

RSDX and POSTX: MODFLOW Packages for In-Line Postprocessing

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1. Introduction

The purpose of this report is primarily to document the in-line postprocessors RSDX and POSTX for the version of MODFLOW-96 that was modified for use in the SWAT-MODFLOW linkage. This report also documents the stand-alone program Cols2mat, a preprocessor to convert arrays from database field format to MODFLOW 2-d array input format.

RSDX calculates hydraulic head residuals based on available observations for each time step. POSTX performs some postprocessing functions. Both RSDX and POSTX operate on MODFLOW's solutions while they exist in memory at the end of each time step, rather than on MODFLOW's standard output after the complete simulation has been run. This feature has been used successfully to eliminate significant computing time and intermediate file storage requirements.

An example of how RSDX and POSTX are invoked is provided by a listing of the Name file Hru1Long.nam, below. It is one of three such Name files (HruNLong.nam for N=1 to 3) in the subdirectory \gh\rep992\hruvirt\hrulong\, which is explained in a SWAT-MODFLOW linkage installation guide (Ch. 4 of P&S, KGS OFR 2000-38). RSDX and POSTX were developed for use in previous modeling studies of the Rattlesnake Creek watershed (S&P, KGS OFR 98-59), Wet Walnut Creek watershed (P&S, KGS OFR 98-60), and the Lower Republican River basin (P&S, KGS OFR 99-24 and 99-25). RSDX and POSTX are packages that were added to MODFLOW-96 (v.3.3) along with the SWBX, STRX, and WELX packages for the SWAT-MODFLOW linkage (documented in P&S, KGS O-F Reports 2000-38, 2000-67, and 2000-68) However, RSDX and POSTX are not involved in the SWAT-MODFLOW linkage, and are not documented in the SWAT-MODFLOW linkage User's Manual (P&S, KGS OFR 2000-68), but instead in this document (P&S, KGS OFR 2000-85, file InPost.doc).

The procedure followed in Modflow-96 as it was adapted by incorporating the above packages, is outlined as follows.

3. Stream-aquifer simulation: MODFLOW-96 (v.3.3)

For each aquifer solution time step:

- Distribute HRU-averaged flow rates for each subbasin over grid to specify recharge, tributary flow, surface and ground water diversions, and max. evaporation for shallow gw (SWBX, STRX and WELX packages).
- Formulate and solve finite difference equations (FM_ and solver routines);
- Write summary of evaporation from shallow ground water to be read by SWAT and SWBAVG on a subsequent run (subr. SWB2BD);
- Call optional packages (invoked by Name file): RSDX (calculate residuals for simulated heads) and POSTX (write postprocessing results).

The added packages SWBX, STRX, and WELX, incorporated for linking Swat and Modflow, are documented separately; see P&S (2000a-c).

In-line "postprocessing" packages developed for use in MODFLOW

Graphical user interfaces are available separately for SWAT and MODFLOW and are widely used; they play a vital role in developing and applying watershed and ground water models. The scope of the current project has been limited largely to the coordination of the watershed and stream-aquifer models themselves and the associated computer code, model input requirements, and data that are passed between SWAT and MODFLOW. However, two packages which we developed for use with earlier versions of the combined SWAT-MODFLOW code were updated as part of this project. Although they are peripheral to the scope summarized above, they are useful in expediting analysis of MODFLOW results, and provide postprocessing capability that could be used with standard Modflow cases. These two packages are summarized as follows.

RSDX calculates residuals, or the errors in simulated heads with respect to ground water elevation measurements, which are specified in chronological order by an input file in a format similar to that used for specifying wells for the WELL package. After MODFLOW's solution has converged for each time step, residuals are calculated for all observations made during that time step.

POSTX provides MODFLOW simulation results in convenient spreadsheet-style formats directly and bypasses the sometimes problematic intermediate steps of writing MODFLOW results in standard output format and then operating on that standard format with postprocessors to extract results of interest. An input file is read by POSTX to specify which results are to be provided. Options include time series (hydrographs) for hydraulic heads at specified grid cells, streamflow at specified stream reaches, hydraulic head solutions for specified time steps, and overall volumetric budget results for each time step.

Data files associated with the in-line postprocessing packages RSDX and POSTX

RSDX data files

- *.obs (In): ground water level measurements associated with grid cell coordinates and solution time step for comparison with simulated hydraulic heads.
- *.rsd (Out): annual summary of ground water residual (error in simulated heads) statistics: mean and std deviation residual; mean dtw; mean saturated thickness.
- *.mea (Out): For each time step of MODFLOW's solution, write a summary of each individual water level residual (= simulated head - measured water level) for all water level measurements specified by the input file (*.obs) during the time step.

POSTX data files

- *.pos (In): Specifies postprocessing options; see the User's Manual for instructions.
- *.bud (Out): Post1rp; summary of MODFLOW's ground water budget in spreadsheet format (one record per solution time step); may specify budget terms as flow rates or cumulative volumes, depending on MODFLOW's option. Inflow and outflow are given as separate terms for each hydrologic component as in MODFLOW's standard output (*.LST).
- *.net (Out): Post1rp; similar to *.bud, but inflow and outflow terms are combined into a single net inflow term for each hydrologic component.

- *.hyd (Out): Hyd1rp, Hyd1ot; time series of hydraulic head or flow rate for specified grid cells or stream reaches.
- *.dat (Out): Hyd1ot; solution arrays of hydraulic head or change in hydraulic head for specified time steps.
- *.ntz (Out): net budget terms for specified grid zones. This capability is provided by a subroutine version of the program ZoneBudget (Harbaugh, 1990), but is not available for the updated MODFLOW-96 version as it was for the MODFLOW-88 version to avoid changing the standard packages in MODFLOW-96.

References

Perkins, S.P. and M.A. Sophocleous, 2000d. Programs to Pre- and Postprocess MODFLOW Data. Open-File Report No. 2000–85, Kansas Geol. Survey, Lawrence, KS, 26 p.

2. RSDX: Residuals package (ground water level observations)

For each stress period, available observations of piezometric heads in the aquifer are read from the input file to this package. Then for each time step, MODFLOW's solution is compared with measurements taken during the time step at corresponding grid locations. Results of this comparison are written to two files. (a) Individual residuals are written to [case].mea; (b) Statistics of residuals are written to [case].rsd. Statistics include residual mean and standard deviation, which are summarized for each stress period and over the cumulative time period of the simulation.

