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Selecting Calibration Values and Formulating Calibration Targets for Ground-Water Flow Simulations

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ABSTRACT

Simulation of ground-water flow is often a desired or promised outcome of many field investigations. Frequently, the study design, and data collection and analysis are performed without regard to the desired accuracy of the modeling results. Rarely are calibration values and targets set prior to simulation or even considered when designing the study. This neglect of fundamental field information needed in model calibration leads to unrealistic expectations from modeling efforts. We suggest a systematic approach to assessing the level of error associated with sample information selected for calibration assessment. It is proposed that this procedure occur prior to the initiation of ground-water flow modeling. Our procedure involves: 1) selecting calibration values, typically heads, fluxes and a water balance; 2) setting calibration targets based on error analysis of calibration values; 3) assessing the results of calibration efforts based on the agreement between simulated values and calibration targets. Application of the procedure is demonstrated using results from a flow model of an unconfined intermontane basin aquifer.

INTRODUCTION

The development and use of numerical ground water flow models has expanded greatly in the last 20 years. Of late, demand for ground-water modeling has been spurred by requests from regulatory agencies for interpretive and predictive ground-water modeling and by private industry's desire to be competitive in a rapidly expanding market, as well as researchers' search for better methods to represent complex hydrogeologic settings. Ground-water flow modeling has become a standard part of resource and contaminant transport analyses. However, there is growing concern over the usefulness and possible misuse of modeling results. This distrust is partly based on: 1) The absence of calibration protocols and poor documentation of the calibration procedure; 2) recognition of uncertainties in parameter values and distributions. As a result, flow modeling results are coming under intense scrutiny (National Research Council, 1990).

It is the intent of this work to propose a calibration protocol that requires the use of field values and their associated error to measure calibration success. In proposing a modeling protocol, we recognize that different levels or degrees of calibration may be appropriate for a particular ground-water setting depending on the hydrogeologic questions being posed and the quality and quantity of field data. For example, construction of an interpretative model to determine the magnitude and location of bedrock recharge to an alluvial aquifer may not require the same level of calibration as a model being used for capture zone analyses. This view of calibration may be unpopular in an era when lawyers and regulatory agencies thirst for a hard and fast set of procedures or rules that will certify that a particular rendition of a field setting in a model is correct. However, we support a more problem specific approach.

THE CALIBRATION PROCESS

The comparison of simulated heads and fluxes with field measured values during the repeated adjustment of aquifer parameters and stresses is the heart of the calibration process. Ground-water models are typically calibrated to steady state conditions, sometimes followed by transient calibration. Some models are only calibrated to transient conditions (Anderson and Woessner, 1992 a). In trail-and-error calibration the process is considered complete when the residual errors between simulated and measured values are subjectively judged "acceptable" (Peters, 1987).

Clearly, subjective judgements must be based on a set of criteria that are easily understood and evaluated. Unfortunately, many model users attempt model calibration without carefully evaluating the quality of their data or setting criteria for an acceptable calibration. This leaves their subjective judgement with a poor foundation. It often appears that criteria used to determine calibration "acceptability" are founded more on the time schedule and budget of a project than on a clearly stated and tested set of calibration values and targets. Obviously, this weakens claims of model calibration.

We propose a four part calibration process that is designed to provide a data set upon which a judgement of acceptability can be based:

1) Selection of pre-simulation calibration values and calibration targets;

2) Setting ranges of aquifer parameter estimates;

3) Fitting of simulated results to calibration targets;

4) Evaluation and documentation of the calibration process.

This paper emphasizes the formulation of calibration values and calibration targets (Table 1). We also include a brief discussion of the methods to document and evaluate the calibration process. Finally, we use a case study to illustrate the setting of calibration targets and their use in assessing model calibration. A more detailed presentation of the complete calibration process is found in Anderson and Woessner (1992 a).

Table 1: Definitions*.

