range. The dds_pertsize is the only algorithm parameter to set in the DDS algorithm (Tolson and Shoemaker, 2007). The default value of 0.2 is recommended by Tolson and Shoemaker (2007). Depending on the study APEX project, the dds_ndraw can be limited to fewer than around 1500. Users can choose to use either the default APEX parameter values provided in the par_calib.csv file (described below) or DDS random sampling values of the APEX parameters as initial parameter values for APEX run (namely, initial solution).

2) par_calib.csv

Figure 2. Example of the par_calib.csv file.

par_n	Symbol	par_f	x0	bl	bu	units	Input_File
1	CN2	1	3	-5	5	-	OPC
2	parm1	0	2	1	2	-	parm0806
3	parm7	0	0.9	0	1	-	parm0806
4	parm8	0	15	10	20	-	parm0806
5	parm12	1	1.5	1.5	2.5	-	parm0806
6	parm14	1	0.2	0.1	1	-	parm0806
7	parm17	1	0.1	0.01	0.5	-	parm0806
8	parm18	0	1.5	1	1.5	-	parm0806
9	parm19	0	0.05	0.005	0.05	-	parm0806
10	parm20	1	0.2	0.05	0.4	-	parm0806
11	parm29	0	0.1	0.1	0.5	-	parm0806
12	parm34	0	0.6	0.5	0.6	-	parm0806
13	parm35	0	0.99	0.9	1.1	-	parm0806
14	parm40	1	0.05	0.001	1	-	parm0806
15	parm42	0	0.5	0.3	2.5	-	parm0806
16	parm46	1	0.5	0.5	1.5	-	parm0806
17	parm47	1	1	0.01	3	-	parm0806
18	parm59	0	2	1	30	-	parm0806
19	parm70	0	1	0.05	1.5	-	parm0806
20	parm72	0	0.15	0.05	0.5	-	parm0806
21	parm74	0	0.2	0	20	-	parm0806
22	parm83	0	4	0.1	10	-	parm0806
23	parm92	1	1	0.8	2	-	parm0806
24	RFTO	1	6	0	50	day	APEXCONT
25	RFPO	1	0.5	0.05	0.98	-	APEXCONT
26	SATO	0	0.95	0.01	1	-	APEXCONT
27	RCCO	0	0.7	0.001	1	-	APEXCONT

par_calib

Ready

The choices of APEX parameters which can be selected for SA and auto-calibration are saved in par_calib.csv (Fig. 2).

par_f: 0 = not considered for SA or calibration; 1 = select for SA or calibration