Input instructions for the Residuals package

1. For each simulation (RSD1AL):

Data: mxobs,iobsch,ioprds,dtwmax
Format: (2I10,f10.0)

2. For each stress period (RSD1RP), read number of water level observations and year:

Data: numobs, iyrper
Format: (2I10)

3. For each observation from 1 to numobs (RSD1RP):

Data: ilay,irow,icol,iyrdtw,imodtw,zw,dtw,elevls
Format: (FREE) --see note below (*) regarding format used to write data set

Definition of Residual package input data

Line 1 (for each simulation).

mxobs: maximum number of water level observations in a stress period.

iobsch: print(<0) simulated heads, measured water levels, and residuals (sim. – meas.)

ioprds: (option) if ioprds > 0 (or igrp > 1; see def. below); then calculate a residual based on each measurement for which dtw < dtwmax.

dtwmax include only water level observations with dtw < dtwmax.

Line 2 (for each stress period).

numobs number of observations to be read for comparison with simulated heads in this stress period.

iyrper calendar year corresponding to stress period.

Line 3 (for each observation of piezometric heads in aquifer): RSD2RP

Definitions of input data, with reference to location in array Gwobs(25)

lay: (1) layer index

row: (2) row index (= row containing rwr; i.e., rwr rounded up)

col: (3) column index (= column containing cwr; i.e., cwr rounded up)

iyrdtw (8) year of measurement (4 digits, e.g. 1992), prev. well(11)
imodtw (9) month of measurement (1=Jan,...,12=Dec), prev. well(12)
zw (4) measured water level, prev. well(10)
dtw (6) depth to water, prev. well(14)
elevwr (5) land surface elevation, prev. well(9)

Additional data included in set (for reference)

cwr (13) column coordinate, prev. well(8)
rwr (12) row coordinate, prev. well(7)
src (10) data source ID (for your own use; codes here are for Wet Walnut Creek): 'KGS'
(KGS measurements 1960-1996); 'WL' (interpolated water level distributions for
1981 and 1996); 'DWR' (taken from DWR water use reports). 'KGS' and 'WL1981'
data sets (1960-1990) were used for calibration; the 'DWR' and 'WL1996' data sets
(1991-1996) were used for verification.
idwell Well ID associated with data base or spreadsheet from which input file was exported.
daydtw day of month of measurement

Other data given for Republican River Basin data set

(14) iappno = application no. (taken from well identifier), prev. well(15)
(15) calculated head at this node (hnew; see WEL1WR), prev. well(16)
(16) istrch = identifier for closest stream reach: index to order in which the reach was read,
prev. well(21); not defined.
(17) dsstrm = approx. distance to stream reach, prev. well(22); not defined.
(18) elev. difference: meas. water level - calc. stream stage, prev. well(24)
(19) elev. difference: calc. water level - calc. stream stage, prev. well(25)
grid cell elev. variation = surf. elev. at center of node - surf. elev. at well

(*) Note: Data are exported from a data base or spreadsheet in the following format; the first few fields may then be read in free format as indicated above:

Data: ilay,irow,icol,iyrdtw,imodtw,zw,dtw,elevls, cwr,rwr,datsrc,idwell,idaywl,legloc
Format: (5i5,5f8.0,1x,a6,2i5,1x,a)

Example Residuals input data file: gwadmnu.obs for Lower Republican River basin

Excrpts from the file are shown, including observations from two data sources: DWR (1981 water use reports) and KGS (1994 field survey).

Column headings corresponding to input:

lay row col yr mon zw dtw ls_elev cwr rwr src idwel day Loc.(PLSS)

Input:

lay	row	col	yr	mon	zw	dtw	ls_elev	cwr	rwr	src	idwel	day	Loc.(PLSS)					
220	-1	1	40	mxobs	iobs	io	dtwmax	gwadmnu.obs										
0	1977	0.293	36.176	1.000	0	numobs	year											
0	1978	0.520	37.427	1.000	0													
0	1979	0.560	38.535	1.000	0													
3	1980	1.001	38.867	1.000	0													
1	5	18	1288	1310	22	80	1980	12	1	3	4.31	17.19	A0041870005S02W2505NCSWNW					
1	11	31	1222	1242	20	57	1980	6	1	3	10.56	30.69	A0045860006S02E3001NENWSE					
1	11	31	1222	1242	20	59	1980	6	1	3	10.31	30.44	A0054750006S02E3002NESENW					
104	1981	0.356	40.695	1.000	0													
1	7	29	1241	1268	27	62	1900	0	1	4	6.20	28.33	VCY00010006S01E020642003550					
1	7	29	1241	1268	27	62	1900	0	1	4	6.20	28.32	VCY00010006S01E020542003600					
1	13	34	1203	1229	26	55	1977	1	1	4	12.99	33.07	VCY00030007S02E030100504920					
79	1994	0.590	52.489	1.000	0													
1	1	4	1380.9	1393	12	1994	11	3	0.59	3.59	5S	4W	3	dbbd	s2	KACKLEY	"	
1	1	4	1373.5	1381	8	1994	11	3	0.97	3.34	5S	4W	3	cdcd	s2a	KACKLEY	"	
1	2	2	1372.2	1392	20	1994	11	3	1.66	1.91	5S	4W	8	dadb	s6a	KACKLEY	"	
1	3	2	1375.0	1389	14	1994	11	3	2.03	1.97	5S	4W17	aaaa	s6b	JAMESTOWN	"		
1	3	3	1370.7	1380	9	1994	11	3	2.03	2.97	5S	4W16	aaaa	s9a	JAMESTOWN	"		
1	4	4	1367.1	1380	13	1994	11	3	3.03	3.59	5S	4W22	abba	s10	JAMESTOWN	"		
1	1	4	1366.4	1385	19	1994	11	3	0.97	3.59	5S	4W	3	dccd	s1a	CONCORDIA	NW	"
1	4	10	1328.6	1337	8	1994	11	3	3.53	9.97	5S	3W22	daaa	55	CONCORDIA	"		
1	4	7	1356.8	1370	13	1994	11	3	3.09	6.34	5S	3W19	babd	50	CONCORDIA	"		
1	3	5	1356.9	1365	8	1994	11	3	2.66	4.84	5S	4W14	daca	s7	CONCORDIA	"		
1	4	6	1350.4	1362	12	1994	11	3	3.59	5.03	5S	4W24	cbbc	s12a	CONCORDIA	"		
1	3	4	1366.0	1375	9	1994	11	3	2.16	3.59	5S	4W15	abca	s8	JAMESTOWN	"		
1	3	7	1353.0	1375	22	1994	11	3	2.97	6.16	5S	3W18	ccdc	47	CONCORDIA	"		
1	3	7	1356.7	1382	25	1994	11	3	2.47	6.03	5S	3W18	bccc	47a	CONCORDIA	"		
1	3	6	1349.7	1377	27	1994	11	3	2.72	5.97	5S	4W13	dadd	47b	CONCORDIA	"		
1	4	7	1347.1	1359	12	1994	11	3	3.84	6.66	5S	3W19	dcac	49	CONCORDIA	"		
1	4	8	1341.5	1350	9	1994	11	3	3.78	7.66	5S	3W20	dcab	49a	CONCORDIA	"		
1	4	9	1328.0	1370	42	1994	11	3	3.03	8.28	5S	3W21	babb	49b	CONCORDIA	"		
1	4	8	1348.3	1370	22	1994	11	3	3.09	7.03	5S	3W20	bbbc	49c	CONCORDIA	"		
1	4	16	1299.7	1312	12	1994	11	3	3.66	15.47	5S	2W22	cada	21a	RICE	"		
1	6	17	1300.5	1323	23	1994	11	3	5.28	16.03	5S	2W35	bcbb	39a	RICE	"		
1	6	14	1309.3	1335	26	1994	11	3	5.53	13.53	5S	2W32	dbbb	39b	RICE	"		
1	4	15	1306.5	1320	14	1994	11	3	3.72	14.03	5S	2W21	cbcc	17a	RICE	"		
1	5	13	1317.0	1327	10	1994	11	3	4.91	12.22	5S	2W30	ccda	69a	RICE	"		
1	4	12	1319.1	1333	14	1994	11	3	3.91	11.03	5S	3W24	cccb	27a	RICE	"		
1	4	12	1315.6	1330	14	1994	11	3	3.84	11.41	5S	3W24	cdac	27b	RICE	"		
1	5	18	1297.7	1317	19	1994	11	3	4.53	17.03	5S	2W25	cbbb	24a	CLYDE	"		
1	5	20	1283.8	1294	10	1994	11	3	4.16	19.03	5S	1W29	bbcb	A	CLYDE	"		