Calibration value:	Field-measured value, typically head, flux and/or a water balance.
Calibration target:	The calibration value and associated error.
Calibration level:	Integer scale indicating the degree of match between the calibration target and the simulated value.

* *modified from Woessner and Anderson (1990 a)*

SELECTING CALIBRATION VALUES

Calibration values include field measured hydraulic heads, fluxes and water balances. It is important to realize that both heads and one or more flux values (i.e., measured stream channel leakage rates) or heads and a water balance should be used when attempting model calibration. Modelers recognize that calibration efforts usually result in a non-unique solution to the inverse problem (Freyberg, 1988). Calibration to a large number of one or more evenly spaced calibration values of head will increase the likelihood of obtaining a unique calibration, as will the use of fluxes as calibration targets.

The objective of calibration is not to reproduce the field measured values exactly, as each measurement has an associated error. The modeler must identify and quantify the error associated with each calibration value, thereby defining a calibration target (Figure 1). This process should take place prior to initiation of numerical simulation as it is the setting of these calibration targets that form a portion of the standard by which the degree of calibration success is assessed. Guidelines for the formulation of calibration targets for head, flux values and water balances follows.

Head

If you ask a hydrogeologist which set of field data is most accurately known in a typical field site the response will be head measurements. Most often the measurement error associated with heads measured using a steel or electric tape is small, i.e. + /- 0.02 ft (Sweet et al., 1990). Furthermore, elevation surveys commonly add less than one tenth of a foot of error to field measurements. Thus, the resulting potentiometric surface contour maps constructed from field head data often are a good representation of the head distribution. However, these heads

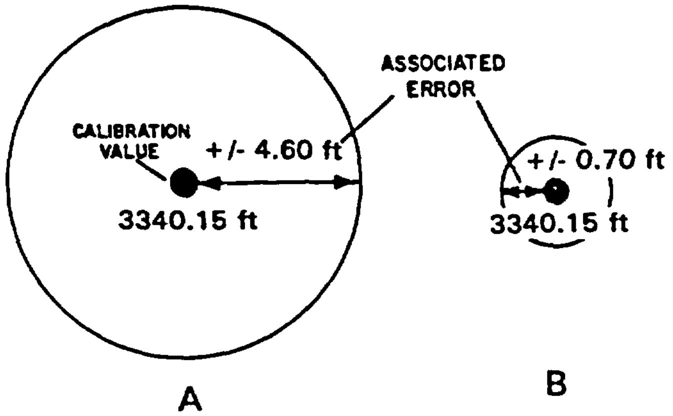

Figure 1: A calibration target is defined as a calibration value and its associated error. A) A target with a large associated error, 3340.15 ft +/- 4.60. B) A target with a small associated error, 3340.15 ft +/- 0.70 ft. (modified from Anderson and Woessner, 1992 a)

typically are not reproduced exactly by a model because of what we might call model error.

The selection of heads as calibration values requires that both measurement error and model error be evaluated. Measurement error encompasses: 1) Operator error; 2) instrument error; 3) survey error. Measurement errors include those introduced by the procedure used by the operator and those attributed to the tape, transducer or recording device. Only the operator error is not easily quantified. This is the first place in the process that a judgement based on knowledge of the field procedures, the type of well being monitored (e.g. with or without a pump, shallow vs. deep wells), the experience of the operator with the instruments and the field conditions at the time of data collection all have to be weighed and a portion of the error attributed to the operator. Each assumption about the nature and amount of error should be clearly stated in the modeling report.

Survey error is defined by the instruments and required accuracy of the survey. Typically, surveys are judged acceptable if some predefined error is not exceeded for a given distance of level line once the survey loop is closed. The calculated total error is then evenly distributed over the number of points surveyed in that particular loop. Hence, survey error is available from the land surveyor's report. If topographic maps are used to estimate well elevations, which is sometimes done for regional studies, the accuracy of the well location and the errors involved in interpolating elevations are used to quantify survey error.