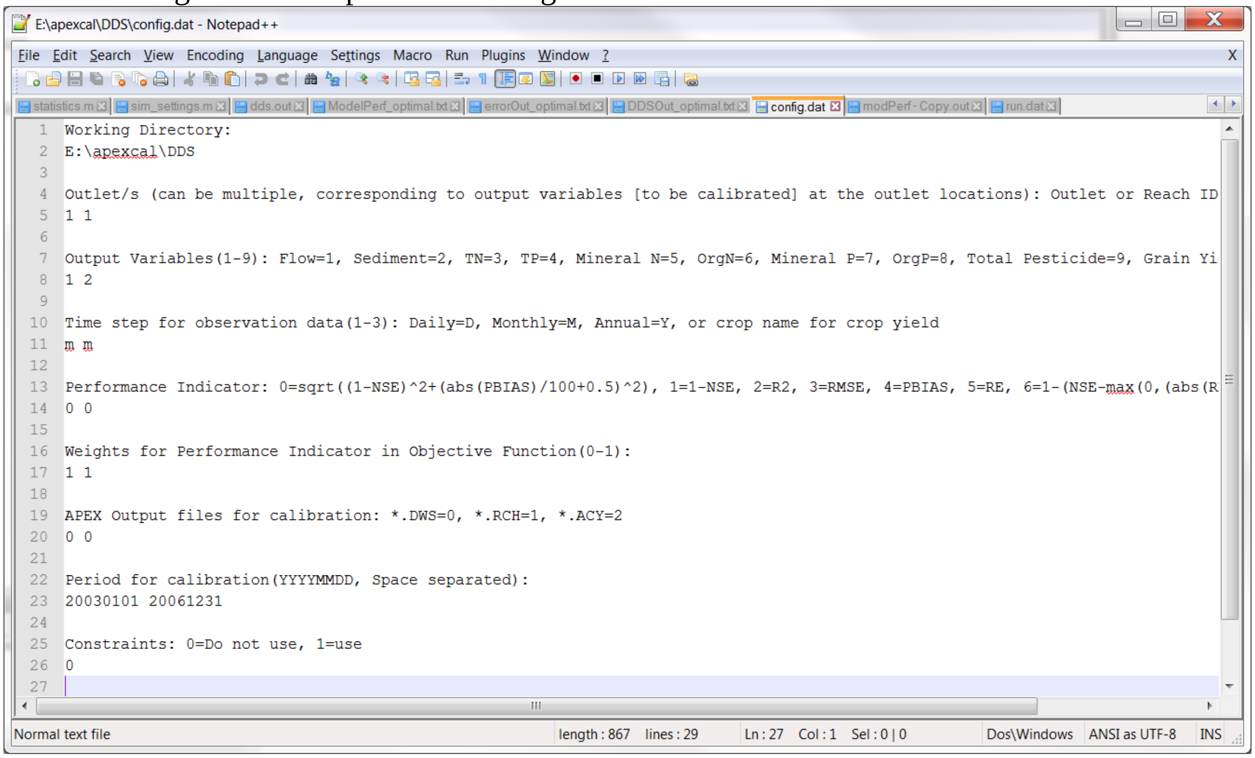
x0: default values of APEX parameters

bl: lower boundary of the parameter value

bu: upper boundary of the parameter value

3) config.dat

Figure 3. Example of the config.dat file.



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Working Directory:
E:\apexcal\DDS

Outlet/s (can be multiple, corresponding to output variables [to be calibrated] at the outlet locations): Outlet or Reach ID
1 1

Output Variables(1-9): Flow=1, Sediment=2, TN=3, TP=4, Mineral N=5, OrgN=6, Mineral P=7, OrgP=8, Total Pesticide=9, Grain Yi
1 2

Time step for observation data(1-3): Daily=D, Monthly=M, Annual=Y, or crop name for crop yield
m m

Performance Indicator: 0=sqrt((1-NSE)^2+(abs(PBIAS)/100+0.5)^2), 1=1-NSE, 2=R2, 3=RMSE, 4=PBIAS, 5=RE, 6=1-(NSE-max(0,(abs(R