1	5	22	1278.9	1288	9	1994	11	3	4.41	21.59	5S 1W27	acca	Cc	CLYDE	"
1	6	23	1270.9	1280	9	1994	11	3	5.09	22.22	5S 1W35	bbad	Cd	CLYDE	"
1	7	23	1270.8	1280	9	1994	11	3	6.09	22.59	6S 1W 2	abbd	Ce	CLYDE	"
1	6	22	1273.9	1285	11	1994	11	3	5.91	21.53	5S 1W34	dccb	Da	CLYDE	"
1	6	20	1282.8	1307	24	1994	11	3	5.84	19.53	5S 1W32	dcbc	Db	CLYDE	"
1	5	23	1241.0	1291	50	1994	11	3	4.47	22.84	5S 1W26	adcd	Ca	CLYDE	"
1	4	22	1258.3	1308	50	1994	11	3	3.03	21.72	5S 1W22	abaa	Cb	CLYDE	"
1	9	31	1229.9	1245	15	1994	11	3	8.72	30.16	6S 2E18	cbdc	R9a	CLIFTON	"
1	9	31	1230.4	1245	15	1994	11	3	8.84	30.22	6S 2E18	ccad	R9b	CLIFTON	"
1	9	30	1230.1	1259	29	1994	11	3	8.47	29.22	6S 1E13	bcdd	5	CLIFTON	"
1	9	30	1231.6	1248	16	1994	11	3	8.22	29.53	6S 1E13	abcc	5a	CLIFTON	"
1	9	29	1232.5	1259	27	1994	11	3	8.97	28.53	6S 1E14	dccc	C4	CLIFTON	"
1	10	29	1233.5	1265	32	1994	11	3	9.47	28.16	6S 1E23	bcdc	C4a	CLIFTON	"
1	10	30	1227.5	1253	26	1994	11	3	9.22	29.22	6S 1E24	bbdd	C4b	CLIFTON	"
1	7	29	1245.5	1264	19	1994	11	3	6.22	28.53	6S 1E 2	abcc	C3a	CLIFTON	"
1	8	28	1246.0	1255	9	1994	11	3	7.28	27.47	6S 1E10	bdaa	21a	CLIFTON	"
1	8	27	1253.0	1262	9	1994	11	3	7.03	26.66	6S 1E 9	abab	21b	CLIFTON	"
1	8	28	1248.9	1259	10	1994	11	3	7.34	27.03	6S 1E10	bcbc	21c	CLIFTON	"
1	6	28	1250.3	1274	24	1994	11	3	5.97	27.53	5S 1E34	dccc	21d	CLIFTON	"
1	7	26	1254.2	1267	13	1994	11	3	6.09	25.03	6S 1E 5	bbbc	C1a	CLIFTON	"
1	7	25	1260.4	1269	9	1994	11	3	6.47	24.53	6S 1E 6	accc	C1b	CLIFTON	"
1	7	25	1261.8	1275	13	1994	11	3	6.03	24.09	6S 1E 6	bbba	C1c	CLIFTON	"
1	10	32	1224.9	1236	11	1994	11	3	9.78	31.03	6S 2E20	ccbb	R14a	LINN SW	"
1	10	31	1225.4	1240	15	1994	11	3	9.28	30.66	6S 2E19	acab	R14b	LINN SW	"
1	18	34	1189.8	1200	10	1994	11	3	17.22	33.03	7S 2E34	bbcc	97	CLAY CTR NW	"
1	17	33	1186.3	1198	12	1994	11	3	16.97	32.97	7S 2E28	dddd	97a	CLAY CTR NW	"
1	17	34	1193.8	1218	24	1994	11	3	16.78	33.47	7S 2E27	cdaa	90	CLAY CTR NW	"
1	18	34	1191.6	1215	23	1994	11	3	17.03	33.72	7S 2E34	abaa	90a	CLAY CTR NW	"
1	17	34	1189.3	1215	26	1994	11	3	16.84	33.97	7S 2E27	dadad	90b	CLAY CTR NW	"
1	18	34	1189.1	1209	20	1994	11	3	17.28	33.97	7S 2E34	adaa	90c	CLAY CTR NW	"
1	18	34	1181.3	1201	20	1994	11	3	17.84	33.97	7S 2E34	dadad	90d	CLAY CTR NW	"
1	19	35	1179.9	1209	29	1994	11	3	18.03	34.91	8S 2E 2	aaab	201	CLAY CTR NW	"
1	19	36	1178.7	1203	24	1994	11	3	18.31	35.69	8S 2E 1	aca	200	CLAY CTR NW	"
1	19	36	1180.4	1206	26	1994	11	3	18.28	35.28	8S 2E 1	bdbb	200a	CLAY CTR NW	"
1	19	36	1182.2	1207	25	1994	11	3	18.72	35.28	8S 2E 1	cacc	200b	CLAY CTR NW	"
1	19	36	1180.4	1205	25	1994	11	3	18.03	35.72	8S 2E 1	abaa	200c	CLAY CTR NW	"
1	16	34	1202.5	1220	17	1994	11	3	15.22	33.91	7S 2E22	aadc	79	CLAY CTR NW	"
1	15	33	1204.8	1215	10	1994	11	3	14.22	32.41	7S 2E16	badc	70	CLAY CTR NW	"
1	15	33	1207.3	1225	18	1994	11	3	14.72	32.97	7S 2E16	dadd	70a	CLAY CTR NW	"
1	15	34	1205.9	1223	17	1994	11	3	14.69	33.44	7S 2E15	cad	64	CLAY CTR NW	"
1	15	34	1208.9	1225	16	1994	11	3	14.34	33.03	7S 2E15	bcbc	64a	CLAY CTR NW	"
1	14	35	1212.0	1227	15	1994	11	3	13.94	34.06	7S 2E11	ccc	57a	CLAY CTR NW	"
1	14	35	1212.9	1231	18	1994	11	3	13.47	34.03	7S 2E11	bccc	57n	CLAY CTR NW	"
1	13	33	1214.3	1240	26	1994	11	3	12.72	32.34	7S 2E 4	cacd	51a	CLAY CTR NW	"
1	13	34	1214.1	1235	21	1994	11	3	12.34	33.03	7S 2E 3	bcbc	51b	CLAY CTR NW	"
1	17	36	1183.9	1210	26	1994	11	3	16.97	35.09	7S 2E25	cccd	85	CLAY CTR NW	"
1	21	36	1184.8	1198	13	1994	11	3	20.69	35.81	8S 2E13	dac	216	CLAY CTR SW	"
1	20	36	1170.6	1200	29	1994	11	3	19.59	35.53	8S 2E12	dbbc	213	CLAY CTR SW	"
1	20	36	1177.6	1205	27	1994	11	3	19.28	35.53	8S 2E12	acbb	213a	CLAY CTR NW	"
1	20	36	1178.3	1205	27	1994	11	3	19.03	35.53	8S 2E12	abbb	213b	CLAY CTR NW	"
1	21	36	1177.8	1190	12	1994	11	3	20.56	35.56	8S 2E13	dbb	W	CLAY CTR SW	"

layer row column wlevel zlnd dtw dtb iyr mon nobs u row column file_id--TspRngSc Subsec obs. map
79 observations written to file dtw94nov.obs

3. POSTX package: postprocessing during Modflow execution

MODFLOW presents a difficult task in data interpretation, due to the complexity of both the data and the model. To help simplify this task, we have developed a MODFLOW package with postprocessing functions to provide results of interest in formats convenient for further analysis and display. The postprocessing functions are based on earlier versions which were designed to extract results from MODFLOW's standard output format. These functions have been combined into a package and revised to provide results in the desired formats as an auxiliary function during MODFLOW's execution, and are written from memory at the end of each solution time step. This eliminates the need for the sometimes cumbersome intermediate steps of first writing MODFLOW's results in its standard format and then reading desired results from the standard output, although MODFLOW's options are kept intact for writing results in its standard format.

Results of interest provided by POSTX include arrays of aquifer heads or drawdowns; time series (hydrographs) of aquifer heads or drawdowns at nodes of interest, or of streamflow or streambed leakage at specified reaches; and aquifer hydrologic budgets. Results are written in formats for import into commercial packages for further analysis and visualization of results.

POSTX is invoked according to MODFLOW's standard conventions, and the user specifies its postprocessing tasks with an input data file, which is described here. POSTX includes some capabilities that take advantage of data available in memory during the simulation that are not written to the standard output file, but would otherwise require invoking MODFLOW's binary output option. These capabilities include writing vectors that describe flow and velocity fields, and zone budgets as defined for the ZONEBUDGET program (McDonald, 1989), which we revised for incorporation into POSTX as a subroutine.

Scope

This package is based on earlier versions of postprocessing programs that operated on standard Modflow output. By invoking this package, some common postprocessing tasks can be accomplished during execution of MODFLOW as an alternative to these postprocessors. These tasks and related postprocessors include the following:

1. volumetric budgets for the entire solution domain (shown in the standard output file under the control of Output Control option **ibudfl**): files are written for import into spreadsheet programs, showing separate sets of columns for elapsed simulated time and for input and output terms of each budget component (constant heads, recharge, evaporation, pumping, streambed leakage (baseflow), etc.). These results are written either as rates $Q [L^3/T]$ or as cumulative volumes $\Sigma Q\Delta t [L^3]$. These options are

also accomplished by postprocessor POSTMD3, which reads the overall hydrologic budgets from MODFLOW's standard output.

Volumetric budgets for zones, i.e. subsets of the grid domain; similar results can be produced by program ZONEBUDGET (specifying that MODFLOW write a binary output file (i.e., "save" results) ;

2. hydrographs (time series), similar to results of postprocessor program MODHYD;
3. solution arrays for selected time steps, similar to results of postprocessor programs POSTMOD (for 2-D, i.e. single layer models), POSTMD3 (for multilayer models), and some related versions.