Modeling errors include: 1) Scaling effects; 2) transient error; 3) interpolation error. Scaling effects include errors introduced by the averaging effects of measuring heads in long well screens and the effect of small scale heterogeneities in the aquifer properties (Gelhar, 1986). Attempts should be made to compare heads measured in wells with different lengths of screens located at approximately the same position in the field so that calculations can be made to assess the magnitude of error introduced by the well design. Ideally the well design should match the dimensionality of the model. Fully penetrating wells are needed for two-dimensional areal models, for example. A three-dimensional array of piezometers is needed for a three-dimensional model. Scaling errors also include errors introduced by representing a heterogeneous aquifer as an equivalent homogeneous porous medium at the scale of the cell or element used in the model. Small scale hetrogenieties not included in the model may affect head measurements.

Transient errors occur when simulated heads are compared with field data collected over a longer period of time than represented by the simulation. Field measurements may reflect the effects of transient pumping, tides, barometric effects and regional variation in head (Sayko et al., 1990).

Interpolation error occurs when the site of the field measurement does not coincide with the nodal point in the model. In this case, an equivalent field measured value is derived for comparison with a simulated nodal value. Typically, an interpolated field head value is derived by linearly interpolating the field measured value to the nodal location based on the measured hydraulic gradient in the vicinity of the cell or element. The magnitude of error associated with this process is proportional to the accuracy with which the location of the field value is known, and accuracy with which the distance to the node and hydraulic gradient can be measured.

Once each source of measurement and model error has been accounted for, the total error is calculated and the head calibration target is defined (Figure 1).

Fluxes

Recharge, baseflow, springflow, evapotranspiration, and infiltration from losing streams may also be used in conjunction with heads to calibrate flow models. Unfortunately, in many cases flux values are much harder to measure than heads. Larger measurement errors for fluxes causes larger calibration targets than those for heads. It is often a goal of flow modeling to estimate particular flux values, but, whenever possible, measurements or estimates of flux values should be used to help constrain the calibration. Baseflow, pumping rates of wells, and springflows are more easily measured than recharge and evapotranspiration. For example, standard procedures to assess stream and spring discharge measurement error are reported in the literature (Linsley et al., 1949). However, operator error and interpolation error as well as measurement error should also be evaluated. Fluxes calculated indirectly by measuring head gradients across boundaries involve estimates of hydraulic conductivity and require error analysis that incorporates the possible ranges of hydraulic conductivity values as well as errors in the hydraulic gradient measurement.

Water Balance

The water balance results from the calibrated model should also be compared with a field-based water balance. The pre-calibration water balance involves quantifying all fluxes across the model's boundaries using field data. Each flux will have associated error depending on the method of measurement or the method of calculating or estimating the water balance component. The total inflow, outflow and/or the volume change related to storage variation are the calibration values. Each of these components is composed of one or more term. For example, the inflow component may consist of the sum of all the following: recharge from precipitation, underflow across a boundary, infiltration from losing streams and water introduced through injection wells. The calibration target becomes the component value plus its error.

Other Values

Investigators have also used the location of gaining and losing streams as calibration targets (Makepeace, 1989), velocities (Duffield et al., 1990) and solute distributions (Krabbenhoft et al., 1990; Medina et al., 1990; Kauffmann et al, 1990; Keidser et al., 1990) in addition to head and water balance calibration targets as calibration targets. Use of each of these values also requires an assessment of error to formulate calibration targets.

In professional practice, calibration is typically performed manually by trial-and-error and the modeler is on "his honor" to perform a complete error analysis prior to calibration. In automated solutions to the inverse problem the modeler is forced to quantify error prior to running the inverse model (Carrera and Neuman, 1986).

