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Analysis Report for Preparation of 2005-2007 Culebra Potentiometric Surface
Contour Maps
Revision 1

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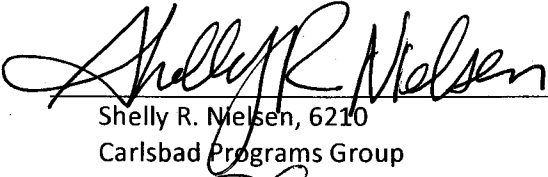

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1 Introduction

This report documents the preparation of three historic potentiometric contour maps and associated particle tracks for the Culebra Member of the Rustler Formation in the vicinity of the Waste Isolation Pilot Plant (WIPP), for submittal to the New Mexico Environment Department (NMED). The driver for this analysis is the draft of the Stipulated Final Order sent to NMED on May 28, 2009 (Moody, 2009). This Analysis Report follows the procedure laid out in procedure SP 9-9 (Kuhlman, 2009), which is based upon this NMED driver. This report is similar to Kuhlman (2011), the same analysis is performed on data from 2005, 2006 and 2007, rather than 2010 data.

Historic data were taken from the Annual Site Environmental Reports (ASERs) to plot freshwater head and density¹ at Culebra wells through time; see (DOE, 2005) through (DOE, 2011) in references. This additional step of plotting time series at each well was done to pick an appropriate month with relatively undisturbed conditions and to assign consistent density data for 2005-2007. This revision includes this additional step because the current procedures related to Culebra densities and contour map creation (SP 9-9 and SP 9-11) were not in place when the historic potentiometric surface contour maps were created.

Beginning with the ensemble of 100 calibrated MODFLOW transmissivity (T), horizontal anisotropy (A), and areal recharge (R) fields (Hart et al., 2009) used in WIPP performance assessment (PA), three average parameter fields are used as input to MODFLOW to simulate freshwater heads within and around the WIPP land withdrawal boundary (LWB). For each year (2005-2007) PEST is used to adjust a subset of the boundary conditions in the averaged MODFLOW model to obtain the best-fit match between the observed freshwater heads and the model-predicted heads. The output of the averaged, PEST-calibrated MODFLOW model is both contoured and used to compute each year's advective particle track forward from the WIPP waste-handling shaft.

This revision (1) fixes an error in the 2007 contour map generation. WQSP-1 was incorrectly included as a well in the group >3 km from the WIPP LWB (zone 2), when it is actually inside the WIPP LWB. WQSP-1 incorrectly had a small weight (0.4), when it should have had a large weight (2.5). After fixing this, the calculations were re-run and the figures for 2007 were all regenerated. The tables of results and predictions of particle path lengths were revised. In general the resulting changes were very small compared to the initial report (revision 0, February 20, 2012). A second minor fix was a correction of the statements regarding boundary conditions that were impacted most by which x- or y-direction related variables. The results were correct, but the text discussion of the results was incorrect.

¹ Density in units of grams/cm³ is numerically equivalent to specific gravity, the ratio of the density of any water to that of fresh water.

2 Scientific Approach

2.1 2005-2007 Freshwater Head and Density Data Review

In previous analysis reports based on the SP 9-9 procedure, recent data from the current ASER were used; plotting of the data was not done independently. Data reported in historic ASERs are being plotted to ensure consistency and explain anomalies. Python scripts and resulting data plots at each well are listed in Section 8.3. Table 1 summarizes freshwater heads, measurement dates, and Culebra groundwater densities for all three years.

Water level and freshwater head values (and measurement dates) were obtained from Table F-8 in the 2004-2010 ASERs. Estimates of Culebra densities from historic Troll data were done for 2005 (Johnson, 2012a) and 2006 (Johnson, 2012b). Culebra midpoint elevations were obtained from Johnson (2008). Historic events (pumping tests, purging events, drilling and plugging & abandonment) were tabulated from ASERs. All of these data were plotted together through time as part of the data review to determine two things. First, were there significant events in a well that warrant assigning a sudden change in fluid density? For example, H-10c was baled to remove fresh water in 2009 (see H-10c plot in Section 8.3). If there was a noticeable change in observed depth-to-water that occurred at the same time as a documented event, a different density is assigned to the periods before and after this event. Secondly, one or more representative densities were chosen for the well, and a start and end time was assigned to each density. If only one density is assigned, then the beginning time is just before the beginning of this analysis (1999), and the end is the current date. There is some variability in the measurements of density in wells. Especially with older data, the variability can become large, due to inaccuracies in recorded Troll installation depths. In January 2007 (beginning with the 2007 ASER) more accurate reference point elevations were used to compute water level and freshwater head elevations. For consistency across years, pre-2007 water level elevations were adjusted to use the newer reference point elevation.

The data review revealed June to be the best month in 2005 to contour (the 2005 ASER used December water levels), because water levels were impacted in many wells due to the large-scale SNL-14 pumping test in the summer of 2005. Some wells took several months to recover from the drawdown caused by this pumping test. June data are more representative of non-testing conditions. WIPP-30 used an August water level, because there was no water level reported in June 2005 at that well.

Table 1. Fresh Water Head (FWH) elevation AMSL and specific gravities used to compute FWH from depth to water observations. Depth to water in each well was measured on the FWH date.

	2005			2006			2007		
	FWH date	FWH	Specific gravity	FWH date	FWH	Specific gravity	FWH date	FWH	Specific gravity
C-2737	6/21/05	920.04	1.019	11/9/06	920.48	1.019	5/9/07	920.71	1.010
ERDA-9	6/20/05	924.18	1.067	11/9/06	924.78	1.067	5/9/07	924.68	1.067
H-02b2	6/20/05	927.24	1.000	11/9/06	928.24	1.000	5/9/07	928.34	1.000
H-03b2	6/21/05	918.53	1.042	11/9/06	918.31	1.042	5/9/07	918.65	1.042
H-04b	6/20/05	916.53	1.015	11/8/06	916.42	1.015	5/9/07	916.35	1.015
H-05b	6/16/05	938.30	1.095	11/6/06	938.96	1.095	5/10/07	939.15	1.095
H-06b	6/13/05	935.43	1.040	11/6/06	936.75	1.040	5/7/07	936.45	1.040
H-07b1	6/13/05	914.63	1.002	11/8/06	914.60	1.002	5/7/07	914.58	1.002
H-09c	6/20/05	913.53	1.001	11/8/06	912.58	1.001	5/8/07	912.78	1.001
H-10c	6/20/05	921.94	1.001	8/14/06	921.93	1.001	5/8/07	922.07	1.001
H-11b4	6/20/05	917.13	1.070	11/9/06	917.07	1.070	5/7/07	917.05	1.070
H-12	6/20/05	916.28	1.097	11/9/06	916.62	1.097	5/8/07	916.54	1.097
H-15	6/20/05	920.82	1.082				5/9/07	920.08	1.053
H-17	6/20/05	916.29	1.133	11/9/06	916.29	1.133	5/7/07	916.29	1.133
H-19b0	6/20/05	918.79	1.068	11/8/06	918.80	1.068	5/9/07	918.83	1.068
I-461	6/13/05	928.57	1.005	11/6/06	929.34	1.005	5/7/07	928.94	1.005
P-17	6/20/05	915.44	1.053						
SNL-01	6/16/05	939.24	1.033	11/6/06	941.47	1.033	5/8/07	941.85	1.033
SNL-02	6/13/05	937.02	1.012	11/6/06	938.35	1.012	5/7/07	937.66	1.012
SNL-03	6/16/05	937.85	1.023	11/6/06	939.47	1.023	5/8/07	939.77	1.023
SNL-05	6/13/05	937.01	1.010	11/6/06	938.61	1.010	5/7/07	938.59	1.010
SNL-08				11/6/06	930.52	1.052	5/7/07	930.01	1.052
SNL-09	6/13/05	931.48	1.024	11/6/06	932.50	1.024	5/7/07	932.03	1.024
SNL-10							5/7/07	931.57	1.011
SNL-12	6/20/05	915.52	1.005	11/6/06	915.22	1.005	5/7/07	915.24	1.005
SNL-13	6/21/05	917.55	1.027	11/6/06	918.00	1.027	5/7/07	918.20	1.027
SNL-14							11/14/07	916.37	1.048
SNL-16				11/8/06	918.43	1.010	9/17/07	918.17	1.010
SNL-17				11/6/06	916.75	1.006	5/7/07	916.78	1.006
SNL-18				11/6/06	939.86	1.028	5/8/07	939.90	1.028
SNL-19				11/6/06	937.92	1.003	5/7/07	937.58	1.003
WIPP-11	6/13/05	938.87	1.038	8/14/06	939.87	1.038	5/9/07	940.65	1.038
WIPP-13	6/13/05	938.33	1.053	11/8/06	939.86	1.053	5/9/07	939.84	1.053
WIPP-19	6/20/05	932.01	1.044	11/8/06	933.51	1.044	5/9/07	933.70	1.044
WIPP-25	6/13/05	935.73	1.011						
WIPP-30	8/17/05	938.35	1.000	11/6/06	939.29	1.000	5/8/07	939.06	1.000
WQSP-1	6/20/05	936.94	1.048	11/8/06	938.58	1.048	5/9/07	938.61	1.048
WQSP-2	6/20/05	939.45	1.048	11/8/06	941.14	1.048	5/9/07	941.20	1.048
WQSP-3	6/20/05	935.46	1.146	11/8/06	936.98	1.146	5/9/07	936.81	1.146
WQSP-4	6/20/05	918.90	1.075	11/8/06	918.97	1.075	5/9/07	918.96	1.075
WQSP-5	6/20/05	918.04	1.025	11/8/06	918.12	1.025	5/9/07	918.18	1.025
WQSP-6	6/20/05	921.54	1.014	11/8/06	921.95	1.014	5/9/07	921.88	1.014

Information Only

The data review revealed November to be a good month in 2006 to contour (which was also used by the 2006 ASER). WIPP-11 used an August 2006 water level because anomalously high water levels were reported October-December, 2006. Similarly, H-10c used an August 2006 water level because of high water levels reported later in the year.

The data review revealed May 2007 to be the best month in 2007 to contour (the 2007 ASER used December). This month also coincides with the month used to pick data for the calibration of the Performance Assessment (PA) Culebra groundwater model. SNL-14 used a November 2007 water level because now water levels were measured January-October 2007 due to pumping and sampling activities in the well. SNL-16 used a September 2007 water level, because there was no May 2007 water recorded and previous to September, the well had anomalously high water levels.

2.2 Modeling Overview

Steady-state groundwater flow simulations are carried out using similar software as was used in the analysis report for AP-114 Task 7 (Hart et al., 2009), which was used to create the input calibrated fields. See Table 2 for a summary of all software used in this analysis. The MODFLOW parameter fields (transmissivity (T), anisotropy (A), and recharge (R)) used in this analysis are ensemble averages of the 100 sets of Culebra parameter fields used for WIPP PA for the 2009 Compliance Recertification Application (CRA-2009) PA baseline calculations (PABC). To clearly distinguish between the two MODFLOW models, the original MODFLOW model, which consists of 100 realizations of calibrated parameter fields (Hart et al., 2009), will be referred to as the "PA MODFLOW model." The model we derive from the PA MODFLOW model, calibrate using PEST, and use to construct the resulting contour map and particle track, is referred to as the "averaged MODFLOW model." The PA MODFLOW model T, A and R input fields are appropriately averaged across 100 realizations, producing a single averaged MODFLOW flow model. This averaged MODFLOW model is used to predict regional Culebra groundwater flow across the WIPP site.

For CRA 2009 PABC, PEST was used to construct 100 calibrated model realizations of the PA MODFLOW model by adjusting the spatial distribution of model parameters (T, A, and R); MODFLOW boundary conditions were fixed. The calibration targets for PEST in the PA MODFLOW model were both May 2007 freshwater heads and transient drawdown to large-scale pumping tests. Hart et al. (2009) describe the calibration effort and results that went into the CRA-2009 PABC. An analogous but much simpler process is used here for the averaged MODFLOW model. We use PEST to modify a subset of the MODFLOW boundary conditions (see red boundaries in Figure 1). The boundary conditions are modified, rather than the T, A, and R parameter fields for simplicity, because re-calibrating the 100 T, A, and R parameter fields would be a significant effort (thousands of hours of computer time). The PEST calibration targets for the averaged MODFLOW model are the 2005-2007 measured annual freshwater heads at Culebra monitoring wells. In the averaged MODFLOW model, boundary conditions are modified while holding model parameters T, A, and R constant. In contrast to this, the PA MODFLOW model used fixed boundary conditions and made adjustments to T, A, and R parameter fields.

Table 2. Software used

Software	Version	Description	Platform	Software QA status
MODFLOW-2000	1.6	Flow model	PA cluster	Acquired; qualified under NP 19-1 (Harbaugh et al., 2000)
PEST	9.11	Inverse model	PA cluster	Developed; qualified under NP 19-1 (Doherty, 2002)
DTRKMF	1.00	Particle tracker	PA cluster	Developed; qualified under NP 19-1
Python	2.3.4	Scripting language (file manipulation)	PA cluster	Commercial off the shelf
Enthought Python	7.2-2	Scripting language (plotting)	Mac desktop	Commercial off the shelf
Bash	3.00.15	Scripting language (file manipulation)	PA cluster	Commercial off the shelf

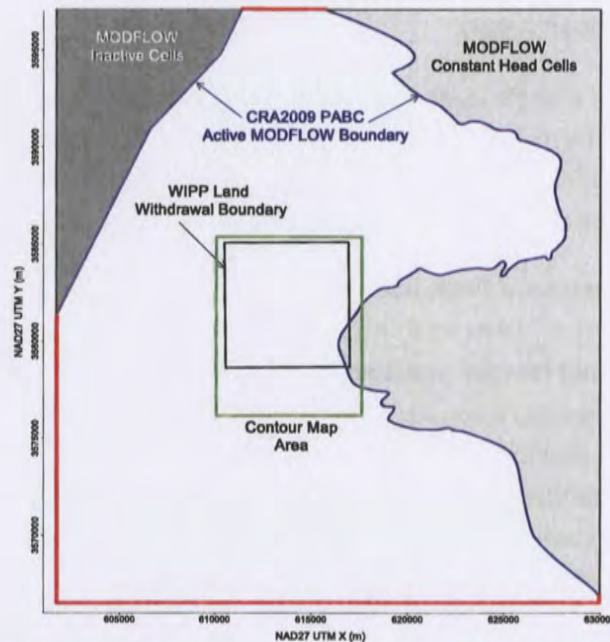


Figure 1. MODFLOW-2000 model domain, adjusted boundary conditions shown in red, contour area outlined in green.

The resulting heads from the PEST-calibrated averaged MODFLOW model are contoured over an area surrounding the WIPP site using matplotlib (a Python plotting library included in the Enthought Python Distribution (EPD)). The figure covers a subset of the complete MODFLOW model domain – see the green rectangle surrounding the WIPP LWB in Figure 1. We compute the path taken by a conservative (i.e., non-dispersive and non-reactive) particle to the WIPP LWB, initially released to the Culebra at the waste-handling shaft. The particle track is computed from the MODFLOW flow field using DTRKMF, these results are also plotted using matplotlib. Scatter plot statistics were computed using NumPy (an array-functionality Python library included in EPD), which summarize the quality of the fit between the averaged MODFLOW model and observed Culebra freshwater heads. MODFLOW, PEST, DTRKMF, and the Bash and Python scripts written for this work were executed on the PA Linux cluster

(alice.sandia.gov), while the plotting and creation of figures was done using Python scripts on an Intel-Xeon-equipped desktop computer running Mac OS X, version 10.6.8.

2.3 Creating Average MODFLOW Simulation

An averaged MODFLOW model is used to compute the freshwater head and cell-by-cell flow vectors. The heads are contoured and the flow vectors are used to compute particle tracks. The ensemble-averaged inputs are used to create a single average simulation that produces a single averaged output, rather than averaging the 100 individual outputs of the Culebra flow model used for WIPP PA. This approach was taken to simplify the contouring process, and create a single contour map that exhibits physically realistic patterns (i.e., its behavior is constrained by the groundwater flow equation). The alternative approach would be to averaging outputs from 100 models to produce a single average result, but the result may be physically unrealistic. The choice to average inputs, rather than outputs, is a simplification (only one model must be calibrated using PEST, rather than 100) that results in smoother freshwater head contours and faster particle tracks, compared to those predicted by the ensemble of fields in AP114 Task 7 (Hart et al., 2009).

The MODFLOW model grid is a single layer, comprised of 307 rows and 284 columns, each model cell being a 100 meter square. The modeling area spans 601,700 to 630,000 meters in the east-west direction, and 3,566,500 to 3,597,100 meters in the north-south direction, both in Universal Transverse Mercator (UTM) North American Datum 1927 (NAD27) coordinates, zone 13.

The calibrated T, A, and R parameter fields from the PA MODFLOW model were checked out of the PA repository using the `checkout_average_run_modflow.sh` script (scripts are listed completely in the Appendix; input and output files are available from the WIPP version control system in the repository `$CVSLIB/Analyses/SP9_9`). Model inputs can be divided into two groups. The first group includes model inputs that are the same across all 100 calibrated realizations; these include the model grid definition, the boundary conditions, and the model solver parameters. The second group includes the T, A, and R fields, which are different for each realization. The constant model inputs in the first group are used directly in the averaged MODFLOW model (checked out from the CVS repository), while the inputs in the second group were averaged across all 100 calibrated model realizations using the Python script `average_realizations.py`. All three averaged parameters were arithmetically averaged in \log_{10} space, since they vary over multiple orders of magnitude.

2.4 Boundary Conditions

The boundary conditions taken from the PA MODFLOW model are used as the initial condition from which PEST calibration proceeds. There are two types of boundary conditions in both MODFLOW models. The first type of condition includes geologic or hydrologic boundaries, which correspond to known physical features in the flow domain. The no-flow boundary along the axis of Nash Draw is a hydrologic boundary (the boundary along the dark gray region in the upper left of Figure 1). The constant-head boundary along the halite margin corresponds to a geologic boundary (the eastern irregular boundary adjoining the light gray region in the right of Figure 1). Physical boundaries are believed to be well known, and are not adjusted in the PEST calibration.

The second type of boundary condition includes the constant-head cells along the rest of the model domain. This type of boundary includes the linear southern, southwestern, and northern boundaries that coincide with the rectangular frame surrounding the model domain (shown as heavy red lines in Figure 1). The value of specified head used along this second boundary type is adjusted in the PEST calibration process.

The Python script `boundary_types.py` is used to distinguish between the two different types of specified head boundary conditions based on the specified head value used in the PA MODFLOW model. All constant-head cells (specified by a value of -1 in the MODFLOW IBOUND array from the PA MODFLOW model) that have a starting head value greater than 1000 meters above mean sea level (AMSL) are left fixed and not adjusted in the PEST optimization, because they correspond to the land surface. The remaining constant-head cells are distinguished by setting their IBOUND array value to -2 (which is still interpreted as a constant-head value by MODFLOW, but allows simpler discrimination between boundary conditions in scripts elsewhere).

Using the output from `boundary_types.py`, the Python script `surface_02_extrapolate.py` computes the heads at active (IBOUND=1) and adjustable constant-head boundary condition cells (IBOUND=-2), given parameter values for the surface to extrapolate.

2.5 PEST Calibration of Averaged MODFLOW Model to Observations

There are three major types of inputs to PEST. The first input type includes the observed freshwater head values, which are used as targets for the PEST calibration. The second input class includes the entire MODFLOW model setup derived from the PA MODFLOW model and described in the previous section, along with any pre- or post-processing scripts or programs needed. These files comprise the forward model that PEST runs repeatedly to estimate sensitivities of model outputs to model inputs. The third input type includes the PEST configuration files, which list parameter and observation groups, observation weights, and indicate which parameters in the MODFLOW model will be adjusted in the inverse simulation. Freshwater head values used as targets for the PEST calibration were taken from published ASERs (2005-2007) and are summarized in Table 1.

To minimize the number of estimable parameters, and to ensure a degree of smoothness in the constant-head boundary condition values, a parametric surface is used to extrapolate the heads to the estimable boundary conditions. The surface is of the same form described in the analysis report for AP-114 Task 7. The parametric surface is given by the following equation:

$$h(x, y) = A + B(y + D \text{sign}(y) \text{abs}(y)^\alpha) + C(Ex^3 + Fx^2 - x) \quad (1)$$

where $\text{abs}(y)$ is absolute value and $\text{sign}(y)$ is the function returning 1 for $y > 0$, -1 for $y < 0$ and 0 for $y = 0$ and x and y are coordinates scaled to the range $-1 \leq \{x, y\} \leq 1$. In Hart et al. (2009), the values $A=928.0$, $B=8.0$, $C=1.2$, $D=1.0$, $\alpha=0.5$, $E=1.0$, and $F=-1.0$ are used with the above equation to assign the boundary conditions.

PEST was then used to estimate the values of parameters A , B , C , D , E , F , and α given the observed heads in Table 1. The Python script `surface_02_extrapolate.py` was used to compute the MODFLOW starting head input file (which is also used to specify the constant-head values) from the parameters A - F and α . Each forward run of the model corresponded to a call to the Bash script `run_02_model`. This script called the `surface_02_extrapolate.py` script, the MODFLOW-2000 executable, and the PEST utility `mod2obs.exe`, which is used to extract and interpolate model-predicted heads from the MODFLOW output files at observation well locations.

The PEST-specific input files (the third type of input) were generated from the observed heads using the Python script `create_pest_02_input.py`. The PEST input files include the instruction file (how to read the model output), the template files (how to write the model input), and the PEST control file (listing the ranges and initial values for the estimable parameters and the weights associated with observations). The wells used in each year's PEST calibration were separated into three groups. Higher weights (2.5) were assigned to wells inside the LWB, and lower weights (0.4) were assigned to wells distant to the WIPP site, while wells in the middle were assigned an intermediate weight (1.0). Additional observations representing the average heads north of the LWB and south of the LWB were used to help prevent over-smoothing of the estimated results across the LWB. The additional observations and weights were assigned to improve the fit in the area of interest (inside the WIPP LWB), possibly at the expense of a somewhat poorer fit closer to the boundary conditions.

2.6 Figures Generated from Averaged MODFLOW Model

The MODFLOW model is run predictively using the averaged MODFLOW model parameters, along with the PEST-calibrated boundary conditions. The resulting cell-by-cell flow budget is then used by DTRKMF to compute a particle track from the waste-handling shaft to the WIPP LWB; particle tracking stops when the particle crosses the WIPP LWB. The Python script `convert_dtrkmf_output_for_surfer.py` converts the MODFLOW cell-indexed results of DTRKMF into a UTM x and y coordinate system, saving the results in the Surfer blanking file format to facilitate plotting with Surfer. The heads in the binary MODFLOW output file are converted to an ASCII matrix file format using the Python script `head_bin2ascii.py`.

The resulting particle track and contours of the model-predicted head are plotted using a matplotlib Python script for an area including the WIPP LWB, corresponding to the region shown in previous versions of the ASER (e.g., see Figure 6.11 in DOE (2008)), specifically the green box in Figure 1. The modeled heads extracted from the MODFLOW output by `mod2obs.exe` are then merged into a common file for plotting using the Python script `merge_observed_modeled_heads.py`.

3 2005 Results

3.1 2005 Freshwater Head Contours

The model-generated freshwater head contours are given in Figure 2 and Figure 3. There is a roughly east-west trending band of steeper gradients, corresponding to lower Culebra transmissivity. The uncountoured region in the eastern part of the figures corresponds to the portion of the Culebra that is located stratigraphically between halite in other members of the Rustler Formation (Tamarisk Member above and Los Medaños Member below). This region east of the "halite margin" has a high freshwater head but extremely low transmissivity, essentially serving as a no-flow boundary in this area.

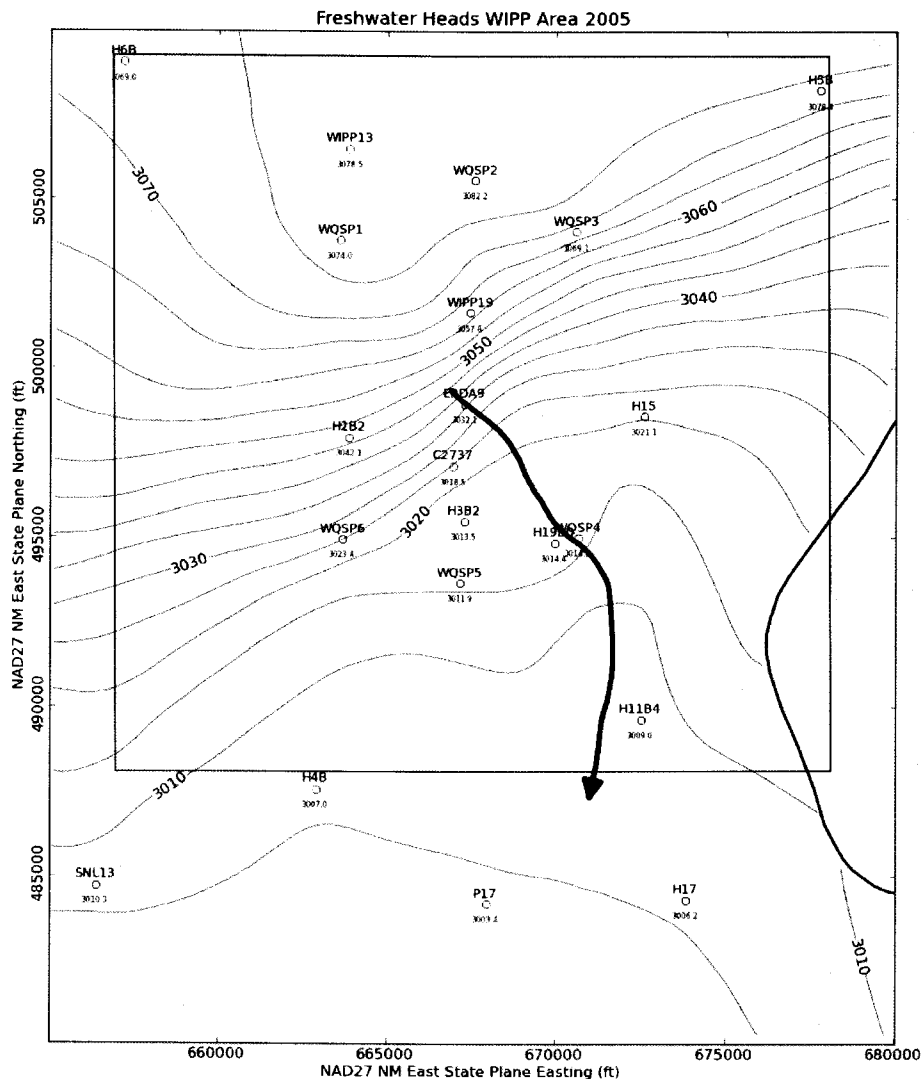


Figure 2. Model-generated June 2005 freshwater head contours with observed head listed at each well (5-foot contour interval) with blue water particle track from waste handling shaft to WIPP LWB

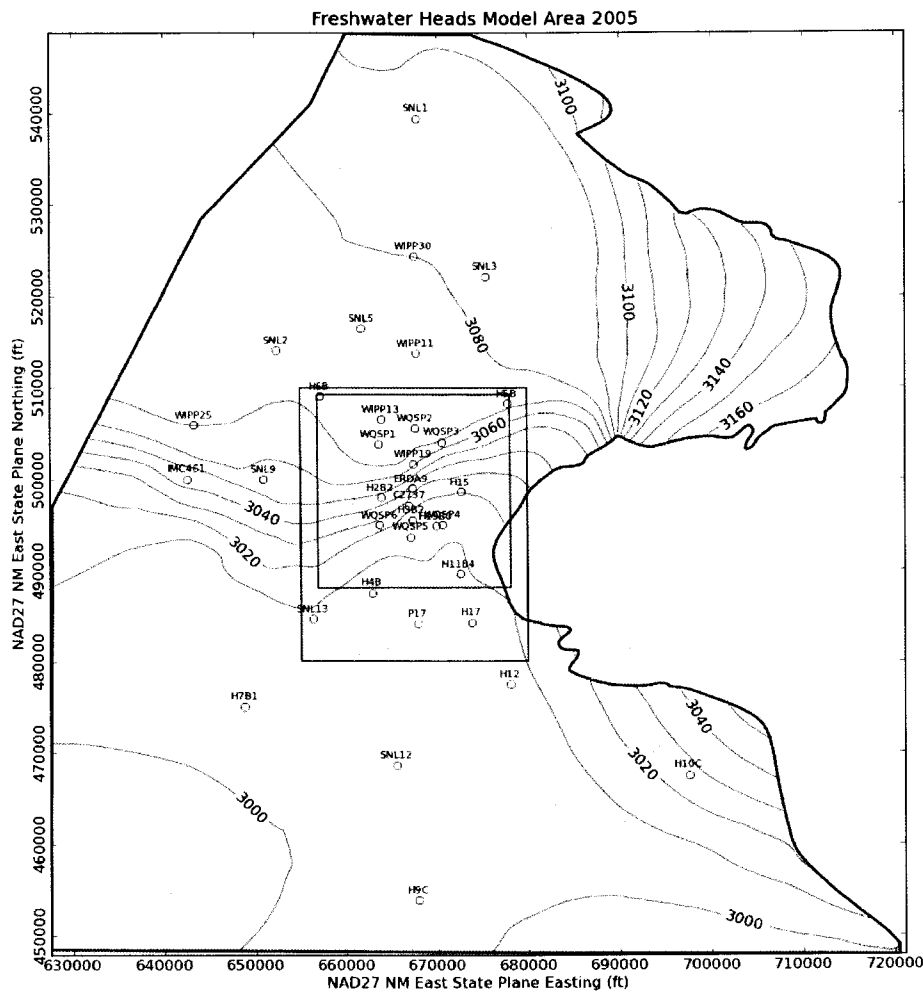


Figure 3. MODFLOW-modeled June 2005 heads for entire model domain (10-foot contour interval). Green rectangle indicates region contoured in Figure 2, black square is WIPP LWB.

3.2 2005 Particle Track

The blue arrow in Figure 2 shows the DTRKMF-calculated path a water particle would take through the Culebra from the coordinates corresponding to the WIPP waste handling shaft to the LWB (a path length of 4083 m). Assuming a 4-m thickness for the transmissive portion of the Culebra and a constant porosity of 16%, the travel time to the WIPP LWB is 6170 years (output from DTRKMF is adjusted from an original 7.75-m Culebra thickness). This is an average velocity of 0.66 m/yr.

3.3 2005 Measured vs. Modeled Fit

The scatter plot in Figure 4 shows measured and modeled freshwater heads at the observation locations used in the PEST calibration. The observations are divided into three groups, based on proximity to the WIPP site. Wells within the LWB are represented by red crosses, wells outside but within 3 km of the LWB are represented with green 'x's, and other wells within the MODFLOW model domain but distant from the WIPP site are given by a blue star. IMC-461 was given a high weight (2.5), treating it as if it was inside the WIPP LWB, to compensate the lack of SNL-16 in the 2005 network. The area at the north end

of the constant head boundary, and the southern end of the no-flow boundary is strongly influenced by the assigned boundary conditions – in 2006 and later SNL-16 is located in this area.

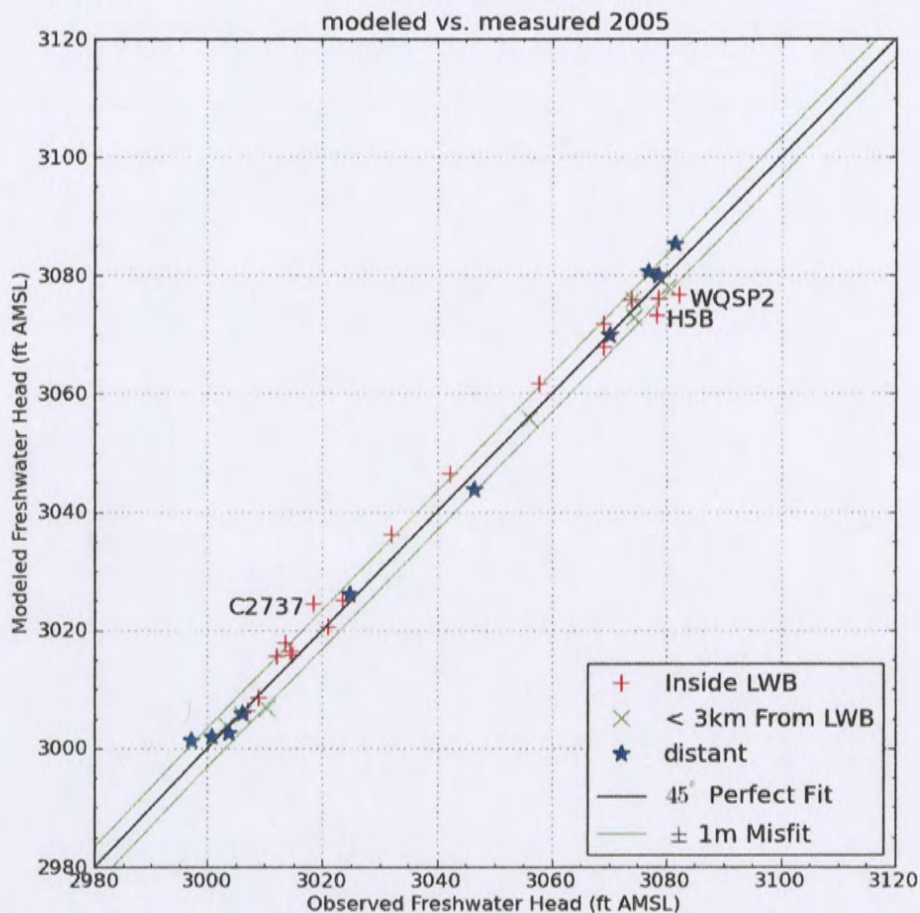


Figure 4. Measured vs. modeled scatter plot for averaged MODFLOW model generated heads and June 2005 observed freshwater heads

The central black diagonal line in Figure 4 represents a perfect model fit (1:1 or 45-degree slope); the two green lines on either side of this represent a 1-m misfit above or below the perfect fit. Wells more than 1.5 m from the 1:1 line are labeled. The calibrated parameters (for equation 1) were $A=928.7$, $B=7.69$, $C=2.26$, $D=0.853$, $E=1.80$, $F=-0.894$, and $\alpha=0.074$. The parameter C, the weight associated with the overall x-direction term, had the largest relative change (88%) compared to the starting values. The parameter E, the weight associated with the cubic variation in the x-direction, also had a large relative change (-85%). The boundary conditions at the west edge of the model domain are impacted most by these parameters.

The squared correlation coefficient (R^2) for the measured vs. modeled data is listed in Table 3. Figure 5 and Figure 6 show the distribution of errors resulting from the PEST-adjusted model fit to observed data. The wells within and near the WIPP LWB have an R^2 of approximately 99%, and the calibration improved the R^2 value very slightly (third decimal place) inside the WIPP LWB. The distribution in Figure 5 does not have a strong bias.

Table 3. 2005 Measured vs. Modeled correlation coefficients

	dataset	measured vs. modeled R ²
Uncalibrated	wells inside WIPP LWB	0.988
	wells <3km from WIPP LWB	0.990
	all wells	0.982
Calibrated	wells inside WIPP LWB	0.989
	wells <3km from WIPP LWB	0.990
	all wells	0.982

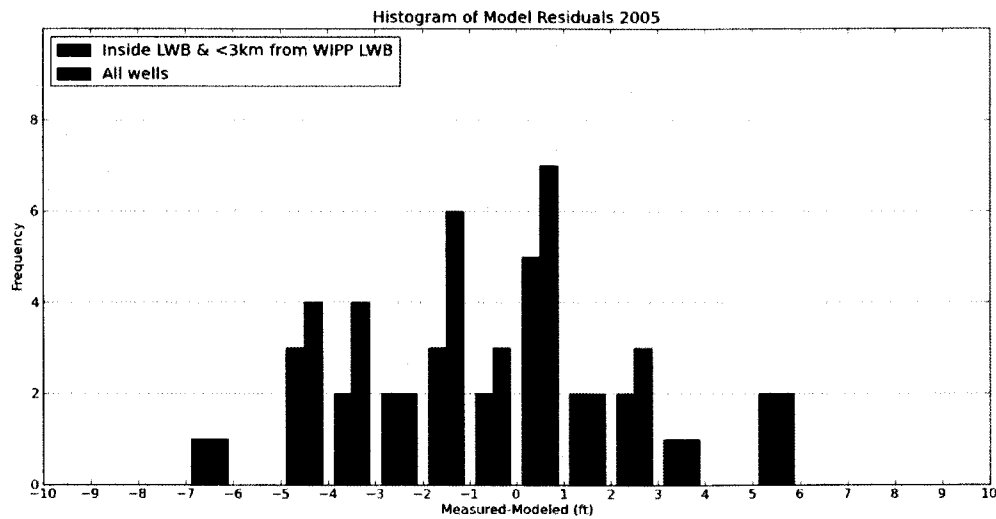


Figure 5. Histogram of Measured-Modeled errors for 2005

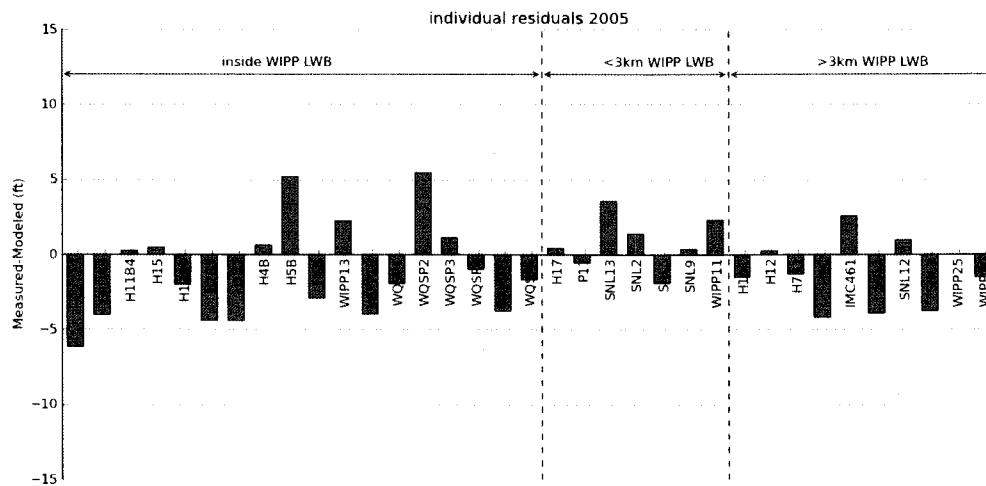


Figure 6. Measured-Modeled errors at each well location for 2005

The model fit to the June 2005 observations is very good. The averaged MODFLOW model captures the bulk Culebra flow behavior, while the PEST calibration improved the model fit to the specific June 2005 observations.

4 2006 Results

4.1 2006 Freshwater Head Contours

The model-generated freshwater head contours are given in Figure 7 and Figure 8. There is a roughly east-west trending band of steeper gradients, corresponding to lower Culebra transmissivity. The uncounted region in the eastern part of the figures corresponds to the portion of the Culebra that is located stratigraphically between halite in other members of the Rustler Formation (Tamarisk Member above and Los Medaños Member below). This region east of the "halite margin" has high freshwater head but extremely low transmissivity, essentially serving as a no-flow boundary in this area.

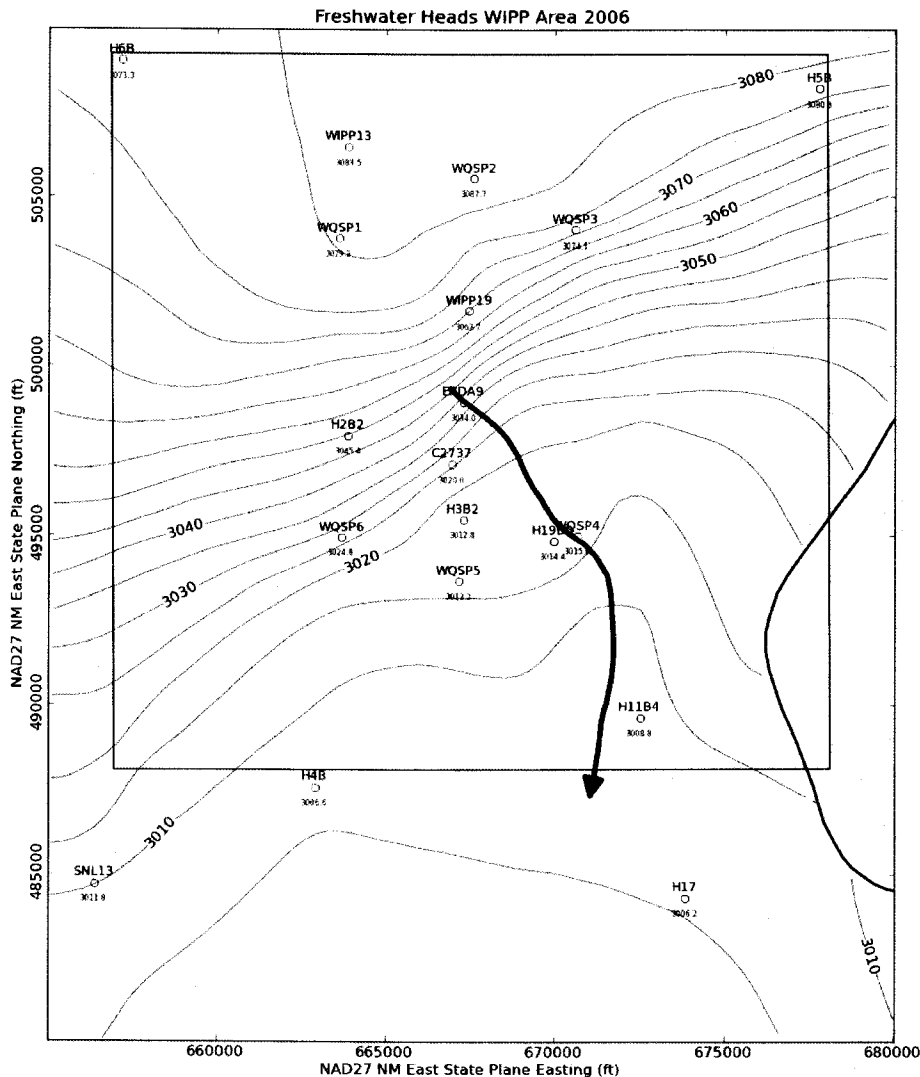


Figure 7. Model-generated November 2006 freshwater head contours with observed head listed at each well (5-foot contour interval) with blue water particle track from waste handling shaft to WIPP LWB

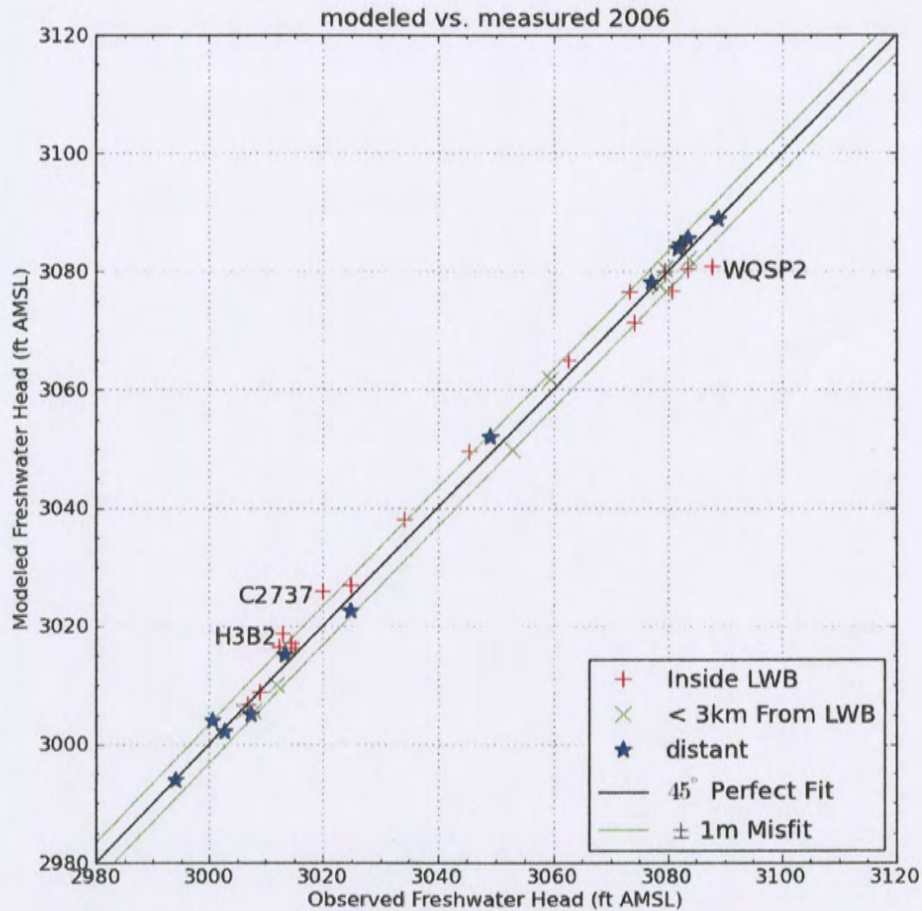


Figure 9. Measured vs. modeled scatter plot for averaged MODFLOW model generated heads and November 2006 observed freshwater heads

The central black diagonal line in Figure 9 represents a perfect model fit (1:1 or 45-degree slope); the two green lines on either side of this represent a 1-m misfit above or below the perfect fit. Wells more than 1.5 m from the 1:1 line are labeled. The calibrated parameters (for equation 1) were $A=927.9$, $B=7.99$, $C=1.16$, $D=1.01$, $E=1.04$, $F=-1.01$, and $\alpha=0.620$. The parameter α , the y-direction exponent, had the largest relative change (24%) compared to the starting values. Overall, the difference between the parameters used in the original model and the calibrated model is slight. The boundary conditions along the northern and southern edges of the model are impacted most by the exponent.