In addition to calculating zone budgets and Darcy flow rates or velocities, POSTX provides the functions of several postprocessors to summarize volumetric budgets, time series, and solution arrays on files in formats that allow import into spreadsheets and contouring programs. These functions are similar to those served by postprocessors that operate on MODFLOW's standard output file with some assistance from the corresponding input, esp. the *.BAS and *.BCF files; see programs POSTMOD, POSTMD3, and MODHYD.

POSTX also calculates volumetric budgets for grid subsets (zones) to produce results comparable to those of program ZONEBUDGET (Harbaugh, 1990), which reads grid cell flow rates from a binary output file written by MODFLOW.

The functions of POSTX are described below.

1. Volumetric budgets for the entire gridded solution domain and for subareas (zones):

POSTX writes mass balance components either as rates Q [L^3/T] to file <case>.rat or as cumulative volumes $\Sigma Q\Delta t$ [L^3] to file <case>.vol. Columns correspond to budgets as read from standard output, showing separate sets of columns for input and output for each budget component (constant heads, recharge, evaporation, pumping, streambed leakage, etc). The same function can be performed by the preprocessor POSTMD3, which reads MODFLOW's standard output file <case>.prm to extract the volumetric budget written by MODFLOW.

MODFLOW's function of calculating the volumetric budget for the total grid domain in each time step is extended to calculating separate volumetric budgets for grid subsets, or zones, including the interactions, i.e. flow rates, between adjacent zones. This function is also served by the postprocessing program ZONEBUDGET, which operates on a binary output file written by MODFLOW for a given case. The example case that accompanies ZONEBUDGET is also run using POSTX to verify that the same results are obtained, and is described below as Example 1. POSTX's version of zone budget calculation also prepares summaries of results for plotting and analysis that are not provided by ZONEBUDGET, including the following:

- a) a matrix of interzonal transfers;
- b) a summary table for all zones and the total grid domain showing input and output flow rates for each hydrologic component;

- c) a separate budget table for each zone (analogous to the standard overall budget table) showing both cumulative volumes and flow rates;
 - d) files that may be imported into a spreadsheet program (e.g. Excel or Quattro) for plotting and analysis, and where the file may be sorted by zone to allow fast plotting of budget results for specified zones. These files include the following:
 - i) file CASE.vlz (cumulative volumes) or CASE.rtz (flow rates) containing input and output terms for each hydrologic component for all zones and for every time step. Analogous summaries of the overall budget are written to CASE.vol (cumulative volumes) or CASE.rat (flow rates).
 - ii) file CASE.ntz containing net flow rates for each hydrologic component for all zones and for every time step. Net flow rates for the overall budget are written to the analogous file CASE.net.
2. Hydrographs, i.e. time series of values at specified aquifer grid or stream reach nodes.
3. Solution arrays for selected time steps

Input instructions for the POSTX package input file (*.pos)

POSTX is invoked in the Basic package input file by IUNIT field 15 (cols. 43-45); subroutines POST1AL, POST1RP, and HYD1RP read the input file described below.

subroutines POST1AL, POST1RP, HYD1RP, POST1OT, POST1OZ. Regarding format requirements:
 FREE refers to the format used for some numerical inputs;
 TEXT identifies records read as alphanumeric text;
 U2DINT refers to MODFLOW's standard input format for 2-D integer arrays.

```

Y      opttim: years (show time in sec, min, hrs, days, or yrs?)
3,    numser (3 time series of values)
R      optvol: write file of [R]ates, cumulative [V]olumes, or [N]either?
0,    iopzon (option to write zone budgets)
21   69   6   streamflow at Nekoma or Rush Ctr (row,col, hydrograph type; see below)
19   89   6   streamflow at Nekoma or Rush Ctr (row,col, hydrograph type; see below)
21  135   6   streamflow at Albert (row,col, hydrograph type; see below)
2,1,1,0      istper,idaxis,islice, iopvec (vector option for cell-by-cell flow)

```

Data for each simulation:

```

POST1AL
(TEXT): opttim      time units for budgets: S M H D Y (sec min hour day year)
(FREE): numser     !no. time series (hydrographs)
(TEXT): optvol     budget option: cumulative [V]olumes, [R]ates, or [N]either
if Zone Budget option is installed (instzn > 0, set in MODFLOW mainline):
(FREE): iopzon     max. budget zone index (zones defined from 0 to iopzon)
(U2DINT): IZONEBD !2-D array of zone indices (0 to numzon)
end if

HYD1RP
do for each time series i=1 to numser: !identify location and type of hydrograph
(FREE):
  if NLAY = 1: irowid, icolid, idser
  if NLAY > 1: layer, irowid, icolid, idtype
end do
(FREE): istper, idaxis, islice, iopfmt
  if (iopfmt = 3) THEN ! proposed option for use with Arc Grid; see limitations
(FREE): XLLCORNER, YLLCORNER, CELL_SIZE, NODATA_VALUE
  if (istper = 1 AND stress period kper = 1) THEN
(FREE) itmstp, iperio, idtype
  if istper = 2) THEN
    DO for every stress period:

```

(FREE) : (ihdstp(j), j=1,nstep)

Input definitions

opttim (TEXT): S M H D Y = time units for budgets (sec, min, hour, day, year)

optvol (TEXT): V = cumulative volumes, R = flow rates, N = none. This controls an option to write separate files describing the overall budget and, optionally, budgets for specified subareas, or zones (see **iopzon**). This optional budget output is in addition to that written to the standard output file, which is controlled by option **ibudfl** from the Output Control file (*.OC); the definition of option **ibudfl** has been extended as described below to control zone budget output.

For options **optvol** = V or R, separate files are written that may be imported into a spreadsheet program (e.g. Excel or Quattro) for plotting and analysis. Files describing the overall hydrologic budget include the following:

- i) file <CASE>.bud: input and output terms for each hydrologic component are given as a flow rate or volume, as in Modflow's volumetric budget summary;
- ii) file <CASE>.net: each hydrologic component is summarized as a net flow rate or volume (input – output).