ASSESSING THE CALIBRATION PROCESS

So far we have discussed calibration values and formulating pre-simulation calibration targets. Determining when to end a trial-and-error calibration requires a subjective judgement. This subjective judgement is defended during calibration assessment. The assessment process includes: 1) Definition of the degree or level of match between simulated values and calibration targets; 2) Evaluation of the sensitivity of the model results to the size of the calibration targets and variability in aquifer parameters; 3) subjective judgement as to the acceptability of the calibration. Detailed documentation of the calibration process is extremely important. Peer review of a modeling application will be based on how successfully the stated objectives were met, the completeness and quality of the calibration procedure and its underlying assumptions. A clear, strong, logical case must be developed to support the modeler's claim that the calibrated model is adequate to address the objective of the project.

In a previous study (Woessner and Anderson, 1990), we proposed defining levels or degrees to which simulated values matched calibration targets. Part of this procedure defines levels of calibration based on the closeness of match with a stated calibration target. A level 1 calibration is achieved when simulated values are within the calibration target. A level 2 calibration is met when simulated values are within two times the error associated with the field value. Higher levels correspond to the multiple of the error within which the simulated value fell (Table 1).

Presentation of the calibration process should include maps and summary tables. The number and distribution of calibration values and the level of calibration achieved for each calibration target set should be shown on a map. A summary table listing the calibration value, the level of calibration achieved and the number and percentage of nodes matching each calibration level should be presented. A table reporting the level of calibration for flux values and the pre-simulation water balance should also be prepared. Maps of the flux residuals in terms of calibration levels also may be appropriate. Additional visual representation of calibration fit should be presented as potentiometric surface contour maps that show both the interpolated field measured head distribution and the simulated head distribution for steady state and for each time step.

Many recent modeling studies present the results of calibration efforts as lumped parameters such as the mean of the absolute value of the differences, root mean squared error, absolute value of the mean differences, or the mean difference between simulated and measured values (e.g., Konikow, 1977; Buckles and Watts, 1988; Yager, 1986; Anderson and Woessner, 1992 a). These values are easy to calculate and are often useful as a way of summarizing a calibration. However, they provide no information on the number and distribution of calibration targets or the spacial distribution of error as does the presentation of calibration levels.

As a final step in the calibration assessment, a detailed sensitivity analysis is required to assess the effect of the size of the calibration targets and uncertainty in the aquifer parameters on model results. Sensitivity analysis consists of varying each parameter value within its estimated error and quantifying the effects on the initial calibrated data set. Results of the sensitivity analysis should be presented graphically to illustrate the changes in the original level of calibration for heads, fluxes and the water balance. Occasionally, best case - worse case scenarios are evaluated by changing a number of parameters at once. Details on sensitivity analysis are presented in Anderson and Woessner (1992 a).

Based on the assessment of the calibration a subjective judgement is made as to the acceptability of the calibration for the objective of the project.

CASE STUDY: AN EXAMPLE OF SETTING CALIBRATION TARGETS AND ASSESSING MODEL CALIBRATION

Unfortunately, detailed documentation of the calibration process used in any particular study is uncommon. In an earlier paper (Woessner and Anderson, 1990), we used a ground-water model of a hydrologically closed basin in Nevada (Thomas et al., 1989) to illustrate the setting of calibration targets and levels. In this paper we use the unpublished work of Miller (1991) who constructed an interpretive model of an intermontane aquifer in western Montana (Figure 2). As with the Nevada study, calibration values and targets were not selected prior to the calibration. However, sufficient error analyses were preformed to derive calibration targets and assess the calibration process ex post facto.

Due to the brevity of this paper we only use a portion of Miller's work to illustrate how calibration targets should be set and reported, and the calibration process assessed. We do not present the procedures for determining field based ranges of aquifer parameter values and their final modeled distribution. Such a process was completed by Miller and modeled aquifer parameter values and their distributions were within pre-simulate set ranges. We also have chosen only to discuss the calibration process used to achieve steady state conditions. Miller's work also included extensive transient calibration using heads, hydrographs, fluxes and an annual field based water balance.