The squared correlation coefficient (R^2) for the measured vs. modeled data is listed in Table 4. Figure 10 and Figure 11 show the distribution of errors resulting from the PEST-adjusted model fit to observed data. The wells within and near the WIPP LWB have an R^2 of greater than 99%, the calibration did not improve the R^2 fit within three significant digits, which can be expected because the original and calibrated model parameters are not dissimilar. The distribution in Figure 10 is roughly symmetric about 0, indicating there is not a strong bias.

Table 4. 2006 Measured vs. Modeled correlation coefficients

	dataset	measured vs. modeled R ²
Uncalibrated	wells inside WIPP LWB	0.991
	wells <3km from WIPP LWB	0.991
	all wells	0.993
Calibrated	wells inside WIPP LWB	0.991
	wells <3km from WIPP LWB	0.991
	all wells	0.993

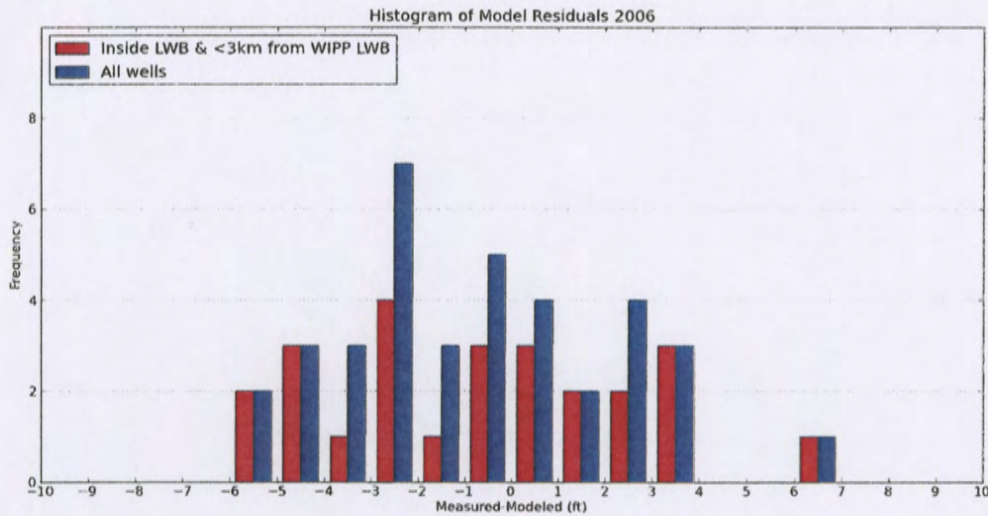


Figure 10. Histogram of Measured-Modeled errors for 2006

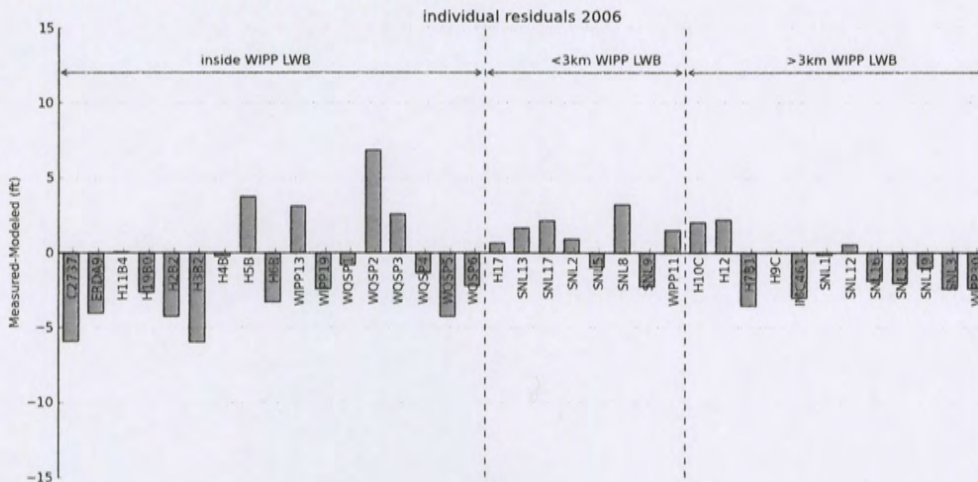


Figure 11. Measured-Modeled errors at each well for 2006

The model fit to the November 2006 observations is very good. The averaged MODFLOW model captures the bulk Culebra flow behavior, while the PEST calibration improved the model fit to the specific November 2006 observations.

5 2007 Results

5.1 2007 Freshwater Head Contours

The model-generated freshwater head contours are given in Figure 12 and Figure 13. There is a roughly east-west trending band of steeper gradients, corresponding to lower Culebra transmissivity. The uncountoured region in the eastern part of the figures corresponds to the portion of the Culebra that is located stratigraphically between halite in other members of the Rustler Formation (Tamarisk Member above and Los Medaños Member below). This region east of the "halite margin" has high freshwater head but extremely low transmissivity, essentially serving as a no-flow boundary in this area.

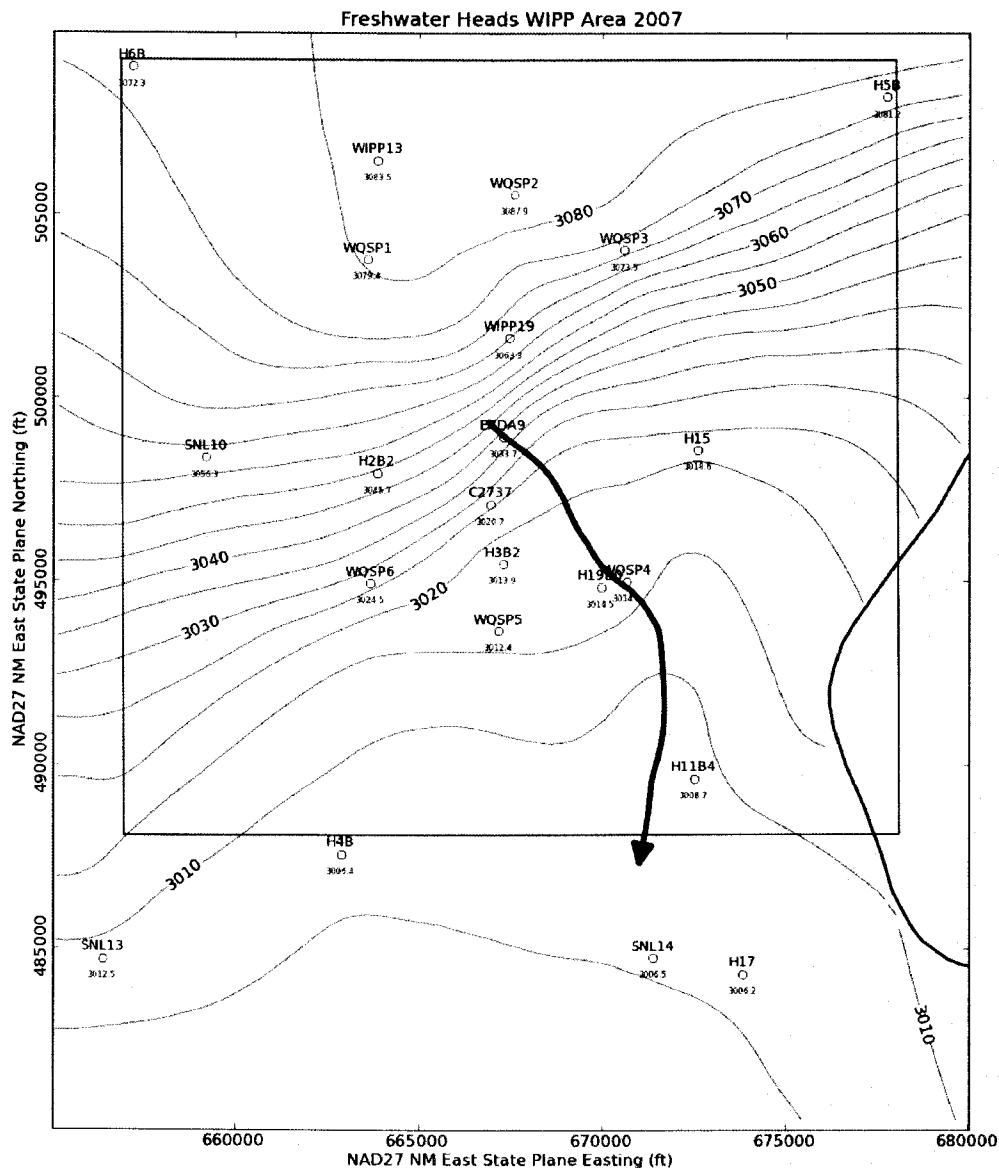
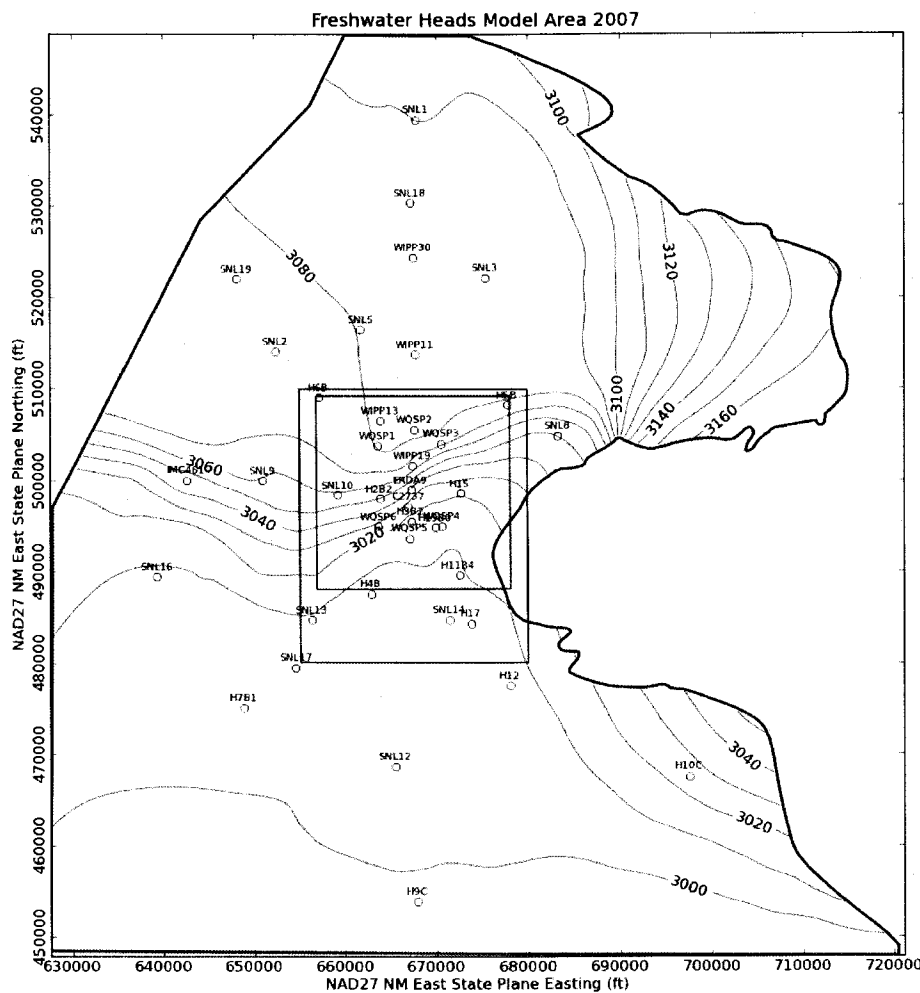


Figure 12. Model-generated May 2007 freshwater head contours with observed head listed at each well (5-foot contour interval) with blue water particle track from waste handling shaft to WIPP LWB

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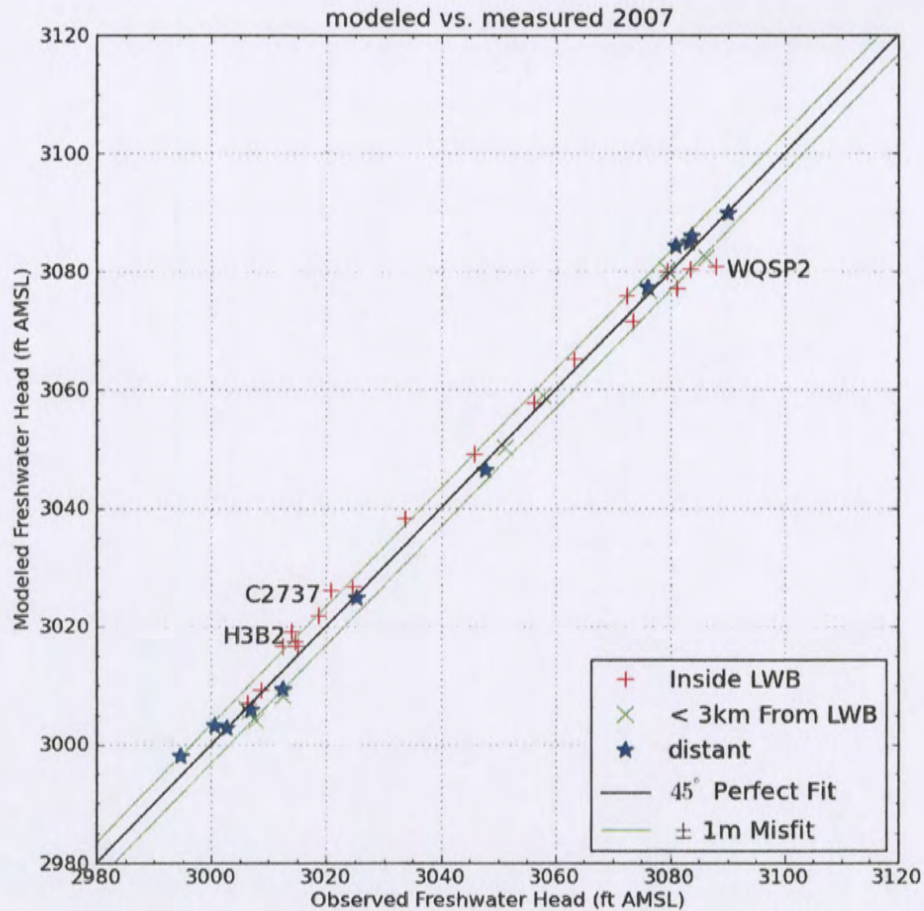


Figure 14. Measured vs. modeled scatter plot for averaged MODFLOW model generated heads and May 2007 observed freshwater heads

The black central diagonal line in Figure 14 represents a perfect model fit (1:1 or 45-degree slope); the two green lines on either side of this represent a 1-m misfit above or below the perfect fit. Wells more than 1.5 m from the 1:1 line are labeled. The calibrated parameters (for equation 1) were $A=928.9$, $B=8.17$, $C=1.40$, $D=0.920$, $E=0.903$, $F=-0.75$, and $\alpha=-0.052$. The parameter α , the y -direction exponent, had the largest relative change (-110%) compared to the starting values. The parameter F , the weight associated with the second-order x -direction term, had the second largest relative change (-25%) compared to the starting values. The boundary conditions along the northern and southern edges of the model are impacted most by the exponent, while the boundary conditions along the western boundary is affected most by changes to the F coefficient.

The squared correlation coefficient (R^2) for the measured vs. modeled data is listed in Table 5. Figure 15 and Figure 16 show the distribution of errors resulting from the PEST-adjusted fit to observed data. The wells within and near the WIPP LWB have an R^2 of greater than 99%, with calibration providing a slight improvement inside the WIPP LWB, at the expense of the fit outside the WIPP LWB (in the third decimal place). The distribution in Figure 15 is roughly symmetric about 0, indicating there is not a strong bias.

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Table 5. 2007 Measured vs. Modeled correlation coefficients

	dataset	measured vs. modeled R ²
Uncalibrated	wells inside WIPP LWB	0.991
	wells <3km from WIPP LWB	0.990
	all wells	0.993
Calibrated	wells inside WIPP LWB	0.992
	wells <3km from WIPP LWB	0.990
	all wells	0.993

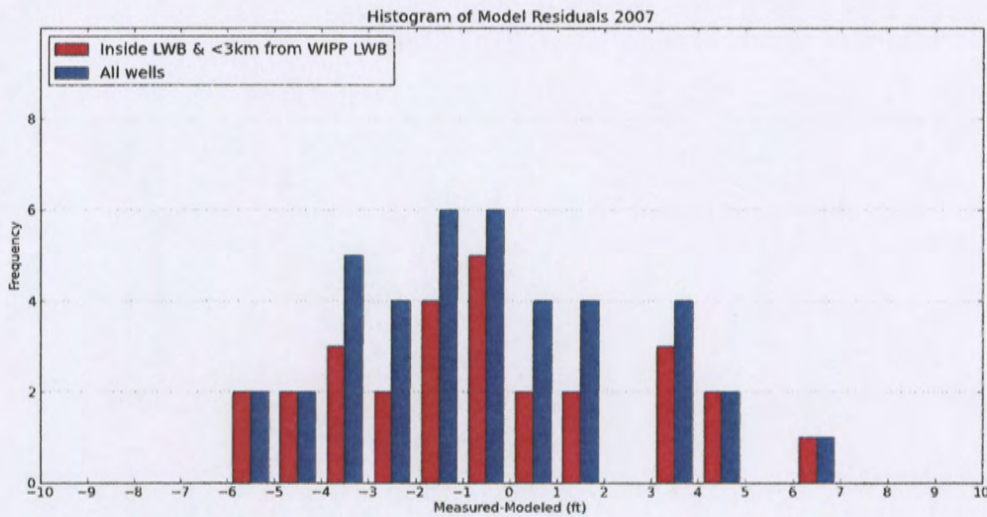


Figure 15. Histogram of Measured-Modeled errors for 2007

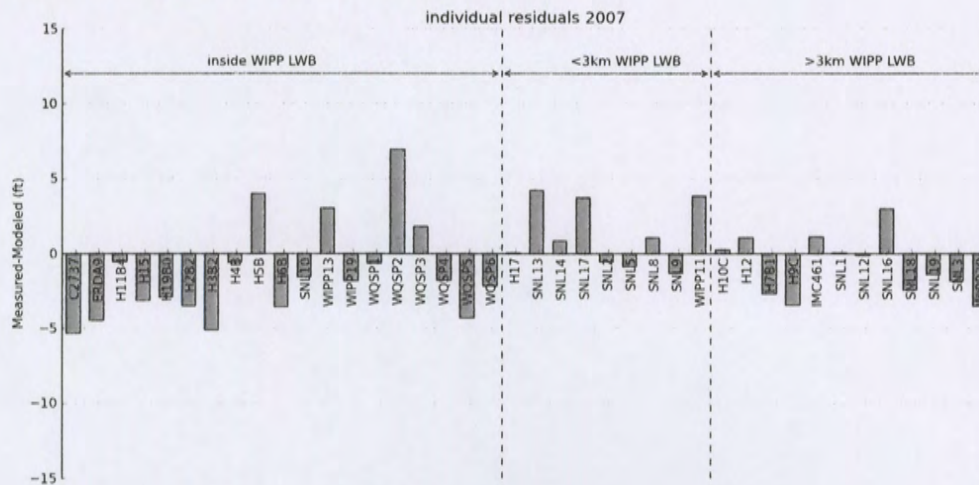


Figure 16. Measured-Modeled errors at each well for 2007

The model fit to the May 2007 observations is excellent, because these heads were the ones used to calibrate the PA MODFLOW model. The averaged MODFLOW model captures the bulk Culebra flow behavior, while the PEST calibration improved model fit to the May 2007 observations.

6 Summary

The development of the 2005-2007 historic Culebra contour maps in general followed quite closely to the procedure used in previous revisions of this report. The main deviations included additional work to gather, plot, and select appropriate freshwater head data for these years. The results of this additional work is presented in Section 8, and gives a unique view of the results presented in previous ASER reports, which is continuous across calendar years.

The average MODFLOW model calibration process resulted in similar (2006) or improved (2005 & 2007) model fits to the data selected for each year. The process of averaging the 100 realizations, and working with a single set of results from the average MODFLOW model creates a simpler result, which is still based upon the PA MODFLOW model.

This work began as part of an effort to create consistent Culebra contour maps for historic data already reported in the ASER. The results of this work (2005-2007) and upcoming work (pre-2005) will be consistency in maps across years and between regulators. The US Environmental Protection Agency and The NM Environment Department now receive compatible hydrology products (PA MODFLOW model and these contour maps) from the WIPP hydrology community.

7 References

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8 Run Control Narrative

This section is a narrative describing the calculation process mentioned in the text, which produced the figures given there.

Figure 17 gives an overview of the driver script `checkout_average_run_modflow.sh` (§A-4.1); this script first exports the 3 parameter fields (transmissivity (T), anisotropy (A), and recharge (R), and storativity (S)) from CVS for each of the 100 realizations of MODFLOW, listed in the file `keepers` (see lines 17-26 of script). Some of the realizations are inside the `Update` or `Update2` subdirectories in CVS, which complicates the directory structure. An equivalent list `keepers_short` is made from `keepers`, and the directories are moved to match the flat directory structure (lines 31-53). At this point, the directory structure has been modified but the MODFLOW input files checked out from CVS are unchanged.

Python script `average_realizations.py` (§A-4.2) is called, which first reads in the `keepers_short` list, then reads in each of the 400 input files and computes the arithmetic average of the base-10 logarithm of the value at each cell across the 100 realizations. The 400 input files are saved as a flattened 2D matrix, in row-major order. The exponentiated result is saved in 4 parameter fields, each with the extension `.avg` instead of `.mod`. A single value from each file, corresponding to either the cell in the southeast corner of the domain (input file row 87188 = model row 307, model column 284 for K and A) or on the west edge of the domain (input file row 45157 = model row 161, model column 1 for R and S) is saved in the text file `parameter_representative_values.txt` to allow checking the calculation in Excel, comparing the results to the value given at the same row of the `.avg` file. The value in the right column of Table 6 can be found by taking the geometric average of the values in the text file, which are the values from the indicated line of each of the 100 realizations.

The input files used by this analysis, the output files from this analysis (including the plotting scripts) are checked into the WIPP version control system (CVS) under the repository `$CVSLIB/Analyses/SP9_9`.

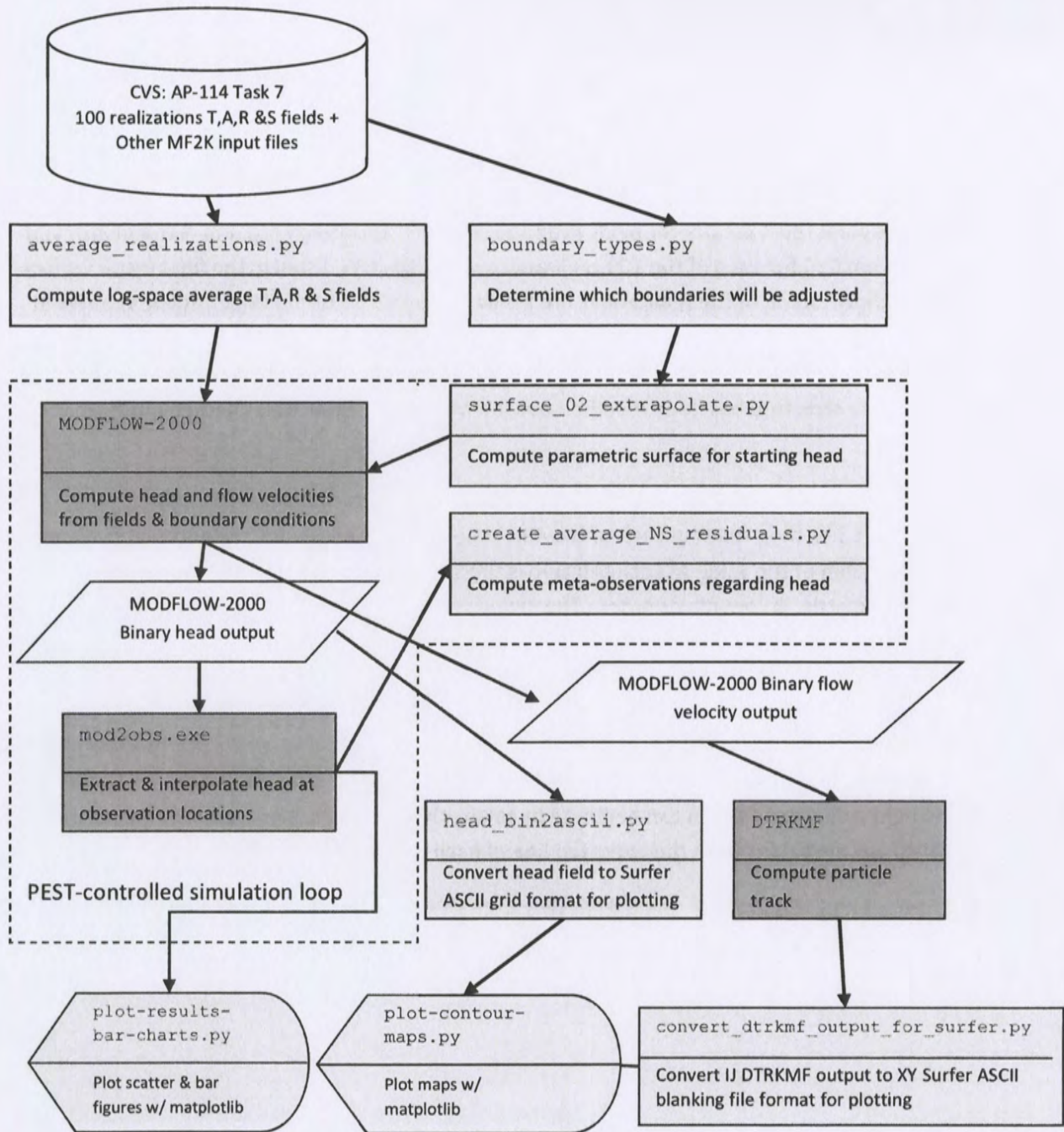


Figure 17. Process flowchart; dark gray indicates qualified programs, light gray are scripts written for this analysis

Table 6. Averaged values for representative model cells

Field	Input file row	Model row	Model column	Geometric average
K	87188	307	284	9.2583577E-09
A	87188	307	284	9.6317478E-01
R	45157	161	1	1.4970689E-19
S	45157	161	1	4.0388352E-03

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Figure 18 shows plots of the average \log_{10} parameters, which compare with similar figures in Hart et al. (2009); inactive regions $<1.0E-15$ were reset to 1.0 to improve the plotted color scale. The rest of the calculations are done with these averaged fields.

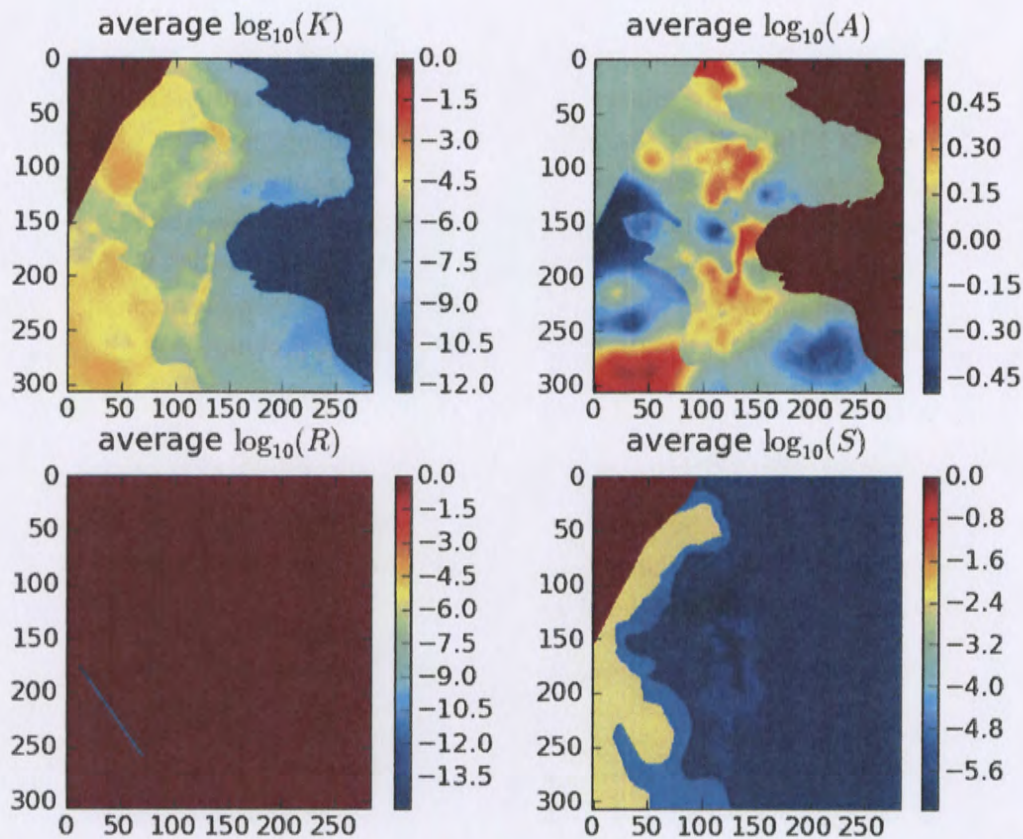


Figure 18. Plots of base-10 logarithms of average parameter fields; rows and columns are labeled on edges of figures.

Next, a subdirectory is created, and the averaged MODFLOW model is run without any modifications by PEST. Subsequently, another directory will be created where PEST will be run to improve the fit of the model to observed heads at well locations.

The next portion of the driving script `checkout_average_run_modflow.sh` links copies of the input files needed to run MODFLOW-2000 and DTRKMF into the `original_average` run directory. Then MODFLOW-2000 is run with the name file `mf2k_head.nam`, producing binary head (`modeled_head.bin`) and binary cell-by-cell flow budget (`modeled_flow.bud`) files, as well as a text listing file (`modeled_head.lst`). DTRKMF is then run with the input files `dtrkmf.in` and `wippctrl.inp`, which utilizes the cell-by-cell budget file written by MODFLOW to generate a particle track output file, `dtrk.out`. The input file `wippctrl.inp` specifies the starting location of the particle in DTRKMF face-centered cell coordinates, the porosity of the aquifer (here 16%), and the

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coordinates of the corners of the WIPP LWB, since the calculation stops when the particle reaches the LWB.

The Python script `head_bin2ascii.py` (§A-4.7) converts the MODFLOW binary head file, which includes the steady-state head at every element in the flow model domain (307 rows × 284 columns) into a Surfer ASCII grid file format. This file is simply contoured in Python using `matplotlib`, no interpolation or gridding is needed. The Python script `convert_dtrkmf_output_for_surfer.py` (§A-4.9) reads the DTRKMF output file `dtrk.out` and does two things. First it converts the row, column format of this output file to an X,Y format suitable for plotting, and second it converts the effective thickness of the Culebra from 7.75m to 4m. The following table shows the first 10 lines of the `dtrk.out` and the corresponding output of the Python script `dtrk_output_original_average.blm`. The first three columns of `dtrk.out` (top half of Table 7) after the header are cumulative time (red), column (blue), and row (green). The three columns in the blanking file (second half of Table 7) after the header are UTM NAD27 X (blue), UTM NAD27 Y (green), and adjusted cumulative time (red, which is faster than the original cumulative travel time by the factor $7.75/4=1.9375$). The conversion from row, column to X, Y is

$$X = 601700.0 + 100.0 * column$$

$$Y = 3597100.0 - 100.0 * row$$

since the I,J origin is the northwest corner of the model domain (601700,3597100), while the X,Y origin is the southwest corner of the domain. The blanking file is plotted directly in Python using `matplotlib`, since it now has the same coordinates as the ASCII head file.

Table 7. Comparison of first 10 lines of DTRKMF output and converted Surfer blanking file for `original_average`

1	159									
0.00000000E+00	118.79	150.21	1.18790000E+04	1.50210000E+04	0.00000000E+00	1.85168267E-01	1.59999996E-01	1.00000000E+00		
5.53946616E+01	118.86	150.29	1.18859872E+04	1.50285080E+04	1.02562574E+01	1.85130032E-01	1.59999996E-01	1.00000000E+00		
1.10789323E+02	118.93	150.36	1.18929942E+04	1.50359947E+04	2.05104788E+01	1.85094756E-01	1.59999996E-01	1.00000000E+00		
1.66017959E+02	119.00	150.43	1.19000000E+04	1.50434379E+04	3.07321029E+01	1.85062532E-01	1.59999996E-01	1.00000000E+00		
3.27990509E+02	119.21	150.62	1.19206651E+04	1.50624751E+04	5.88294962E+01	1.73534671E-01	1.59999996E-01	1.00000000E+00		
4.89963060E+02	119.42	150.81	1.19415109E+04	1.50813473E+04	8.69490492E+01	1.73684593E-01	1.59999996E-01	1.00000000E+00		
6.51450155E+02	119.62	151.00	1.19624759E+04	1.51000000E+04	1.15010608E+02	1.73860152E-01	1.59999996E-01	1.00000000E+00		
7.40581455E+02	119.75	151.10	1.19749757E+04	1.51102419E+04	1.31170520E+02	1.81333000E-01	1.59999996E-01	1.00000000E+00		
8.29712755E+02	119.87	151.20	1.19874963E+04	1.51204665E+04	1.47335525E+02	1.81390626E-01	1.59999996E-01	1.00000000E+00		
159,1										
613579.0,3582079.0,			0.00000000E+00							
613586.0,3582071.0,			2.85907931E+01							
613593.0,3582064.0,			5.71815861E+01							
613600.0,3582057.0,			8.56866885E+01							
613621.0,3582038.0,			1.69285424E+02							
613642.0,3582019.0,			2.52884160E+02							
613662.0,3582000.0,			3.36232338E+02							
613675.0,3581990.0,			3.82235590E+02							
613687.0,3581980.0,			4.28238841E+02							

The PEST utility script `mod2obs.exe` is run to extract and interpolate the model-predicted heads at observation locations. The input files for `mod2obs.exe` were taken from AP-114 Task 7 in CVS. The observed head file has the wells and freshwater heads, but is otherwise the same as that used in the model calibration in AP-114. The Python script `merge_observed_modeled_heads.py` (§A-4.9) simply puts the results from `mod2obs.exe` and the original observed heads in a single file together for easier plotting and later analysis.

cells as constant head which have an IBOUND entry < 0, so both -2 and -1 are the same to MODFLOW, but allow distinguishing between them in the Python script which extrapolates the heads to the boundaries.

The required PEST input files are created by the Python script `create_pest_02_input.py` (§A-4.4). This script writes **1)** the PEST instruction file (`modeled_head.ins`), which shows PEST how to extract the model-predicted heads from the `mod2obs.exe` output; **2)** the PEST template file (`surface_par_params.ptf`), which shows PEST how to write the input file for the surface extrapolation script; **3)** the PEST parameter file (`surface_par_params.par`), which lists the starting parameter values to use when checking the PEST input; **4)** the PEST control file (`bc_adjust_2009ASER.pst`), which has PEST-related parameters, definitions of extrapolation surface parameters, and the observations and weights that PEST is adjusting the model inputs to fit. The observed heads are read as an input file in the PEST borehole sample file format (`meas_head_2009ASER.smp`), and the weights are read in from the input file (`obs_loc_2009ASER.dat`).

PEST runs the “forward model” many times, adjusting inputs and reading the resulting outputs using the instruction and template files created above. The forward model actually consists of a Bash shell script (`run_02_model`) that simply calls a pre-processing Python script `surface_02_extrapolate.py` (§A-4.5), the MODFLOW-2000 executable, the Python script `create_average_NS_residuals.py`, and the PEST utility `mod2obs.exe` as a post-processing step. The script redirects the output of each step to `/dev/null` to minimize screen output while running PEST, since PEST will run the forward model many dozens of times.

The Python script `create_average_NS_residuals.py` takes the output from the PEST utility `mod2obs.exe` and creates a meta-observation that consists of the average residual between measured and model-prediction, only averaged across the northern or southern WIPP wells (the wells in the center of the WIPP site are not included in either group). This was done to minimize cancelation of the errors north (where the model tended to underestimate heads) and south (where the model tended to overestimate heads) of the WIPP. The results of this script are read directly by PEST and incorporated as four additional observations (mean and median errors, both north and south of WIPP).

The pre-processing Python script `surface_02_extrapolate.py` reads the new IBOUND array created in a previous step (with -2 now indicating which constant-head boundaries should be modified), the initial head file used in AP-114 Task 7 (`init_head_orig.mod`), two files listing the relative X and Y coordinates of the model cells (`rel_{x,y}_coord.dat`), and an input file listing the coefficients of the parametric equation used to define the initial head surface. This script then cycles over the elements in the domain, writing the original starting head value if the IBOUND value is -1 or 0, and writing the value corresponding to the parametric equation if the IBOUND value is -2 or 1. Using the parameters corresponding to those used in AP-114 Task 7, the output starting head file should be identical to that used in AP-114 Task 7.

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After PEST has converged to the optimum solution for the given observed heads and weights, it runs the forward model one more time with the optimum parameters. The post-processing Python scripts for creating the Surfer ASCII grid file and Surfer blanking file from the MODFLOW and DTRKMF output are run and the results are plotted using additional Python scripts that utilize the plotting and map coordinate projection functionality of the matplotlib library.

These two plotting scripts (`plot-contour-maps.py` and `plot-results-bar-charts.py`) are included in the appendix for completeness, but only draw the figures included in this report, and passed on to WRES for the ASER. These two scripts automate the plotting process and take the place of the Microsoft Excel, USACE Corpscon, and Golden Software Surfer input files that were previously used.