These files describe the volumetric budget for the entire gridded solution domain in each time step.

- iii) If zones are specified (see **iopzon**), budget summaries analogous to those above for each zone are written to file <CASE>.vlz (cumulative volumes) or <CASE>.rtz (flow rates).

numser: number of time series (hydrographs); $0 \leq \text{numser} \leq 15$.

iopzon: option to calculate zone budgets (see output option **ibudfl** definition below):

=0: no zone budgets are calculated;

>0: maximum number of budget zones $\text{mxzone} = \text{iopzon} + 1$ with allowable indices from 0 to **iopzon**; zone 0 is treated the same as zones 1 through **iopzon**. (Note: this is consistent with tests of postprocessing program ZONEBUDGET (Harbaugh, 1990), in spite of ZONEBUDGET documentation that states the contrary.) Zone budget results are optionally summarized on MODFLOW's standard output file under the control of output option **ibudfl**, specified in the output control (*.OC) input file, with the extended definition shown below.

ibudfl: This budget output option is set in MODFLOW's output control (*.OC) input file. Its definition has been modified as shown below.

= 0: no budget summary output to standard output file.

= 1: write overall budget summary table to standard output;

= 2: in addition to the above, write zone budget summary arrays to standard output showing interzone transfers and hydrologic components of budget;

≥ 3: in addition to the above, write a budget summary table to standard output for each zone.

izonbd: 2-D integer array of budget zone indices, with allowable values from 0 to **iopzon**; read only if **iopzon** > 0. This array is read using MODFLOW's U2DINT utility routine in the same way as array **ibound** from the Basic package input file (*.BAS) and array **ibshed** from the soil water balance input file (*.SWB).

(**layer, irowid, icolid**): indices to grid cell location of hydrograph j for j = 1 to numser.

idtype: index to type of results (0 to 8):

- 0: no results
- 1: head $h(\mathbf{x},t)$, $\mathbf{x} = (x,y,z)$
- 2: change in head $h(\mathbf{x},t) - h(\mathbf{x},0)$, where $h(\mathbf{x},0)$ represents starting heads;
- 3: drawdown $h(\mathbf{x},0) - h(\mathbf{x},t)$, the negative of (2);
- 4: saturated thickness
- 5: baseflow (streambed leakage)
- 6: streamflow
- 7: flow rate through cells, $Q = KAdh/dl$
- 8: Darcy velocity (specific flow rate) through cells, $q=Q/A$

istper: option for specifying when to write solution arrays to a separate file according to a format specified by **iopfmt** (below):

- 0: Write solution for NO time steps according to option **iopfmt**;
- 1: Specify solution option for only one time step (**itmstp**, **iperio**, **idtype**);
- 2: Specify option **ihdstp(j)** for each time step $j=1$ to $nstp$ in each stress period;
- 3: Write results for ALL time steps.

idaxis: option to write a LAYER ($idaxis=1$), ROW ($idaxis=2$), or COLUMN ($idaxis=3$) of the solution array for each specified time step according to option **istper**.

islice: index to the layer (1 to $nlay$), row (1 to $nrow$), or column (1 to $ncol$) of the plane to be written, depending on option **idaxis**.

iopfmt: format option for solution arrays:

iopfmt = 0: matrix form, Modflow input format; see also **iopfmt**=3, below.

iopfmt = 1: single node/record as follows:

- if $nlay = 1$: "x, y, f(x,y)";
- if $nlay > 1$: "x, y, z, f(x,y,z)"

iopfmt = 2: flow vector format (applicable only for **idtype** = 7 or 8) as follows:

The flow rate for each cell is described by a magnitude (for either flow rate Q or darcy velocity q) and direction indicated by unit vector components (u_x, u_y, u_z); both magnitude and direction are written for options **iopfmt** > 0. For **iopfmt** = 2, a position vector's beginning and ending points are written to represent each flow vector in a format that can be imported into a spreadsheet and plotted as a flow field. The vector originates at the center of node (j,i,k) for column j , row i , and layer k at location (x_c, y_r, z_l) , where $x_c = xx(j)$, location of column j center, $y_r = yy(i)$, row i center, and $z_l =$ location of layer k center, represented by $z_l = (nlay - k + 1) - 0.5$. The vector ends at location $(x_c + x_q, y_r + y_q, z_l + z_q)$, where $x_q = u_x * delx(j)/2$, $y_q = u_y * dely(i)/2$, and $z_q = u_z * dz/2$, where $dz = 1$ represents layer k thickness.

iopfmt = 3 (proposed option): Arc Grid format for import using the command `AsciiGrid`. This option is not implemented yet, but is planned as part of the Swat-Modflow upgrade. One way to implement this option is described as follows. If **iopfmt** = 3, then four additional data records will be read to specify the data required for import to Arc Grid. These four lines are denoted by items b-d in the description given below of the required format for an Ascii file to be imported to

Arc Grid; items a and e are not specified in the POSTX input file, since they are passed to POSTX from Modflow for the case being simulated. Note: this option is available only for a regular grid of square cells, since that is the only option for representing a cell grid in Arc Grid.

Required format of Ascii file for import to Arc Grid as a grid coverage using AsciiGrid is listed below, and describes the format POSTX must follow in writing an array for import to Arc Grid. Note: a-e refer to explanations below; for further explanation, see ArcInfo's documentation on the AsciiGrid command. Angle brackets (<) refer to required input (to Arc Grid); the other brackets ({}) refer to optional input.

```
<NCOLS xxx> (a*)
<NROWS xxx> (a*)
<XLLCENTER xxx | XLLCORNER xxx> (b)
<YLLCENTER xxx | YLLCORNER xxx> (b)
<CELLSIZE xxx> (c)
{NODATA_VALUE xxx} (d)
row 1 (e)
row 2 (e)
...
row n (e)
```

Notes on definitions for writing results as Ascii files for import to Arc Grid:

- (a) no. grid rows and columns. (*) Note: these are not to be specified in the POSTX input file, since they are already known for the case being run according to their definition in the Basic package.
- b) (x,y) coordinates for either the center or lower left corner of the lower left grid cell, in terms of the projection coordinates to be used for the grid coverage in ArcInfo.
- c) cell size, i.e., cell side length for a regular grid of square cells, in terms of units to be used for the grid coverage. Note: this should equal the column and row widths as specified in the BCF file, but does not need to be in the same units; e.g., for the Republican River basin case, column and row widths are specified as 5280 ft in the BCF file, but may correspond to a cell size of 1609 m if the ArcInfo grid coverage has units of meters.
- (d) optional; NODATA_VALUE defaults to -9999)
- (e) Cell value in row order (all cells of row 1, then all cells of row 2,..., to row n), with values delimited by a space. Carriage return is not required at the end of each row.

itmstp: time step for solution option idtype for istper = 1;

iperio: stress period for solution option idtype for istper = 1;

ihdstp(j), j = 1 to nstep: vector of solution options (idtype) for each time step; read for each stress period kper = 1 to nper.