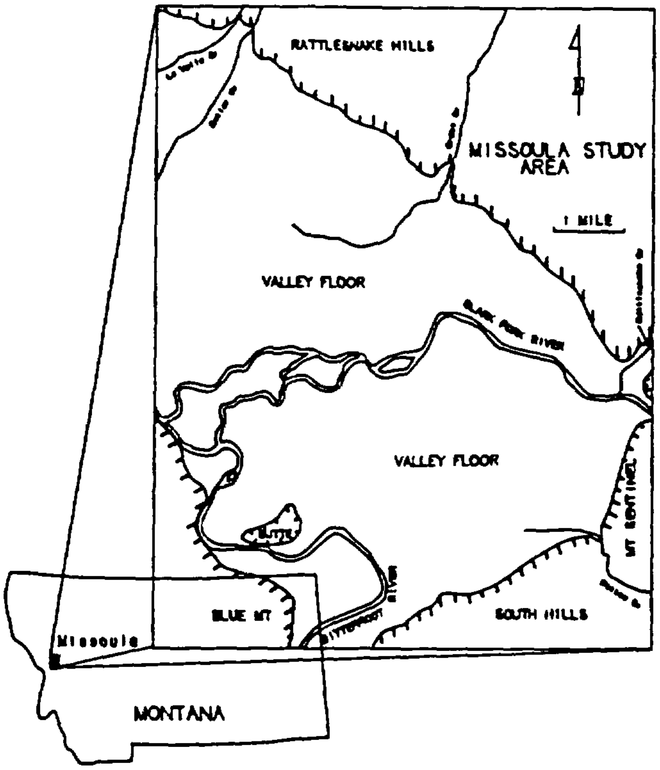

Figure 2: Location map of the valley floor Missoula Aquifer (Miller, 1991)

A two-dimensional finite difference model of the Missoula Aquifer, an unconfined sand, gravel and boulder aquifer, was formulated (Figure 3) for MODFLOW (McDonald and Harbaugh, 1988). Modeling objectives included interpreting boundary conditions and assessing the magnitude of recharge from the channel of the Clark Fork River.

The model grid consisted of 56 columns by 68 rows with square cells 660 ft by 660 ft (Figure 3). After boundary assignment a total of 2,460 nodes were active. The Clark Fork River has an average flow of 3,000 cfs and is a losing stream over the first four and to six miles of channel length. Hydraulic conductivity distributions were determined from evaluations of specific capacity data, the results of six classic aquifer tests (discharge was typically 1000 gpm), and interpretation of the geologic setting using facies models. Potentiometric surface contour maps were generated from head values measured monthly at 78 wells from five separate sources for the period February 1, 1986, to January 1, 1987. Steady state conditions were represented by February water levels, a period during which water levels stabilize.

The location and distribution of 15 wells with the most complete set of monthly head measurements for the study period were selected to provide head calibration values (Figure 3).