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9 Appendix: Water Level and Density Data Listing

9.1 Input files for plotting water levels and densities

bytes	description	file name
2.3K	Culebra midpoint elevations	culebra-midpoint-elevations.csv
4.8K	UTM X and Y coordinates for wells	well-coordinates.csv
0.9K	reference point change for pre-2007 elevations	reference-point-change-2007.dat
43K	data from Table-F.8 of 2004 ASER	ASER-2004-waterlevel-data.csv
40K	data from Table-F.8 of 2005 ASER	ASER-2005-waterlevel-data.csv
41K	data from Table-F.8 of 2006 ASER	ASER-2006-waterlevel-data.csv
42K	data from Table-F.8 of 2007 ASER	ASER-2007-waterlevel-data.csv
43K	data from Table-F.8 of 2008 ASER	ASER-2008-waterlevel-data.csv
43K	data from Table-F.8 of 2009 ASER	ASER-2009-waterlevel-data.csv
42K	data from Table-F.8 of 2010 ASER	ASER-2010-waterlevel-data.csv
15K	summary of events in wells from ASERs	well-events.csv
23K	data from Table-6.3 of ASERs	reported-density-values.csv
2.9K	designated densities to use at wells	densities-to-use.csv

9.1.1 densities-to-use.csv input file

well	begin date	end date	density	source
C-2737	1/1/1998	5/12/2003	1.000	ASER
	11/19/2003	2/1/2007	1.019	TROLL2005
	2/1/2007	6/28/2008	1.010	JOHNSON2009
	6/28/2008	1/1/2012	1.029	TROLL2008
ERDA-9	1/1/1998	1/1/2012	1.067	JOHNSON2009
H-02B2	1/1/1998	4/12/2005	1.014	JOHNSON2009
	4/12/2005	2/24/2009	1.000	SNL notebooks
	2/24/2009	1/1/2012	1.011	TROLL2010
H-03B2	1/1/1998	1/1/2012	1.042	JOHNSON2009
H-04B	1/1/1998	6/14/2009	1.015	JOHNSON2009
H-05B	1/1/1998	6/11/2005	1.104	ASER
	6/11/2005	1/1/2012	1.095	JOHNSON2009
H-06B	1/1/1998	2/19/2008	1.040	JOHNSON2009
H-07B1	1/1/1998	1/1/2012	1.002	JOHNSON2009
H-09C	1/1/1998	1/1/2012	1.001	JOHNSON2009
H-10C	2/19/2002	7/12/2009	1.001	JOHNSON2009
	7/12/2009	1/1/2012	1.089	TROLL2009
H-11B4	1/1/1998	1/1/2012	1.070	JOHNSON2009
H-12	1/1/1998	12/1/2003	1.083	SNL notebooks
	4/12/2005	11/24/2008	1.097	JOHNSON2009
	11/24/2008	1/1/2012	1.096	TROLL2008
H-15	1/1/1998	2/1/2001	1.154	SAND89-7068/2
	11/18/2003	4/10/2006	1.082	TROLL2005
	4/10/2006	3/5/2008	1.053	JOHNSON2009
H-17	1/1/1998	1/1/2012	1.133	JOHNSON2009
H-19B0	1/1/1998	1/1/2012	1.068	JOHNSON2009
I-461	10/15/2003	1/1/2012	1.005	JOHNSON2009
P-17	1/1/1998	6/17/2005	1.070	PDS 2004 2005 avg
	6/17/2005	8/18/2006	1.053	SGR 2006 SNL SURVEY
SNL-01	3/25/2004	1/1/2012	1.033	JOHNSON2009
SNL-02	4/28/2003	1/1/2012	1.012	JOHNSON2009
SNL-03	8/14/2003	1/1/2012	1.023	JOHNSON2009
SNL-05	4/26/2004	1/1/2012	1.010	JOHNSON2009
SNL-08	6/14/2005	8/28/2007	1.052	JOHNSON2009
	8/28/2007	1/1/2012	1.103	TROLL2007
SNL-09	5/17/2003	1/1/2012	1.024	JOHNSON2009
SNL-10	5/31/2006	1/1/2012	1.011	JOHNSON2009
SNL-12	6/25/2003	1/1/2012	1.005	JOHNSON2009
SNL-13	4/11/2005	1/1/2012	1.027	JOHNSON2009
SNL-14	5/3/2005	1/1/2012	1.0480	JOHNSON2009
SNL-16	4/11/2006	1/1/2012	1.010	JOHNSON2009
SNL-17	4/25/2006	1/1/2012	1.006	JOHNSON2009
SNL-18	6/20/2006	1/1/2012	1.028	JOHNSON2009
SNL-19	5/5/2006	1/1/2012	1.003	JOHNSON2009
WIPP-11	9/7/2004	1/1/2012	1.038	JOHNSON2009
WIPP-13	1/1/1998	1/1/2012	1.053	JOHNSON2009
WIPP-19	1/1/1998	1/1/2012	1.044	JOHNSON2009
WIPP-21	1/1/1998	1/1/2012	1.071	ASER
WIPP-22	1/1/1998	1/1/2012	1.087	ASER
WIPP-25	1/1/1998	6/12/2009	1.011	JOHNSON2009
WIPP-29	1/1/1998	1/1/2012	1.180	ASER
WIPP-30	1/1/1998	6/22/2005	1.018	SAND89-7068/2
	6/22/2005	3/1/2008	1.000	JOHNSON2009
WQSP-1	1/1/1998	1/1/2012	1.048	SGR ROUNDS 23 to 25
WQSP-2	1/1/1998	1/1/2012	1.048	SGR ROUNDS 23 to 25
WQSP-3	1/1/1998	1/1/2012	1.146	SGR ROUNDS 23 to 25
WQSP-4	1/1/1998	1/1/2012	1.075	SGR ROUNDS 23 to 25
WQSP-5	1/1/1998	1/1/2012	1.025	SGR ROUNDS 23 to 25
WQSP-6	1/1/1998	1/1/2012	1.014	SGR ROUNDS 23 to 25


```

252     # some SNL wells are not zero padded some years
253     # therefore they appear as different wells
254     num = well.split('-')[1]
255     if len(num) == 1:
256         well = 'SNL-0' + num
257
258     if zone == 'SRD':
259         zone = 'SRDL'
260     elif 'RUSS' in zone:
261         zone = 'RS'
262
263     if len(r) < 8 or r[7].strip() == "":
264         fwh = -999.0
265     else:
266         fwh = float(r[7])*0.3048
267
268     wlem = float(r[6])
269     if year < 2007 and well in rpcorr:
270         cwlem = wlem + rpcorr[well]
271     else:
272         cwlem = wlem
273
274     data.append((well, zone, dt, float(r[4]), wlem, cwlem, fwh))
275
276 data = np.array(data, dtype=wldtype)
277 data = np.sort(data, order=('dt', 'zone', 'well'))
278
279
280 # wells reported by WRES (doesn't include Gnome wells)
281 wells = list(set(data[:, 'well']))
282 wells.sort()
283
284 # can plot all wells reported by WRES
285 zones = list(set(data[:, 'zone']))
286 for zone in zones:
287     zmask = data['zone'] == zone
288     zwells = list(set(data[zmask]['well']))
289     zwells.sort()
290
291 # months used for creating ASER contour maps (no apparent ranges for 2003 & 2004)
292 # NB: 2003, 2004, 2005 & 2006 are my choice, not necessarily what used in ASER
293 cmonths = {2001:(datetime.datetime(2001,12,1), datetime.datetime(2001,12,31)),
294            2002:(datetime.datetime(2002,12,1), datetime.datetime(2002,12,31)),
295            2003:(datetime.datetime(2003,9,1), datetime.datetime(2003,9,30)),
296            2004:(datetime.datetime(2004,9,1), datetime.datetime(2004,9,30)),
297            2005:(datetime.datetime(2005,6,1), datetime.datetime(2005,6,30)),
298            2005:(datetime.datetime(2005,6,1), datetime.datetime(2005,6,30)),
299            2006:(datetime.datetime(2006,11,1), datetime.datetime(2006,11,30)),
300            2007:(datetime.datetime(2007,5,1), datetime.datetime(2007,5,31)),
301            2008:(datetime.datetime(2008,9,1), datetime.datetime(2008,9,30)),
302            2009:(datetime.datetime(2009,6,1), datetime.datetime(2009,6,30)),
303            2010:(datetime.datetime(2010,2,1), datetime.datetime(2010,2,28))}
304
305 # exceptions to the above rules, based on looking closer at data
306 cexceptions = {'WIPP-11':{2006:(datetime.datetime(2006,8,1),
307                               datetime.datetime(2006,8,31))},
308               'H-10C':{2006:(datetime.datetime(2006,8,1),
309                               datetime.datetime(2006,8,31))},
310               'SNL-14':{2005:(None, None),
311                          2007:(datetime.datetime(2007,11,1),
312                               datetime.datetime(2007,11,30))},
313               'SNL-16':{2007:(datetime.datetime(2007,9,1),
314                               datetime.datetime(2007,9,30))},
315               'WIPP-26':{2005:(None, None)},

```

```

316         'WIPP-30':{2005:(datetime.datetime(2005,8,1),
317                     datetime.datetime(2005,8,31))}}
318
319
320 newfwhfh = {}
321 newfwhfh[2005] = open('meas_head_2005ASER.smp','w')
322 newfwhfh[2006] = open('meas_head_2006ASER.smp','w')
323 newfwhfh[2007] = open('meas_head_2007ASER.smp','w')
324
325 # minimum density range for plot
326 denmax = 1.100
327 denmin = 1.000
328 denrange = denmax - denmin
329
330 #@#fhrpchange = open('reference-point-change-2007.dat','w')
331
332 # %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
333 # $$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
334 # cycle over all Culebra wells, plotting figures for each
335 zone = 'CUL'
336 zmask = data['zone'] == zone
337 zdat = data[zmask]
338 for well in wells:
339     wm = zdat['well'] == well
340     if wm.sum() == 0:
341         continue # no data for this well
342     else:
343         print 'processing', zone, well
344
345     fig = plt.figure(1, figsize=(11,8.5))
346     ax1 = fig.add_subplot(211)
347
348     # plot reported (adjusted) WRES depth-to-water measurements (small red circles)
349     ax1.plot_date(zdat[wm]['dt'], zdat[wm]['dtwm'], 'ro', markersize=2, markeredgecolor='red')
350
351     # invert depth-to-water axis (bigger numbers on bottom)
352     ymin, ymax = ax1.get_ylim()
353     ax1.set_ylim([ymax, ymin])
354
355     pmask = zdat[wm]['fwhm'] > 0.0
356     pdata = (zdat[wm])[pmask]
357
358     # uncomment below and run once on data to generate corrections file
359     #@#pre2007mask = pdata['dt'] < datetime.datetime(2007,1,1)
360     #@#post2007mask = np.logical_not(pre2007mask)
361     #@## only compute correction to reference point elevation if data straddles January/1/2007
362     #@#if pre2007mask.sum() > 0 and post2007mask.sum() > 0:
363     #@#     oldrpelev = (pdata[pre2007mask]['dtwm'] + pdata[pre2007mask]['wlem']).mean()
364     #@#     newrpelev = (pdata[post2007mask]['dtwm'] + pdata[post2007mask]['wlem']).mean()
365     #@#     earlyrpcorr = newrpelev - oldrpelev
366     #@#else:
367     #@#     earlyrpcorr = 0.0
368     #@#fhrpchange.write('%s\t%.2f\n' % (well, earlyrpcorr))
369
370     # plot freshwater heads on second y-axis
371     ax2 = ax1.twinx()
372
373     # plot freshwater head data as reported in ASER (small blue stars)
374     ax2.plot_date(pdata[:, 'dt'], pdata[:, 'fwhm'], 'b*', markersize=3, markeredgecolor='blue')
375
376     # correct FWH for densities chosen as "correct" densities over a given time range
377     fdmask = finden[:, 'well'] == well
378     fdata = finden[fdmask]
379

```

```

380 for dval in fdata:
381     # mask off ASER values in the date range associated with this density value
382     datemask = np.logical_and(pdata['dt'] >= dval['dt0'],
383                               pdata['dt'] <= dval['dt1'])
384
385     newfwhdates = pdata[datemask]['dt']
386
387     # compute new fwh using consistent density
388     newfwh = (pdata[datemask]['cwlem']-midpt[well])*dval['den'] + midpt[well]
389
390     # plot consistent freshwater heads (large blue x's)
391     ax2.plot_date(newfwhdates, newfwh, 'bx', markersize=5)
392
393     # save 2005, 2006, and 2007 fwh to file for use by PEST
394     for yr in [2005,2006,2007]:
395         exception = False
396         skipwell = False
397         if well in cexceptions:
398             if yr in cexceptions[well]:
399                 exception = True
400                 if cexceptions[well][yr][0] == None:
401                     # skip this well this year, even though there is data
402                     skipwell = True
403                 else:
404                     # use a different month than the one selected for all other wells
405                     maskyrfwh = np.logical_and(newfwhdates >= cexceptions[well][yr][0],
406                                                 newfwhdates <= cexceptions[well][yr][1])
407             if not exception:
408                 # use the standard month selected for all other wells
409                 maskyrfwh = np.logical_and(newfwhdates >= cmonths[yr][0],
410                                           newfwhdates <= cmonths[yr][1])
411
412             if maskyrfwh.sum() > 0 and not skipwell:
413                 # use the same name if this well was used before,
414                 # otherwise strip hyphen and go for it
415                 if well.upper() in aserfwh[2010]:
416                     wname = aserfwh[2010][well]['name']
417                 elif well.upper() in aserfwh[2009]:
418                     wname = aserfwh[2009][well]['name']
419                 elif well.upper() in aserfwh[2008]:
420                     wname = aserfwh[2008][well]['name']
421                 else:
422                     wname = well.replace('-0', '-') # remove leading zero
423                     wname = wname.replace('-', '') # remove hyphen
424
425                 # if there are more than one fwh during that month, select the first one
426                 newfwhfh[yr].write('%s\t%s\t12:00:00\t%.3f\t%.4f\n' %
427                                   (wname, newfwhdates[maskyrfwh][0].strftime("%m/%d/%Y"),
428                                   newfwh[maskyrfwh][0], dval['den']))
429
430     ax1.xaxis.set_major_formatter(NullFormatter())
431     ax1.set_title('%s water levels and specific gravities' % well)
432     ax2.xaxis.set_major_locator(YearLocator())
433     ax2.xaxis.set_minor_locator(MonthLocator())
434     ax2.xaxis.set_major_formatter(DateFormatter('%Y'))
435     ax1.set_ylabel('ASER depth to water (m BTOC)', color='red', fontsize=9)
436
437     ax2.set_ylabel('freshwater head (ASER=*, this rept=x) (m AMSL)',
438                   color='blue', fontsize=9)
439
440     # add date ranges used for contouring
441     for yr in cmonths.keys():
442         exception = False
443         if well in cexceptions:

```



```

444     if yr in cexceptions[well]:
445         exception = True
446         if cexceptions[well][yr][0] == None:
447             # don't use this well this year
448             continue
449         else:
450             # use a different month for this well this year
451             ax2.axvspan(cexceptions[well][yr][0], cexceptions[well][yr][1],
452                       alpha=0.25, color='green')
453     if not exception:
454         # use the standard month for this well and year
455         ax2.axvspan(cmonths[yr][0], cmonths[yr][1], alpha=0.25, color='blue')
456 axd = fig.add_subplot(212)
457
458 # aparent specific gravity is (fwh-el - midpt-el)/(wl-el - midpt-el)
459 # computed from wl elevation and freshwater head reported by WRERS +
460 # Culebra midpoint elevations (small green circles)
461 specgrav = (((zdat[wm])[pmask]['fwhm'] - midpt[well])/
462             ((zdat[wm])[pmask]['wlem'] - midpt[well]))
463 axd.plot_date((zdat[wm])[pmask]['dt'], specgrav, 'go',
464              markersize=2, markeredgecolor='green')
465
466 fdmask = finden[:, 'well'] == well
467 fdata = finden[fdmask]
468 for dval in fdata:
469     # plot the "final" gravity as a line across the figure (solid green line)
470     axd.plot_date([dval['dt0'], dval['dt1']], [dval['den'], dval['den']], 'g-')
471
472 # plot reported density values; different symbols
473 dm = den['well'] == well
474 ddat = den[dm]
475 setsrc = set(ddat[:, 'src'])
476 sources = list(setsrc)
477
478 # change TROLLYYYY to just TROLL
479 for src in sources:
480     if 'TROLL' in src:
481         setsrc.remove(src)
482         setsrc.add('TROLL')
483     if 'PDS' in src:
484         setsrc.remove(src)
485         setsrc.add('PDS')
486     if 'SGR' in src:
487         setsrc.remove(src)
488         setsrc.add('SGR')
489
490 sources = list(setsrc)
491 for src in sources:
492     # densities from this sources (all TROLLYYY just count as TROLL, etc.)
493     mddat = npchar.find(ddat[:, 'src'], src) >= 0 # find returns -1 if not found
494     sddat = ddat[mddat]
495
496     # densities since cutoffdate
497     msddat = sddat['dt'] > firstplot
498     dsddat = sddat[msddat]
499     nrecent = msddat.sum()
500
501     if src == 'TROLL':
502         if nrecent > 0:
503             tmpden = dsddat[msddat]['den']
504             # move any troll-computed densities below 1.0 to fresh water (1.0)
505             tmpden[tmpden < 1.0] = 1.0
506             # troll densities plot as a date range
507             axd.plot_date([sddat[msddat]['dt'], sddat[msddat]['dt2']], [tmpden, tmpden],

```

```

508         srcsymb[src], linestyle='solid', color=srccolor[src],
509         linewidth=2.0, label=src, markersize=9)
510
511     else:
512         if nrecent > 0:
513             tmpden = sddat[msddat]['den']
514             # move any densities below 1.0 to fresh water (1.0)
515             tmpden[tmpden < 1.0] = 1.0
516             # non-troll densities plot as a single date
517             axd.plot_date(sddat[msddat]['dt'], tmpden, srcsymb[src],
518                         color=srccolor[src], label=src, markersize=9)
519
520             # densities before cutoff date (plot on edge with left-pointing triangle)
521             msddat = sddat['dt'] < firstplot
522             nold = msddat.sum()
523
524             if nold > 0:
525                 axd.plot_date([firstplot]*nold, sddat[msddat]['den'], '<',
526                             color='yellow', label='pre-2005', markersize=9)
527
528             # make range of density plots at least a minimum range
529             ymin, ymax = axd.get_ylim()
530             if ymax < denmax:
531                 ymax = denmax
532
533             if ymin > denmin:
534                 ymin = denmin
535
536             axd.set_ylim((ymin, ymax))
537
538             # add pumping, drilling, and pluggin events located at the current well
539             em = events[:, 'well'] == well
540             if em.sum() > 0:
541                 ee = events[em]
542                 ymin, ymax = axd.get_ylim()
543                 yann = ymax - (ymax - ymin)/5.0
544                 for ev in ee:
545                     if ev['dt1'] == None:
546                         # no ending date
547                         axd.axvline(ev['dt0'], alpha=0.5, color=ev['c'])
548                         axd.annotate(ev['s'], (ev['dt0'], yann),
549                                   rotation='vertical', fontproperties=AnnFontP)
550                     else:
551                         axd.axvspan(ev['dt0'], ev['dt1'], alpha=0.25, color=ev['c'])
552                         axd.annotate(ev['s'], (ev['dt0']+(ev['dt1']-ev['dt0'])/2, yann),
553                                   rotation='vertical', fontproperties=AnnFontP)
554
555             # add drilling and P&A events for wells within 500 m (i.e., same pad)
556             for other in evwells:
557                 if not other == well:
558                     em = events[:, 'well'] == other
559                     ee = events[em]
560                     om = np.logical_or(ee[:, 'c'] == 'red', ee[:, 'c'] == 'green')
561                     dist = np.sqrt((xyz[well]['x']-xyz[other]['x'])**2 +
562                                   (xyz[well]['y']-xyz[other]['y'])**2)
563                     # does other well have drilling or p&a activities?
564                     if om.sum() > 0:
565                         if dist < 500:
566                             for ev in ee[om]:
567                                 if ev['dt1'] == None:
568                                     # no ending date
569                                     axd.axvline(ev['dt0'], alpha=0.5,
570                                               linestyle='dashed', color=ev['c'])

```

```

572         else:
573             axd.axvspan(ev['dt0'], ev['dt1'], alpha=0.25,
574                       linestyle='dashed', color=ev['c'])
575             axd.annotate('%s (%im) %s' % (ev['well'], dist, ev['s']), (ev['dt0'], yann),
576                          rotation='vertical', fontproperties=AnnFontP, color='gray')
577
578         # nearby pumping tests (not slug tests) within 5.0 km
579         # npchar.find() returns -1 for not found
580         om = np.logical_and(ee[:, 'c'] == 'cyan',
581                             npchar.find( ee[:, 's'], 'slug') == -1)
582         if om.sum() > 0:
583             if dist < 5000:
584                 for ev in ee[om]:
585                     if ev['dt1'] == None:
586                         # no ending date
587                         axd.axvline(ev['dt0'], alpha=0.5,
588                                   linestyle='dashed', color=ev['c'])
589                     else:
590                         axd.axvspan(ev['dt0'], ev['dt1'], alpha=0.25,
591                                   linestyle='dashed', color=ev['c'])
592                         axd.annotate('%s (%.1fkm) %s' % (ev['well'], dist/1000.0, ev['s']),
593                                     (ev['dt0'], yann), rotation='vertical',
594                                     fontproperties=AnnFontP, color='gray')
595
596
597         ax2.set_xlim(left=datetime.datetime(2004,11,1))
598         ax2.set_xlim(right=datetime.datetime(2011,1,1))
599
600         # force subplots to have same data range
601         axd.set_xlim(ax2.get_xlim())
602         axd.set_ylabel('specific gravity')
603
604         # legend for type of density measurement
605         # while removing duplicate entries from legend
606         handles, labels = axd.get_legend_handles_labels()
607         newhandles = []
608         newlabels = []
609         if len(handles) > 0:
610             for h,l in zip(handles, labels):
611                 if not l in newlabels:
612                     newhandles.append(h)
613                     newlabels.append(l)
614
615         leg = axd.legend(newhandles, newlabels, loc=0, prop=LegFontP, numpoints=1, scatterpoints=1)
616
617         axd.xaxis.set_major_locator(YearLocator())
618         axd.xaxis.set_minor_locator(MonthLocator())
619         axd.xaxis.set_major_formatter(DateFormatter('%Y'))
620         plt.savefig('%s-%s-ASER-waterlevels.png' % (zone, well), dpi=150)
621         plt.close(1)
622
623         newfwhf[2005].close()
624         newfwhf[2006].close()
625         #@#rhrpchange.close()

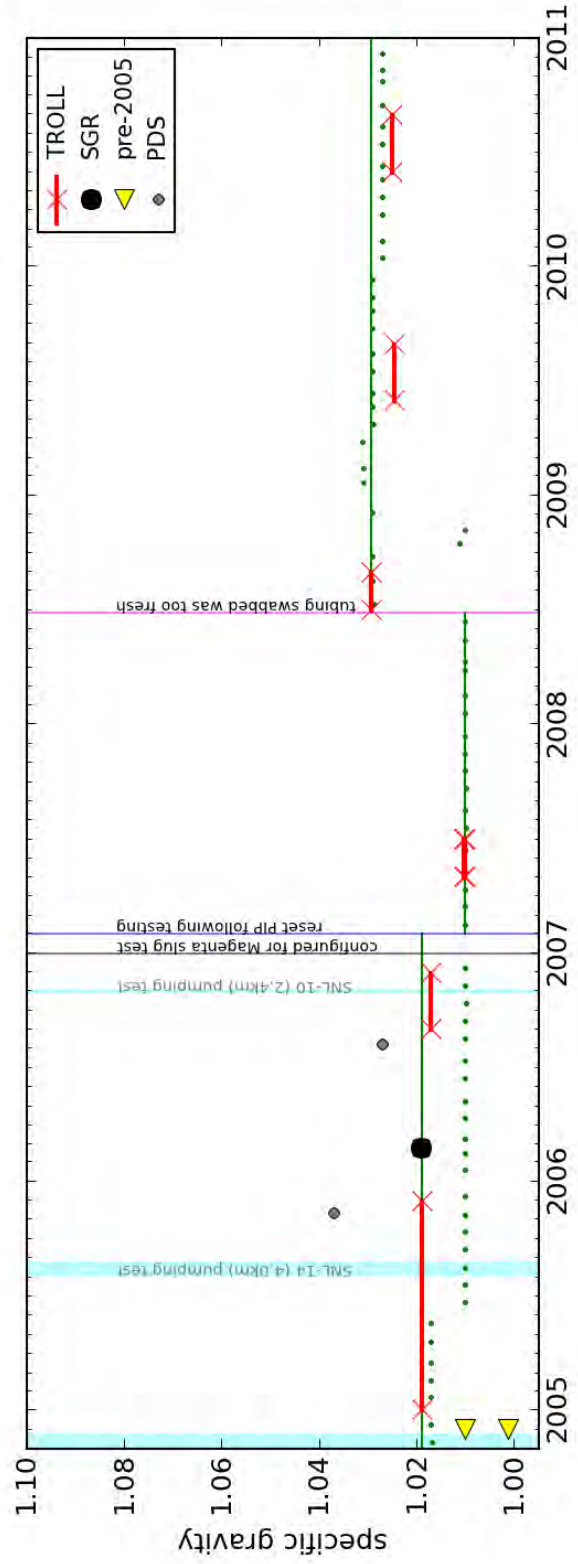
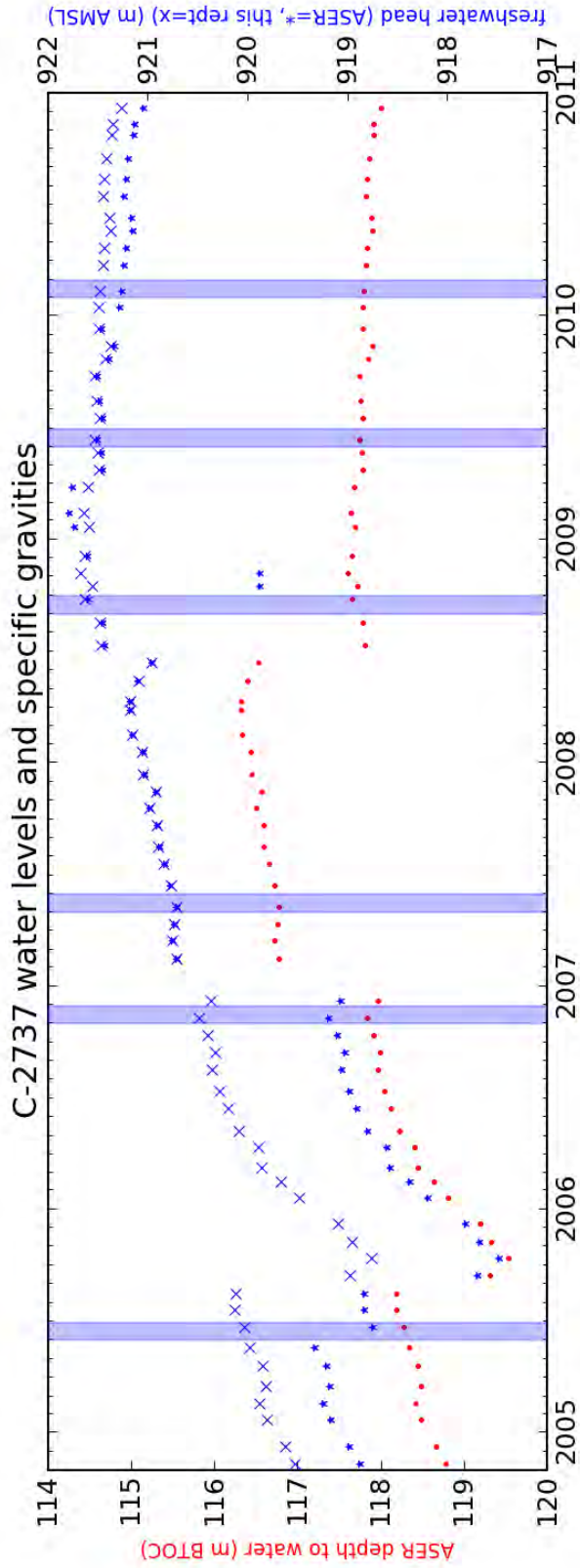
```

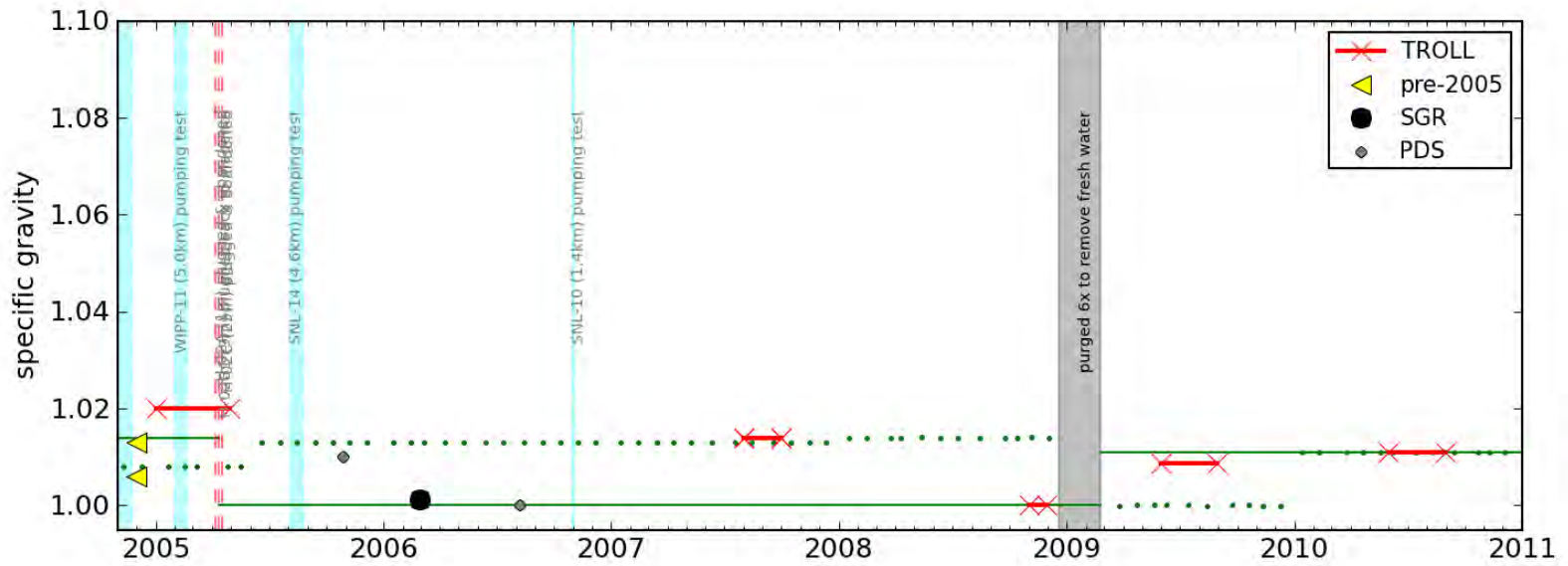
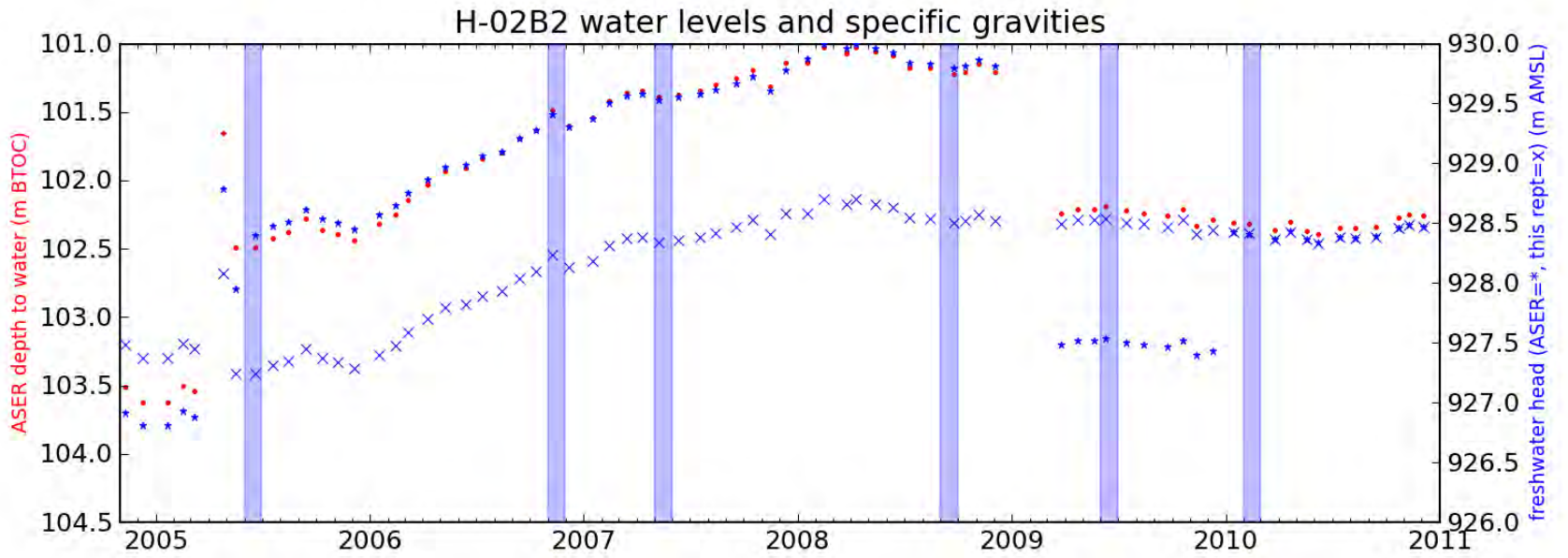
9.3 Figures Generated by Python Water Level Script

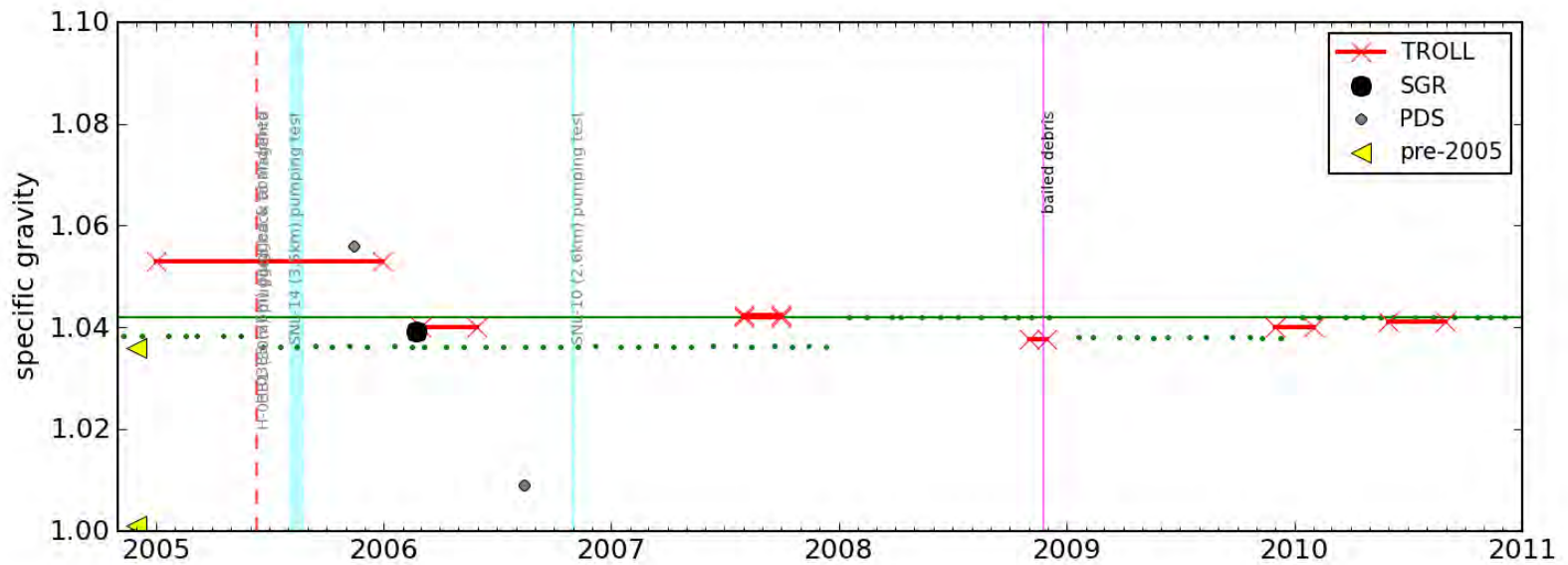
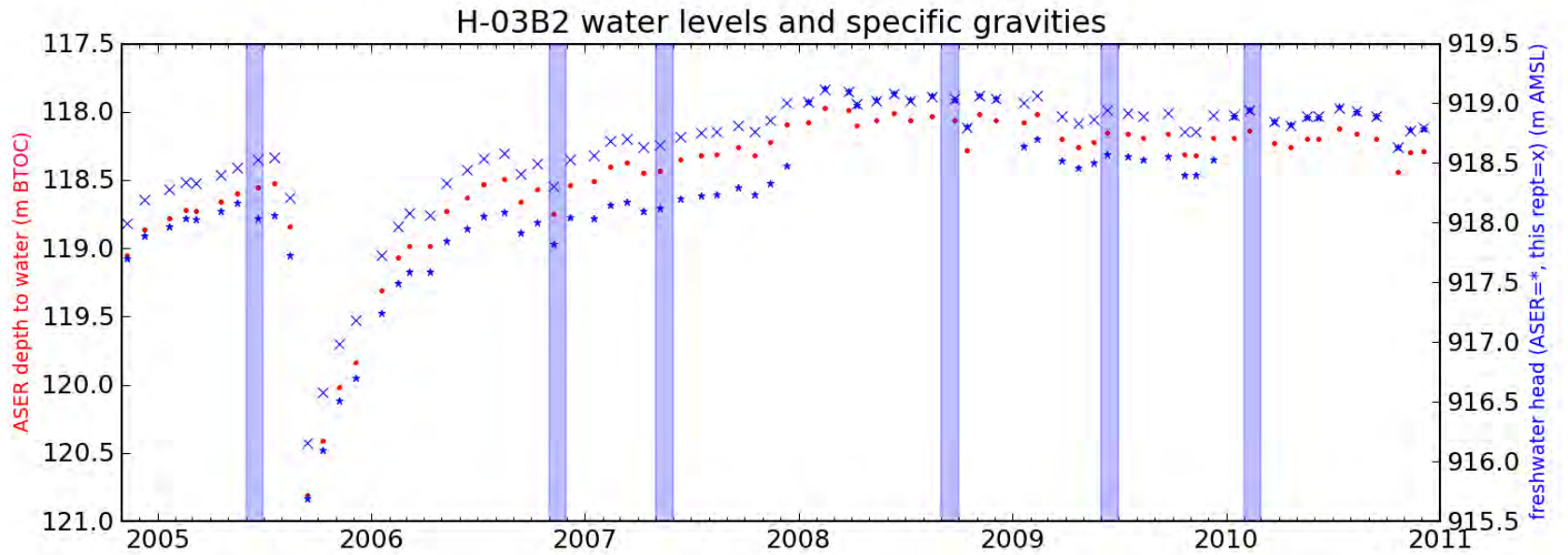
The following figures were generated by the Python script `plot-waterlevels.py` and represent the water level, density (aka specific gravity), and well-event data listed in the 2004-2010 ASERs.

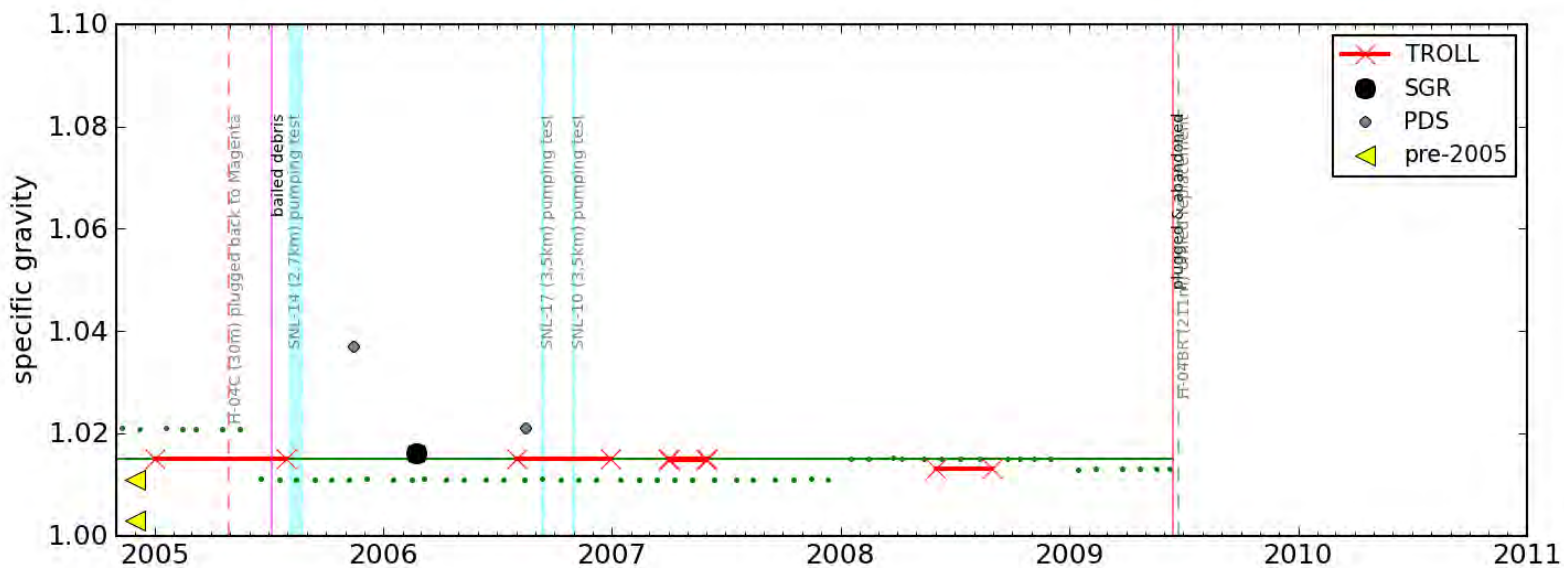
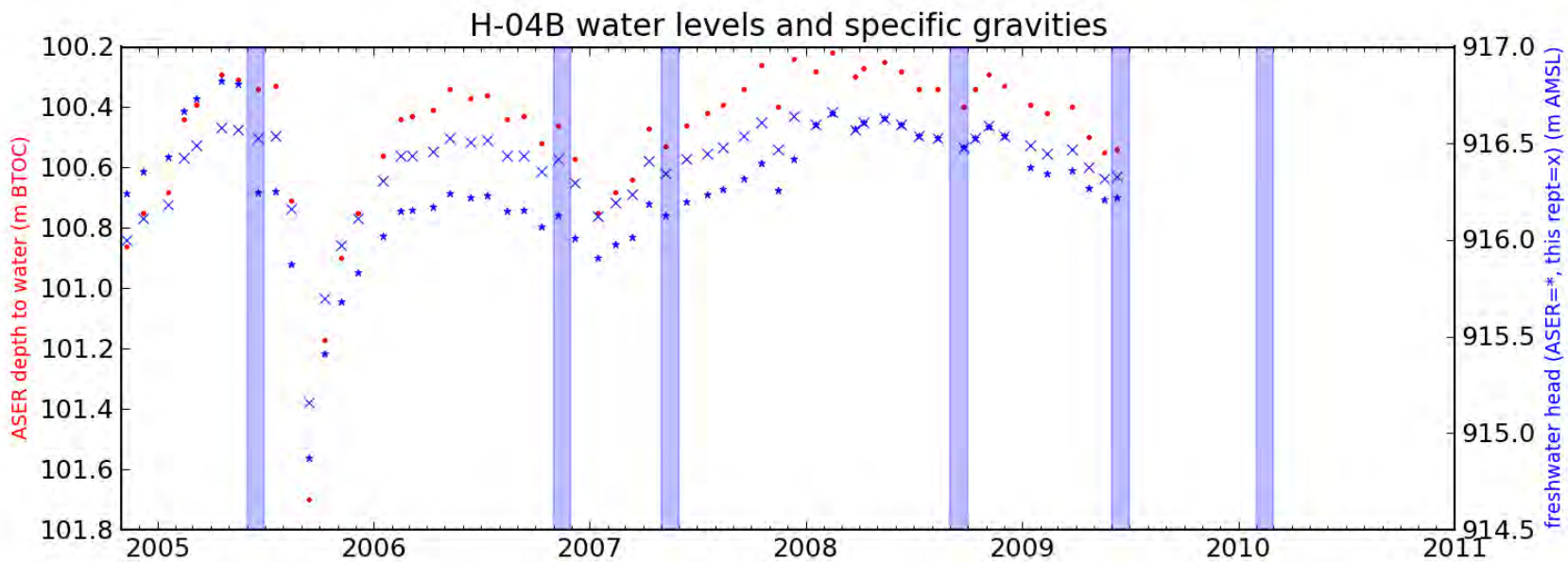
Each page represents the 2005-current ASER data for a given Culebra well. In the water level plots (top), filled red circles are reported depths to water (meters below top of casing (BTOC)), filled blue stars are ASER-reported freshwater head elevations (meters above mean sea level (AMSL)), and the blue \times 's are the freshwater head elevations (AMSL) computed using the density values recommended in the file `densities-to-use.csv`. Adjustments to pre-2007 water level elevations to use better-surveyed modern reference point elevations are reflected in the re-computed freshwater heads (blue \times 's), but not in the ASER-reported freshwater heads (blue stars). Vertical bands indicate the months that were used for contouring heads.

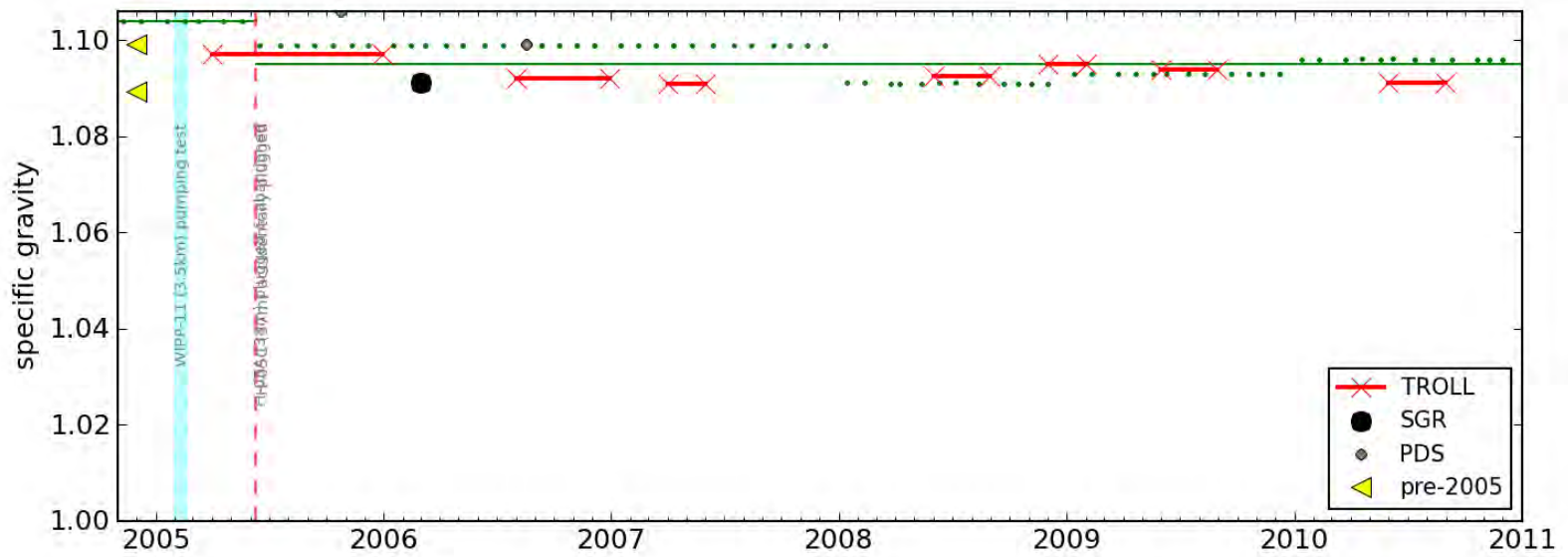
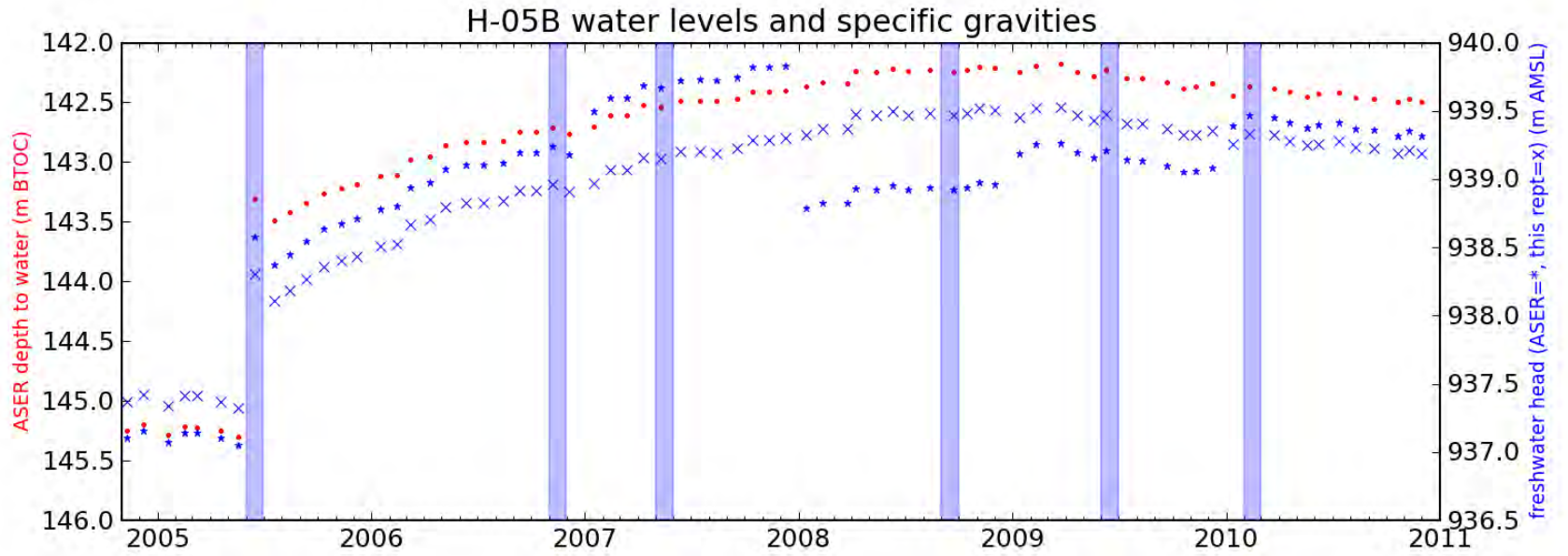
In the density plots (bottom), horizontal green lines indicate the density/specific gravity values chosen to be used at a given time (`densities-to-use.csv`), vertical lines are events in current or nearby wells (nearby wells are gray text and indicate the distance between the wells, while the current well is in black text). Red \times 's with connecting red lines are density values computed from Troll data (representing the date range used to compute the density), gray circles indicate reported pressure-density surveys (PDS), large black circles are field specific gravity readings (SGR), and small green dots are densities back-calculated from the freshwater head elevations and water level elevations reported in the ASERs.