Example 1. Application to a case from the Republican River Basin study

This example illustrates many of the capabilities of POSTX, including zone budgets for all nine subbasins, hydrographs (time series) for nodes of interest; and solution arrays for time steps of interest. Note: the Zone Budget capability has not been included with the update to MODFLOW-96 in order to avoid changes to standard packages that are peripheral to the objective of providing an updated SWAT-MODFLOW linkage.

Result files:

Basecase.net: net flow into aquifer for each overall budget component, i.e. the input and output columns shown in file basecase.bud are subtracted as (input - output).

Basecase.ntz net flow into aquifer for each zone and budget component.

Basecase.hyd: hydrographs for streamflow, head, and change in head at various nodes of interest. Up to 20 hydrographs may be written to this file.

Basecase.dat (concatenated files h00s00p.dat): solutions for each time step s and stress period p , written in "x,y,f(x,y)" format (results for one node per record).

Columns of file:

- 1 x-coordinate of cell
- 2 y-coordinate of cell
- 3 head
- 4 head change
- 5 saturated thickness
- 6 row index
- 7 column index
(additional columns for long form)
- 8 cell activity (value of ibound array)
- 9 delx (column width)
- 10 dely (row width)

The response file for the base case, rpbse.rsp, specifies input file names for each package, the unit device number to be associated with the input file, an abbreviation for the package, and a description of the package; In its 1988 version, we modified Modflow to read the file names; the corresponding unit device numbers are specified by input to the Basic package to be read into the Iunit array. In the standard 1996 version of MODFLOW, both the file name and associated unit device number may be specified by a response file in essentially the format of the one shown below.

The case name, rpbse, given by the first record of the response file, is incorporated into the names of files written by MODFLOW. The local directory should contain the response file and a subdirectory, inbase, which contains the input files named in the response file. Two additional input files to be read during execution but not named in the response file are inbase\rpbse.bal, identified at the bottom of the SWB package input file (rpbse.swb); and ..\exe\newbase, identified in the PLT package input file (basecase.plt). The executable file MODFLOW.EXE and associated files (f7713.eer) are

Example 2. Invoking RSDX and POSTX with the Name file (Modflow-96)

The Name file Hru1Long.nam is listed below. This example is for the Lower Republican River basin model used for testing of the updated SWAT-MODFLOW linkage (see Introduction and Installation Guide, P&S, KGS OFR 2000-38)

```
LIST 6  hrulvirt.lst                case name (~.log, ~.prn, ~.rsp)
BAS  1  ..\inbase\bcase_t4.bas      Monthly Basic package
OC   69 ..\inbase\rbase.oc          Output control
BCF  61 ..\inbase\kbase20b.bcf     Block-centered flow
RCH  67 ..\inbase\matrix1.rch      67 Recharge
EVT  65 ..\inbase\repsurf.evt      Evapotranspiration
PCG  68 ..\inbase\model1bs.pcg     preconditioned conjugate gradient
#
# Non-standard Modflow-88 modules substituted for standard Modflow-96 modules,
# modified for coordination with the added SWB module:
#
WEL  62 ..\inbase\wrrepub.wel      Well: groundwater use
STR  70 ..\inbase\rpctest.str      monthly Streamflow, Ks=0.54 ft/day
#
# If invoking WELX and STRX to be used with SWB (below), open:
# 2, iostrm: Str2fm (stream routing details for istrbd = 0 or 2)
DATA 117 hrulvirt.stm
# 3, ioreg: Str2fm, Wel2stp: record of pumping rates that have been
# reduced due to low saturated thickness or streamflow.
DATA 218 hrulvirt.reg
#
# Modules added to Modflow-96:
#
# SWB: 2 input files are specified, *.swb and *.bal:
SWB  66 ..\inbase\rpctest96.swb     Soil water balance
# 1, iobal: Soil Water Balance simulation produced by SWAT and SWBAVG:
DATA 116 ..\hrulvirt.bal
# 5, ioshl: Swb2bd, summary of evaporation from shallow gw for each subbasin.
# This file can be used as input to a subsequent watershed simulation
# (e.g. by SWAT) to implement a two-way coupling by successive approximation.
DATA 220 hrulvirt.shl
# 4, ioswm: Swb2bd, combined surface & gw budget terms
DATA 219 hrulvirt.swm
#
# RSD: Calculate gw residuals during simulation.
RSD  72 ..\inbase\gwuadmnu.obs      gw level measurements
# Output files associated with the RSD package:
# 11, iorsd: Rsd1wl, annual summary of residuals for measured water levels
DATA 226 hrulvirt.rsd
# 12, iomeas: Rsd1wl, observed and simulated heads and difference for each
obs.
DATA 227 hrulvirt.mea
#
# POS: Postprocessor
POS  64 ..\inbase\nozones.pos      Postprocessor
# 6, iobud: Post1rp, Post1ot: Summary of budget terms
DATA 221 hrulvirt.bud
# 7, ionet: Post1rp, Post1ot: Summary of net budget terms
DATA 222 hrulvirt.net
# 8, ionetz: net budget terms requires ZoneBudget option to be installed)
DATA 223 hrulvirt.ntz
# 9, iohyd: Hyd1rp, Hyd1ot: time series of heads and flow rates
DATA 224 hrulvirt.hyd
# 10, iodat: Hyd1ot: solution arrays for specified time steps
DATA 225 hrulvirt.dat
```

Example 3. Use of Rsdx and Postx with Swbx, Strx, and Welx (MODFLOW-96)

MODFLOW is used as modified for the SWAT-MODFLOW linkage (P&S, 2000a). From the subdirectory \gh\test99_2\modflw\, run \gh\modflx96 with the following command:

```
\gh\test99_2\modflw> \gh\modflx96
```

MODFLOW prompts for the Name file, and the name HRU1.NAM is entered for this case. The Name file specifies all of the packages and the associated input and output data files required to run this case. The file Hru1.nam is listed below.

