MEMO

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Date:	6 January 2012
To:	ESHMC
From:	IDWR Allan Wylie
cc:	SV Sean Vincent, Rick Raymondi RR
Subject:	IDWR contribution to the Uncertainty White Paper

This memo is prepared in response to a request to discuss the predictive uncertainty protocol and determine whether the current process has value. This memo will discuss: 1) the reasons for conducting a predictive uncertainty analysis, 2) how the current procedure was developed, 3) the current procedure selected by the Eastern Snake Hydrologic Modeling Committee (ESHMC), and 4) the results of the analyses conducted to date.

Reasons for conducting a predictive uncertainty analysis
Ground water models have been used in hydrologic studies for several decades. Many post audits during that time show that model predictions are not always accurate due to use of inaccurate data during model calibration and parameter correlations resulting in non-unique calibrations (Konikow, 1986; Steward and Langevin, 1999; Andersen and Lu, 2003). One way to evaluate this problem is to conduct a predictive uncertainty analysis. The suite of analyses proposed for version two of the Eastern Snake Plain Aquifer Model (ESPAM2) will estimate predictive uncertainty. Predictive uncertainty analyses are conducted to: 1) establish the precision for key model predictions (Meyer and others, 2007); 2) help identity where more data can reduce predictive uncertainty (Dausman and others, 2010) and; 3) document the limitations of the model (Doherty and others, 2011). Along with these technical reasons to conduct a predictive uncertainty analysis, the ESHMC received requests from others. Hearing Officer Schroeder (2008) requested an uncertainty analysis, Director Tuthill requested an uncertainty analysis during the January 2009 ESHMC meeting, and Director Spackman requested an uncertainty analysis in his June 9, 2011 letter to the EHSMC.

Doherty and others (2011) indicate that there are two sources of error in ground water models:

1) Measurement noise – Noise is inherent in all measurements and observations used for calibration. This includes components of the water budget, river gains, spring discharges, aquifer water levels, etc.
2) Failure to capture the more important components of the hydrogeologic system integral to key predictions – The simplifications inherent in creating ground water

models due to incomplete or inaccurate knowledge of the system can contribute to predictive uncertainty.

During model development, efforts were made to reduce model uncertainty by including calibration targets, or field observations, that the ESHMC thought would constrain the adjustable parameters. There are numerous calibration targets within the model, and the committee has reviewed modeled vs. measured data to assess the general success of calibration. Of course even with the calibration targets, there is still some degree of model uncertainty, but model uncertainty is only a problem if it significantly impacts an important prediction. For example, parameter correlations may result in a non-unique calibration, however, if none of the predictions from the suite of models with an acceptable calibration are significantly different, then the non-uniqueness does not pose a problem. Thus a model may have a high degree of uncertainty, but low predictive uncertainty. The ESHMC chose to evaluate predictive uncertainty, the uncertainty in key predictions due to poorly constrained parameters, not model uncertainty. Doherty and others (2011) state that predictive uncertianty analyses are "fundamental to the use of modeling in support of decision making".

How the current procedure was selected

In 2007, the ESHMC identified goals for development and calibration of ESPAM2 and individual committee members ranked the components that they considered most important. That exercise resulted in the ranking shown in Figure 1. An uncertainty analysis was ranked as the third most important improvement to ESPAM2. In the November 2009 meeting, the ESHMC chose to evaluate predictive uncertainty using PEST (Doherty, 2010) following the procedure outlined by Doherty (2003). This decision was modified to use the nonlinear analysis proposed by James and others (2009) in the February 2010 meeting. During the March 2011 meeting, the ESHMC unanimously agreed to proceed with a predictive uncertainty analysis immediately after calibration of ESPAM2 was complete. In the June 2011 meeting, the committee chose to reduce the scope of the analysis because an exhaustive analysis of a complex model like the ESPAM2 would take far too long. The committee chose a limited predictive uncertainty analysis that involved imposing a stress at the centroid within each of eight water districts and determining uncertainty for the impact of the stress on each of four spring/river reaches. The eight water districts are Water District 100, 110, 120, 130, 140, 33, 34, and the Rexburg Bench. The four spring/river reaches are Clear Lakes, Blue Lakes, nr Blackfoot to Minidoka, and Ashton to Rexburg.