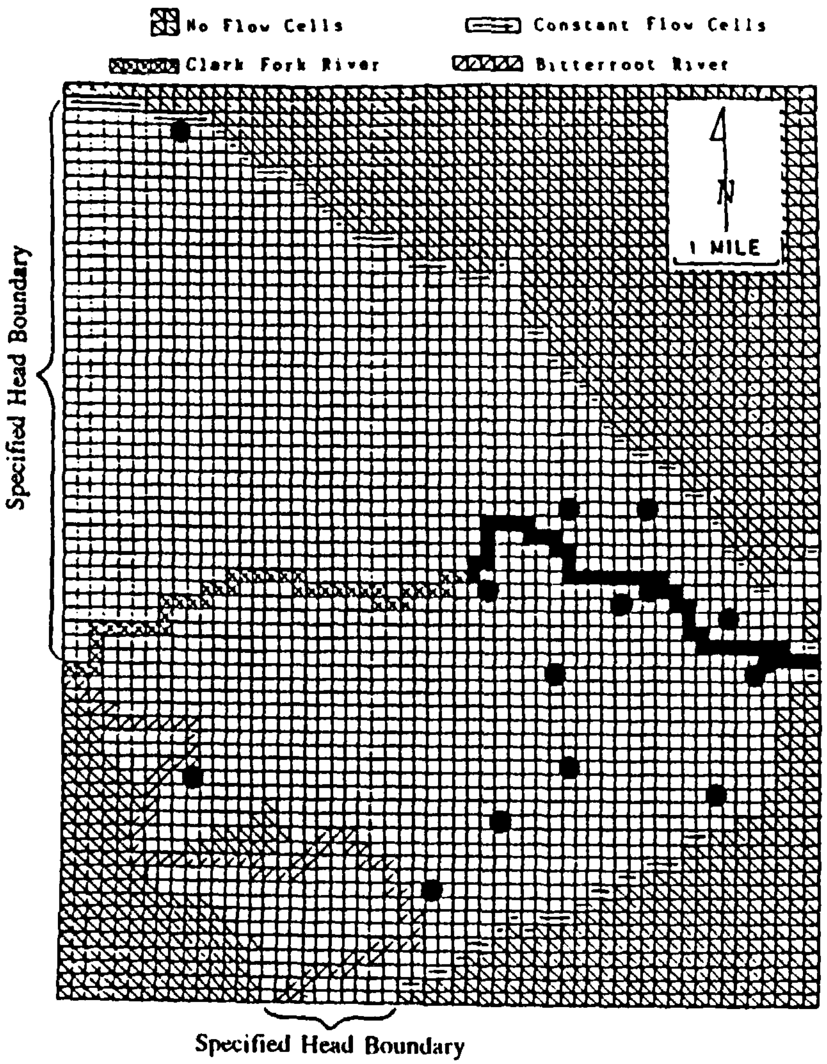

Figure 3: Model grid indicating the location of calibration targets (shaded circles) and the losing reach of the Clark Fork River (shaded squares) (modified from Miller, 1991).