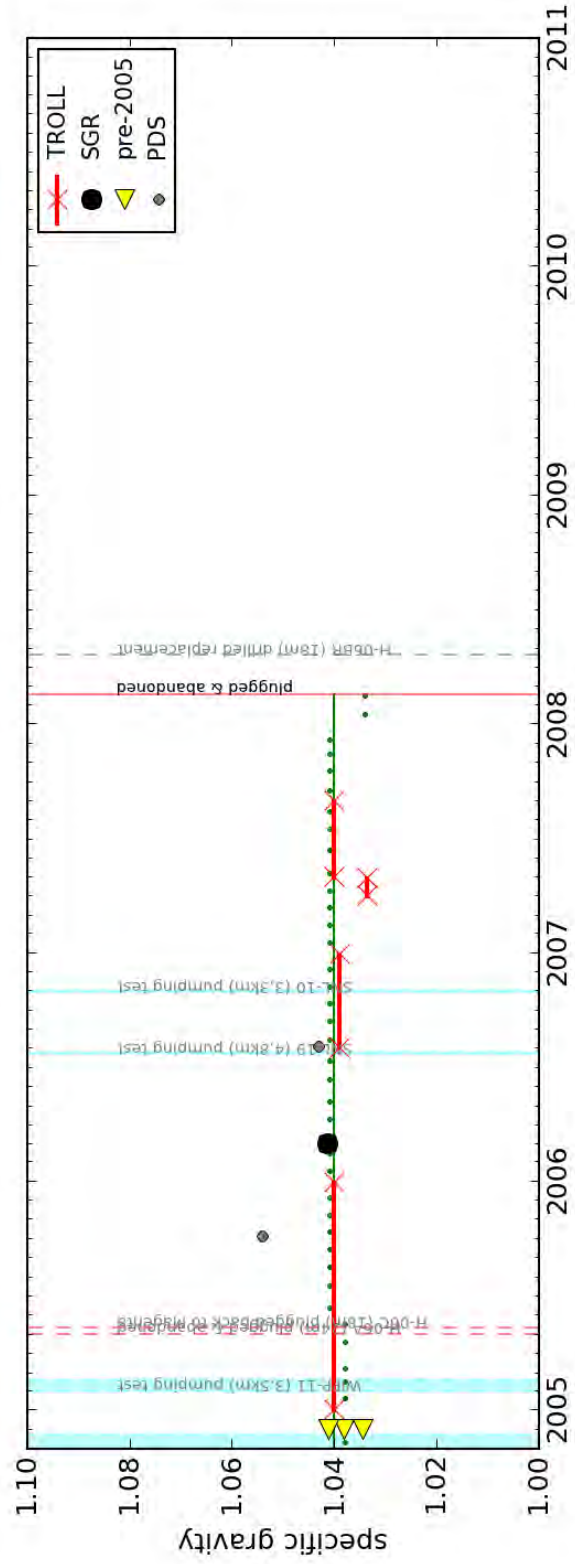
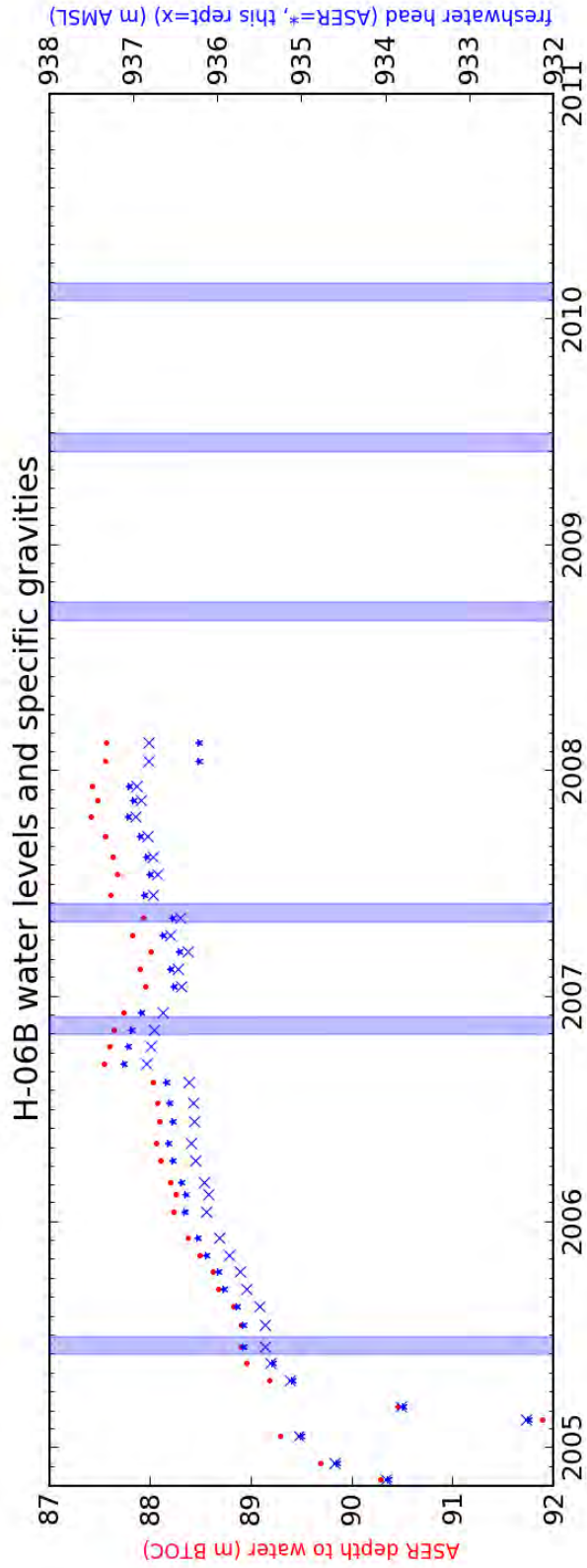


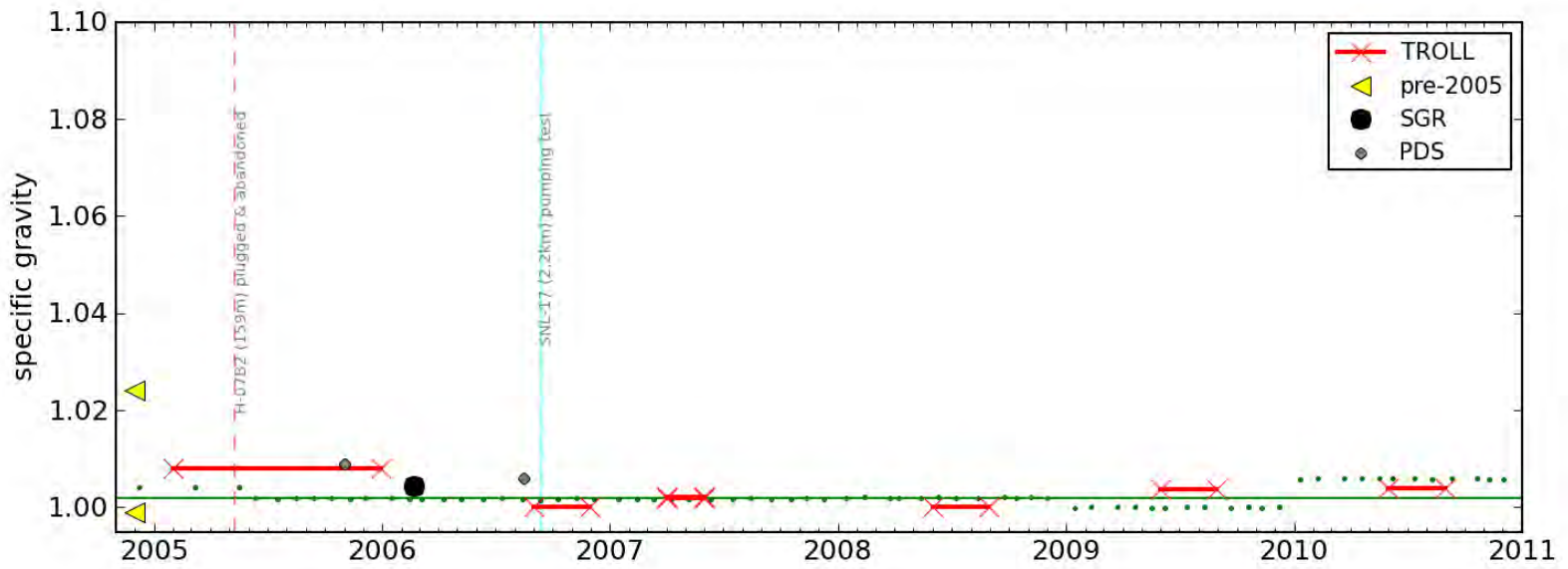
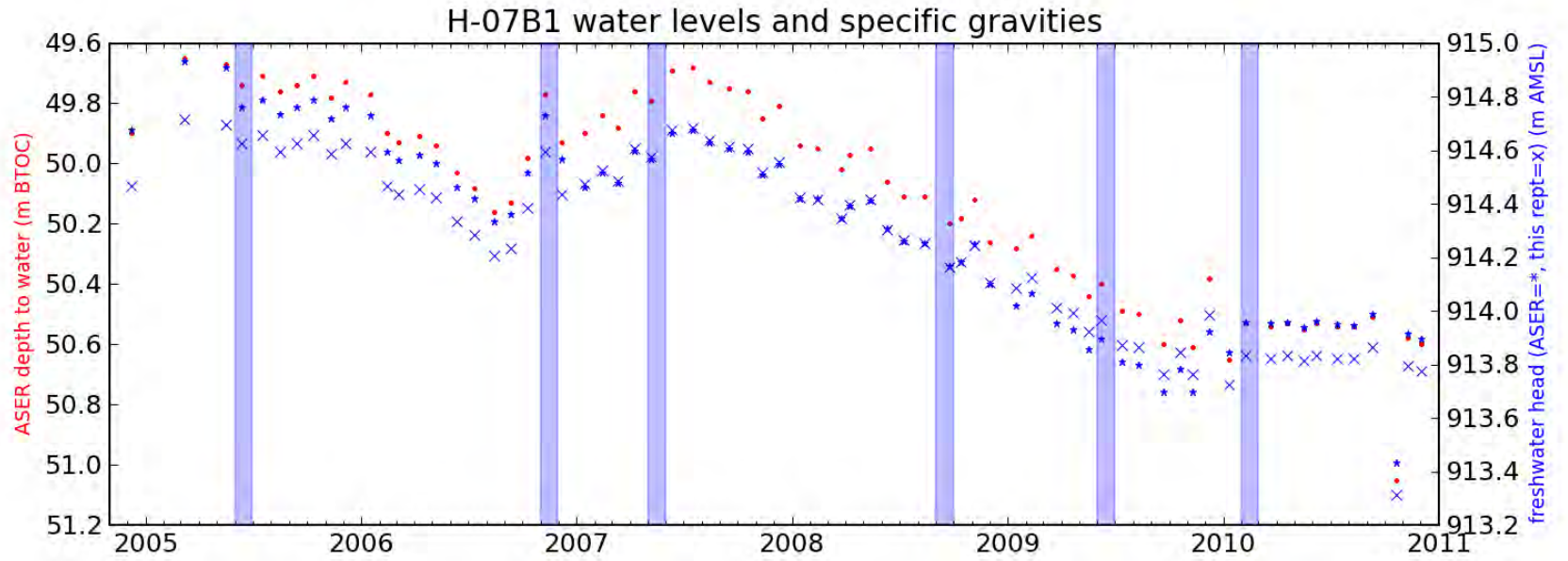


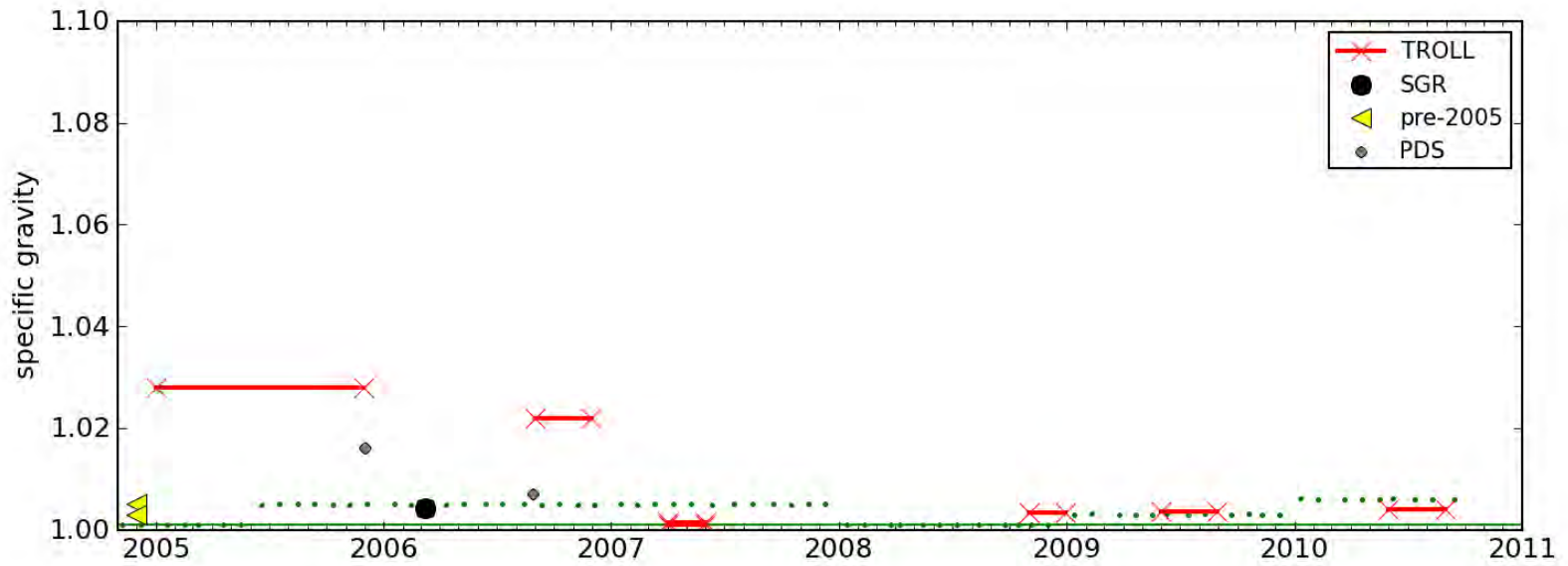
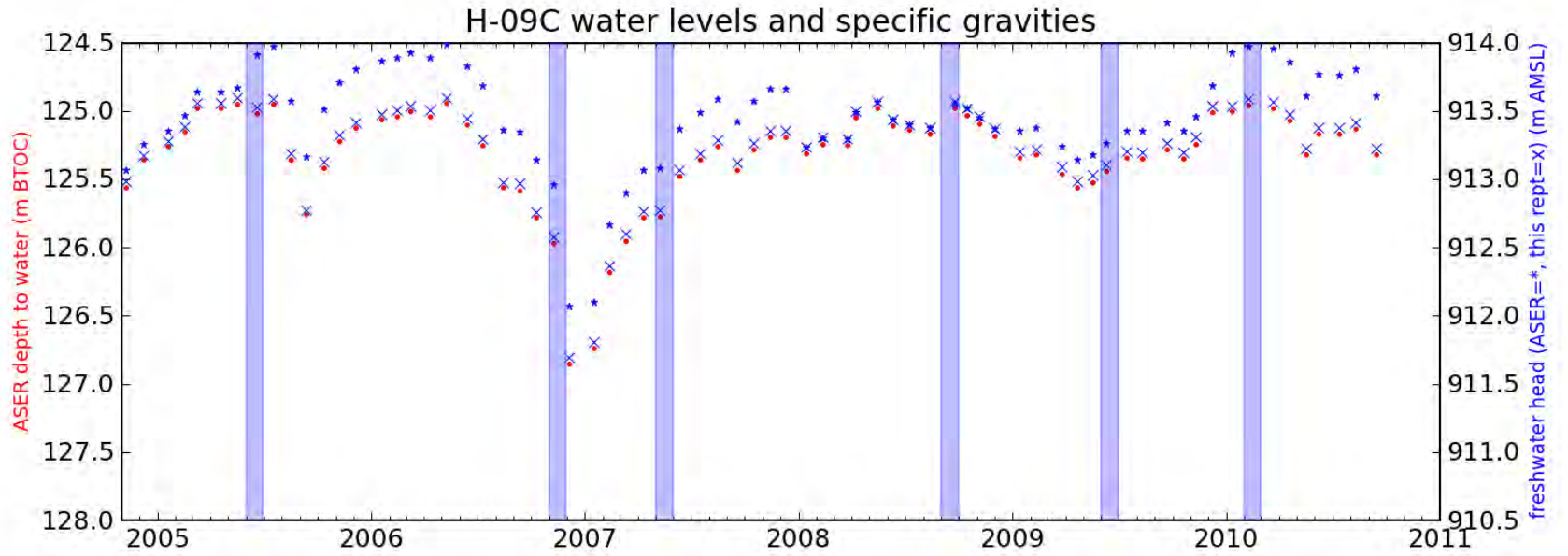


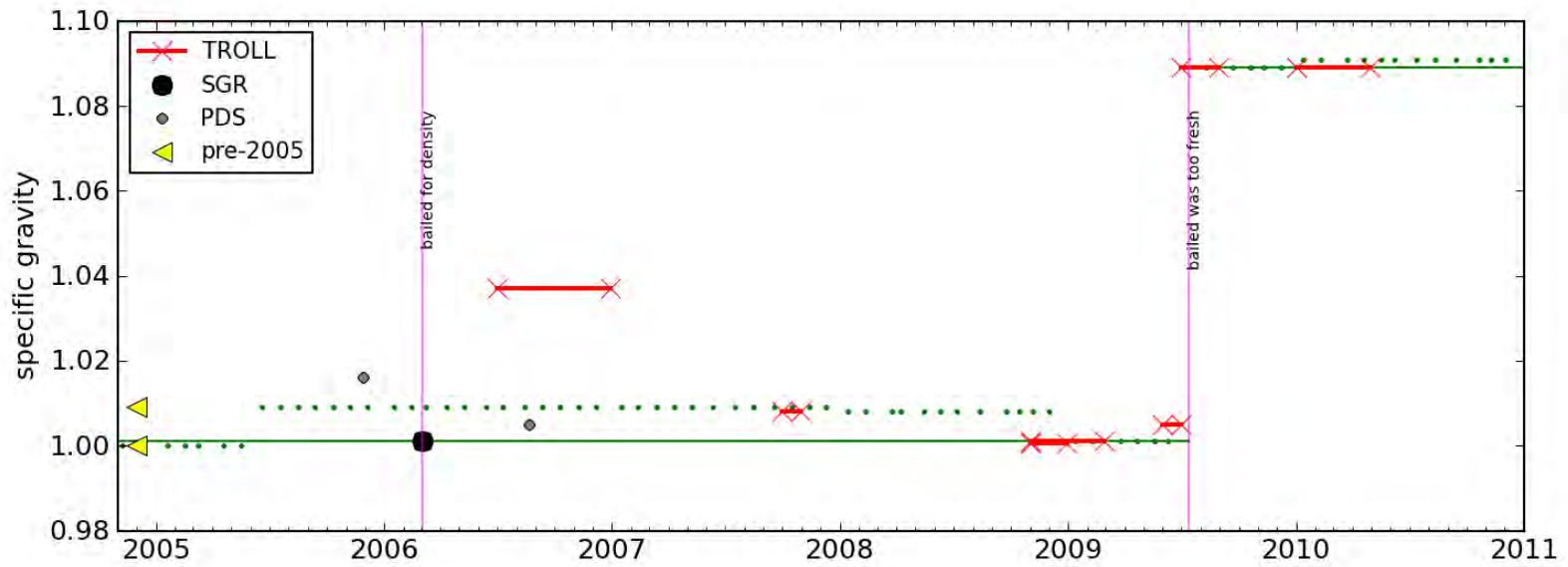
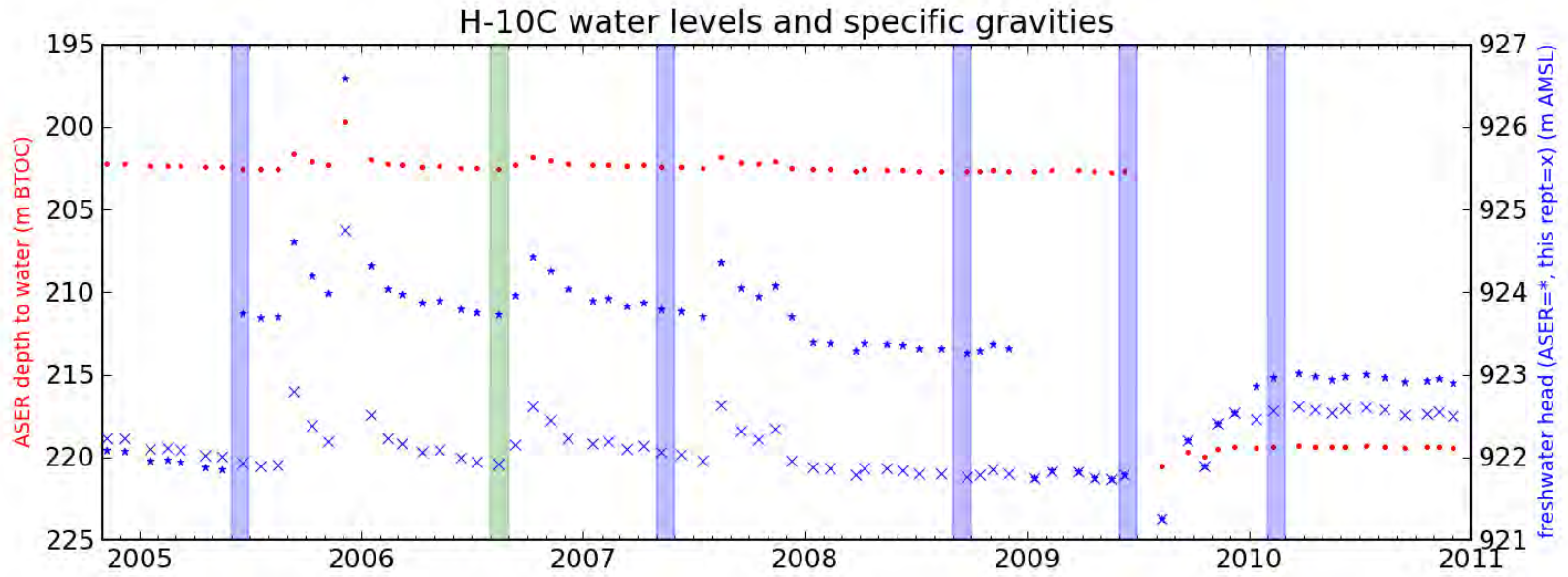


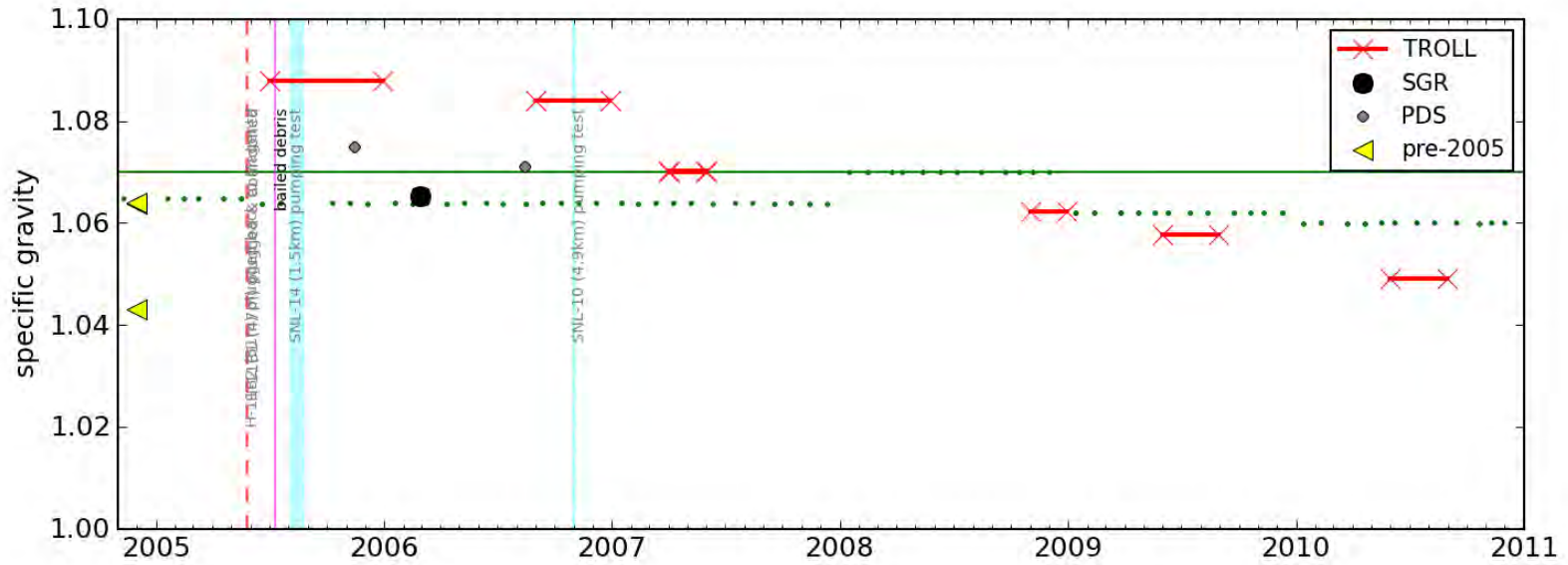
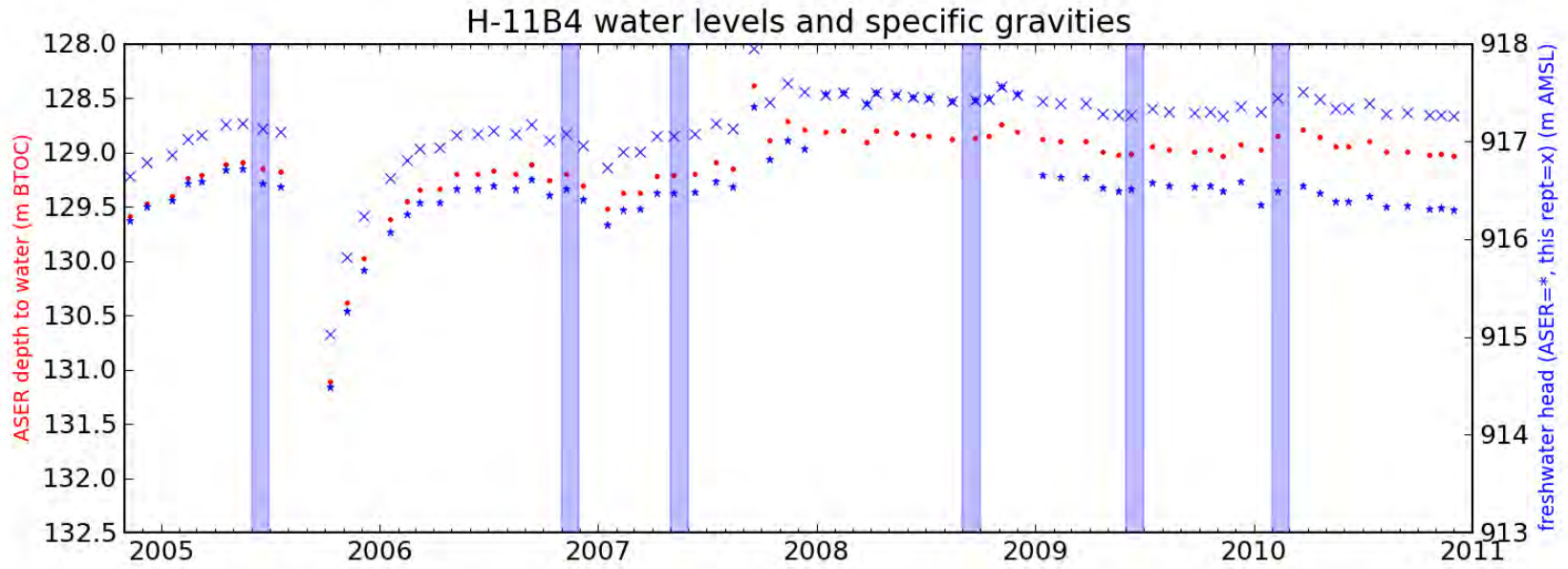


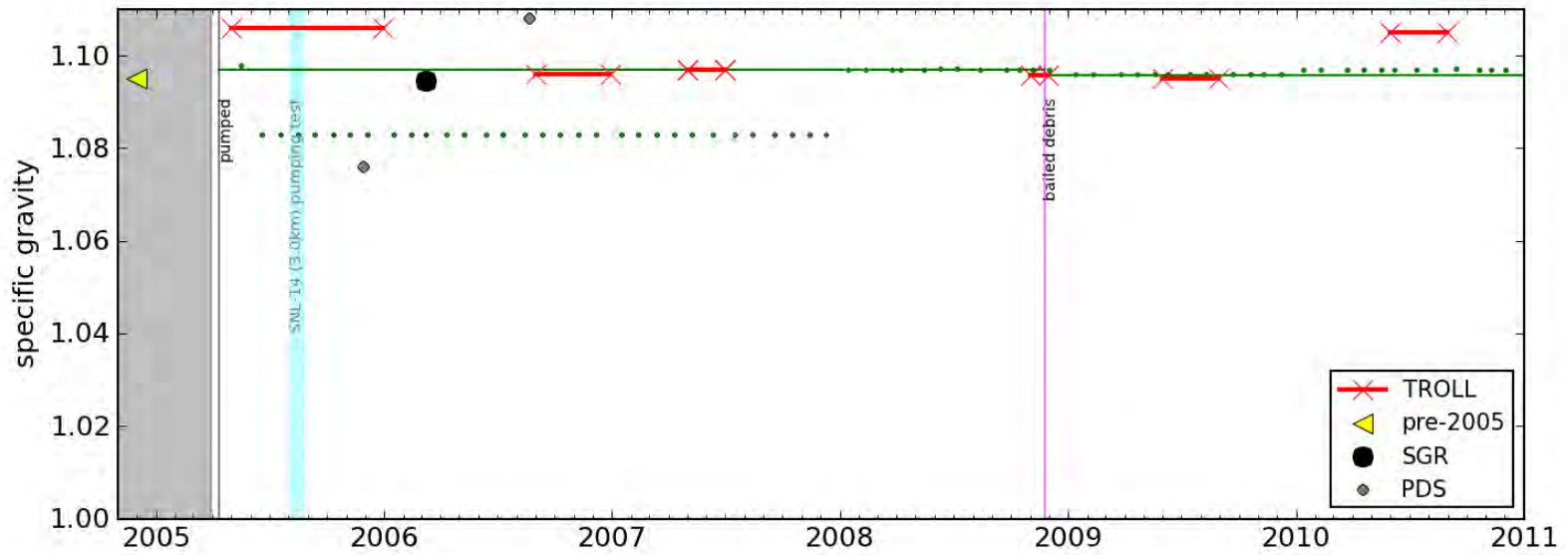
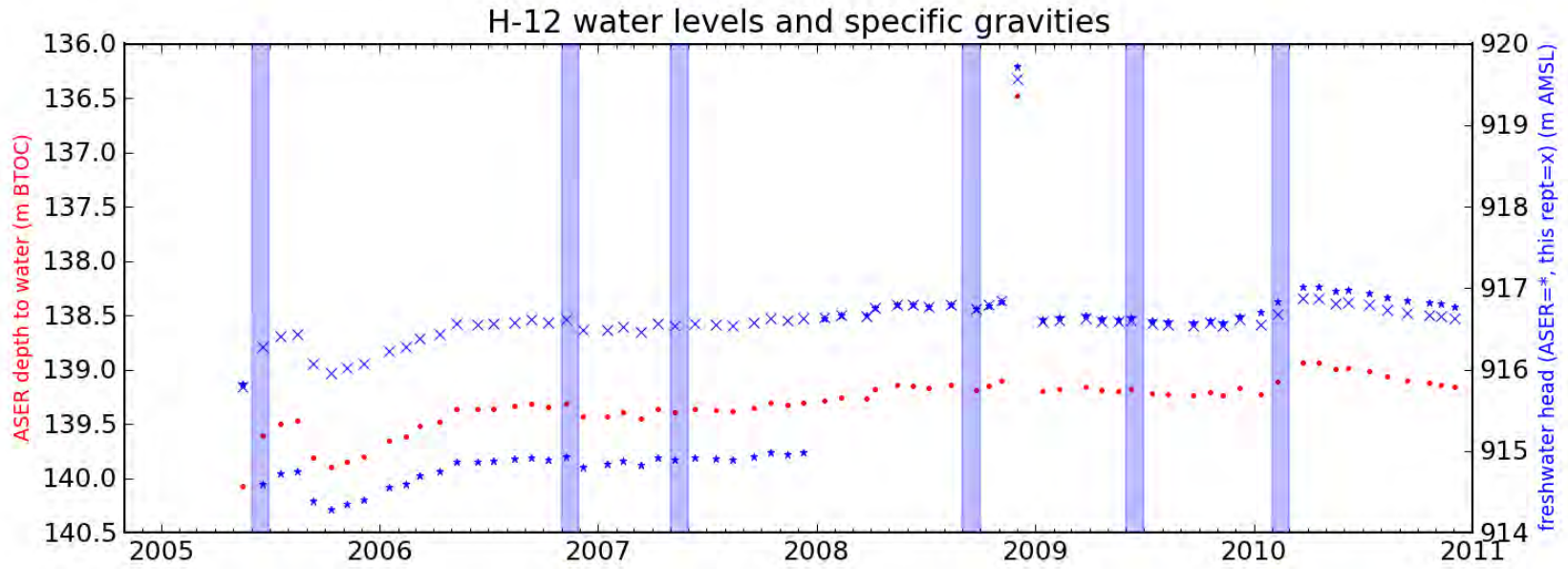


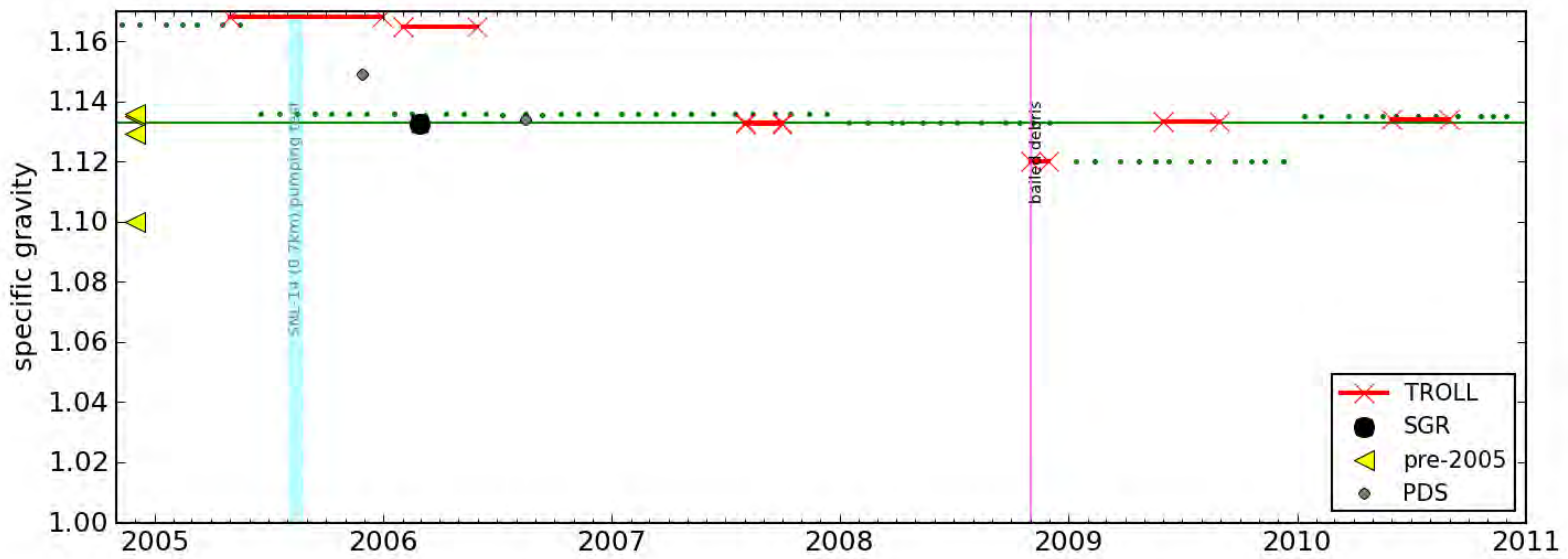
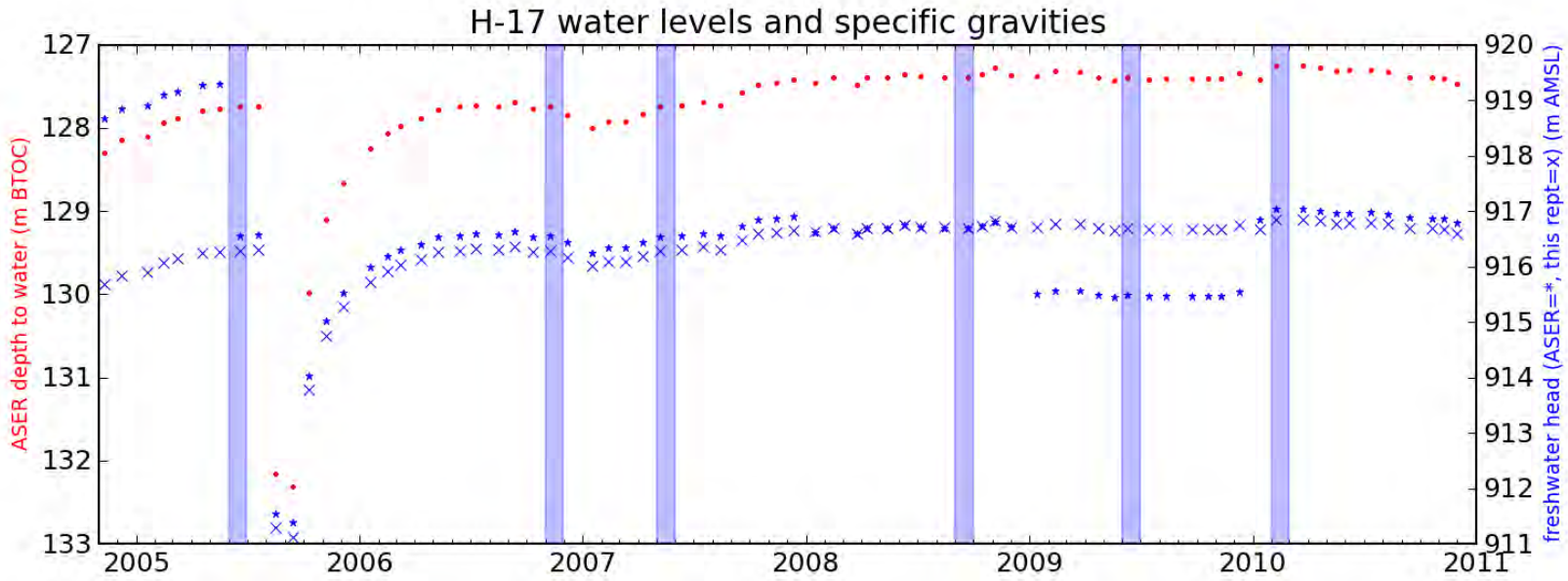