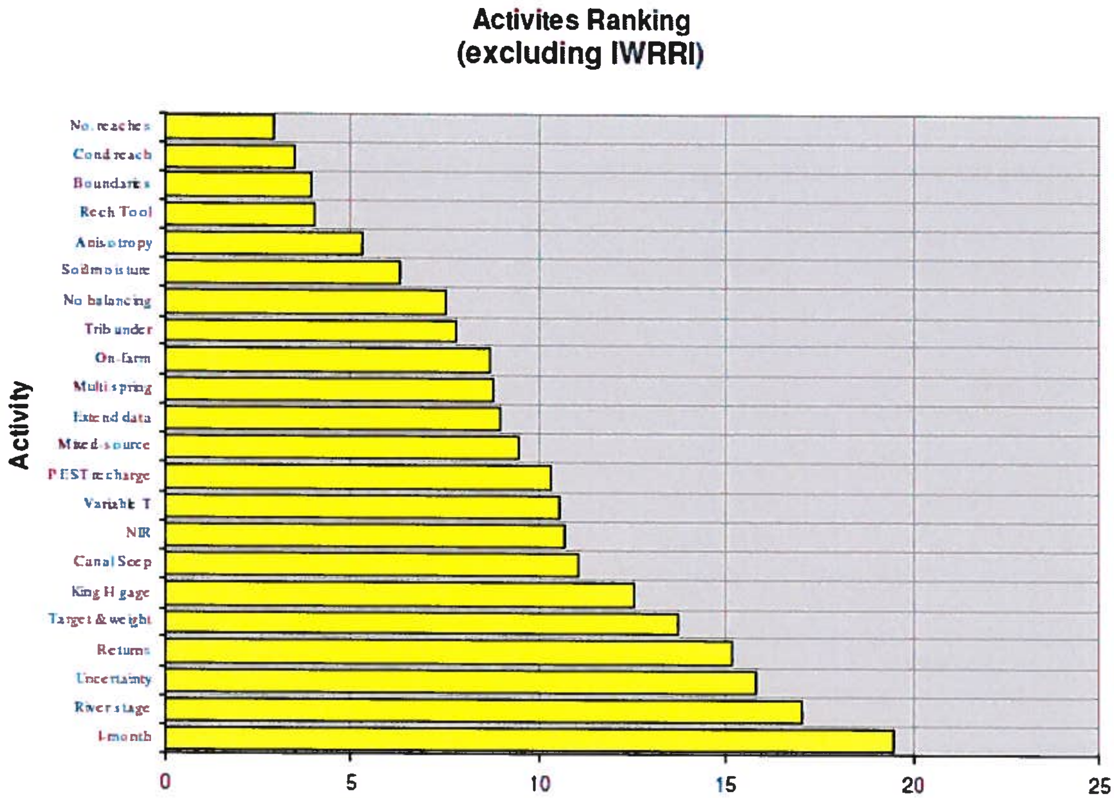

Figure 1. Ranking of proposed improvements for ESPAM2. (From Contor 2008)

The analysis chosen by the ESHMC will interrogate the collective impact of the following components of the ESPAM2 model on predictive uncertainty: 1) uncertainty in adjustable components of the water budget, 2) physical parameter uncertainty, and 3) measurement uncertainty. During calibration PEST is allowed to adjust many components of the water budget, so the contributions to predictive uncertainty from the adjustable components of the water budget are incorporated in the predictive uncertainty analysis. All physical properties adjustable during calibration are also adjustable during the predictive uncertainty analysis (e.g. transmissivity, specific yield, drain conductance, riverbed conductance, etc), so the contribution to predictive uncertainty by physical properties also is included in the analysis. The ESHMC often assigned weights for field observations based on their confidence in the measurements. Weighting more uncertain measurements less allows for more misfit between model output and field observations. Thus, to the extent that the weighting scheme takes into account measurement uncertainty, measurement uncertainty's contribution is also incorporated in the predictive uncertainty analysis.