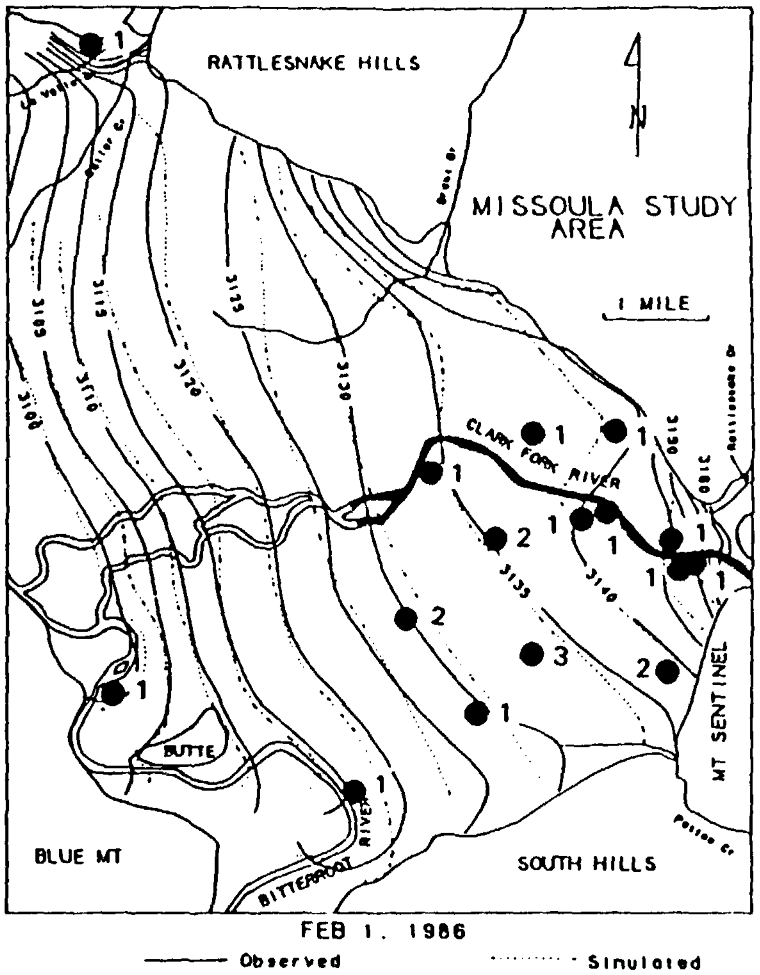

Figure 4: Observed vs. simulated potentiometric surface contours, the location of calibration targets (shaded circles) and associated calibration levels (1, 2 or 3, see Table 3), and the simulated length (4.5 mi) of losing river channel (shaded) (modified from Miller, 1991).

The error analysis performed on the head values is presented in Table 2. The largest error was attributed to transient effects that resulted from the author's attempt to normalize head values collected at different times during the month to the first of the month using monthly regional water level trend analysis.

Table 2. Head error analysis.

Source of error	magnitude
well survey elevations	+/- 0.12 ft
water level measurement	+/- 0.02 ft*
scaling effects	#
transient interpolation	+/- 0.30 ft
interpolation error	+/- 0.14 ft**
Total error	+/- 0.58 ft

** combines operator and instrument error, # judged to be insignificant, ** ranged from +/- 0.05 to +/- 0.14 ft, (modified from Miller, 1991)*

Table 3 defines the calibration levels for heads and the length of losing river reach. The percent of measured heads that fell in each level is also indicated. Figure 4 shows the distribution of calibration values and levels. Calibration values are sparse in the western and northern portions of the modeled area. If poor field matches between field and simulated values occur in these regions, they are probably sufficiently removed from the Clark Fork River so as not to compromise river leakage estimates. The match of interpolated field measurements with the simulated head contours (Figure 4) provides qualitative support of the calibration process as summarized in Table 3. The mean absolute error for the 15 wells used as calibration targets was 0.46 ft.

Table 3. Calibration levels for the case study, steady state

Calibration Value	Level 1	Level 2	Level 3
Head (15 nodes)	+/- 0.58* (73%)#	+/- 1.16 (20%)	+/- 1.74 (7%)
Length of Losing Channel	+/- 0.5** (100%)	+/- 1.0	+/- 1.5

** ft, # percent of nodal values falling within a given level, ** mi*

Miller also attempted to calibrate the steady state model to the length of the losing reach of Clark Fork River channel. Prior to model development the losing length of Clark Fork River channel was estimated from the February potentiometric surface contour map and river stage elevations to be 4.7 miles measured from where the river enters the east boundary of the model (Figure 3). The calibration target, 4.7 mi +/- 0.5 mi, was formulated by accounting for the measurement and interpolation error associated with the river stage and the potentiometric surface contour map. Steady state model calibration resulted in a losing channel length of 4.5 miles, a level 1 calibration level (Figure 4).

A sensitivity analysis was performed by varying the hydraulic conductivity, bottom elevation of the aquifer, river bottom conductance, stage of both rivers, well withdrawal rates, and the storage coefficient for transient simulations. Results are shown in Figure 5 and reported as percent change in input data and the resulting average absolute error. Modeled heads were most sensitive to the +/- 20 % variation in hydraulic conductivity and the +/- 20% variation of river bottom conductance, which controls the leakage rate from the river. Sensitivity results indicate that though the absolute mean error increased for maximum variations in some parameters, differences between simulated and measured heads remained small, a desired outcome.