0 0

Weights for Performance Indicator in Objective Function(0-1):
1 1

APEX Output files for calibration: *.DWS=0, *.RCH=1, *.ACY=2
0 0

Period for calibration(YYYYMMDD, Space separated):
20030101 20061231

Constraints: 0=Do not use, 1=use
0

```
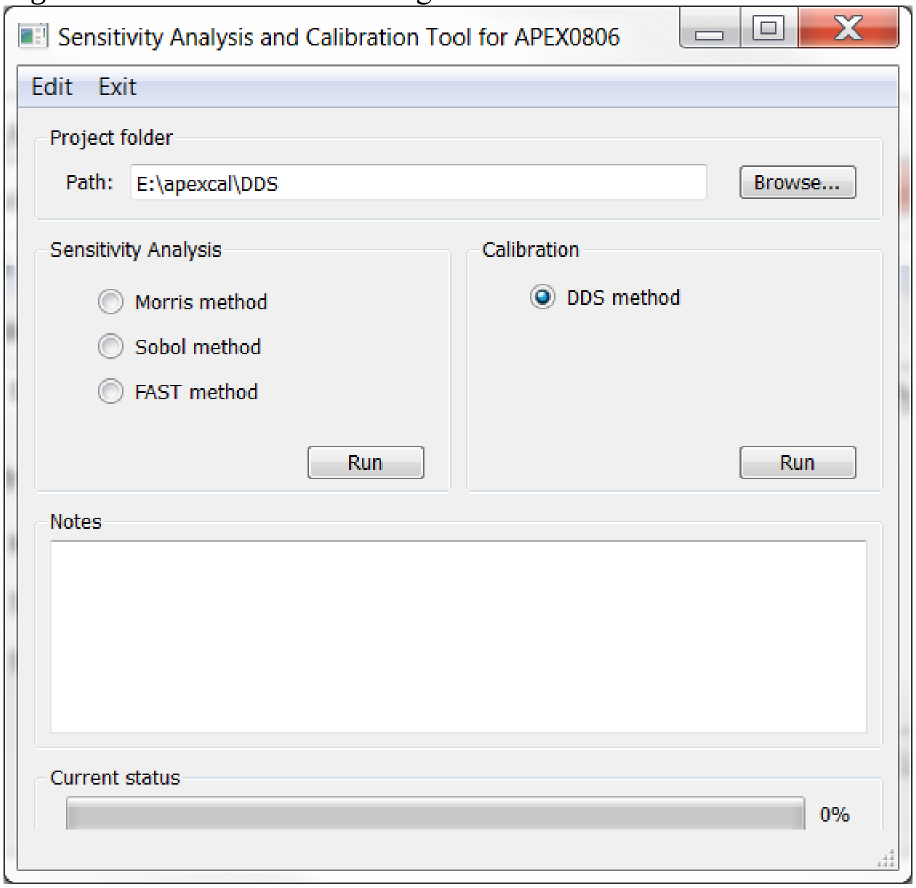

The config.dat file provides the APEX-CUTE working directory where the 3 required setup files: DDS.set, par_calib.csv, and config.dat, are saved (Fig. 3). This should also be the APEX-CUTE *project folder path* while running the tool (Fig. 4). The other variables in the config.dat should be self-explained (Fig. 3).

Figure 4. APEX-CUTE's starting GUI.



In addition to the above 3 files, the core APEX input files should be saved in the TxtInOut folder under the APEX-CUTE project folder path, e.g., C:\APEX-CUTE\Project\TxtInOut\ in the example case (Figs 3 and 4). While running APEX-CUTE, the APEX input files will be copied to E:\apexcal\DDS\TxtWork\ folder for APEX-CUTE to work on SA or auto-calibration. This is to reserve ("backup") the original APEX dataset.

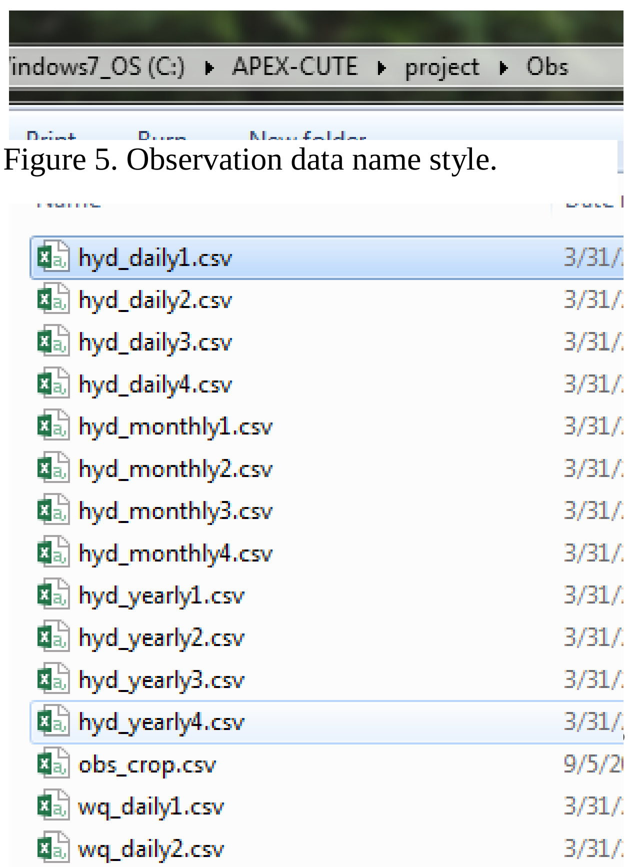


Figure 5. Observation data name style.

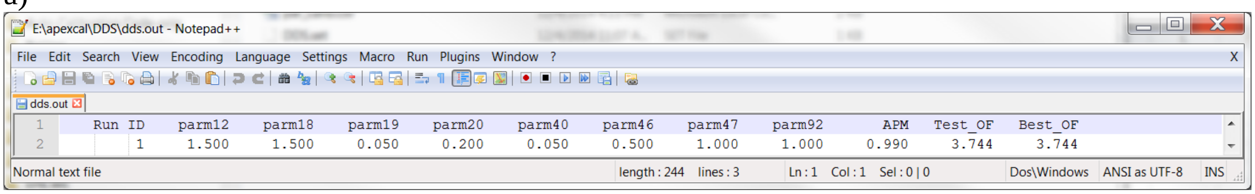
For calibration purpose, observed data will also need to be prepared following the template in the default example files. They should be saved in the Obs foloder under the APEX-CUTE project folder path, e.g., C:\APEX-CUTE\DDS\Obs\ in the example case (Figs 3 and 4). They should be named following the name style as in Fig. 5, where "hyd_" means flow data, "wq_" means water quality data, "*yearly2*" means yearly interval