The procedure

The following is the procedure used to prepare a PEST predictive uncertainty run to identify how correlations in adjustable parameters can impact the selected predictions.

1) Identify the centroid of the irrigated lands within the water district (this can be done in GIS).
2) Prepare the model files necessary to run the prediction, including a well file constructed using the 3x3 cell centriod identified in step one (1).

3) Make a copy of the PEST control file. The PEST control file contains all of the adjustable parameters and their bounds, and all the field observations. Since we are copying the control file, every parameter adjustable in our calibration run will also be adjustable in our predictive uncertainty analysis, and every field observation used as a calibration target will also be used as a target in our predictive uncertainty analysis. The following adjustments (items 4 – 12) need to be made to the PEST control file.
4) Replace the word 'regularization' with the word 'prediction' on the third line.
5) Increase the number of observations by one (1) because the prediction will be a new observation.
6) Increase the number of observation groups by one (1) because there will now be an observation group 'predict'.
7) Increase the number of instruction files by one (1) because PEST will now be required to monitor the prediction.
8) Add 'predict' to the list of observation groups.
9) Add an additional observation to the observation section. At this time I expect these will be called 'Predict_CRL' for the Clear Lakes impact, 'Predict_BLK' for the Blue Lakes impact, and 'Predict_nBMin' for impact to the nr Blackfoot-Minidoka reach. Any weight and target observation value can be provided because PEST ignores the weight and target observation value for any observation in the 'predict' group when it is run in predictive analysis mode.
10) Change the model command line to reflect the name of the batch file used to run the model and the prediction.
11) Add the name of the new instruction file and the output file it will read to the list of files used to read model output. I expect the instruction file will be called 'Predict.ins' and the file it will read will be called 'Predict.smp'
12) Add a 'predictive analysis' section to the control file. This will include NPREDMAXMIN, PD0, PD1, and PD2. NPREDMAXMIN tells PEST whether to maximize (+1) or minimize (-1) the prediction of interest. PD0 is a value of the objective function (phi) which is considered calibrated. Naturally, PD0 must be greater than phi for the calibrated model, but only a little greater. Because the shape of the PD0 envelope can be complex, it is extremely hard for PEST to find a parameter set which lies exactly on the boundary. The value supplied for PD1 (which must be slightly higher than PD0) is a value PEST will consider "close enough". If the sum of the squared residuals is above PD2, PEST tries to minimize the objective function until the objective function is below PD2, at which point PEST begins searching for either the maximum or minimum value for the prediction at PD0.

Thus, during a predictive uncertainty analysis run PEST will: A) run MKMOD, B) run MODFLOW, C) compare model output with field observations exactly like in a calibration run, D) compare the sum of the squared residuals (phi) from this run with PD0, E) make a model run in superposition mode containing only the 3x3 well file constructed during steps 1 and 2, F) collect the predicted impact at the target spring or river reach, and G) compare this prediction with the previous maximum (or minimum) prediction and save the value if it is a new maximum (or minimum) and phi for this run is less than PD1.

The Doherty (2010) recommends that phi from the calibrated model <PD0 < PD1 < PD2 and further states that PD0 should only be slightly larger than phi for the calibrated model (1or 2% larger), and PD1 should only be slightly larger than PD0 (1 or 2% larger), and PD2 is generally 1.5 to 2 times PD0. Functionally, assigning PD0 and PD1 values a little larger than the calibrated phi allows PEST enough elbow room to explore parameter space and locate correlated parameters that potentially could impact the selected prediction.

Results

As of December 2011, three analyses have been completed using calibration run E110712A_002. Once calibration is complete, at least some of these analyses will be checked with the updated model. The completed analyses are: centroid of WD130 to Clear Lakes, centroid of WD110 to Clear Lakes, and centroid of WD120 to Clear Lakes (Figure 2).