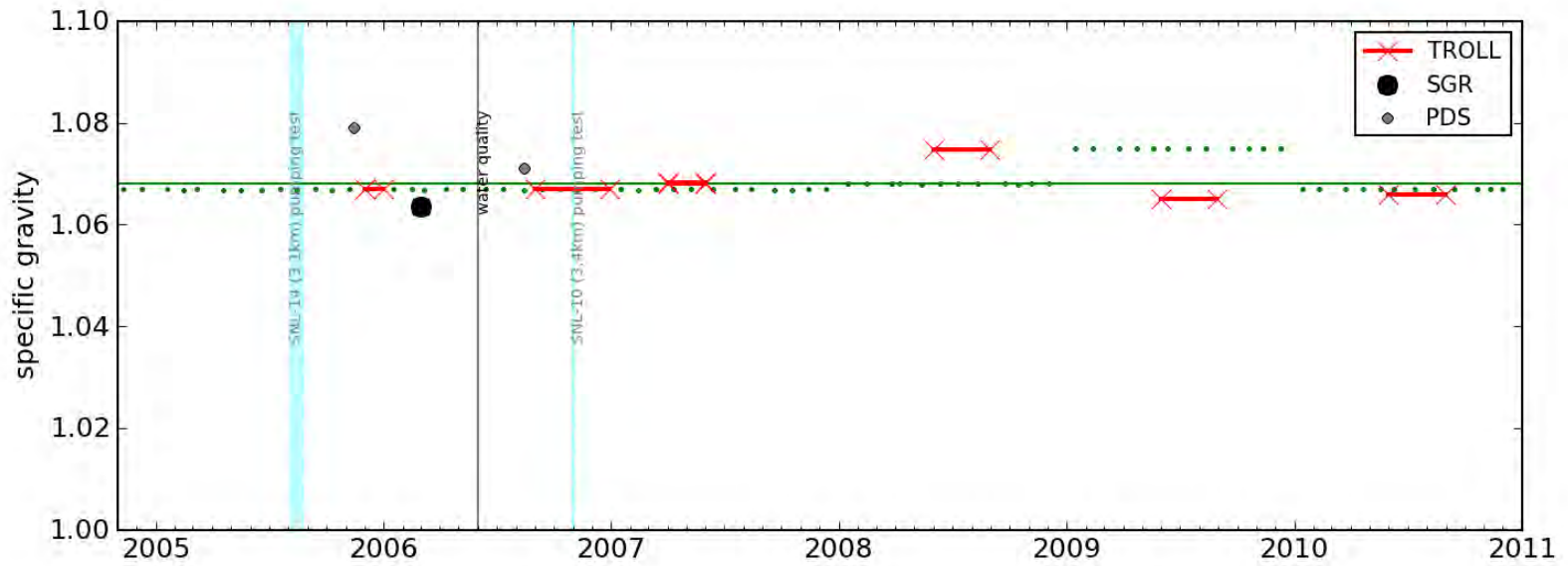
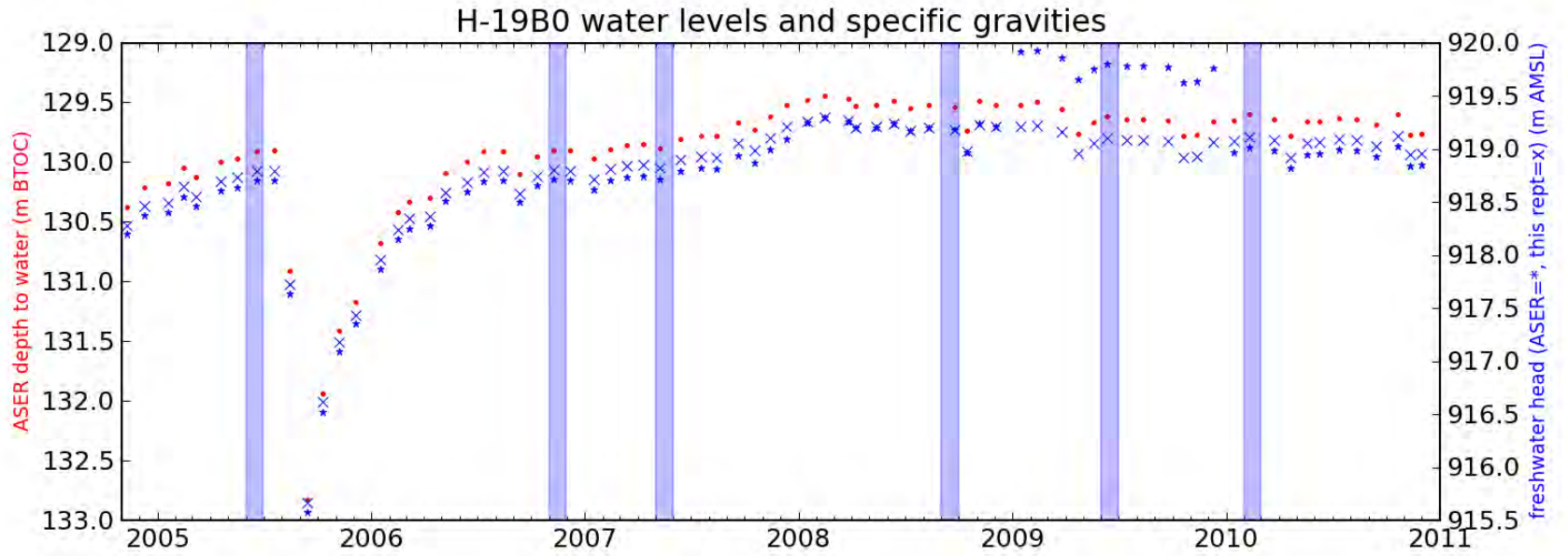


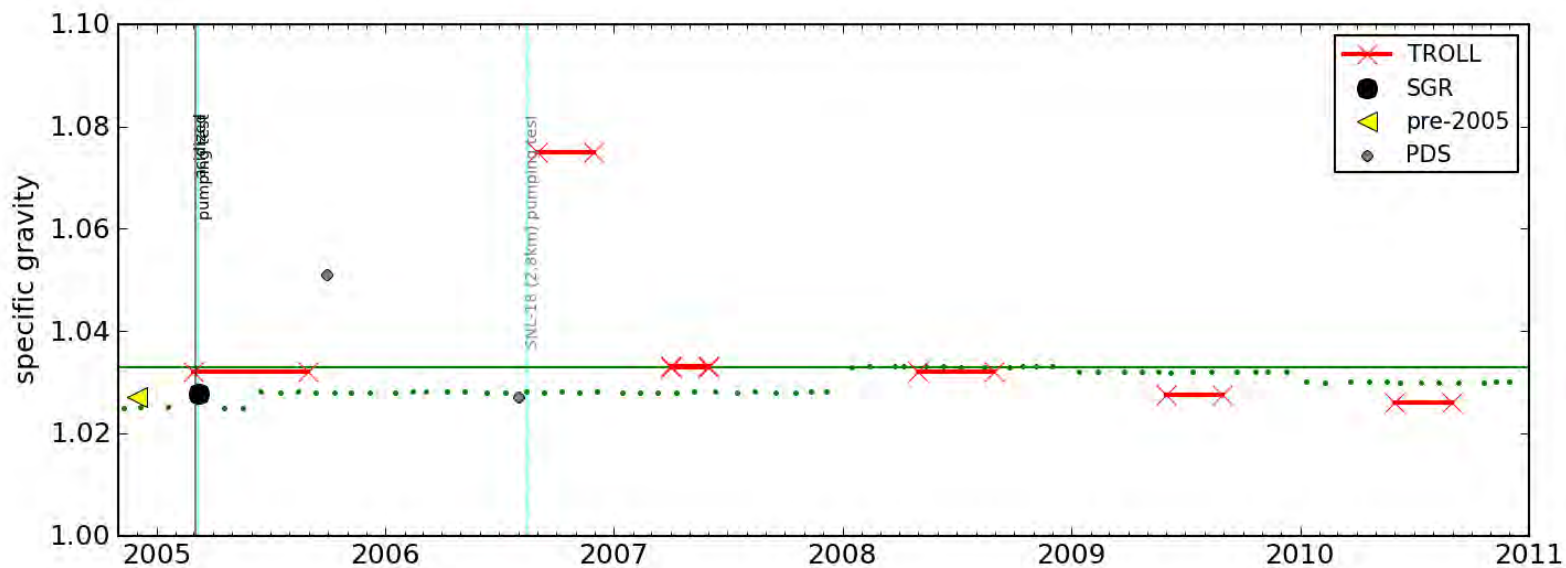
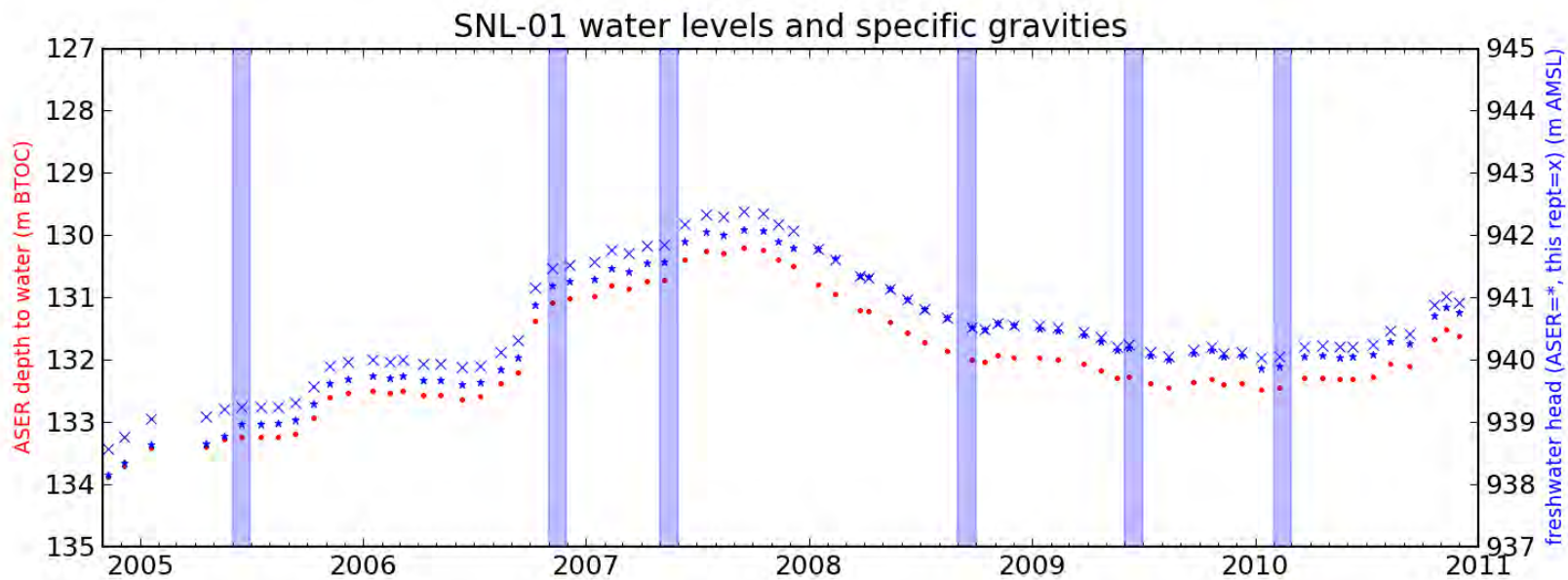


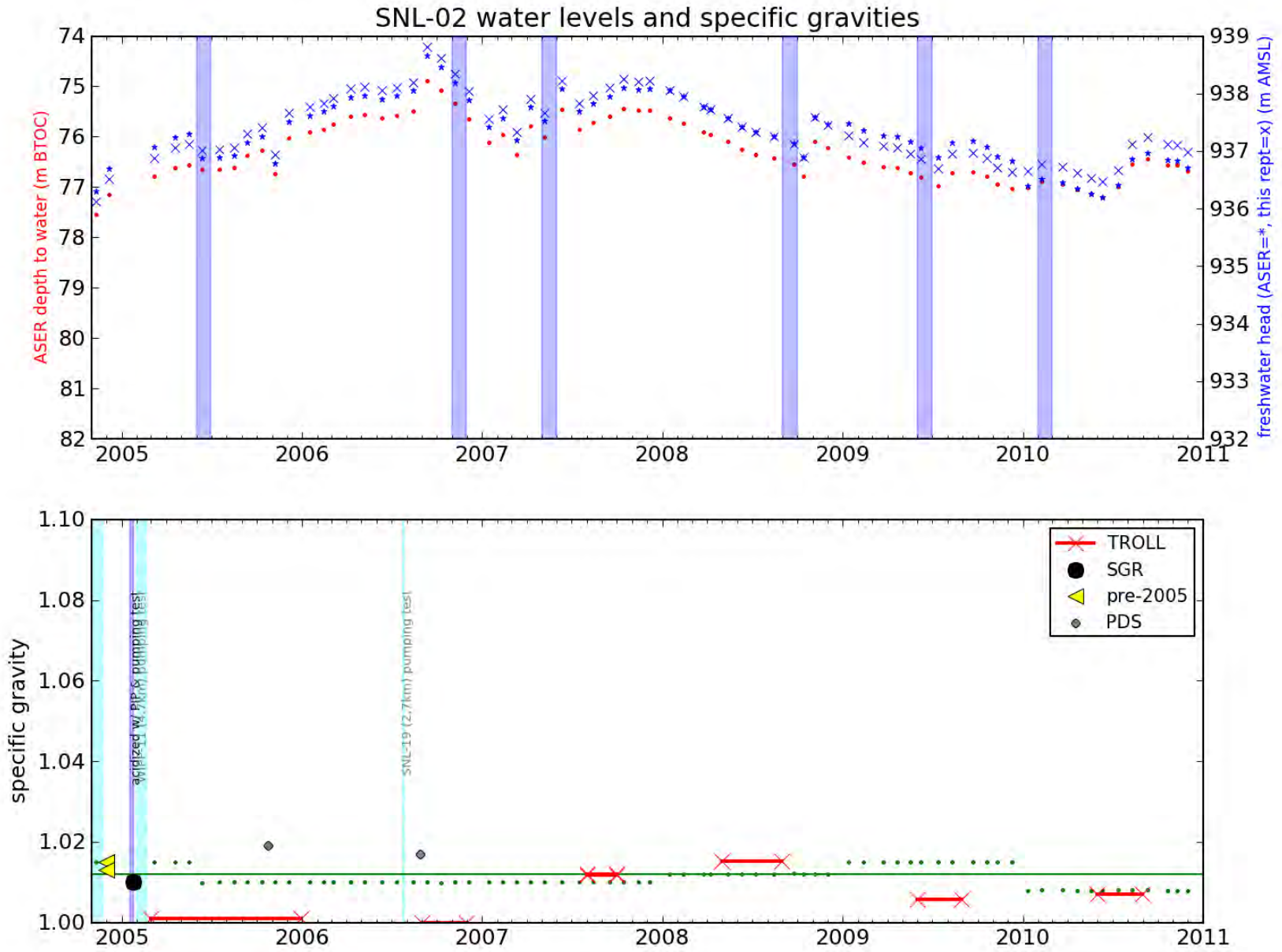


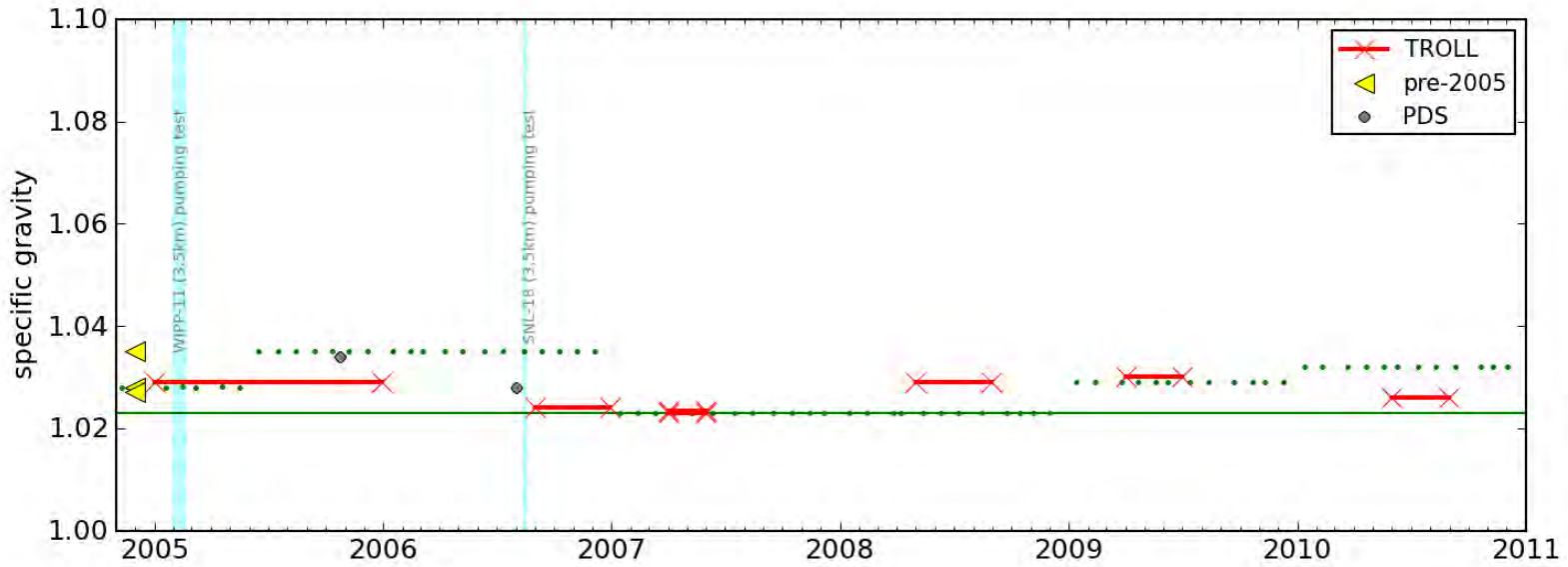
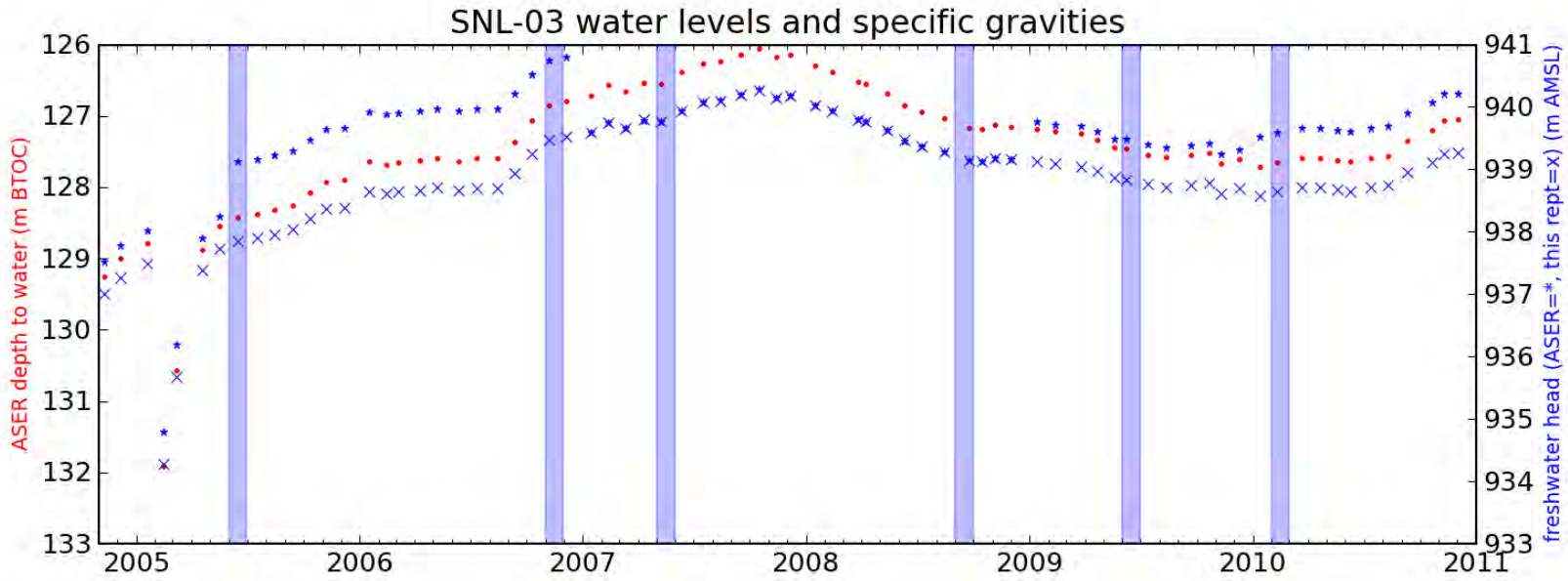


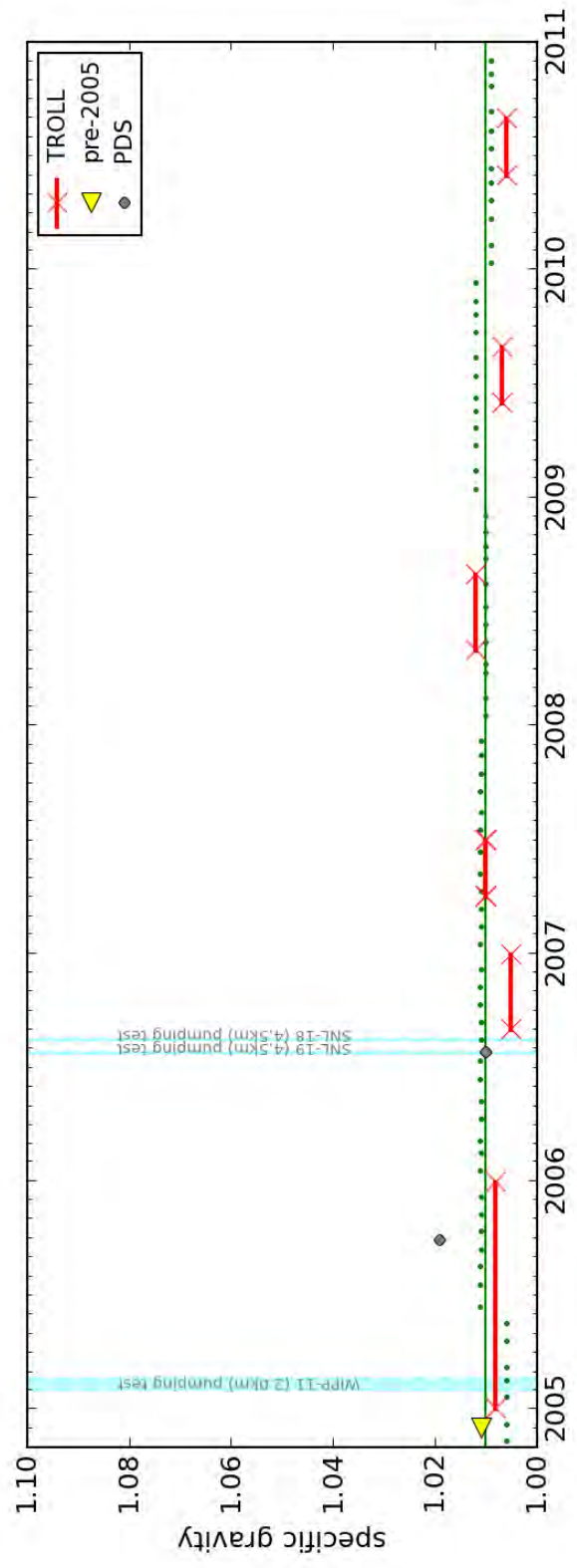
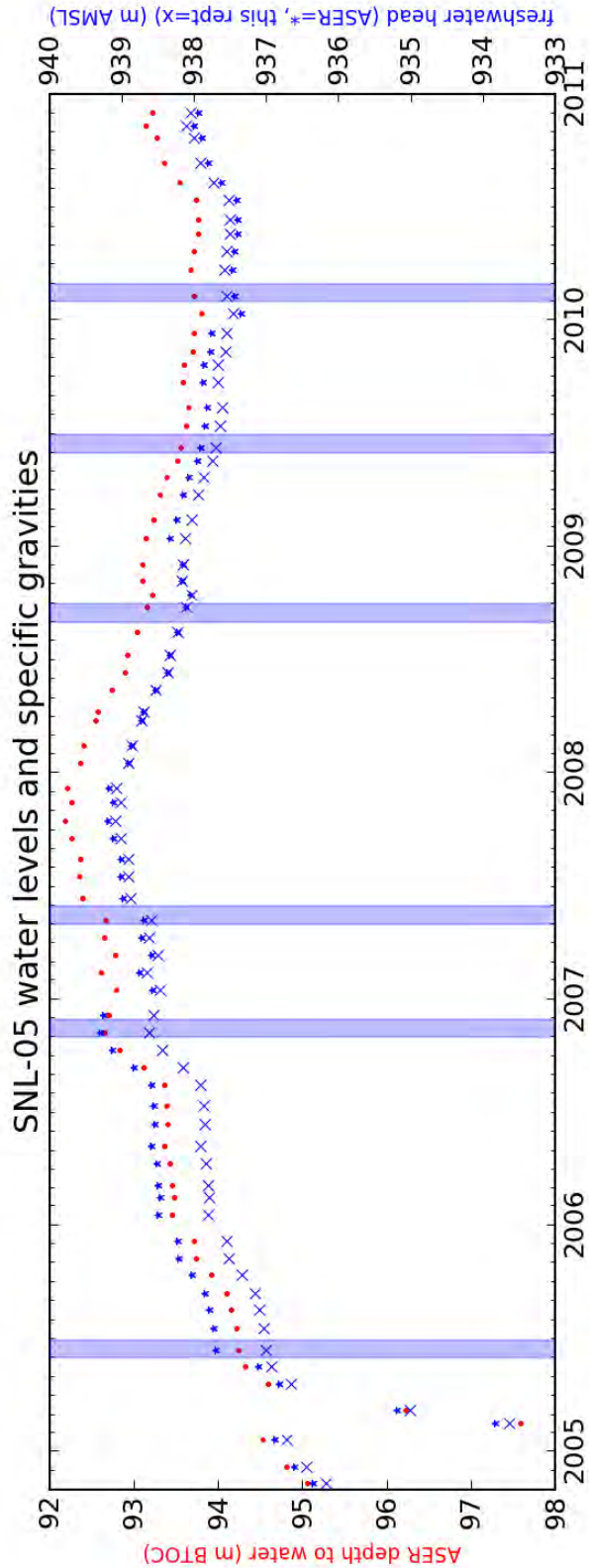


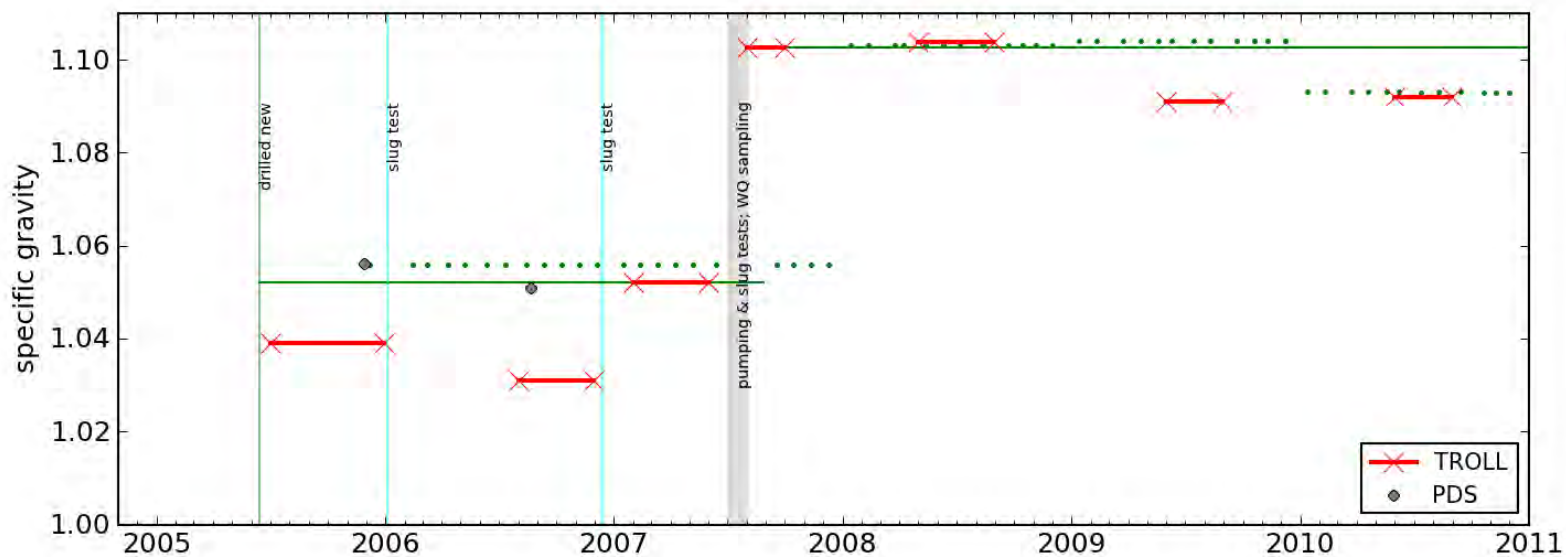
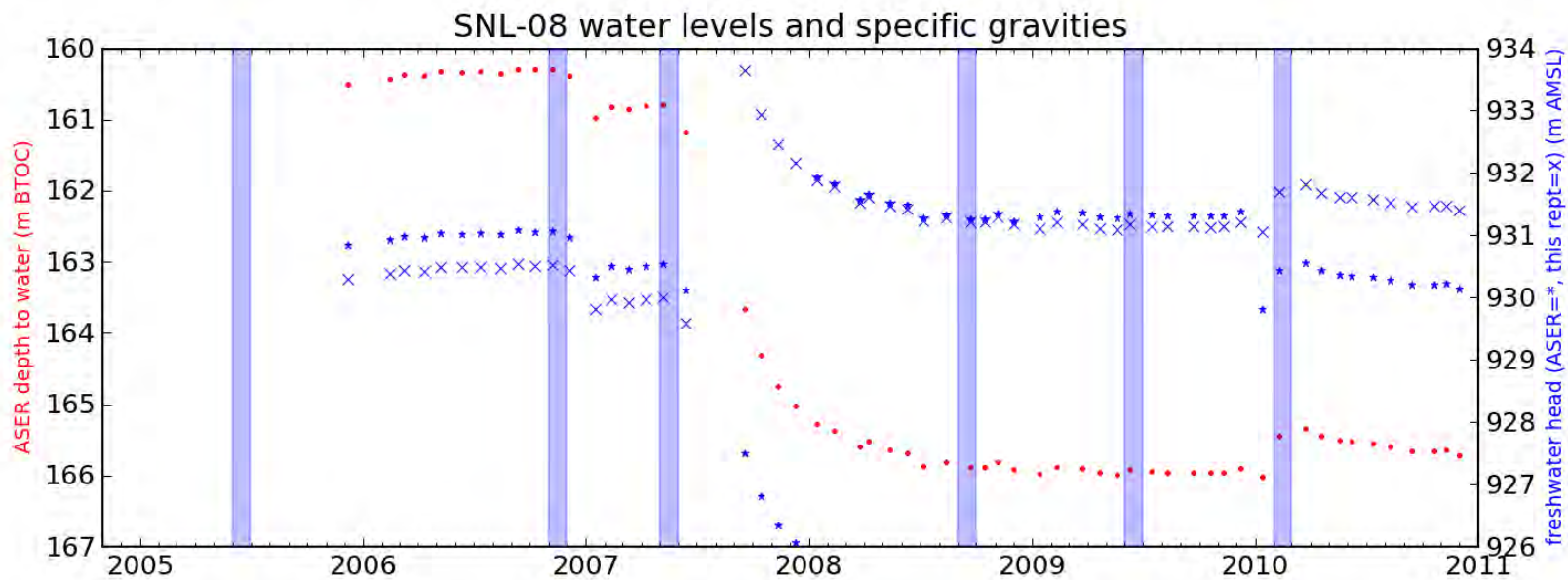


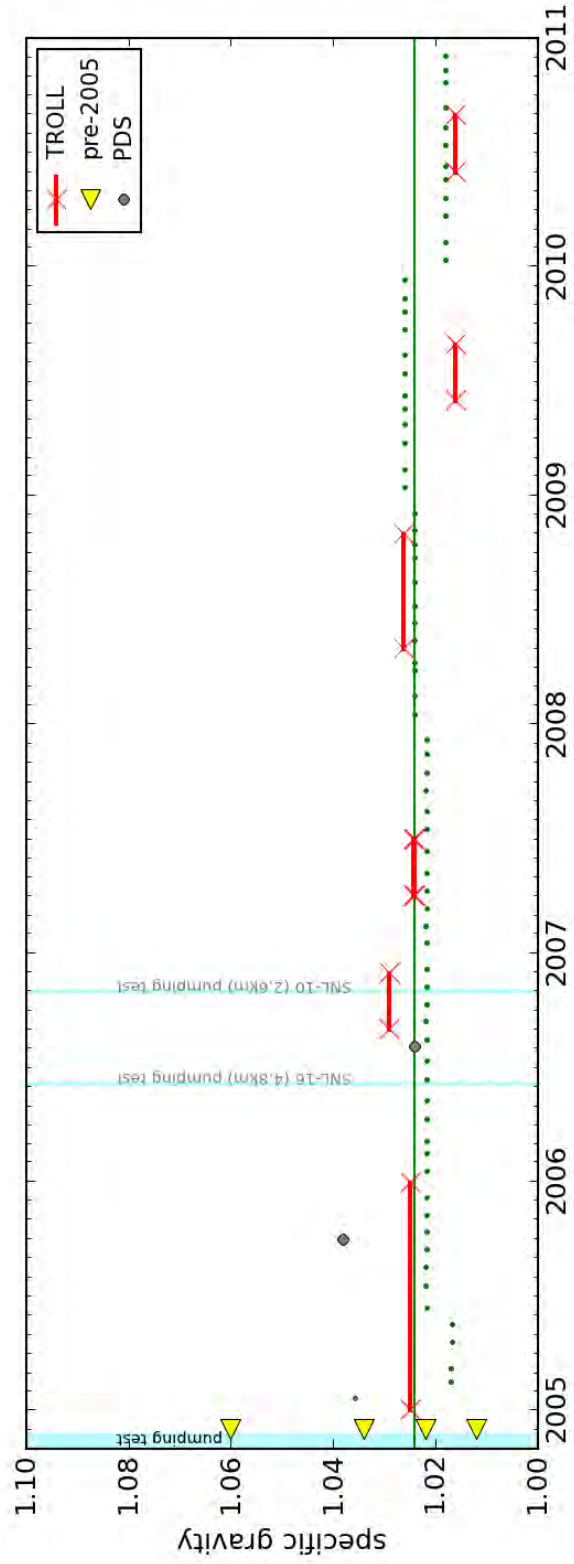
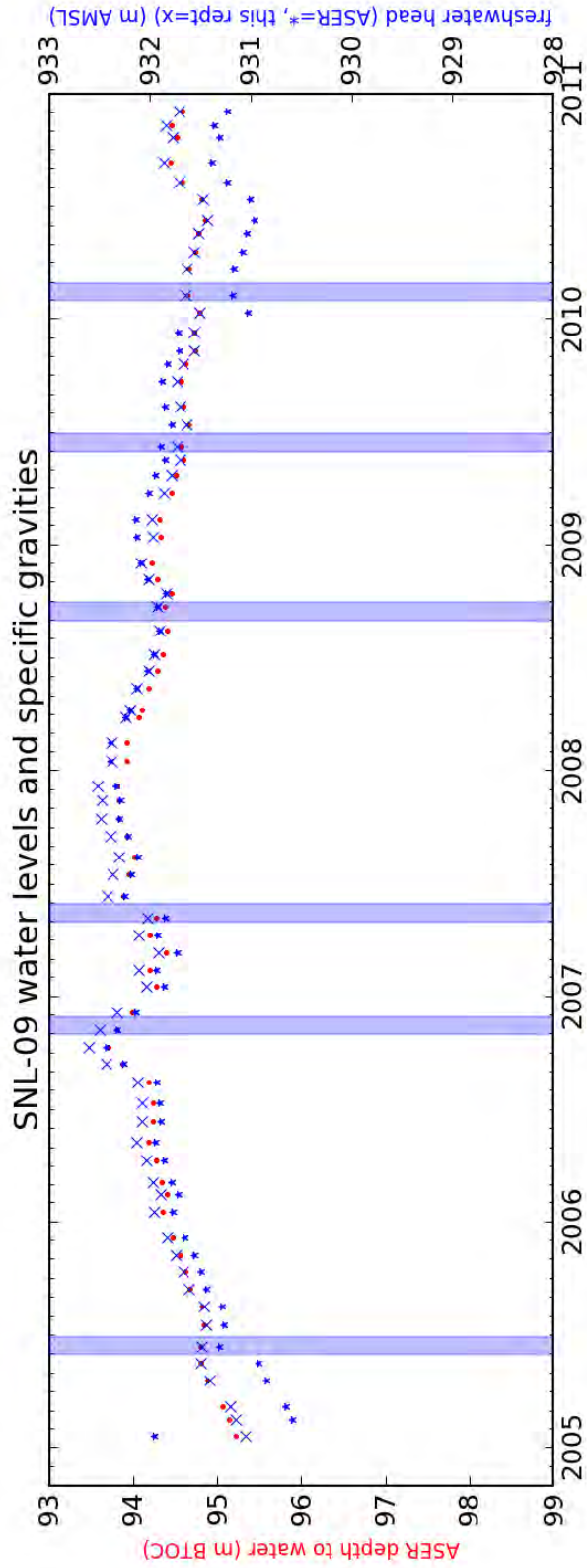


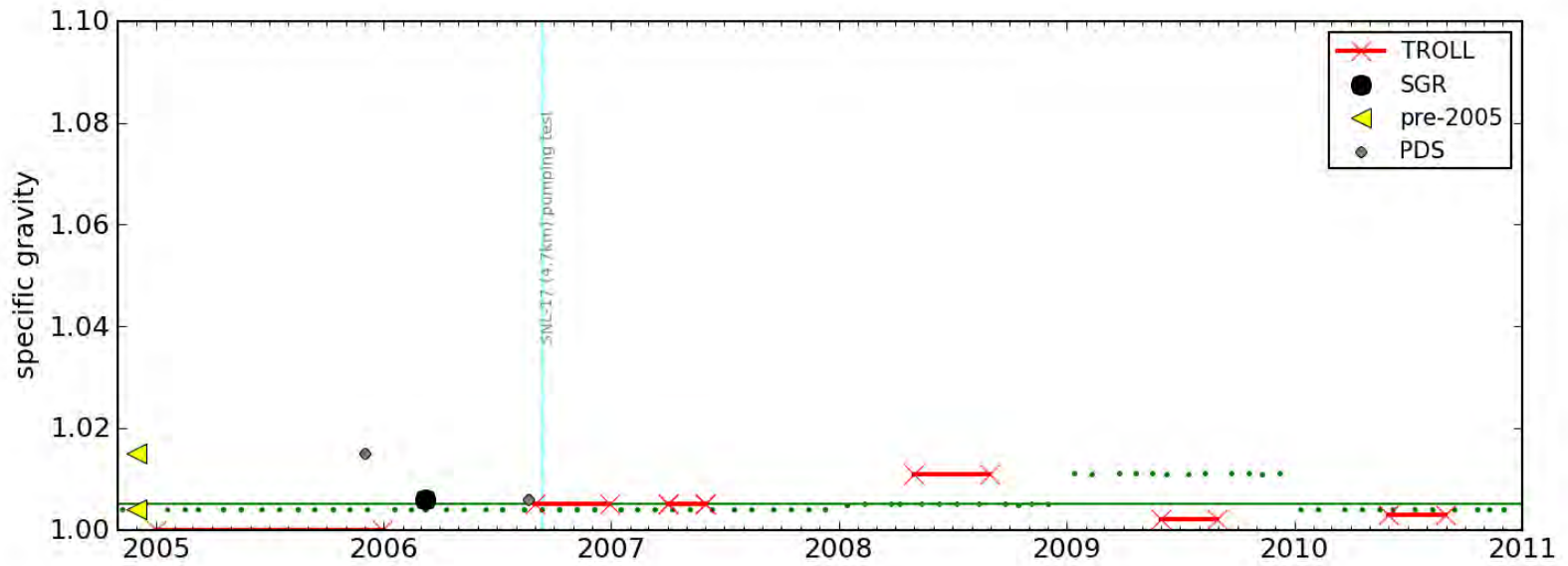
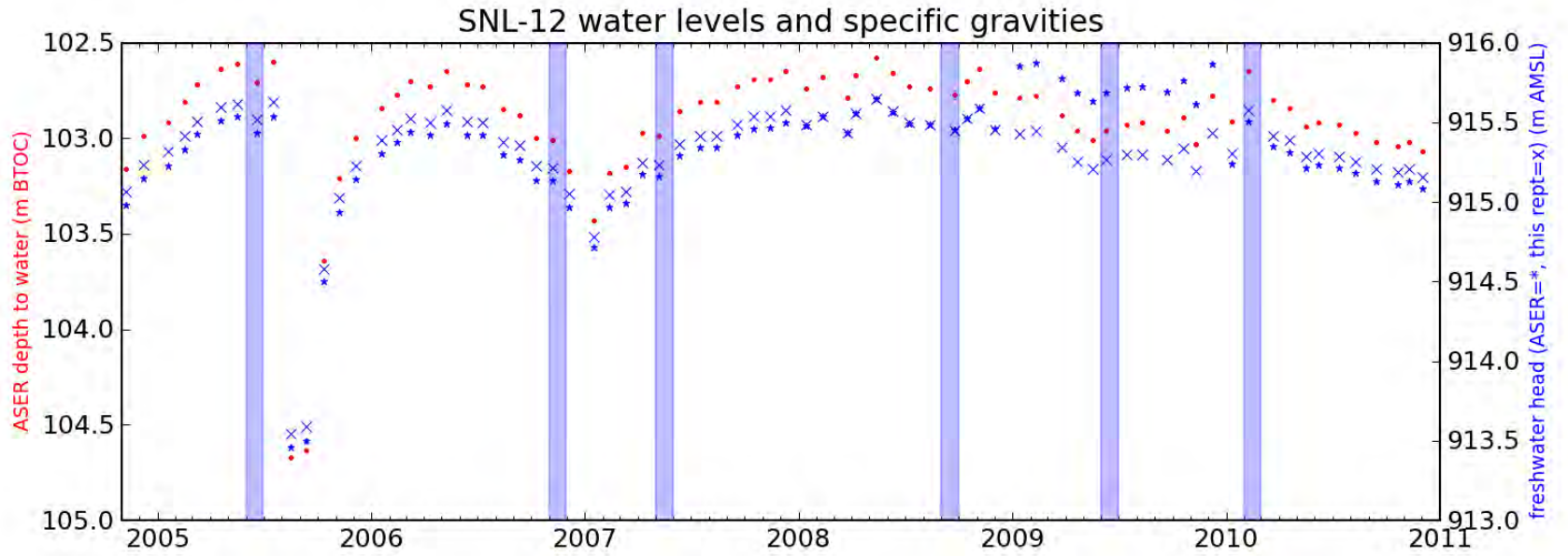


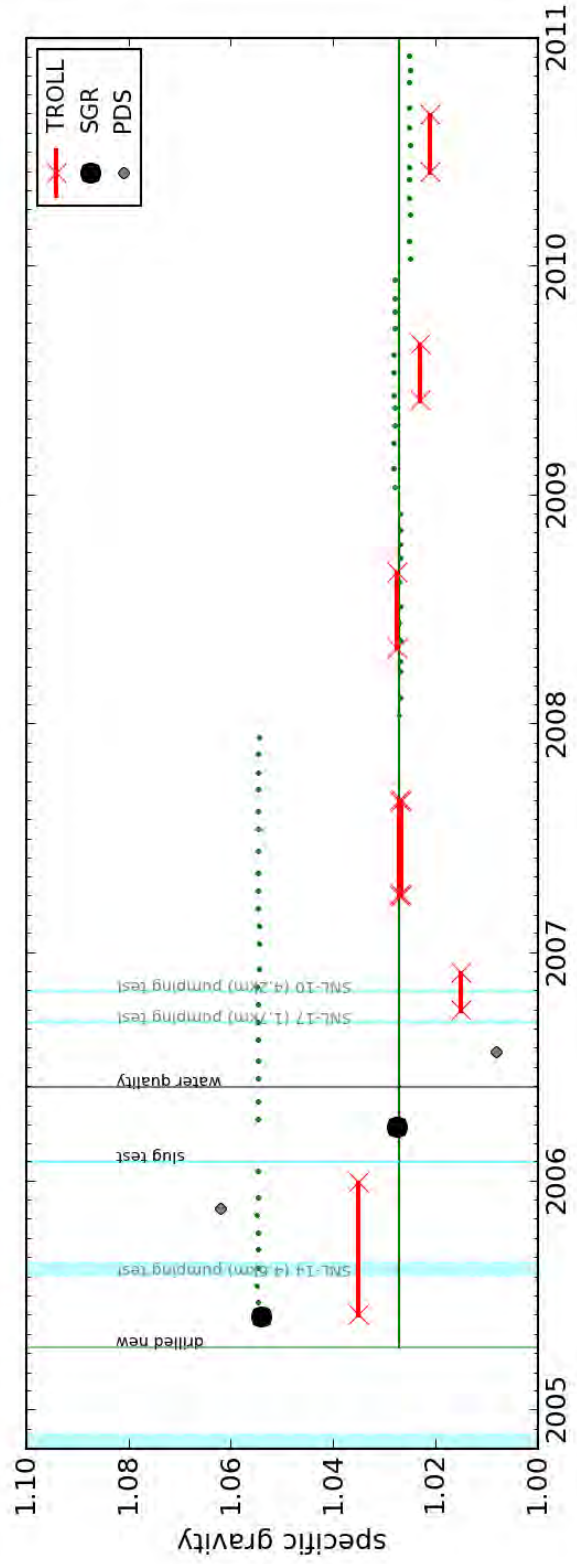
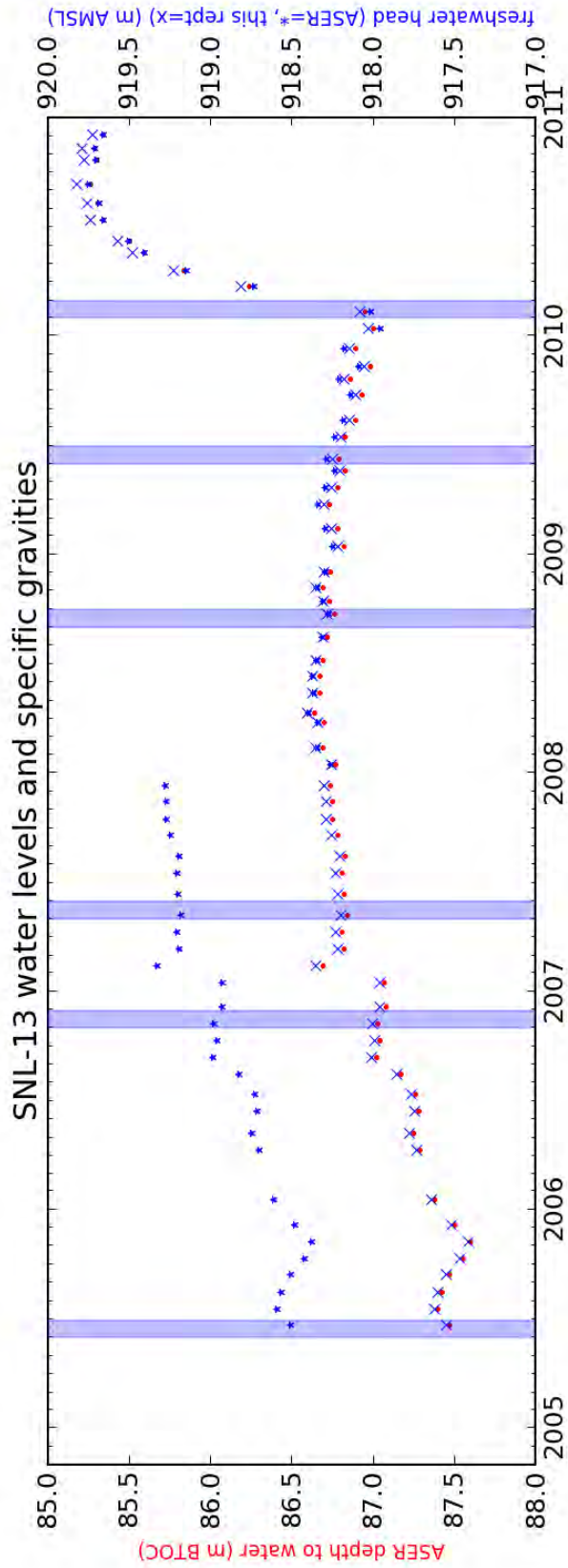