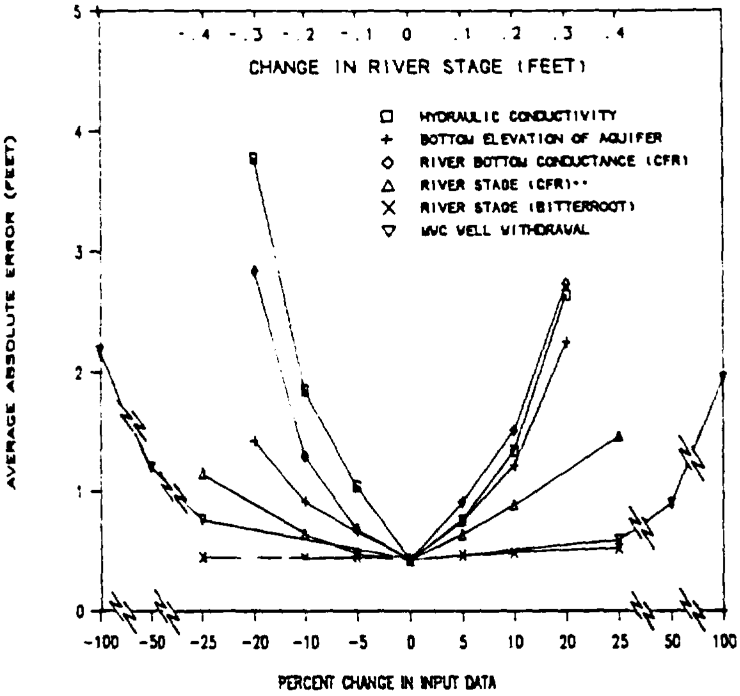

Figure 5: Sensitivity analysis for steady state simulation (modified from Miller, 1991).

Based on the small error associated with head calibration values (i.e., small calibration targets) and the match to calibrated levels 1, 2 and 3, the level 1 match with the length of losing stream reach target and the results of the sensitivity analysis, the steady state model calibration was judged acceptable for the stated purpose of estimating the magnitude of recharge from the influent Clark Fork River. Further calibration included transient simulations that were calibrated to hydrographs, fluxes and water balance estimates, though results are not reported in this paper. Additional sensitivity analyses including a low range-high range of values were also preformed. This calibration process was also judged acceptable for the author's stated goal.

SUMMARY AND CONCLUSIONS

Results of ground-water flow modeling have come under increasing scrutiny partly because of poor documentation of the process used for calibration. We propose a calibration process that includes the setting of calibration values, calibration targets and ranges of aquifer parameters prior to initiating a simulation, fitting of simulated results to calibration targets and the evaluation of the calibration process. The formulation of calibration targets and setting of calibration levels used in assessment of the calibration process are critical aspects of the calibration process.

Calibration targets are derived from field measured values of heads, fluxes and water balances and the error associated with determining these values. For example, head values contain measurement errors, and scaling, transient and interpolation errors (modeling errors). Simulated values are compared to calibration targets and a quantitative assessment of the match made. Sensitivity analyses are used to evaluate the effect of the size of the calibration targets on the model results and uncertainties in the aquifer parameters values.

The case study illustrated the setting of calibration targets for an interpretative ground-water flow model. Model calibration was assessed using our protocol and judged acceptable for the modeling questions posed.

It is important to note that in the case study over 90% of the calibration targets were matched to level 1 or level 2. However, this high level of match in itself does not guarantee an acceptable calibration has been achieved. For our example, the error associated with each calibration value was relatively small so that the calibration targets themselves were small, thus adding support to our judgement of an acceptable calibration. However, modelers could propose sufficiently large calibration targets that would always make it possible to calibrate all the targets to level one. Hence, we emphasize that the use of calibration levels is simply a quantitative way of displaying the results of the calibration and does not singularly imply an acceptable calibration has been achieved. The subjective judgement on the worth of the calibration must be based on a consideration of the error analysis, the results of the calibration as viewed in terms of calibration levels, and the results of the sensitivity analysis.

Deciding whether a model is calibrated well enough for the problem being addressed is a difficult judgement to make. Recognition of this difficulty gives rise to calls for model validation and modeling postaudits. Although worthwhile such efforts will not be practical in most modeling studies (Anderson and Woessner, 1992 b). The guidelines presented in this paper provide a standardized framework upon which to make and support what necessarily will remain a subjective judgement regarding the worth of a calibration.

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