calibration at *reach 2* and so on for the monthly or daily calibrations. Note that the number 2 should be consistent with the ID# provided in line 5 of the config.dat file (Fig. 3). This way APEX-CUTE will be able to find the corresponding observation files to use. If a user calibrates outlets 1 and 2 at the same time, APEX-CUTE will know which observation file is for outlet 1 and which one is for outlet 2. If the APEX project is only for one subarea, user may use 1 as the ID#.

Output

For calibration, three output files will be generated. The contents of these files should be self-explained as in Fig. 6.

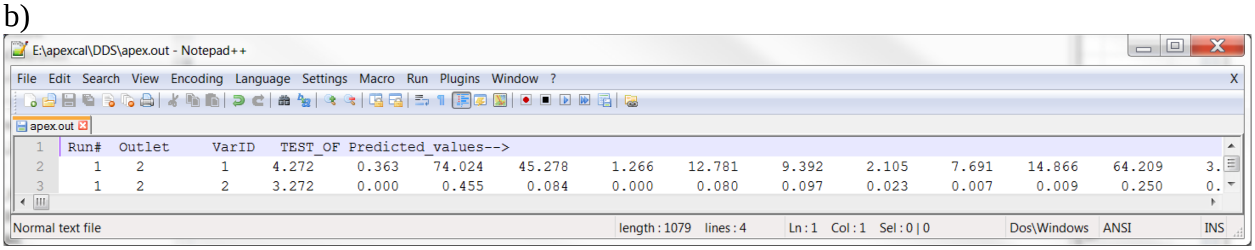
Figure 6. Calibration output files: a) dds.out; b) apex.out; and c) modPerf.out.

a)



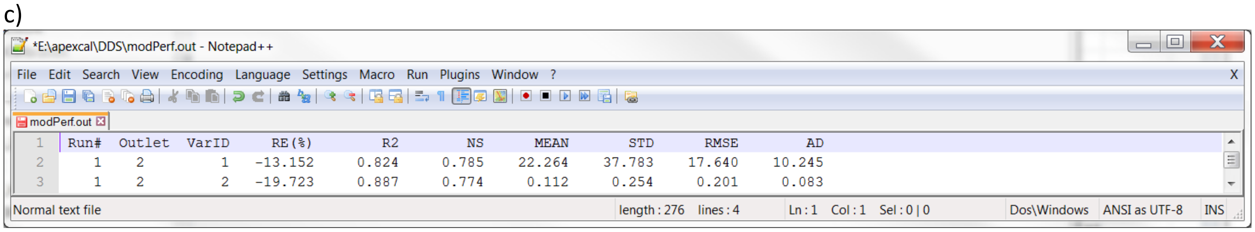
Run ID	parm12	parm18	parm19	parm20	parm40	parm46	parm47	parm92	APM	Test_OF	Best_OF
1	1.500	1.500	0.050	0.200	0.050	0.500	1.000	1.000	0.990	3.744	3.744

b)



Run#	Outlet	VarID	TEST_OF	Predicted_values-->									
1	2	1	4.272	0.363	74.024	45.278	1.266	12.781	9.392	2.105	7.691	14.866	64.209	3.
1	2	2	3.272	0.000	0.455	0.084	0.000	0.080	0.097	0.023	0.007	0.009	0.250	0.

c)



Run#	Outlet	VarID	RE(%)	R2	NS	MEAN	STD	RMSE	AD
1	2	1	-13.152	0.824	0.785	22.264	37.783	17.640	10.245
1	2	2	-19.723	0.887	0.774	0.112	0.254	0.201	0.083

References

Tolson, B. A., & Shoemaker, C. A. (2007). Dynamically dimensioned search algorithm for computationally efficient watershed model calibration. *Water Resources Res.*, *43*(1), W01413. http://dx.doi.org/10.1029/2005WR004723.

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