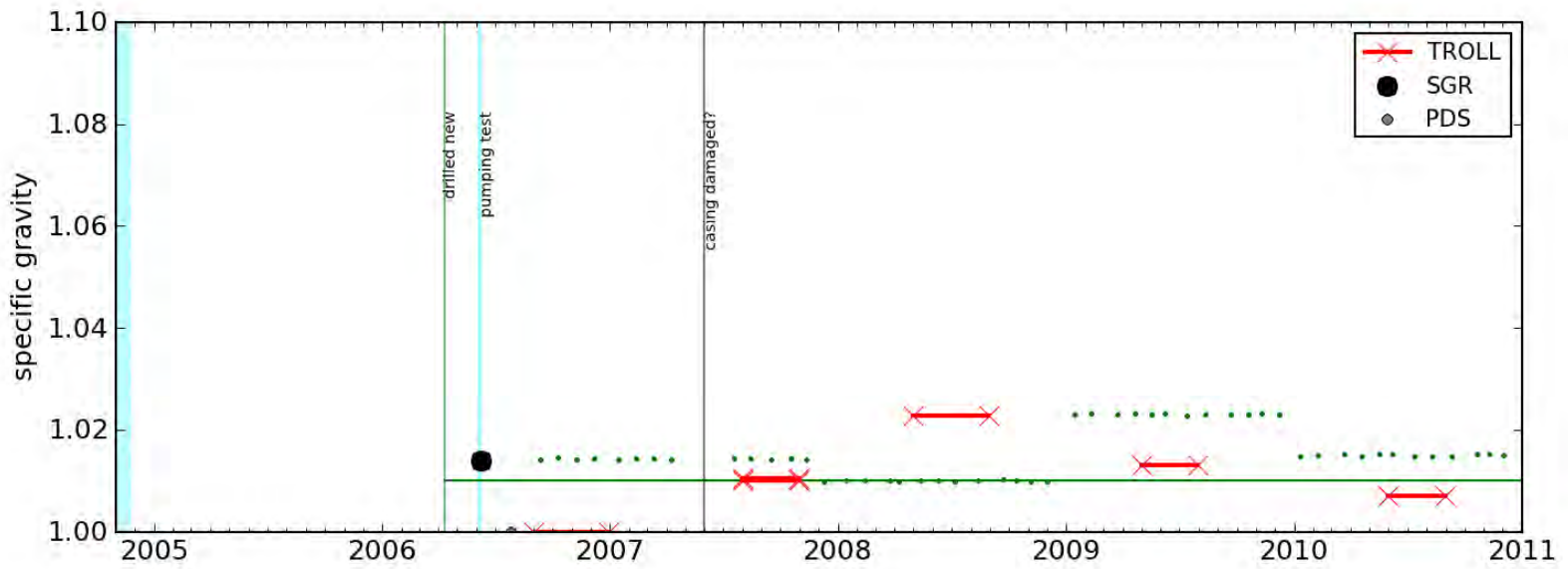
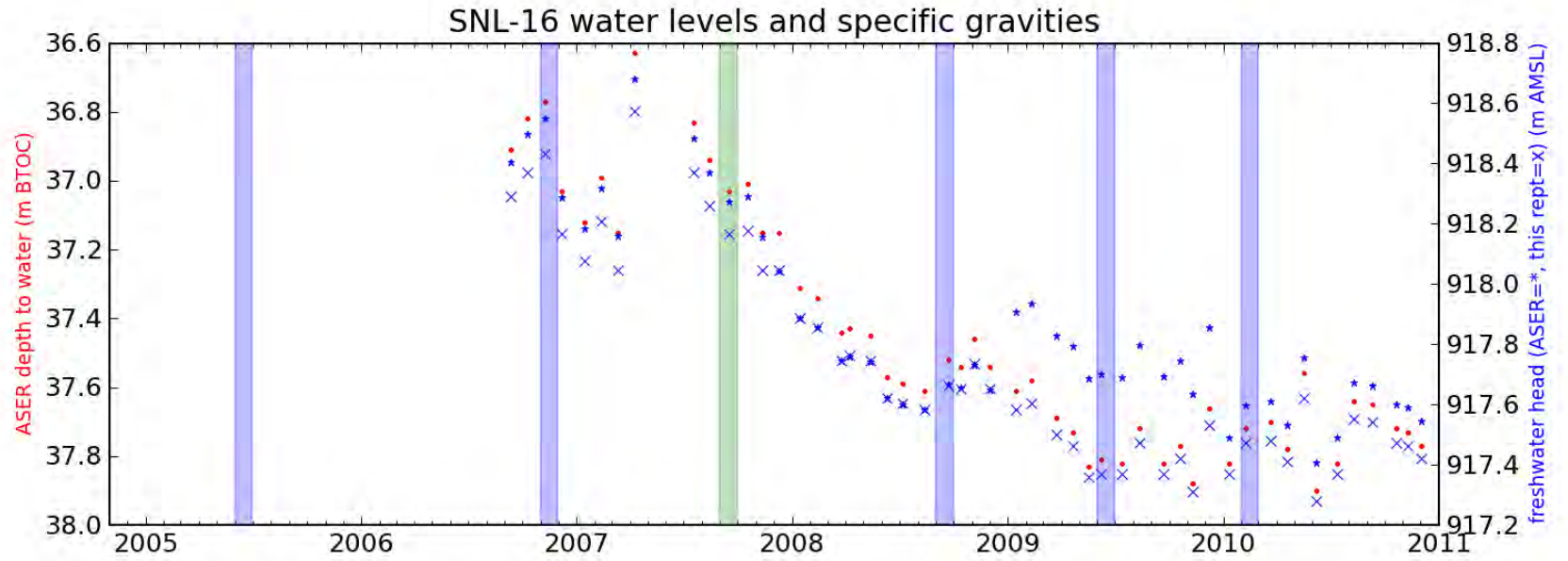


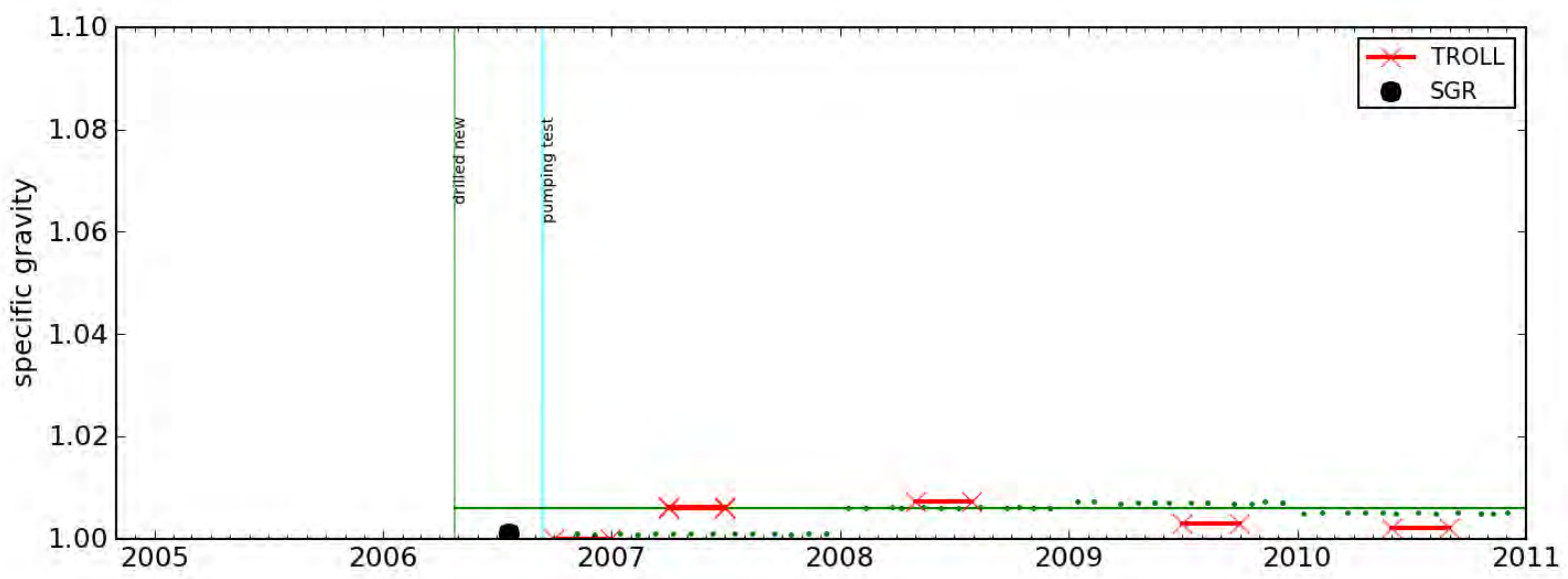
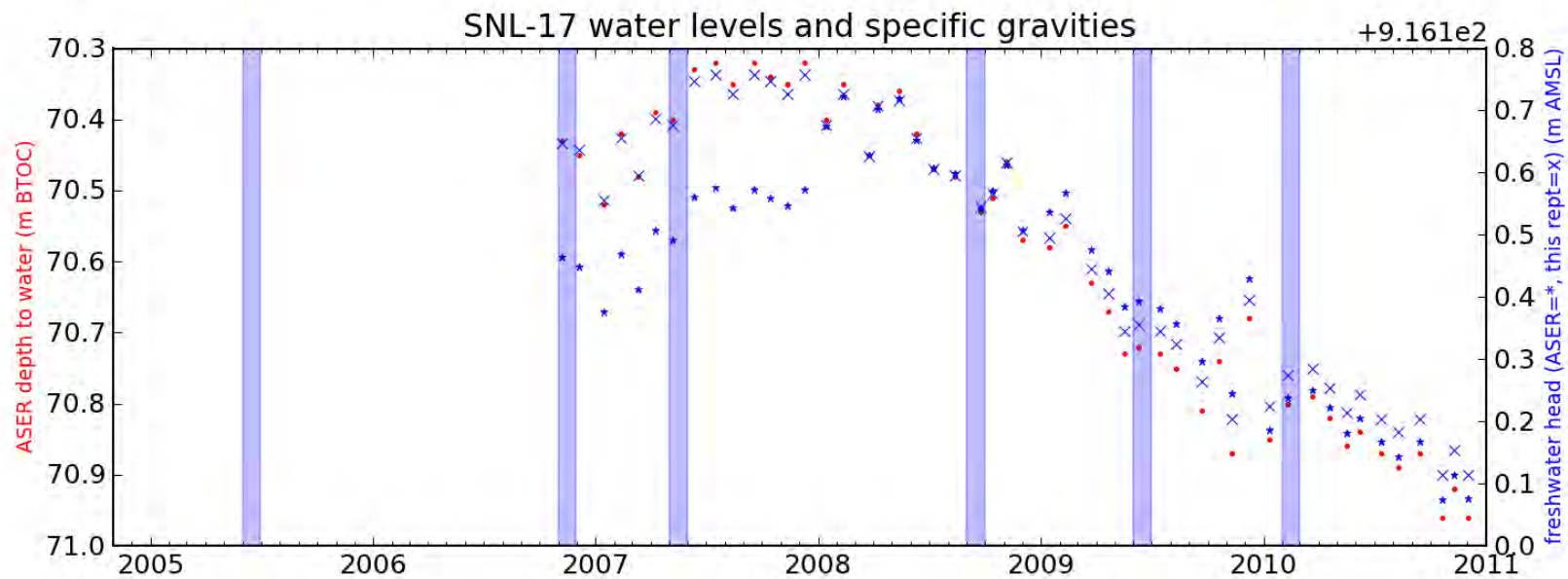


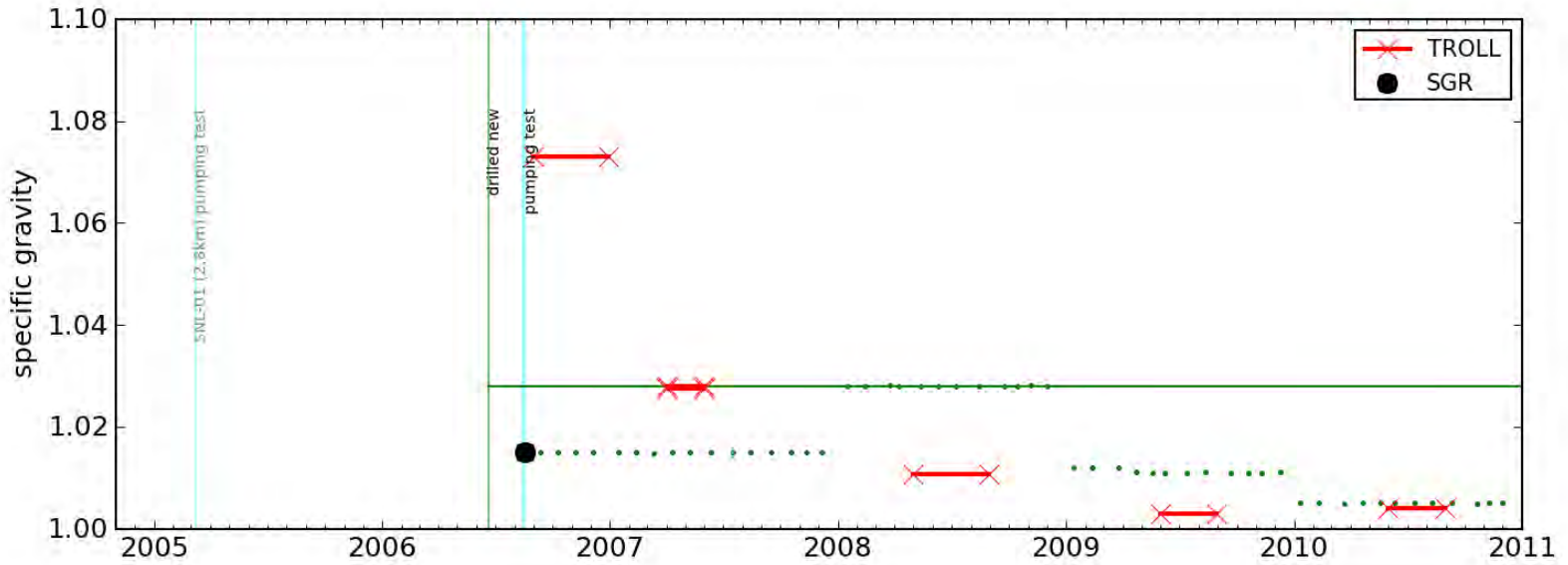
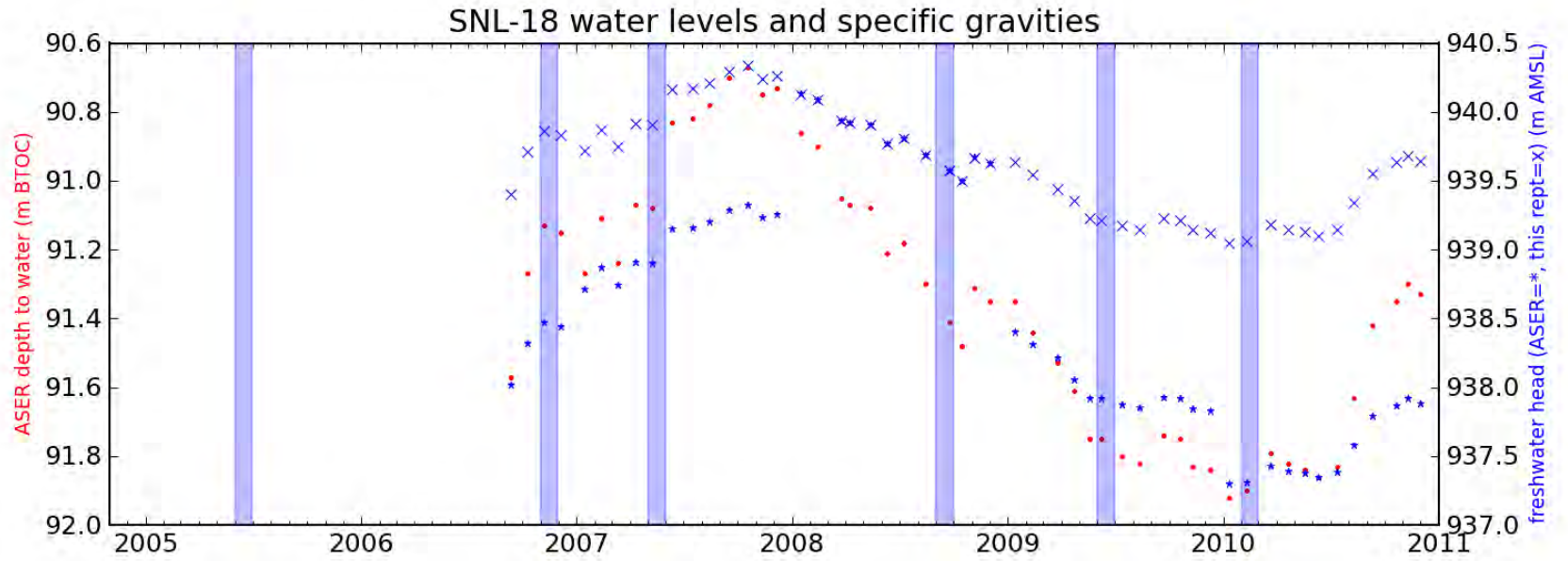


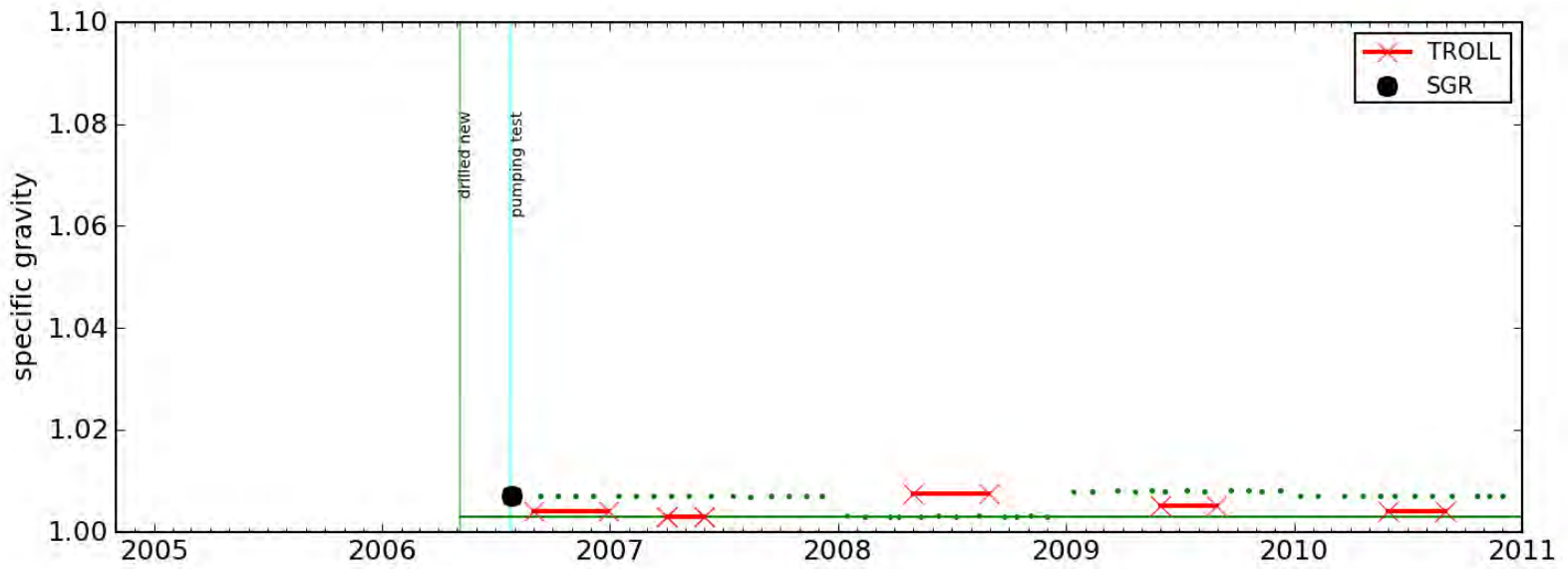
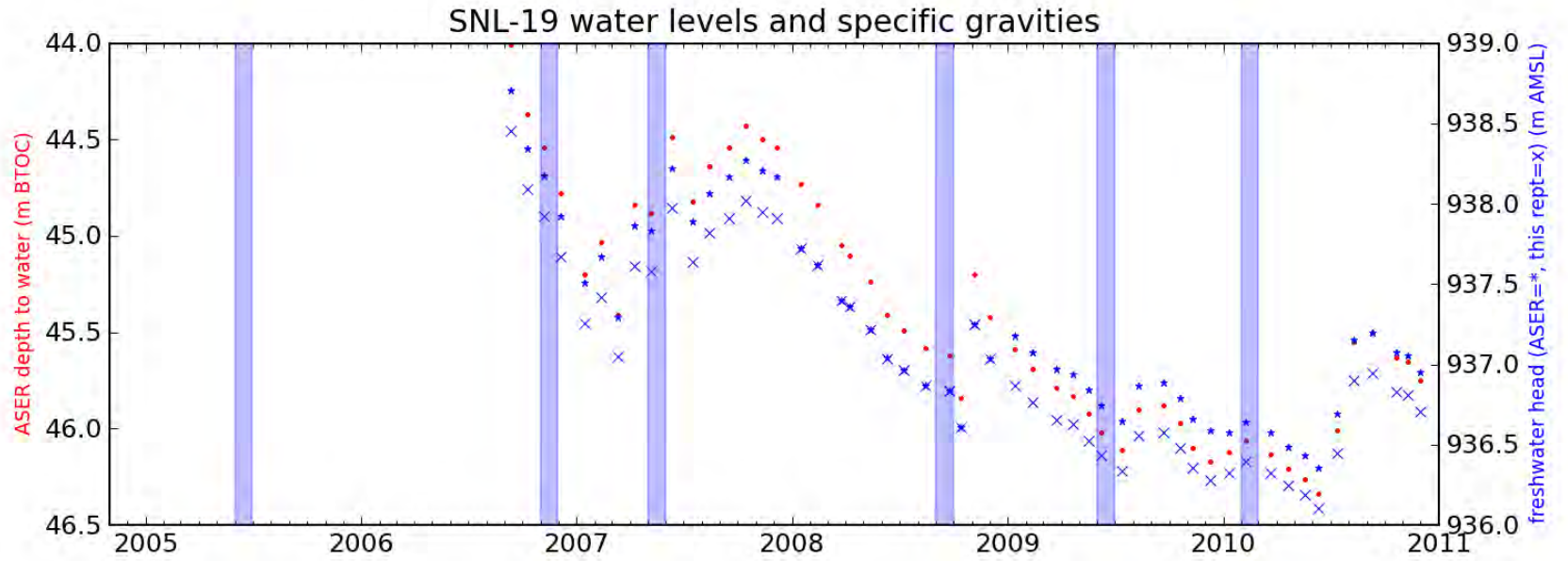


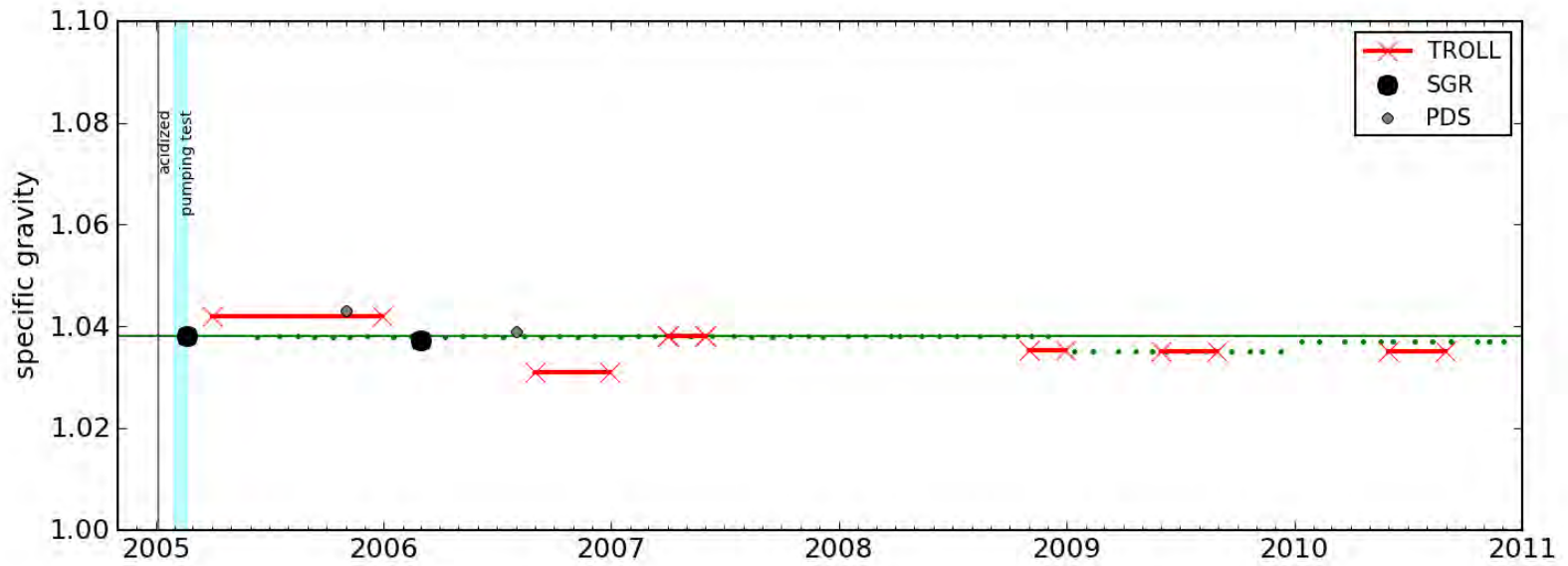
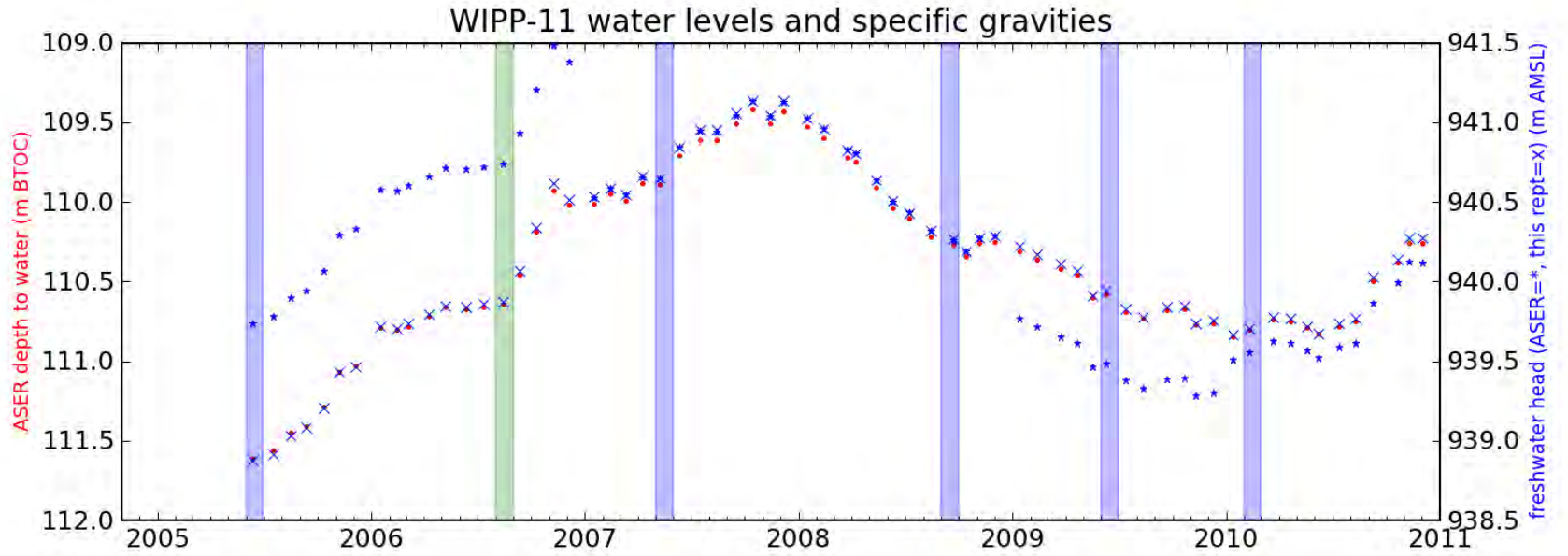


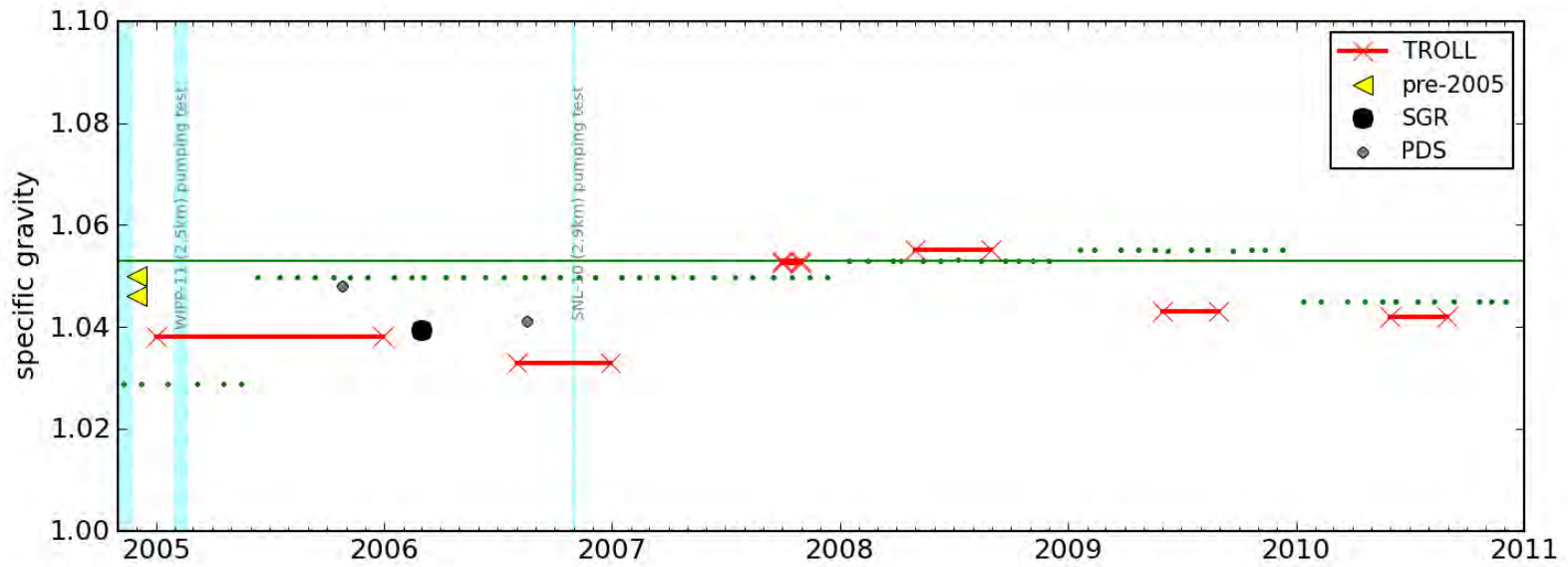
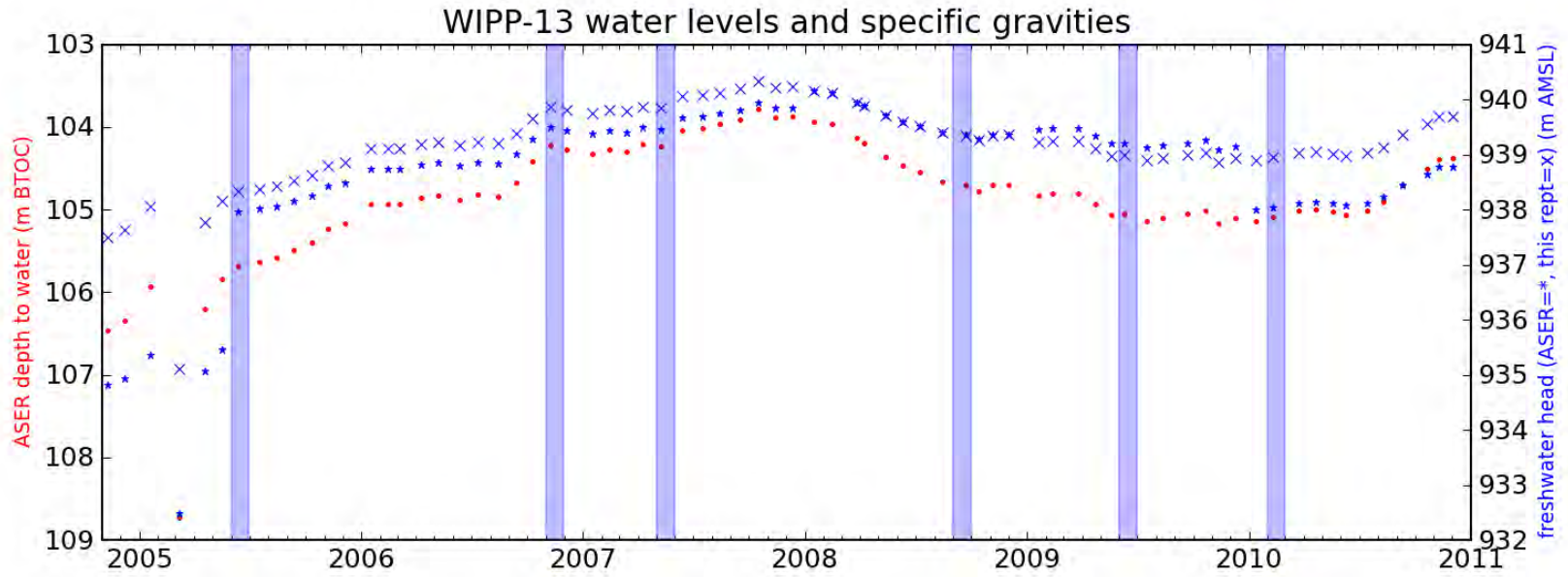


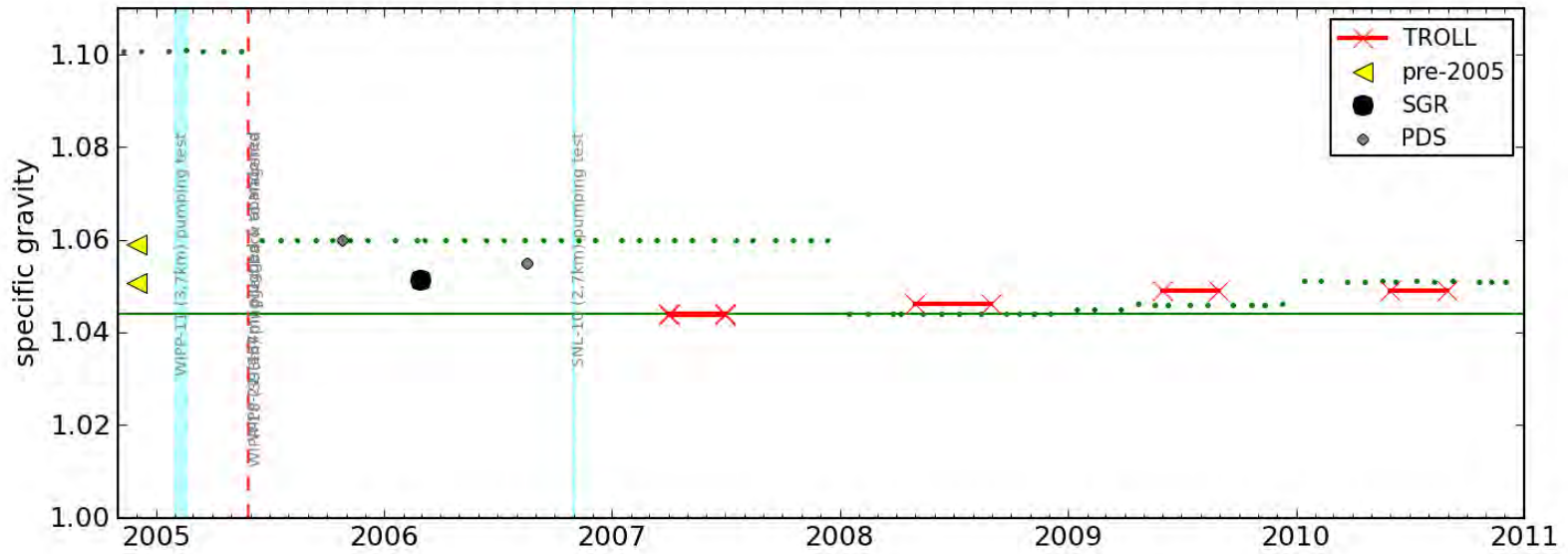
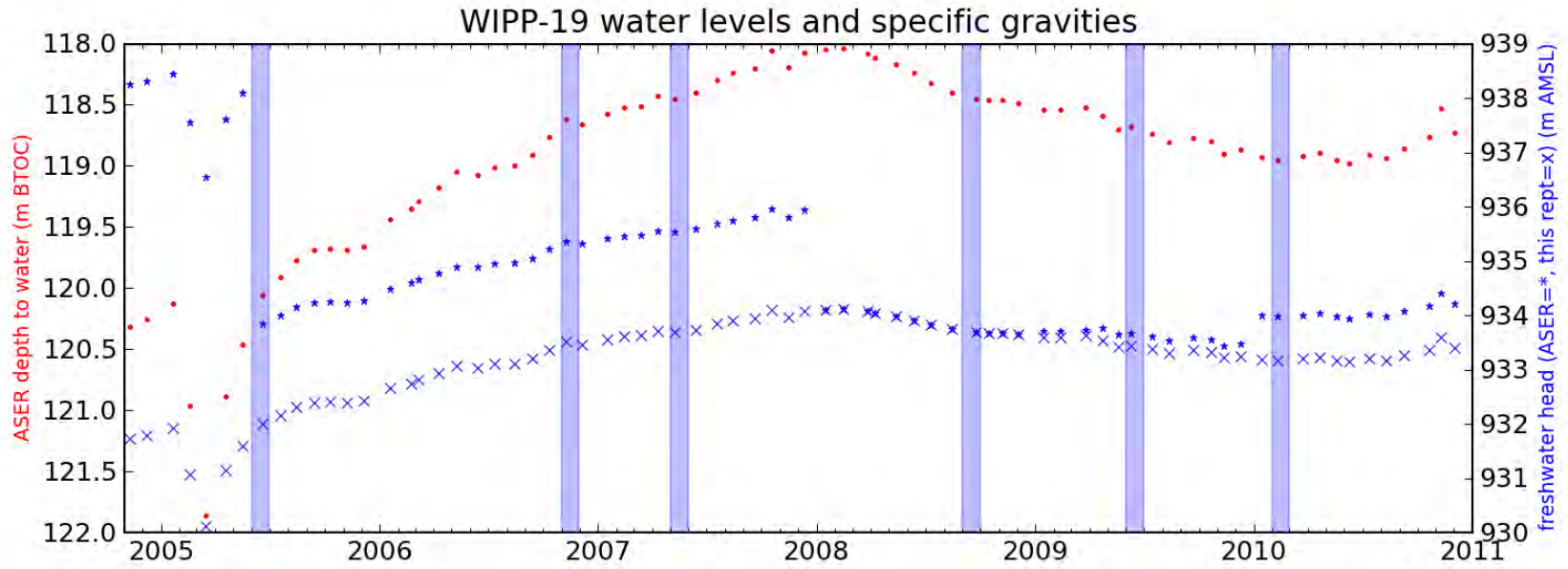