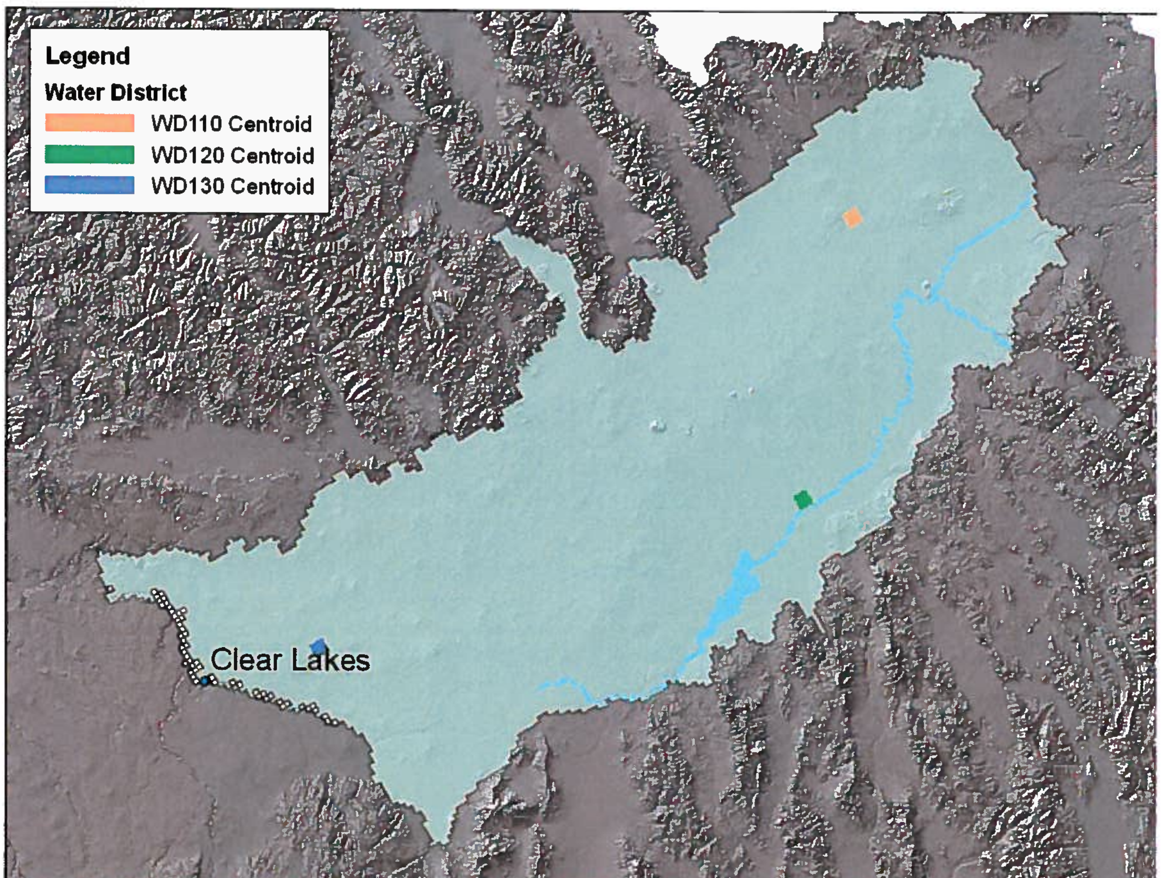

Figure 2. Locations of centroids and spring evaluated to date.

Thus far, the analyses have not identified any significant issues. Largely unknown parameters such as tributary valley underflow have not significantly impacted predictive uncertainty in any of the analyses conducted to date. Table 1 shows the variability in the impact each centroid can have on Clear Lakes Spring. Figure 3 shows the change in the calibrated discharge at Clear Lakes Spring. Figure 3 emphasizes that the calibration is nearly unchanged when the model maximizes or minimizes the impact because of correlations in adjustable parameters. An alternative perspective is that the more important parameters tend to be constrained by relevant field observations.

Table 1. Predicted impact at Clear Lakes as percentage of applied stress.