The first six packages (BAS, OC, BCF, RCH, EVT, and PCG) specified by the Name file are standard MODFLOW packages. The next commands, WEL and STR, invoke the modified packages WELX and STRX, respectively. As noted above, the nonstandard WELX and STRX packages are required and automatically invoked instead of the standard WEL5 and STR1 packages because the SWBX package is invoked. The added nonstandard packages SWBX, RSDX, and POSTX are invoked by the commands SWB, RSD, and POS, respectively. The RSDX and POSTX packages are not involved in the SWAT-MODFLOW linkage, but provide useful postprocessing functions (see the Final Report and User's Manual).

See the MODFLOW-96 User's Manual for further explanation of the Name file and of all standard MODFLOW packages, and notes below regarding nonstandard packages.

```
LIST 6  hru1.lst                                case name (~.log, ~.prn, ~.rsp)
BAS  1  ..\inbase\bcase_t4.bas                   Monthly Basic package
OC   69 ..\inbase\rbpbase.oc                     Output control
BCF  61 ..\inbase\kbase20b.bcf                   Block-centered flow
RCH  67 ..\inbase\matrix1.rch                    67 Recharge
EVT  65 ..\inbase\repsurf.evt                   Evapotranspiration
PCG  68 ..\inbase\model1bs.pcg                  preconditioned conjugate gradient
#
# Non-standard Modflow-88 modules substituted for standard Modflow-96 modules,
# modified for coordination with the added SWB module:
#
WEL  62 ..\inbase\wrrepub.wel                   Well: groundwater use
STR  70 ..\inbase\rpctest.str                   monthly Streamflow, Ks=0.54 ft/day
#
# If invoking WELX and STRX to be used with SWB (below), open:
# 2, iostrm (OUT) Str2fm (stream routing details for istrbd = 0 or 2)
DATA 117  hru1.stm
#
# 3, ioreg (OUT) from Str2fm, Wel2stp: record of pumping rates that have been
# reduced due to low saturated thickness or streamflow.
DATA 218  hru1.reg
#
# Modules added to Modflow-96: SWB, RSD, POS
#
# SWB: 2 input files are specified, *.swb and *.bal:
SWB  66 ..\inbase\rpctest96.swb                 Soil water balance
# 1, iobal (IN) Soil Water Balance simulation produced by SWAT and SWBAVG:
DATA 116  hru1.bal
#
# 5, ioshl (OUT) Swb2bd, summary of evaporation from shallow gw for each subbasin.
# This file can be used as input to a subsequent watershed simulation
```

```

# (e.g. by SWAT) to implement a two-way coupling by successive approximation.
DATA 220 hrul.shl
#
# 4, ioswm (OUT) Swb2bd, combined surface & gw budget terms
DATA 219 hrul.swm

# RSD: Calculate gw residuals during simulation.
RSD 72 ..\inbase\gwuadmmu.obs gw level measurements
# Output files associated with the RSD package:
# 11, iorsd (OUT) Rsd1wl, annual summary of residuals for measured water levels
DATA 226 hrul.rsd
#
# 12, iomeas (OUT) Rsd1wl, observed and simulated heads and difference for each obs.
DATA 227 hrul.mea
#
# POS: Postprocessor
POS 64 ..\inbase\nozones.pos Postprocessor
#
# 6, iobud (OUT) Post1rp, Post1ot: Summary of budget terms
DATA 221 hrul.bud
#
# 7, ionet (OUT) Post1rp, Post1ot: Summary of net budget terms
DATA 222 hrul.net
#
# 8, ionetz (OUT) net budget terms requires ZoneBudget option, which is not installed)
DATA 223 hrul.ntz
# 9, iohyd: Hyd1rp, Hyd1ot: time series of heads and flow rates
# DATA 224 hrul.hyd (disabled by "#" in col. 1)
#
# 10, iodat (out) Hyd1ot: solution arrays for specified time steps
DATA 225 hrul.dat

```

Execution of the modified version of MODFLOW-96 was tested by comparison with the previous version based on MODFLOW-88. This version was executed for the same case using redirected keyboard input from the following "response" file, which is shown here for comparison to the Name file (above):

```

hrul
..\inbase\bcase_t4.bas case name (~.log, ~.prn, ~.rsp)
..\inbase\kbase20b.bcf .bas unit 1 Monthly Basic pkg
..\inbase\wrrepub.wel .bcf unit 61 Block-centered flow
..\inbase\repsurf.evt .wel unit 62 Well: gw, surf. use
..\inbase\rptest.swb .evt unit 65 Evaporation from gw
..\inbase\matrix1.rch .swb unit 66 Soil water balance
..\inbase\model1bs.pcg .rch unit 67 Recharge
..\inbase\rbbase.oc .pcg unit 68 precond. conj. grad.
..\inbase\rptest.str .oc unit 69 Output control
..\inbase\basecase.pos .str unit 70 Stream package
..\inbase\gwuadmmu.obs .pos unit 64 Postprocessor
..\inbase\gwuadmmu.obs .obs unit 72 gw level obs.

```

The SWAT-MODFLOW linkage based on SWAT-94.2 and MODFLOW-88 is documented in Perkins and Sophocleous (1999b-c).

Input file for the SWBX package

The following input file is read for the updated HRU schemes 1-3 by the SWBX package, which is documented in the Swat-Modflow linkage User's Manual (P&S, 2000b). It specifies execution options and initializes associations of subbasin outflows with stream reaches, and subbasin domains with grid cells.

```

9, nwshed (balance file: use case name); file c:\gh\test\inbase\rptest.swb
' ', 1 3 1 1 0.00 1 0 0.0 nambal,irropt,ievopt,ioprch,rchmpy,
evapir,welmpy,iadcod,frseep
sub act row col sbnxt tributary

```