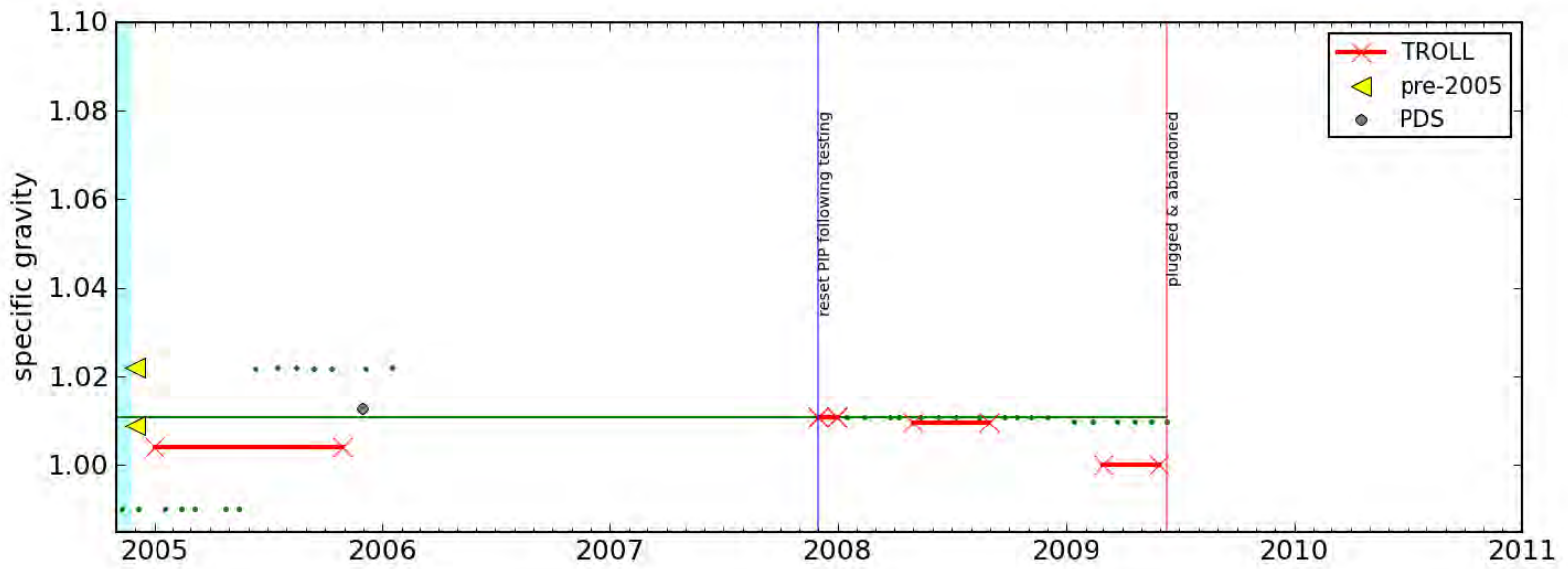
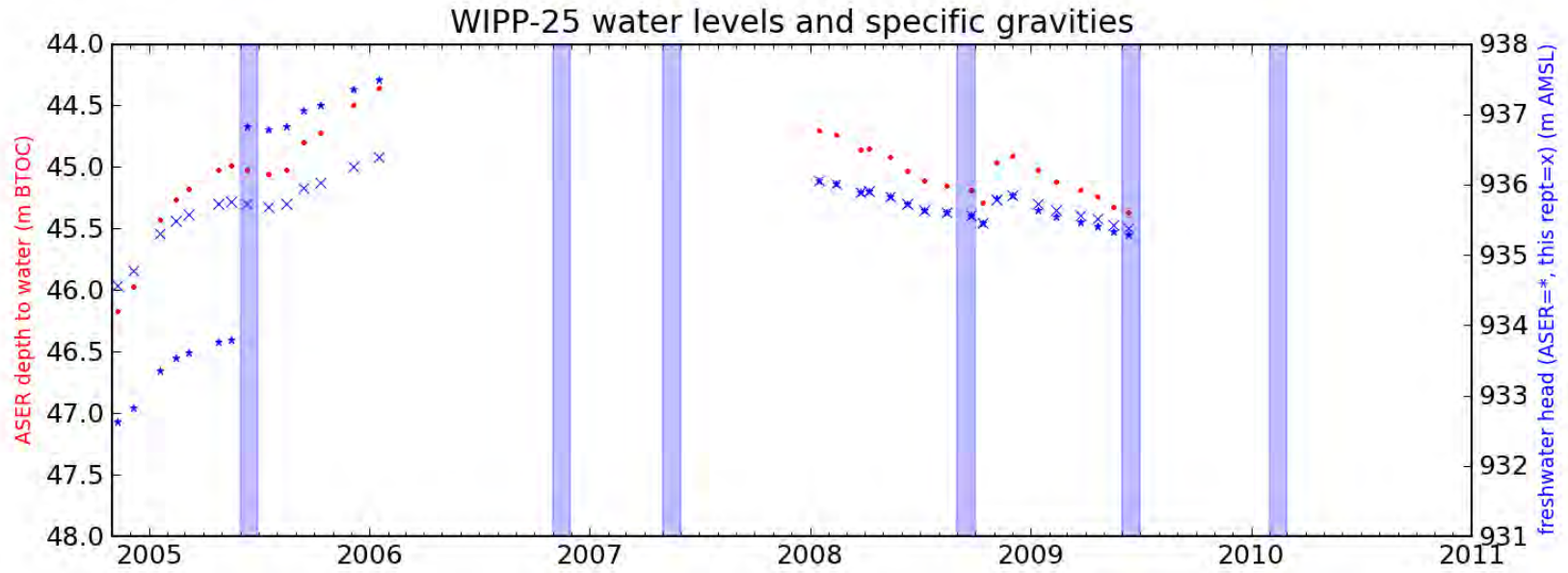


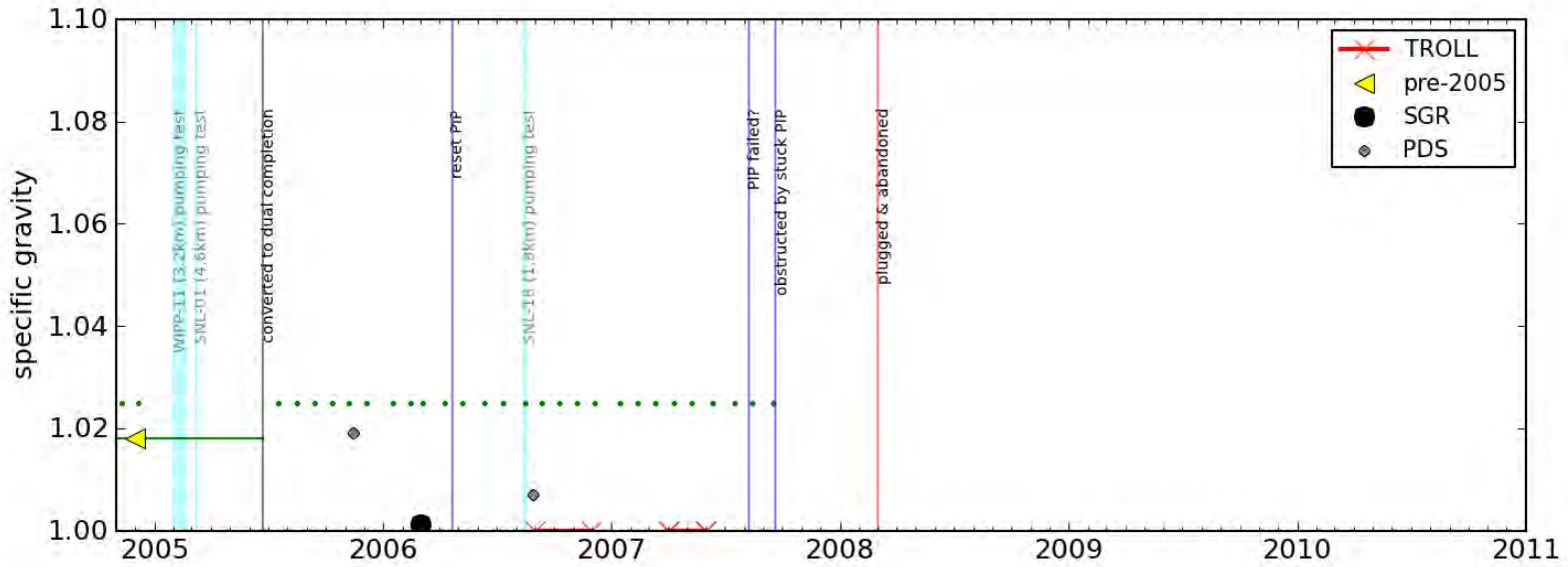
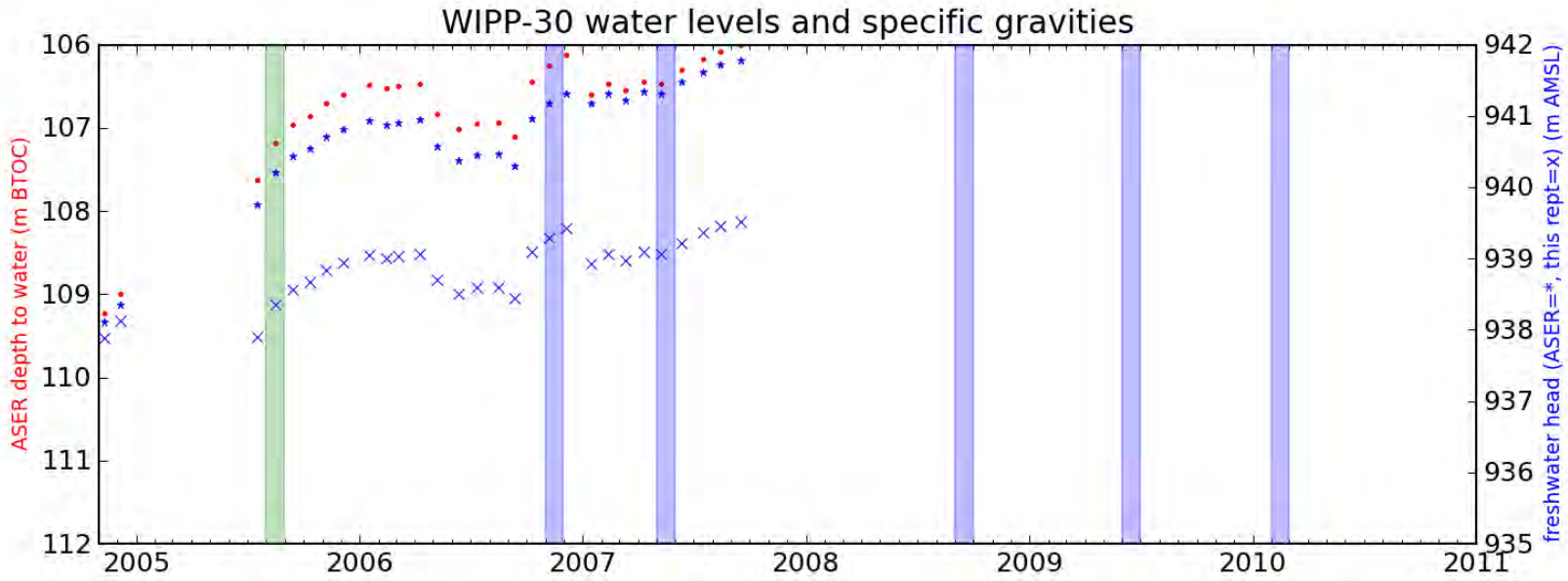


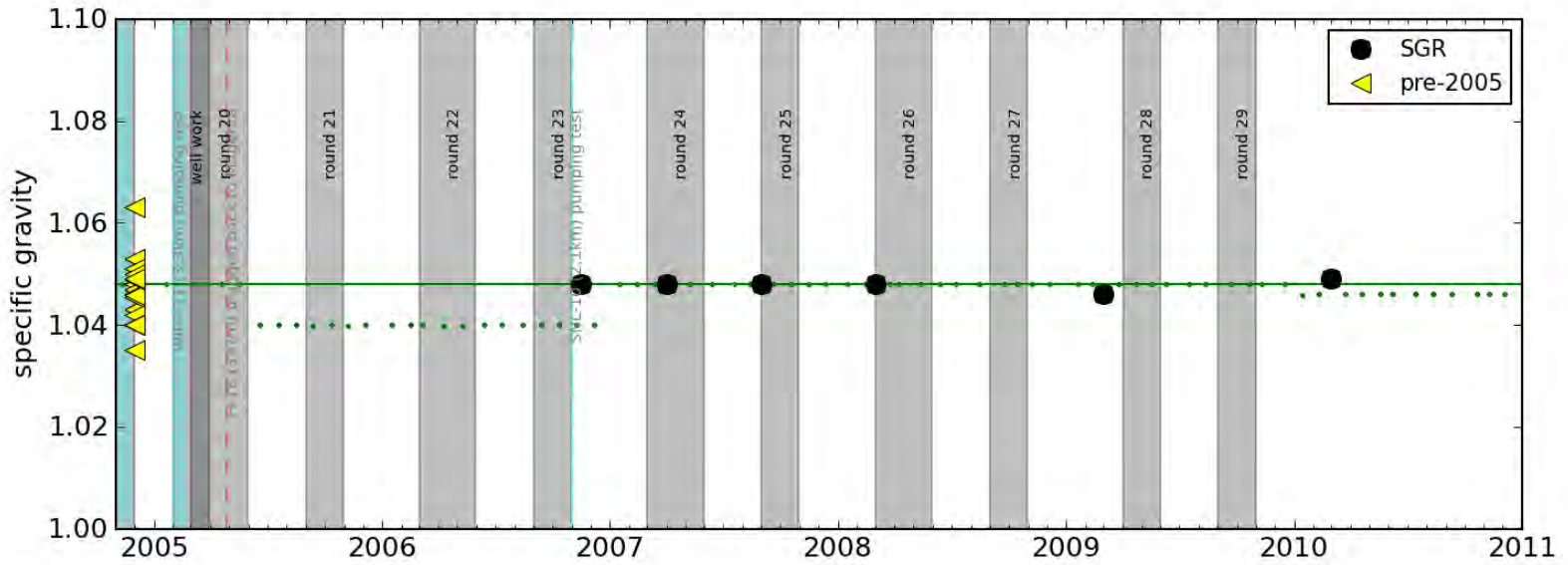
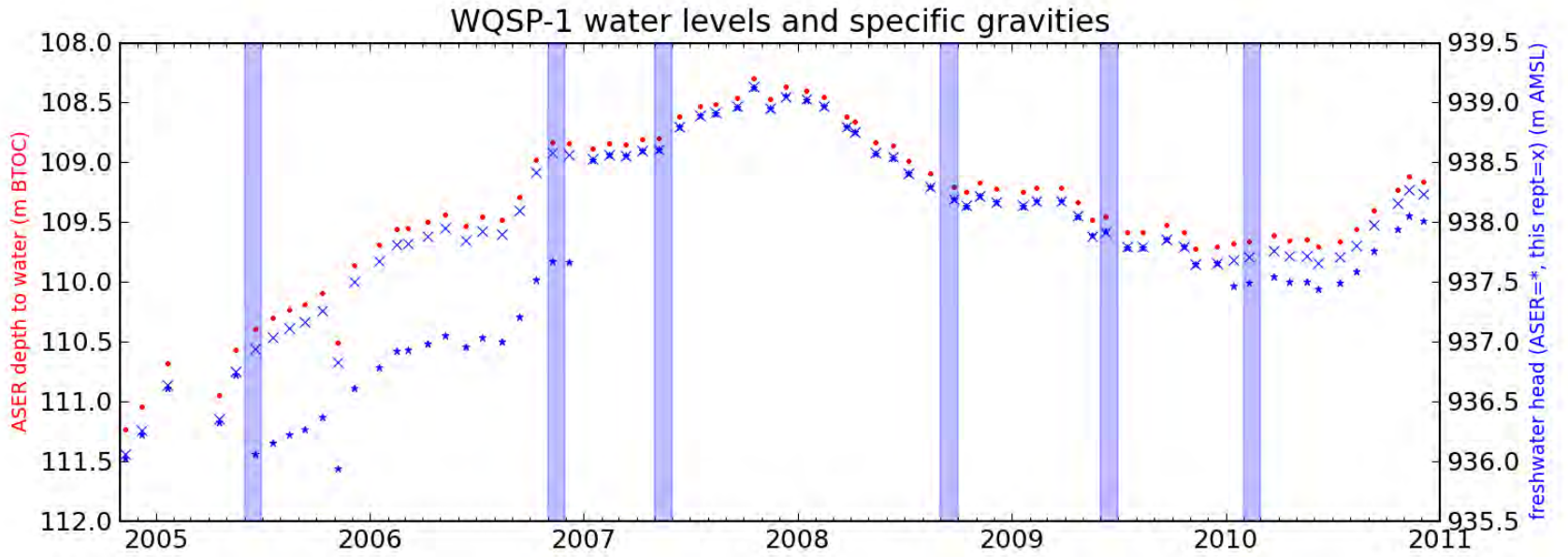


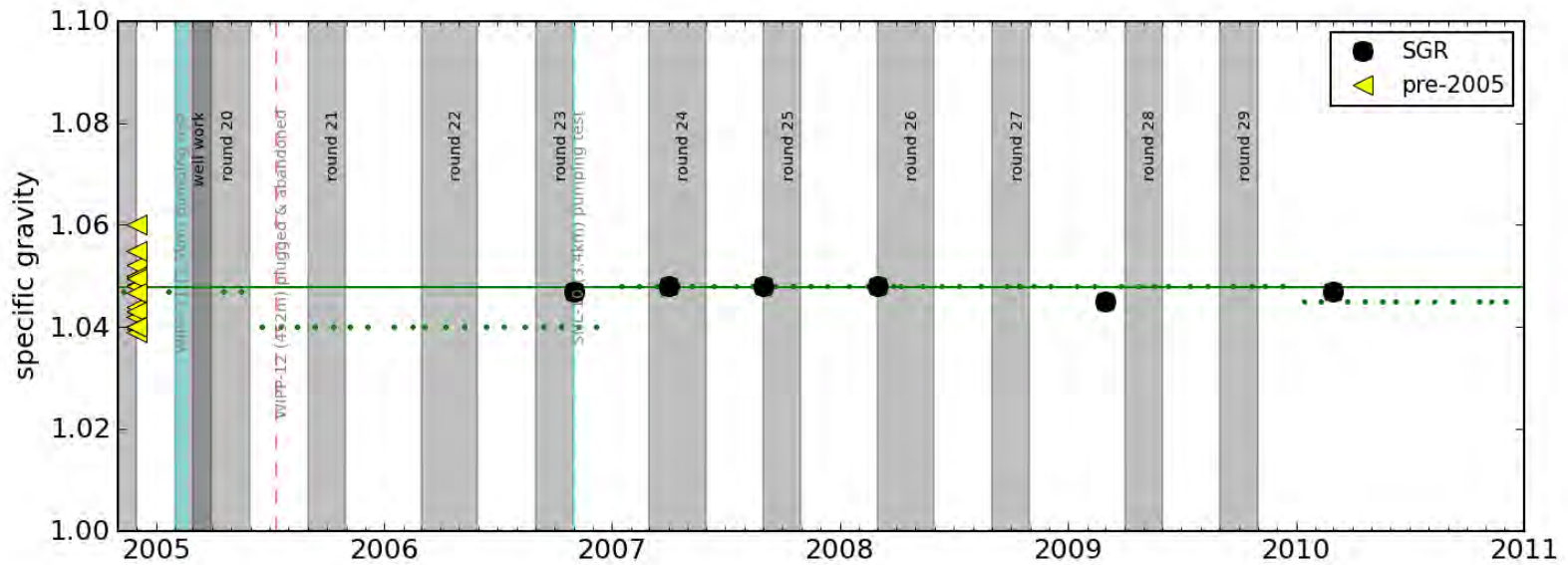
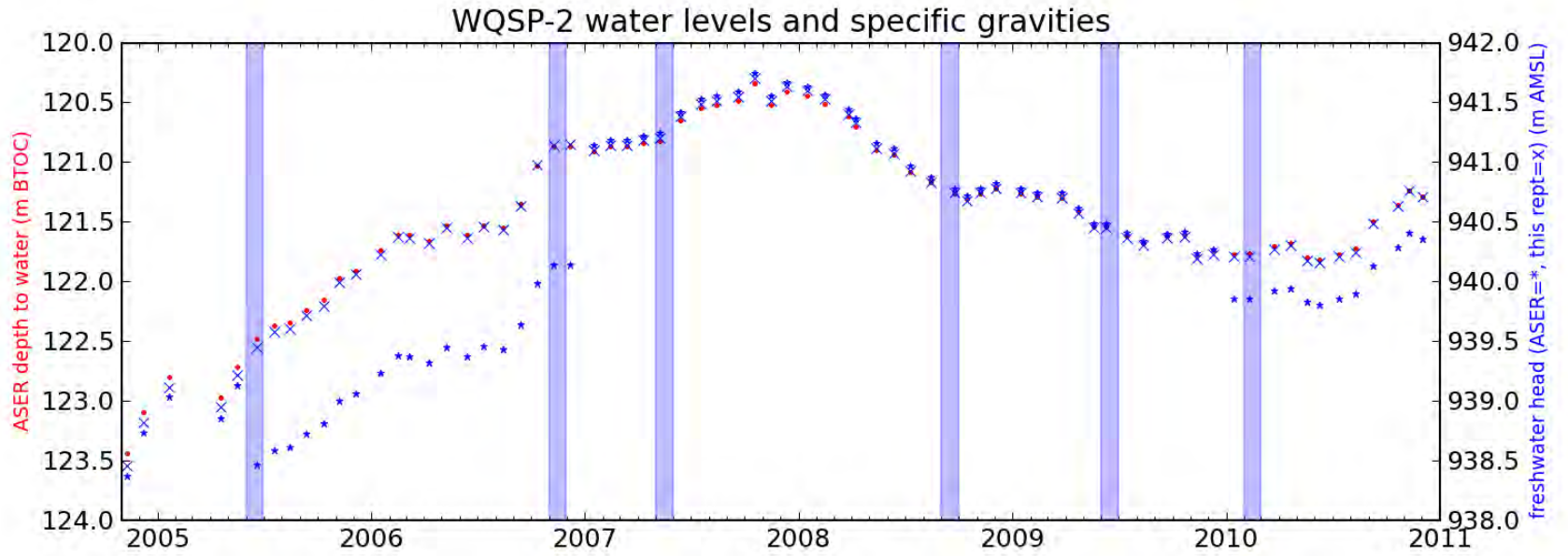


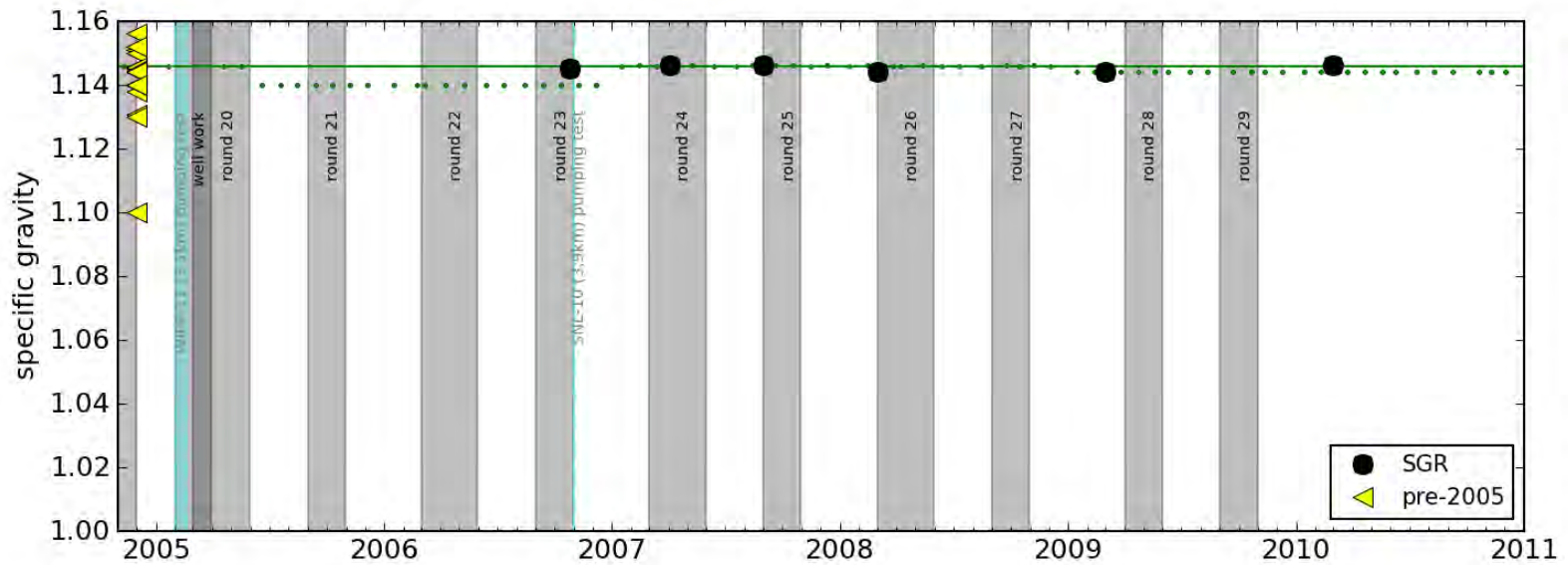
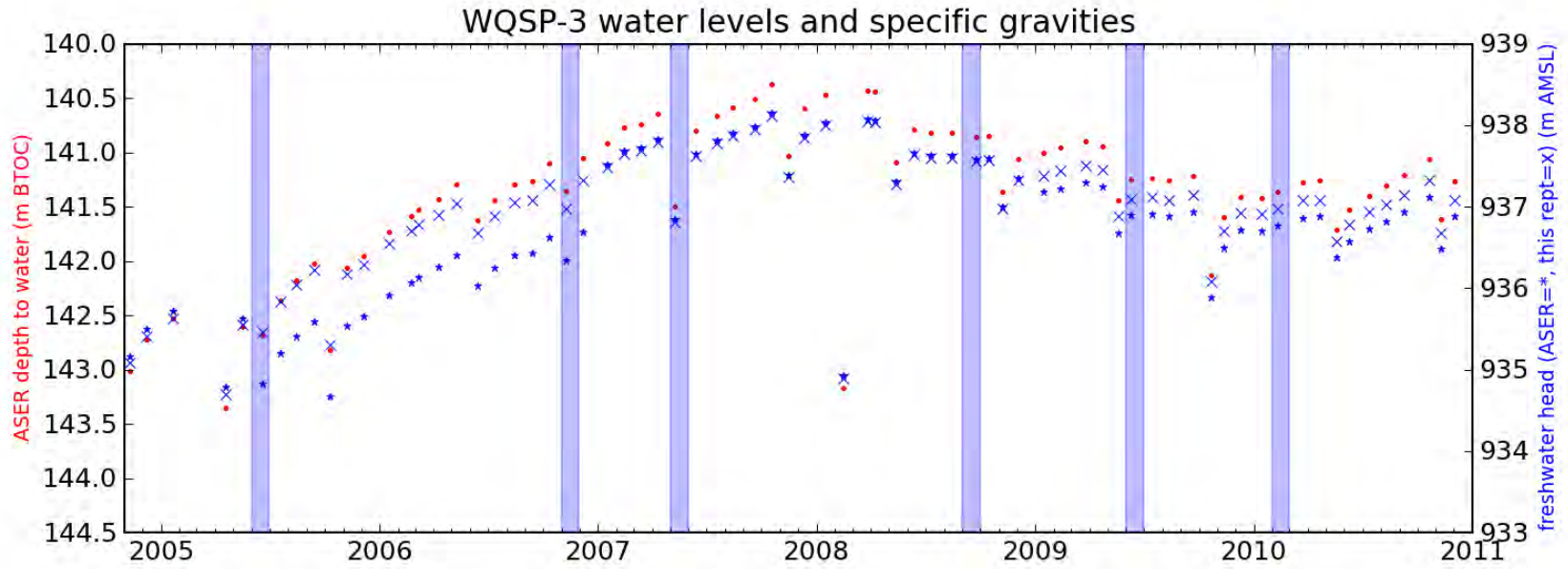


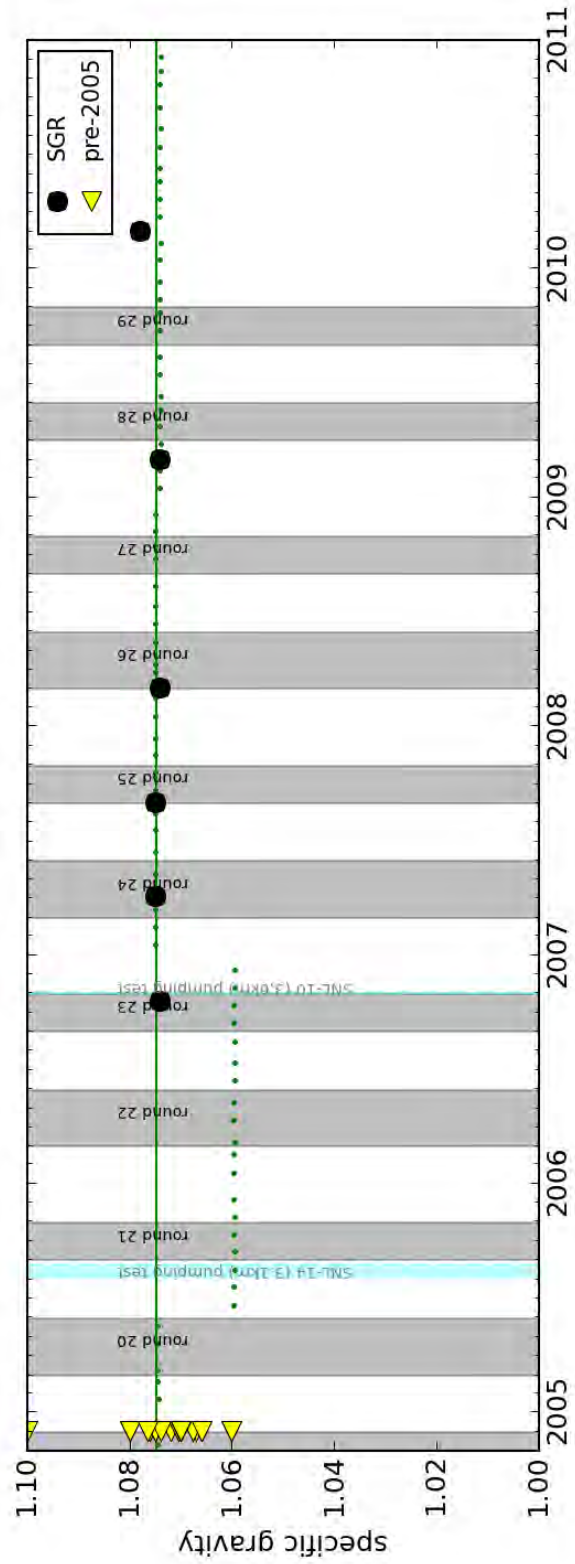
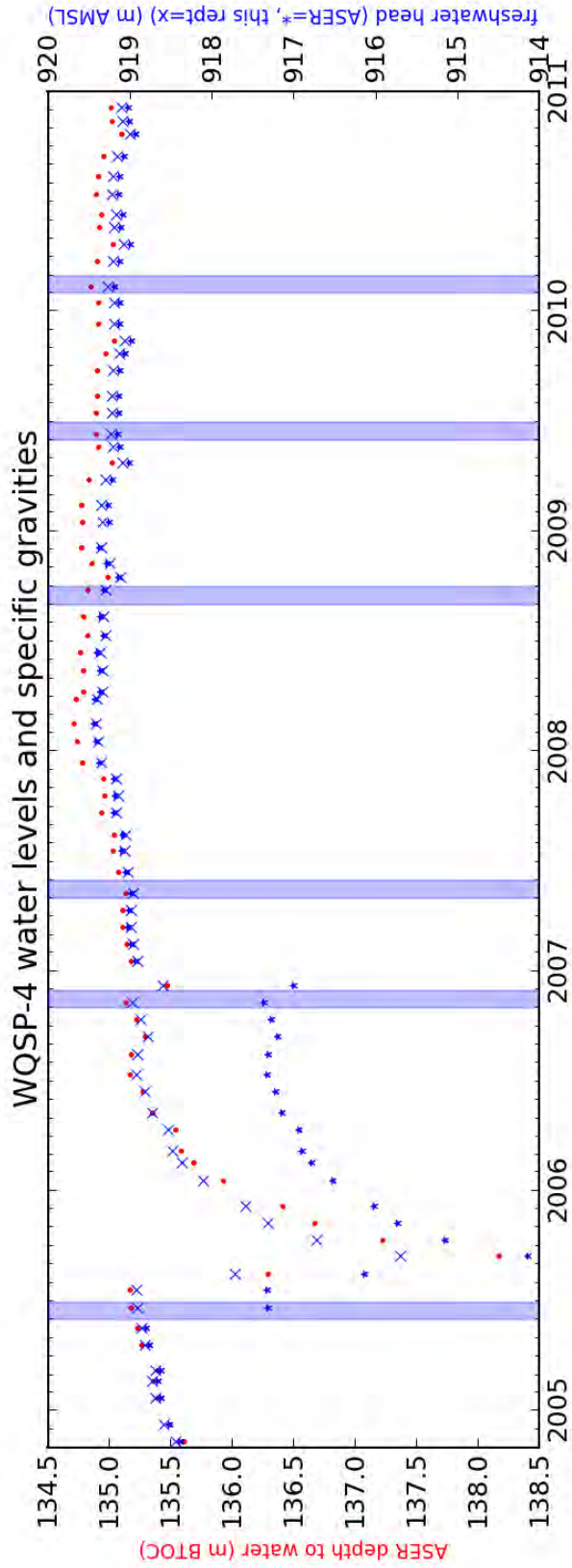


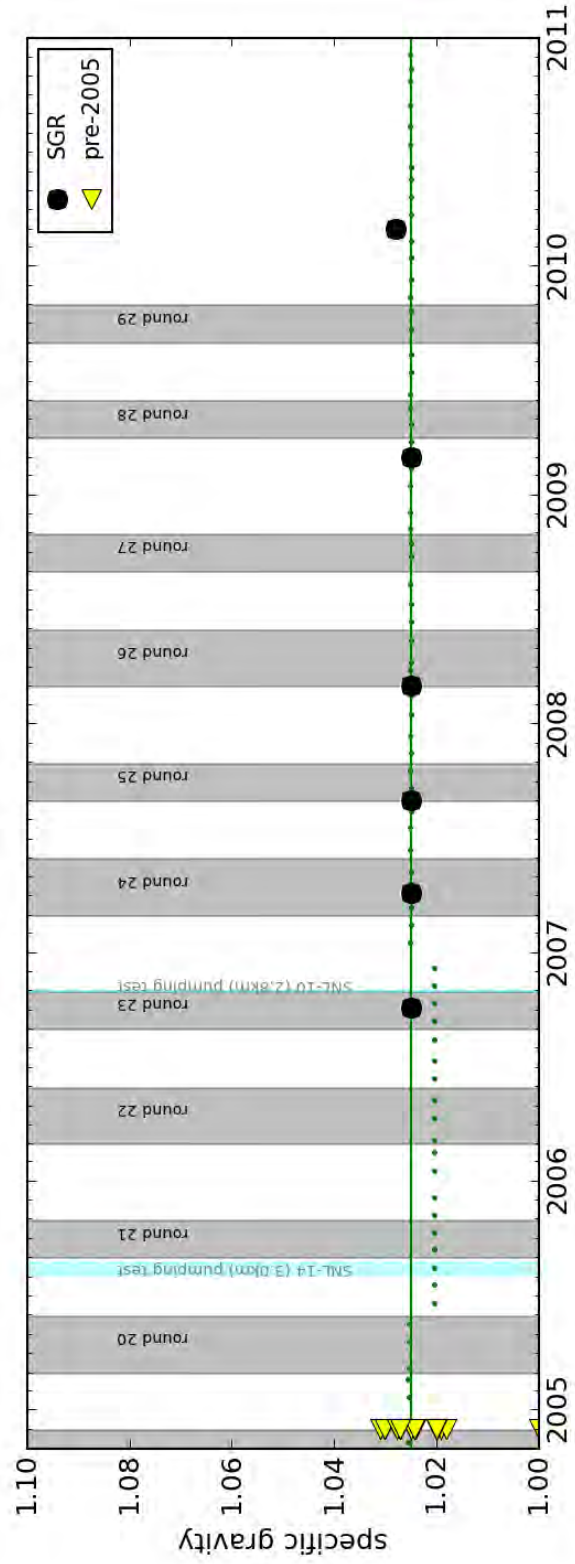
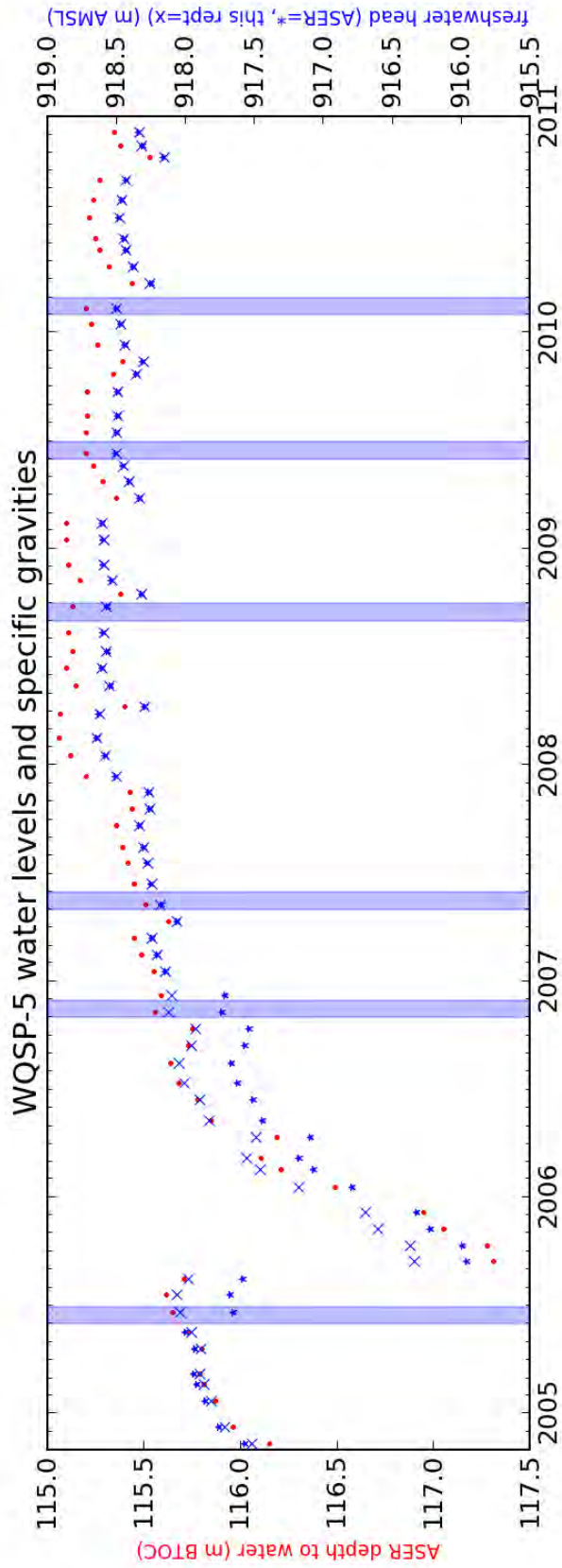


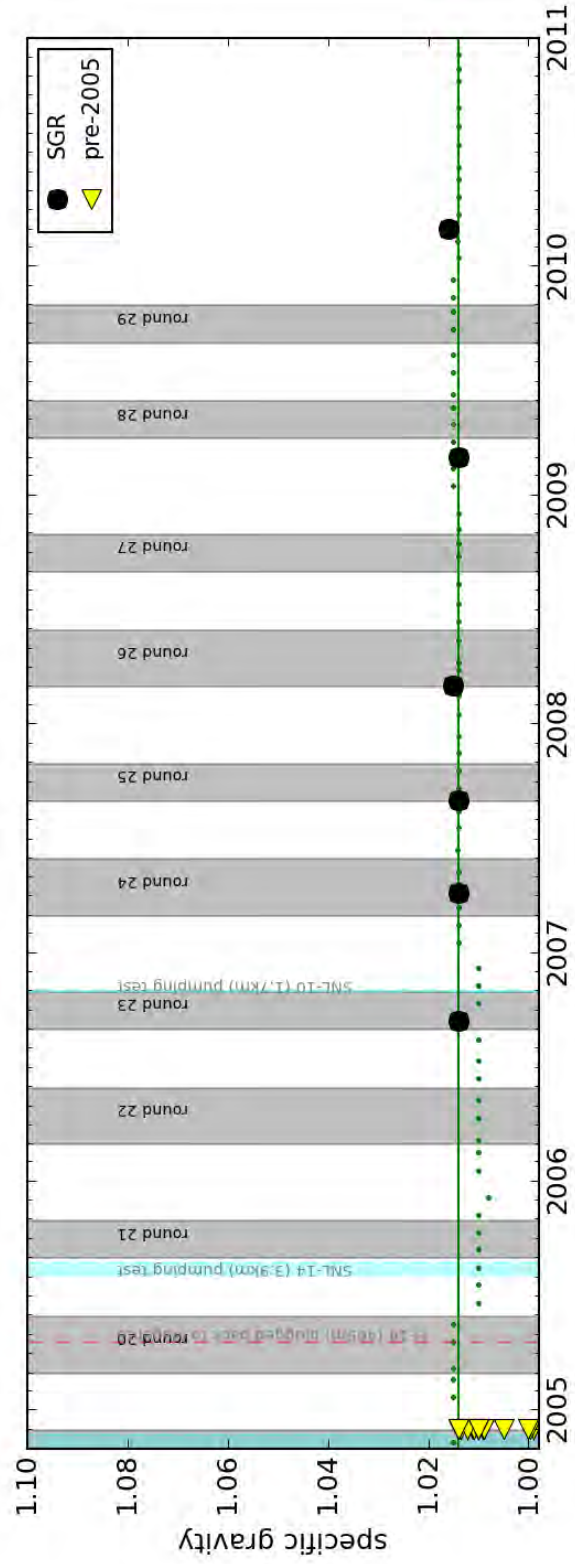
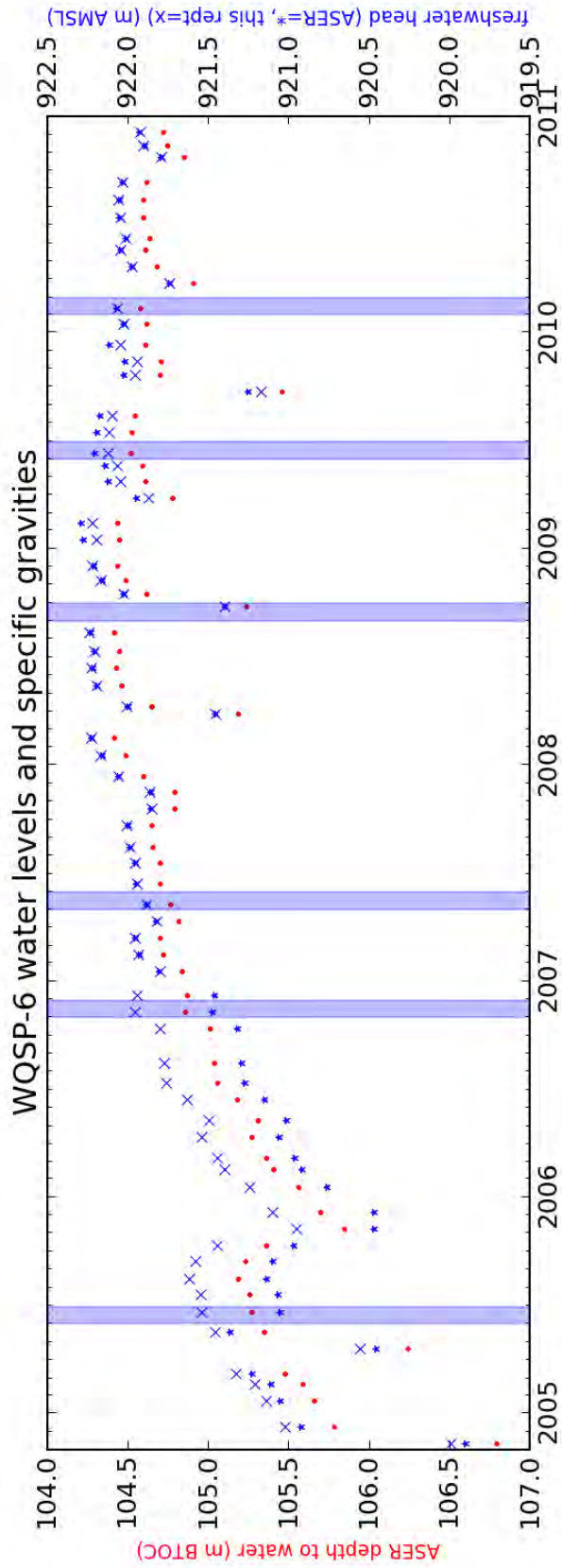












10 Appendix: MODFLOW and Pest Files and Script Source Listings

10.1 Input File Listing

The following table lists the input files for the 2005 contour map. The 2006 and 2007 contour maps have the same files with analogous names.