Centroid	Calibrated Impact	Maximized Impact	Minimized Impact
WD110	0.170%	0.170%	0.164%
WD120	0.450%	0.930%	0.390%
WD130	7.110%	7.360%	6.930%

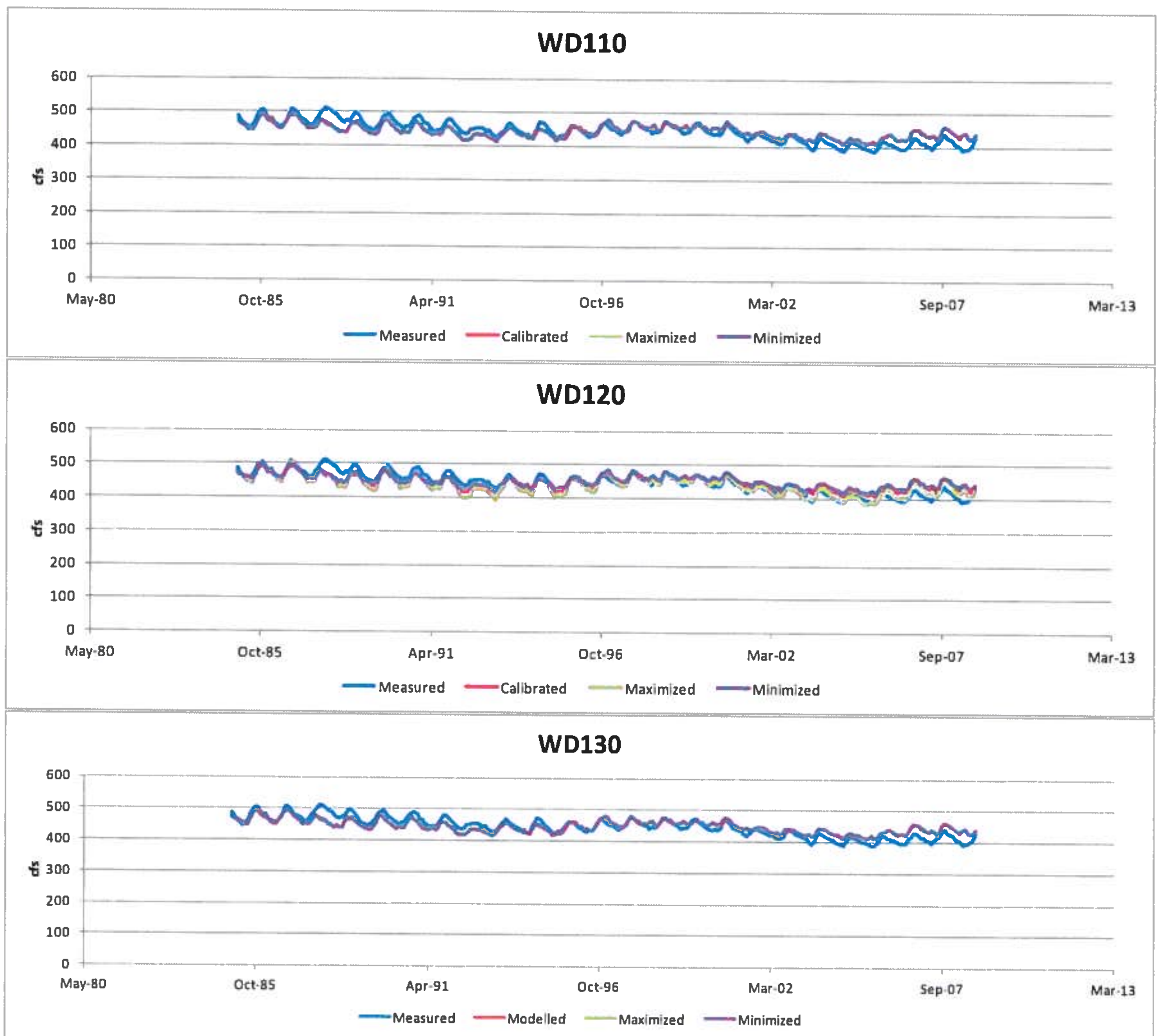

Figure 3. Measured and calibrated discharge, and modeled discharge when impact is maximized and minimized for Clear Lakes.

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