bytes	file type	description	file name
2.1K	Python script	average 100 realizations	average_realizations.py
2.3K	Python script	distinguish different BC types	boundary_types.py
6.6K	Bash script	main routine: checkout files,run MODFLOW run PEST, call Python scripts	checkout_average_run_modflow.sh
809	Python script	convert DTRKMF IJ output to Surfer X,Y blanking format	convert_dtrkmf_output_for_surfer.py
3.2K	Python script	create PEST input files from observed data	create_pest_02_input.py
48	input listing	responses to DTRKMF prompts	dtrkmf.in
4.2K	Python script	convert MODFLOW binary output to Surfer ASCII grid format	head_bin2ascii.py
1.1K	input	listing of 100 realizations from CVS	keepers
1.4K	input	observed heads in mod2obs.exe bore sample file format	meas_head_2010ASER.smp
1.2K	Python script	paste observed head and model-generated heads into one file	merge_observed_modeled_heads.py
76	file listing	files needed to run mod2obs.exe	mod2obs_files.dat
138	input listing	responses to mod2obs.exe prompts	mod2obs_head.in
372	file listing	files needed to run MODFLOW	modflow_files.dat
401	input	listing of wells and geographic groupings	obs_loc_2010ASER.dat
215	file listing	files needed to run PEST	pest_02_files.dat
2.3M	input	relative coordinate $1 \leq x \leq 1$	rel_x_coord.dat
2.3M	input	relative coordinate $1 \leq y \leq 1$	rel_y_coord.dat
389	Bash script	PEST model: execute MODFLOW and do pre- and post-processing	run_02_model
26	input	mod2obs.exe input file	settings.fig
47	input	mod2obs.exe input file	spec_domain.spc
1.7K	input	mod2obs.exe input file	spec_wells.crd
2.7K	Python script	compute starting head from parameter and coordinate inputs	surface_02_extrapolate.py
506	input	DTRKMF input file	wippctrl.inp
5.6K	Python script	plot contour map figures	plot-contour-maps.py
6.7K	Python script	plot bar and scatter figures	plot-results-bar-charts.py
90	plotting data	UTM coordinates of ASER map area	ASER.boundary.csv
9.2K	plotting data	UTM coordinates of MODFLOW model area	total_boundary.dat
6.7K	plotting data	UTM coordinates of WIPP LWB	wipp_boundary.csv

Table 1: Listing of Input Files

10.2 Output File Listing

The following table lists the input files for the 2005 contour map. The 2006 and 2007 contour maps have the same files with analogous names.

bytes	file type	description	file name
19K	DTRKMF output	particle track results	dtrk.out
16K	DTRKMF output	particle track debug	dtrk.dbg
2.0K	script output	heads at well locations	modeled_vs_observed_head_pest_02.txt
1.1M	script output	formatted MODFLOW heads	modeled_head_pest_02.grd
5.3K	script output	formatted DTRKMF particle	dtrk_output_pest_02.blm
16K	PEST output	matrix condition numbers	bc_adjust_2010ASER.cnd
2.7K	PEST output	binary intermediate file	bc_adjust_2010ASER.drf
7.4K	PEST output	binary intermediate file	bc_adjust_2010ASER.jac
7.5K	PEST output	binary intermediate file	bc_adjust_2010ASER.jco
9.9K	PEST output	binary intermediate file	bc_adjust_2010ASER.jst
3.8K	PEST output	parameter statistical matrices	bc_adjust_2010ASER.mtt
477	PEST output	parameter file	bc_adjust_2010ASER.par
62K	PEST output	optimization record	bc_adjust_2010ASER.rec
4.6K	PEST output	model outputs for last iteration	bc_adjust_2010ASER.rei
8.4K	PEST output	summary of residuals	bc_adjust_2010ASER.res
28	PEST output	binary restart file	bc_adjust_2010ASER.rst
24K	PEST output	relative parameter sensitivities	bc_adjust_2010ASER.sen
4.0K	PEST output	absolute parameter sensitivities	bc_adjust_2010ASER.seo
213K	png image	matplotlib plot (Fig. 2)	aser-area-contour-map.png
223K	png image	matplotlib plot (Fig. 3)	large-area-contour-map.png
33K	png image	matplotlib plot (Fig. 5)	model-error-histogram.png
55K	png image	matplotlib plot (Fig. 6)	model-error-residuals.png
93K	png image	matplotlib plot (Fig. 4)	scatter_pest_02.png

Table 2: Listing of Output Files

10.3 Individual MODFLOW and Pest Script Listings

10.3.1 Bash shell script checkout_average_run_modflow.sh

```
1  #!/bin/bash
2
3  set -o nounset # explode if using an un-initialized variable
4  set -o errexit # exit on non-zero error status of sub-command
5
6  # this script makes the following directory substructure
7  #
8  # current_dir \----- Outputs (calibrated parameter fields - INPUTS)
9  #              \----- Inputs (other modflow files - INPUTS)
10 #              \----- original_average (foward sim using average fields)
11 #              \----- bin (MODFLOW and DTRKMF binaries)
12 #              \----- pest_0? (pest-adjusted results)
13
14 ##set -o xtrace # loads of verbose debugging info
15
16 echo " ~~~~~~ "
17 echo " checking out T fields"
18 echo " ~~~~~~ "
19
20 # these will checkout the calibrated parameter-field data into subdirectories
21 # checkout things that are different for each of the 100 realizations
22 for d in `cat keepers`
23 do
24 cvs -d /nfs/data/CVSLIB/Tfields checkout Outputs/${d}/modeled_{K,A,R,S}_field.mod
25 done
26
27 ## checkout MODFLOW input files that are constant for across all realizations
28 cvs -d /nfs/data/CVSLIB/Tfields checkout Inputs/data/elev_{top,bot}.mod
29 cvs -d /nfs/data/CVSLIB/Tfields checkout Inputs/data/init_{bnds.inf,head.mod}
30 cvs -d /nfs/data/CVSLIB/Tfields checkout Inputs/modflow/mf2k_culebra.{lmg,lpf}
31 cvs -d /nfs/data/CVSLIB/Tfields checkout Inputs/modflow/mf2k_head.{ba6,nam,oc,dis,rch}
32
33 ## modify the path of "updated" T-fields, so they are all at the
34 ## same level in the directory structure (simplifying scripts elsewhere)
35
36 if [ -a keepers_short ]
37 then
38 rm keepers_short
39 fi
40 touch keepers_short
41
42 for d in `cat keepers`
43 do
44 bn=`basename ${d}`
45 # test whether it is a compound path
46 if [ ${d} != ${bn} ]
47 then
48 dn=`dirname ${d}`
49 mv ./Outputs/${d} ./Outputs/
50
51 # put an empty file in the directory to indicate
52 # what the directory was previously named
53 touch ./Outputs/${bn}/${dn}
54 fi
55
56 # create a keepers list without directories
57 echo ${bn} >> keepers_short
58 done
59
60 # -----
61 # the averaging was a slow step, when done in python
```



```

62
63 echo " ~~~~~ "
64 echo " perform averaging across all realizations "
65 echo " ~~~~~ "
66
67 python average_realizations.py
68
69 # checkout MODFLOW / DTRKMF executables
70 cvs -d /nfs/data/CVSLIB/MODFLOW2K checkout bin/mf2k/mf2k_1.6.release
71 cvs -d /nfs/data/CVSLIB/MODFLOW2K checkout bin/dtrkmf/dtrkmf_v0100
72
73 # check out pest and obs2mod binaries
74 cd bin
75 cvs -d /nfs/data/CVSLIB/PEST checkout Builds/Linux/pest.exe
76 cvs -d /nfs/data/CVSLIB/PEST checkout Builds/Linux/mod2obs.exe
77 cd ..
78
79 # -----
80
81 echo " ~~~~~ "
82 echo " setup copies of files constant between all realizations "
83 echo " ~~~~~ "
84
85 # directory for putting original base-case results in
86 od=original_average
87
88 if [ -d ${od} ]
89 then
90     echo ${od}" directory exists: removing and re-creating"
91     rm -rf ${od}
92 fi
93
94 mkdir ${od}
95 cd ${od}
96 echo `pwd`
97
98 # link to unchanged input files
99 for file in `cat ../modflow_files.dat`
100 do
101     ln -sf ${file} .
102 done
103
104 # link to averaged files computed in previous step
105 for f in {A,R,K,S}
106 do
107     ln -sf ../modeled-${f}_field.avg ./modeled-${f}_field.mod
108 done
109
110 ln -sf elev_top.mod fort.33
111 ln -sf elev_bot.mod fort.34
112
113 echo " ~~~~~ "
114 echo " run original MODFLOW and DTRKMF and export results for plotting "
115 echo " ~~~~~ "
116
117 # run MODFLOW, producing average head and CCF
118 ../bin/mf2k/mf2k_1.6.release mf2k_head.nam
119
120 # run DTRKMF, producing particle track (from ccf)
121 ../bin/dtrkmf/dtrkmf_v0100 <dtrkmf.in
122
123 # convert binary MODFLOW head output to Surfer ascii grid file format
124 ln -sf ../head_bin2ascii.py .
125 python head_bin2ascii.py

```

```

126 mv modeled_head_asciied.grd modeled_head- $\{od\}$ .grd
127
128 # convert DTRKMF output from cells to X,Y and
129 # save in Surfer blanking file format
130 ln -sf ../convert_dtrkmf_output_for_surfer.py .
131 python convert_dtrkmf_output_for_surfer.py
132 mv dtrk_output.blm dtrk_output- $\{od\}$ .blm
133
134 # extract head results at well locations and merge with observed
135 # head file for easy scatter plotting in Excel (tab delimited)
136 for file in `cat ../mod2obs_files.dat`
137 do
138     ln -sf  $\{file\}$  .
139 done
140
141 ln -sf ../meas_head_2005ASER.smp .
142 ln -sf ../obs_loc_2005ASER.dat .
143 ../bin/Builds/Linux/mod2obs.exe <mod2obs_head.in
144 ln -sf ../merge_observed_modeled_heads.py
145 python merge_observed_modeled_heads.py
146 mv both_heads.smp modeled_vs_observed_head- $\{od\}$ .txt
147
148
149 # go back down into root directory
150 cd ..
151 echo `pwd`
152
153 echo " ~~~~~~"
154 echo " setup and run PEST to optimize parametric surface to set BC "
155 echo " ~~~~~~"
156
157 for p in pest_02
158 do
159
160     if [ -d  $\{p\}$  ]
161     then
162         echo  $\{p\}$ " directory exists: removing and re-creating"
163         rm -rf  $\{p\}$ 
164     fi
165
166     mkdir  $\{p\}$ 
167     cd  $\{p\}$ 
168     echo `pwd`
169
170     # link to unchanged input files
171     for file in `cat ../modflow_files.dat`
172     do
173         ln -sf  $\{file\}$  .
174     done
175
176     # link to averaged files computed in previous step
177     for f in {A,R,K,S}
178     do
179         ln -sf ../modeled- $\{f\}$ _field.avg ./modeled- $\{f\}$ _field.mod
180     done
181
182     # link to mod2obs files (needed for pest)
183     for file in `cat ../mod2obs_files.dat`
184     do
185         ln -sf  $\{file\}$  .
186     done
187
188     # link to pest files
189     for file in `cat ../ $\{p\}$ _files.dat`

```

```

190     do
191         ln -s ${file} .
192     done
193
194     # rename 'original' versions of files to be modified by pest
195     rm init_head.mod
196     ln -sf ../Inputs/data/init_head.mod ./init_head_orig.mod
197     rm init_bnds.inf
198     ln -sf ../Inputs/data/init_bnds.inf ./init_bnds_orig.inf
199
200     # create new ibound array for easier modification during PEST
201     # optimization iterations
202     python boundary_types.py
203
204     # create the necessary input files from observations
205     python create_${p}_input.py
206
207     # run pest
208     ../bin/Builds/Linux/pest.exe bc_adjust_2005ASER
209
210     # last output files should be best run
211     # extract all the stuff from that output
212     #####
213
214     ln -sf elev_top.mod fort.33
215     ln -sf elev_bot.mod fort.34
216
217     ../bin/dtrkmf/dtrkmf_v0100 <dtrkmf.in
218
219     ln -sf ../head_bin2ascii.py .
220     python head_bin2ascii.py
221     mv modeled_head_asciihed.grd modeled_head_${p}.grd
222
223     ln -sf ../convert_dtrkmf_output_for_surfer.py .
224     python convert_dtrkmf_output_for_surfer.py
225     mv dtrk_output.blm dtrk_output_${p}.blm
226
227     for file in `cat ../mod2obs_files.dat`
228     do
229         ln -sf ${file} .
230     done
231
232     ../bin/Builds/Linux/mod2obs.exe <mod2obs_head.in
233     ln -sf ../merge_observed_modeled_heads.py
234     python merge_observed_modeled_heads.py
235     mv both_heads.smp modeled_vs_observed_head_${p}.txt
236
237     cd ..
238     done

```

10.3.2 Python script average_realizations.py

```
1 from math import log10 ,pow
2
3 nrow = 307
4 ncol = 284
5 nel = nrow*ncol
6 nfr = 100 # number of fields (realizations)
7 nft = 4 # number of field types
8
9 def floatload(filename):
10     """Reads file (a list of strings, one per row) into a list of strings."""
11     f = open(filename, 'r')
12     m = [float(line.rstrip()) for line in f]
13     f.close()
14     return m
15
16 types = ['K', 'A', 'R', 'S']
17
18 # get list of 100 best calibrated fields
19 flist = open('keepers_short', 'r')
20 runs = flist.read().strip().split('\n')
21 flist.close()
22
23 # initialize to help speed lists up a bit
24 # nfr (100) realizations of each
25 fields = []
26 for i in xrange(nft):
27     fields.append([None]*nfr)
28     for i in xrange(nfr):
29         # each realization being nel (87188) elements
30         fields[-1][i] = [None]*nel
31
32 # read in all realizations
33 print 'reading ...'
34 for i,run in enumerate(runs):
35     print i,run
36     for j,t in enumerate(types):
37         fields[j][i][0:nel] = floatload('Outputs/'+ run +'/modeled_'+ t +'_field.mod')
38
39 # open up files for writing
40 fh = []
41 for t in types:
42     fh.append(open('modeled_'+ t +'_field.avg', 'w'))
43
44 # transpose fields to allow slicing across realizations, rather than across cells
45 for j in range(len(types)):
46     fields[j] = zip(*(fields[j]))
47
48 print 'writing ...'
49 # do averaging across 100 realizations
50 for i in xrange(nel):
51     if i%10000 == 0:
52         print i
53     for h,d in zip(fh, fields):
54         h.write('%18.11e\n' % pow(10.0, sum(map(log10, d[i]))/ nfr) )
55
56 for h in fh:
57     h.close()
```

10.3.3 Python script boundary_types.py

```
1 nx = 284          # number columns in model grid
2 ny = 307          # number rows
3 nel = nx*ny
4
5 def intload(filename):
6     """Reads file (a 2D integer array) as a list of lists.
7     Outer list is rows, inner lists are columns."""
8     f = open(filename, 'r')
9     m = [[int(v) for v in line.rstrip().split()] for line in f]
10    f.close()
11    return m
12
13 def intsave(filename,m):
14    """Writes file as a list of lists as a 2D integer array, format '%3i'.
15    Outer list is rows, inner lists are columns."""
16    f = open(filename, 'w')
17    for row in m:
18        f.write(' '.join(['%2i' % col for col in row]) + '\n')
19    f.close()
20
21 def floatload(filename):
22    """Reads file (a list of real numbers, one number each row) into a list of floats."""
23    f = open(filename, 'r')
24    m = [float(line.rstrip()) for line in f]
25    f.close()
26    return m
27
28 def reshapev2m(v):
29    """Reshape a vector that was previously reshaped in C-major order from a matrix,
30    back into a matrix (here a list of lists)."""
31    m = [None]*ny
32    for i,(lo,hi) in enumerate(zip(xrange(0, nel-nx+1, nx), xrange(nx, nel+1, nx))):
33        m[i] = v[lo:hi]
34    return m
35
36 #####
37
38 # read in original MODFLOW IBOUND array (only 0,1, and -1)
39 ibound = intload('init_bnds_orig.inf')
40
41 # read in initial heads
42 h = reshapev2m(floatload('init_head_orig.mod'))
43
44 # discriminate between two types of constant head boundaries
45 # -1) CH, where value > 1000 (area east of halite margin)
46 # -2) CH, where value < 1000 (single row/column of cells along edge of domain)
47
48 for i,row in enumerate(ibound):
49     for j,val in enumerate(row):
50         # is this constant head and is starting head less than 1000m ?
51         if ibound[i][j] == -1 and h[i][j] < 1000.0:
52             ibound[i][j] = -2
53
54 # save new IBOUND array that allows easy discrimination between types in python script during
55 # PEST optimization runs, and is still handled the same by MODFLOW
56 # since all ibound values < 0 are treated as constant head.
57 intsave('init_bnds.inf',ibound)
```

10.3.4 Python script create_pest_02_input.py

```
1 prefix = '2005ASER'
2
3 #####
4 ## pest instruction file reads output from mod2obs
5 fin = open('meas_head_%s.smp' % prefix, 'r')
6
7 # each well is a [name,head] pair
8 wells = [[line.split()[0], line.split()[3]] for line in fin]
9 fin.close()
10
11 fout = open('modeled_head.ins', 'w')
12 fout.write('pif @\n')
13 for i, well in enumerate(wells):
14     fout.write("l1 [%s]39:46\n" % well[0])
15 fout.close()
16
17 # exponential surface used to set initial head everywhere
18 # except east of the halite margins, where the land surface is used.
19 # initial guesses come from AP-114 Task report
20 params = [928.0, 8.0, 1.2, 1.0, 1.0, -1.0, 0.5]
21 pnames = ['a', 'b', 'c', 'd', 'e', 'f', 'exp']
22
23 fout = open('avg_NS_res.ins', 'w')
24 fout.write("""pif @
25 l1 [medianN]1:16
26 l1 [medianS]1:16
27 l1 [meanN]1:16
28 l1 [meanS]1:16
29 """)
30 fout.close()
31
32
33 #####
34 ## pest template file
35 ftmp = open('surface_par_params.ptf', 'w')
36 ftmp.write('ptf @\n')
37 for n in pnames:
38     ftmp.write('@ %s @\n' % n)
39 ftmp.close()
40
41
42 #####
43 ## pest parameter file
44
45 fpar = open('surface_par_params.par', 'w')
46 fpar.write('double point\n')
47 for n,p in zip(pnames, params):
48     fpar.write('%s %.2f 1.0 0.0\n' % (n,p))
49 fpar.close()
50
51
52 #####
53 ## pest control file
54
55 f = open('bc_adjust_%s.pst' % prefix, 'w')
56
57 f.write("""pcf
58 * control data
59 restart estimation
60 %i %i 1 0 2
61 1 2 double point 1 0 0
62 5.0 2.0 0.4 0.001 10
63 3.0 3.0 1.0E-3
```

```

64 0.1
65 30 0.001 4 4 0.0001 4
66 1 1 1
67 * parameter groups
68 bc relative 0.005 0.0001 switch 2.0 parabolic
69 """ % (len(params), len(wells)+4))
70
71 f.write('* parameter data\n')
72 for n,p in zip(pnames, params):
73     if p > 0:
74         f.write('%s none relative %.3f %.3f %.3f bc 1.0 0.0 1\n' %
75                (n, p, -2.0*p, 3.0*p))
76     else:
77         f.write('%s none relative %.3f %.3f %.3f bc 1.0 0.0 1\n' %
78                (n, p, 3.0*p, -2.0*p))
79
80 f.write("""* observation groups
81 ss_head
82 avg_head
83 * observation data
84 """)
85
86 ## read in observation weighting group definitions
87 fin = open('obs_loc_%s.dat' % prefix, 'r')
88 location = [line.rstrip().split()[1] for line in fin]
89 fin.close()
90
91 weights = []
92
93 for l in location:
94     # inside LWB
95     if l == '0':
96         weights.append(2.5)
97     # near LWB
98     if l == '1':
99         weights.append(1.0)
100    # distant to LWB
101    if l == '2':
102        weights.append(0.4)
103    if l == '99':
104        weights.append(0.01) # AEC-7
105
106
107 for name, head, w in zip(zip(*wells)[0], zip(*wells)[1], weights):
108     f.write('%s %s %.3f ss_head\n' % (name, head, w))
109
110 # one fewer N observation (WIPP-25 removed), there were 13
111 # there are 12 N observations in the average and 11 S, therefore
112 # split the weight between the mean and median
113 f.write("""medianN 0.0 18.0 avg_head
114 medianS 0.0 16.5 avg_head
115 meanN 0.0 18.0 avg_head
116 meanS 0.0 16.5 avg_head
117 """)
118
119 f.write("""* model command line
120 ./run_02_model
121 * model input/output
122 surface_par_params.ptf surface_par_params.in
123 modeled_head.ins modeled_head.smp
124 avg_NS_res.ins avg_NS_res.smp
125 """)
126 f.close()

```

10.3.5 Python script surface_02_extrapolate.py

```
1 from itertools import chain
2 from math import sqrt
3
4 def matload(filename):
5     """Reads file (a 2D string array) as a list of lists.
6     Outer list is rows, inner lists are columns."""
7     f = open(filename, 'r')
8     m = [line.rstrip().split() for line in f]
9     f.close()
10    return m
11
12 def floatload(filename):
13     """Reads file (a list of real numbers, one number each row) into a list of floats."""
14     f = open(filename, 'r')
15     m = [float(line.rstrip()) for line in f]
16     f.close()
17    return m
18
19 def reshapem2v(m):
20     """Reshapes a rectangular matrix into a vector in same fashion as numpy.reshape().
21     which is C-major order"""
22    return list(chain(*m))
23
24 def sign(x):
25     """ sign function """
26     if x<0:
27         return -1
28     elif x>0:
29         return +1
30     else:
31         return 0
32
33 #####
34
35 # read in modified IBOUND array, with the cells to modify set to -2
36 ibound = reshapem2v(matload('init_bnds.inf'))
37
38 h = floatload('init_head_orig.mod')
39
40 # these are relative coordinates, -1 <= x,y < +1
41 x = floatload('rel_x_coord.dat')
42 y = floatload('rel_y_coord.dat')
43
44 # unpack surface parameters (one per line)
45 # z = A + B*(y + D*sign(y)*sqrt(abs(y)))+C*(E*x**3 - F*x**2 - x)
46
47 finput = open('surface_par_params.in', 'r')
48 try:
49     a,b,c,d,e,f,exp = [float(line.rstrip()) for line in finput]
50 except ValueError:
51     # python doesn't like 'D' in 1.2D-4 notation used by PEST sometimes.
52     finput.seek(0)
53     lines = [line.rstrip() for line in finput]
54     for i in range(len(lines)):
55         lines[i] = lines[i].replace('D','E')
56     a,b,c,d,e,f,exp = [float(line) for line in lines]
57
58 finput.close()
59
60 # file to output initial/boundary head for MODFLOW model
61 fout = open('init_head.mod', 'w')
62 for i in xrange(len(ibound)):
63     if ibound[i] == '-2' or ibound[i] == '1':
```



```

64     # apply exponential surface to active cells (ibound=1) -> starting guess
65     # and non-geologic boundary conditions (ibound=-2) -> constant head value
66     if y[i] == 0:
67         fout.write('%.7e \n' % (a + c*(e*x[i]**3 + f*x[i]**2 - x[i])))
68     else:
69         fout.write('%.7e \n' % (a + b*(y[i] + d*sign(y[i])*abs(y[i])**exp) +
70                                 c*(e*x[i]**3 + f*x[i]**2 - x[i])))
71 else:
72     # use land surface at constant head east of halite boundary
73     # ibound=0 doesn't matter (inactive)
74     fout.write('%.7e\n' % h[i])
75
76 fout.close()

```

10.3.6 Bash shell script run_02_model

```
1  #!/bin/bash
2
3  #set -o xtrace
4
5  #echo 'step 1: surface extrapolate'
6  python surface_02_extrapolate.py
7
8  # run modflow
9  #echo 'step 2: run modflow'
10 ./bin/mf2k/mf2k_1.6.release mf2k_head.nam >/dev/null
11
12 # run mod2obs
13 #echo 'step 3: extract observations'
14 ./bin/Builds/Linux/mod2obs.exe < mod2obs_head.in >/dev/null
15
16 # create meta-observations of N vs. S
17 python create_average_NS_residuals.py
```

10.3.7 Python script head_bin2ascii.py

```
1 import struct
2 from sys import argv, exit
3
4 class FortranFile(file):
5     """ modified from May 2007 Enthought-dev mailing list post by Neil Martinsen-Burrell """
6
7     def __init__(self, fname, mode='r', buf=0):
8         file.__init__(self, fname, mode, buf)
9         self.ENDIAN = '<' # little endian
10        self.di = 4 # default integer (could be 8 on 64-bit platforms)
11
12    def readReals(self, prec='f'):
13        """Read in an array of reals (default single precision) with error checking"""
14        # read header (length of record)
15        l = struct.unpack(self.ENDIAN+'i', self.read(self.di))[0]
16        data_str = self.read(l)
17        len_real = struct.calcsize(prec)
18        if l % len_real != 0:
19            raise IOError('Error reading array of reals from data file')
20        num = l/len_real
21        reals = struct.unpack(self.ENDIAN+str(num)+prec, data_str)
22        # check footer
23        if struct.unpack(self.ENDIAN+'i', self.read(self.di))[0] != 1:
24            raise IOError('Error reading array of reals from data file')
25        return list(reals)
26
27    def readInts(self):
28        """Read in an array of integers with error checking"""
29        l = struct.unpack('i', self.read(self.di))[0]
30        data_str = self.read(l)
31        len_int = struct.calcsize('i')
32        if l % len_int != 0:
33            raise IOError('Error reading array of integers from data file')
34        num = l/len_int
35        ints = struct.unpack(str(num)+'i', data_str)
36        if struct.unpack(self.ENDIAN+'i', self.read(self.di))[0] != 1:
37            raise IOError('Error reading array of integers from data file')
38        return list(ints)
39
40    def readRecord(self):
41        """Read a single fortran record (potentially mixed reals and ints)"""
42        dat = self.read(self.di)
43        if len(dat) == 0:
44            raise IOError('Empty record header')
45        l = struct.unpack(self.ENDIAN+'i', dat)[0]
46        data_str = self.read(l)
47        if len(data_str) != l:
48            raise IOError('Didn't read enough data')
49        check = self.read(self.di)
50        if len(check) != 4:
51            raise IOError('Didn't read enough data')
52        if struct.unpack(self.ENDIAN+'i', check)[0] != 1:
53            raise IOError('Error reading record from data file')
54        return data_str
55
56    def reshapev2m(v, nx, ny):
57        """Reshape a vector that was previously reshaped in C-major order from a matrix,
58        back into a C-major order matrix (here a list of lists)."""
59        m = [None]*ny
60        n = nx*ny
61        for i, (lo, hi) in enumerate(zip(xrange(0, n-nx+1, nx), xrange(nx, n+1, nx))):
62            m[i] = v[lo:hi]
63        return m
```

```

64
65 def floatmatsave(filehandle,m):
66     """Writes array to open filehandle, format '568%e12.5'.
67     Outer list is rows, inner lists are columns."""
68
69     for row in m:
70         f.write(''.join([' %12.5e' % col for col in row]) + '\n')
71
72 # open file and set endian-ness
73 try:
74     infn,outfn = argv[1:3]
75 except:
76     print '2 command-line arguments not given, using default in/out filenames'
77     infn = 'modeled_head.bin'
78     outfn = 'modeled_head_asciihed.grd'
79
80 ff = FortranFile(infn)
81
82 # currently this assumes a single-layer MODFLOW model (or at least only one layer of output)
83
84 # format of MODFLOW header in binary layer array
85 fmt = '<2i2f16s3i'
86 # little endian, 2 integers, 2 floats,
87 # 16-character string (4 element array of 4-byte strings), 3 integers
88
89 while True:
90     try:
91         # read in header
92         h = ff.readRecord()
93
94     except IOError:
95         # exit while loop
96         break
97
98     else:
99         # unpack header
100         kstp,kper,pertim,totim,text,ncol,nrow,ilay = struct.unpack(fmt,h)
101
102         # print status/confirmation to terminal
103         print kstp,kper,pertim,totim,text,ncol,nrow,ilay
104
105         h = ff.readReals()
106
107     ff.close()
108
109     xmin,xmax = (601700.0,630000.0)
110     ymin,ymax = (3566500.0,3597100.0)
111     hmin = min(h)
112     hmax = max(h)
113
114     # write output in Surfer ASCII grid format
115     f = open(outfn,'w')
116     f.write("DSAA\n%i %i\n%.1f %.1f\n%.1f %.1f\n%.8e %.8e" %
117           (ncol,nrow,xmin,xmax,ymin,ymax,hmin,hmax) )
118     hmat = reshapev2m(h,ncol,nrow)
119
120     # MODFLOW starts data in upper-left corner
121     # Surfer expects data starting in lower-left corner
122     # flip array in row direction
123
124     floatmatsave(f,hmat[::-1])
125     f.close()

```

10.3.8 Python script merge_observed_modeled_heads.py

```
1 fobs = open('meas_head_2005ASER.smp','r') # measured head
2 fmod = open('modeled_head.smp','r') # modeled head
3 fwgt = open('obs_loc_2005ASER.dat','r') # weights
4 fdb = open('spec_wells.crd','r') # x/y coordinates
5
6 fout = open('both_heads.smp','w') # resulting file
7
8 # read in list of x/y coordinates, key by well name
9 wells = {}
10 for line in fdb:
11     well,x,y = line.split()[0:3] # ignore last column
12     wells[well.upper()] = [x,y]
13 fdb.close()
14
15 fout.write('\t'.join(['#NAME','UTM-NAD27-X','UTM-NAD27-Y',
16                     'OBSERVED','MODELED','OBS-MOD','WEIGHT'])+'\n')
17
18 for sobs,smod,w in zip(fobs,fmod,fwgt):
19     obs = float(sobs.split()[3])
20     mod = float(smod.split()[3])
21     name = sobs.split()[0].upper()
22     fout.write('\t'.join([name,wells[name][0],wells[name][1],
23                         str(obs),str(mod),str(obs-mod),
24                         w.rstrip().split()[1]])+'\n')
25
26 fobs.close()
27 fmod.close()
28 fwgt.close()
29 fout.close()
```

10.3.9 Python script `convert_dtrkmf_output_for_surfer.py`

```
1
2 # grid origin for dtrkmf cell -> x,y conversion
3 x0 = 601700.0
4 y0 = 3597100.0
5
6 dx = 100.0
7 dy = 100.0
8
9 fout = open('dtrk_output.blm', 'w')
10
11 # read in all results for saving particle tracks
12 fin = open('dtrk.out', 'r')
13 results = [l.split() for l in fin.readlines()[1:]]
14 fin.close()
15
16 npts = len(results)
17
18 # write Surfer blanking file header
19 fout.write('%i,1\n' % npts)
20
21 # write x,y location and time
22 for pt in results:
23     x = float(pt[1])*dx + x0
24     y = y0 - float(pt[2])*dy
25     t = float(pt[0])/7.75*4.0 # convert to 4m Cuelbra thickness
26     fout.write('%0.1f,%0.1f,%0.8e\n' % (x,y,t))
27
28 fout.close()
```

10.3.10 Python script plot-results-bar-charts.py

This script is not run on the QA linux cluster, `alice.sandia.gov`. This script is run on a desktop PC, but is only used to create figures for the analysis report. This script is only included here for completeness.

```
1 import numpy as np
2 import matplotlib
3 matplotlib.use('Agg')
4 import matplotlib.pyplot as plt
5
6 fprefix = 'pest_02/'
7 mprefix = '../wipp-polyline-data/'
8 fname = fprefix + 'modeled_vs_observed_head_pest_02.txt'
9
10 ofname = 'original_average/modeled_vs_observed_head_original_average.txt'
11
12 M2FT = 0.3048
13 year = '2005'
14
15 # load in observed, modeled, obs-mod, (all in meters)
16 res = np.loadtxt(fname, skiprows=1, usecols=(3,4,5))
17 ores = np.loadtxt(ofname, skiprows=1, usecols=(3,4,5))
18
19 # load in weights
20 weights = np.loadtxt(fname, skiprows=1, usecols=(6,), dtype='int')
21 # load in names
22 names = np.loadtxt(fname, skiprows=1, usecols=(0,), dtype='|S6')
23
24 ## checking locations / zones
25 # *****
26 wipp = np.loadtxt(mprefix+'wipp_boundary.dat')
27 x,y = np.loadtxt(fname, skiprows=1, usecols=(1,2), unpack=True)
28
29 fig = plt.figure(2, figsize=(18,12))
30 ax1 = fig.add_subplot(121)
31 ax1.plot(x,y, 'k*') # wells
32 ax1.plot(wipp[:,0], wipp[:,1], 'r-') # WIPP LWB
33 buff = np.loadtxt(mprefix+'wipp_boundary.dat')
34 buff[1:3,0] -= 3000.0
35 buff[0,0] += 3000.0
36 buff[3:,0] += 3000.0
37 buff[2:4,1] -= 3000.0
38 buff[0:2,1] += 3000.0
39 buff[-1,1] += 3000.0
40 ax1.plot(buff[:,0], buff[:,1], 'g--') # WIPP LWB+3km
41 for xv,yv,n,w in zip(x,y,names,weights):
42     plt.annotate('%s %i'%(n,w), xy=(xv,yv), fontsize=8)
43 plt.axis('image')
44 ax1.set_xlim([x.min()-1000,x.max()+1000])
45 ax1.set_ylim([y.min()-1000,y.max()+1000])
46 ax2 = fig.add_subplot(122)
47 ax2.plot(x,y, 'k*') # wells
48 ax2.plot(wipp[:,0], wipp[:,1], 'r-') # WIPP LWB
49 ax2.plot(buff[:,0], buff[:,1], 'g--') # WIPP LWB+3km
50 for xv,yv,n,w in zip(x,y,names,weights):
51     plt.annotate('%s %i'%(n,w), xy=(xv,yv), fontsize=8)
52 plt.axis('image')
53 ax2.set_xlim([wipp[:,0].min()-100,wipp[:,0].max()+100])
54 ax2.set_ylim([wipp[:,1].min()-100,wipp[:,1].max()+100])
55 plt.suptitle('well weights check '+year)
56 plt.savefig('check-well-weights-'+year+'.png')
57
58 # convert lengths to feet
59 res /= M2FT
60 ores /= M2FT
61
```

```

62 # create the histogram of residuals for ASER
63 # *****
64
65 # -10,-9,...8,9,10
66 bins = np.arange(-10,11)
67 rectfig = (15,7)
68 squarefig = (8.5,8.5)
69
70 fig = plt.figure(1,figsize=rectfig)
71 ax = fig.add_subplot(111)
72 # all the data, all but distant wells
73 ax.hist([res[weights<2,2],res[:,2]],bins=bins,range=(-10.0,10.0),
74         rwidth=0.75,align='mid',
75         color=['red','blue'],
76         label=['Inside LWB & <3km from WIPP LWB','All wells'])
77 ax.set_xlabel('Measured-Modeled (ft)')
78 ax.set_ylabel('Frequency')
79 ax.set_xticks(bins)
80 ax.set_ylim([0,10])
81 ax.set_yticks(np.arange(0,10,2))
82 plt.grid()
83 ax.yaxis.grid(True,which='major')
84 ax.xaxis.grid(False)
85 plt.legend(loc='upper left')
86 plt.title('Histogram of Model Residuals '+year)
87 plt.savefig('model-error-histogram-'+year+'.png')
88 plt.close(1)
89
90 # create bar chart plot of individual residual for ASER
91 # *****
92
93 # separate wells into groups
94 resin = res[weights==0,2]
95 resnear = res[weights==1,2]
96 resfar = res[weights==2,2]
97
98 nin = resin.size
99 nnear = resnear.size
100 nfar = resfar.size
101
102 # separate names into groups
103 namin = names[weights==0]
104 namnear = names[weights==1]
105 namfar = names[weights==2]
106
107 # get indices that sort vectors
108 ordin = np.argsort(namin)
109 ordnear = np.argsort(namnear)
110 ordfar = np.argsort(namfar)
111
112 # put vectors back together (groups adjacent and sorted inside each group)
113 resagg = np.concatenate((resin[ordin],resnear[ordnear],resfar[ordfar]),axis=0)
114 namagg = np.concatenate((namin[ordin],namnear[ordnear],namfar[ordfar]),axis=0)
115
116 fig = plt.figure(1,figsize=rectfig)
117 ax = fig.add_subplot(111)
118
119 wid = 0.6
120 shift = 0.5 - wid/2.0
121 ab = np.arange(res.shape[0])
122
123 ax.bar(left=ab+shift,height=resagg,width=0.6,bottom=0.0,color='gray')
124 ax.set_ylim([-15.0,15.0])
125 ax.spines['bottom'].set_position('zero')

```



```

126 ax.spines['top'].set_color('none')
127 ax.xaxis.set_ticks_position('bottom')
128 plt.xticks(ab+wid,namagg,rotation=90)
129 # vertical lines dividing groups
130 ax.axvline(x=nin,color='black',linestyle='dashed')
131 ax.axvline(x=nin+nnear,color='black',linestyle='dashed')
132 ax.axhline(y=0,color='black',linestyle='solid')
133 ax.axhline(y=-15,color='black',linestyle='dotted')
134 plt.grid()
135 ax.yaxis.grid(True,which='major')
136 ax.xaxis.grid(False)
137 ax.set_xlim([0,res.shape[0]])
138
139 plt.annotate('',xy=(0.0,12.0),xycoords='data',
140             xytext=(nin,12.0),textcoords='data',
141             arrowprops={'arrowstyle':'<->'})
142 plt.annotate('inside WIPP LWB',xy=(nin/3.0,12.5),xycoords='data')
143
144 plt.annotate('',xy=(nin,12.0),xycoords='data',
145             xytext=(nin+nnear,12.0),textcoords='data',
146             arrowprops={'arrowstyle':'<->'})
147 plt.annotate('<3km WIPP LWB',xy=(nin+nnear/3.0,12.5),xycoords='data')
148
149 plt.annotate('',xy=(nin+nnear,12.0),xycoords='data',
150             xytext=(nin+nnear+nfar,12.0),textcoords='data',
151             arrowprops={'arrowstyle':'<->'})
152 plt.annotate('>3km WIPP LWB',xy=(nin+nnear+nfar/3.0,12.5),xycoords='data')
153
154 ax.set_ylabel('Measured-Modeled (ft)')
155 ax.set_title('individual residuals '+year)
156 plt.savefig('model-error-residuals-'+year+'.png')
157 plt.close(1)
158
159
160 # create scatter plot of measured vs. modeled
161 # *****
162 m = 1.0/M2FT
163 sr = [2980,3120]
164
165 print 'modeled-vs-measured correlation coefficients'
166 print 'all data: %.4f' % np.corrcoef(res[:,0],res[:,1])[1,0]**2
167 print 'inside WIPP: %.4f' % np.corrcoef(res[weights==0,0],res[weights==0,1])[1,0]**2
168 print 'inside 3km: %.4f' % np.corrcoef(res[weights<2,0],res[weights<2,1])[1,0]**2
169
170 print 'uncalibrated model'
171 print 'all data: %.4f' % np.corrcoef(ores[:,0],ores[:,1])[1,0]**2
172 print 'inside WIPP: %.4f' % np.corrcoef(ores[weights==0,0],ores[weights==0,1])[1,0]**2
173 print 'inside 3km: %.4f' % np.corrcoef(ores[weights<2,0],ores[weights<2,1])[1,0]**2
174
175
176 fig = plt.figure(1,figsize=squarefig)
177 ax = fig.add_subplot(111)
178 ax.plot(res[weights==0,0],res[weights==0,1],color='red',markersize=10,
179         marker='+',linestyle='none',label='Inside LWB')
180 ax.plot(res[weights==1,0],res[weights==1,1],color='green',markersize=10,
181         marker='x',linestyle='none',label='< 3km From LWB')
182 ax.plot(res[weights==2,0],res[weights==2,1],color='blue',markersize=10,
183         marker='*',linestyle='none',label='distant')
184 ax.plot(sr,sr,'k-',label='$45^\{\degree\}$ Perfect Fit')
185 ax.plot([sr[0],sr[1]],[sr[0]+m,sr[1]+m],'g-',linewidth=0.5,label='$\pm$ 1m Misfit')
186 ax.plot([sr[0],sr[1]],[sr[0]-m,sr[1]-m],'g-',linewidth=0.5,label='__nolegend__')
187 ax.set_xticks(np.linspace(sr[0],sr[1],8))
188 ax.set_yticks(np.linspace(sr[0],sr[1],8))
189 ax.set_xlim(sr)

```

```

190 ax.set_ylim(sr)
191 plt.minorticks_on()
192 plt.legend(loc='lower right', scatterpoints=1, numpoints=1)
193 plt.grid()
194 for j, lab in enumerate(names):
195     if res[j,2] < -1.5*m:
196         # plot labels to left of value far above 45-degree line
197         plt.annotate(lab, xy=(res[j,0], res[j,1]),
198                     xytext=(res[j,0]-(2.9*len(lab)), res[j,1]-2.0), fontsize=14)
199     elif res[j,2] > 1.5*m:
200         # plot labels to right of value far below 45-degree line
201         plt.annotate(lab, xy=(res[j,0], res[j,1]),
202                     xytext=(res[j,0]+2.0, res[j,1]-2.0), fontsize=14)
203 ax.set_xlabel('Observed Freshwater Head (ft AMSL)')
204 ax.set_ylabel('Modeled Freshwater Head (ft AMSL)')
205 ax.set_title('modeled vs. measured '+year)
206 plt.savefig('scatter_pest_02_'+year+'.png')

```

10.3.11 Python script plot-contour-maps.py

This script is not run on the QA linux cluster, `alice.sandia.gov`. This script is run on a desktop PC, but is only used to create figures for the analysis report. This script is only included here for completeness.

```
1 import numpy as np
2 #import matplotlib
3 #matplotlib.use('Agg')
4 import matplotlib.pyplot as plt
5 from mpl_toolkits.basemap import pyproj
6
7 # http://spatialreference.org/ref/epsg/26713/
8 # http://spatialreference.org/ref/epsg/31013/
9 putm = pyproj.Proj(init='epsg:26713') # UTM Zone 13N NAD27 (meters)
10 pstp = pyproj.Proj(init='epsg:32012') # NM state plane east NAD27 (meters)
11
12 def transform(xin, yin):
13     """does the default conversion from utm -> state plane
14     then also convert to feet from meters"""
15     xout, yout = pyproj.transform(putm, pstp, xin, yin)
16     xout /= M2FT
17     yout /= M2FT
18     return xout, yout
19
20 year = '2005'
21 fprefix = 'pest_02/'
22 mprefix = '../wipp-polyline-data/'
23 cfname = fprefix + 'modeled_head_pest_02.grd'
24 pfname = fprefix + 'dtrk_output_pest_02.blm'
25 wfname = fprefix + 'modeled_vs_observed_head_pest_02.txt'
26
27 M2FT = 0.3048
28
29 # read in well-related things
30 # %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
31 # load in observed, modeled, obs-mod, (all in meters)
32 res = np.loadtxt(wfname, skiprows=1, usecols=(3, 4, 5))
33 res /= M2FT # convert heads to feet
34 wellx, welly = transform(*np.loadtxt(wfname, skiprows=1, usecols=(1, 2), unpack=True))
35 names = np.loadtxt(wfname, skiprows=1, usecols=(0, ), dtype='|S6')
36
37 # read in head-related things
38 # %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
39 h = np.loadtxt(cfname, skiprows=5) # ASCII matrix of modeled head in meters AMSL
40 h[h<0.0] = np.NaN # no-flow zone in northeast
41 h[h>1000.0] = np.NaN # constant-head zone in east
42 h /= M2FT # convert elevations to feet
43
44 # surfer grid is implicit in header
45 # create grid from min/max UTM NAD27 coordinates (meters)
46 utmy, utmx = np.mgrid[3566500.0:3597100.0:307j, 601700.0:630000.0:284j]
47
48 # head contour coords
49 hx, hy = transform(utmx, utmy)
50 del utmx, utmy
51
52 # read in particle-related things
53 # %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
54 px, py = transform(*np.loadtxt(pfname, skiprows=1, delimiter=',',
55                             usecols=(0, 1), unpack=True))
56 part = np.loadtxt(pfname, skiprows=1, delimiter=',', usecols=(2,))
57
58 # read in MODFLOW model, WIPP LWB & ASER contour domain (UTM X & Y)
59 # %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
60 modx, mody = transform(*np.loadtxt(mprefix+'total_boundary.dat',
61                             unpack=True))
```