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MODEL CALIBRATION TASK OBJECTIVE AND TECHNICAL APPROACH (TO/TA), FEMP, DOE FERNALD FIELD OFFICE, CINCINNATI, OH - (USED AS A REFERENCE IN OU 5 RI REPORT - APPENDIX F)

10/04/93

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REPORT

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Fernald Environmental

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October 4, 1993

U. S. Department of Energy
Fernald Environmental Management Project
Letter No. C:OP:93-1452

Mr. J. Phil Hamric, Manager
Department of Energy
Fernald Field Office
P. O. Box 398705
Cincinnati, Ohio 45239-8705

Dear Mr. Hamric:

CONTRACT DE-AC05-92OR21972, "MODEL CALIBRATION TASK OBJECTIVE AND TECHNICAL APPROACH"

Reference: "Groundwater Modeling Evaluation Report and Improvement Plan, April 1993"

This letter serves to transmit a copy of the Model Calibration Task Objective/ Technical Approach (TO/TA) document. The Model Calibration TO/TA describes the second groundwater modeling improvement activity outlined in the referenced document. With DOE concurrence, the TO/TA will be provided to the Ohio EPA and U.S. EPA at an October 5 Technical Information Exchange Meeting. A draft of the Model Calibration TO/TA was provided to Kathi Nickel of your staff on Thursday, September 30, 1993 for review.

If you have any questions or require more information, please contact Mark Cherry at 738-6816 or Ron White at 738-6506.

Sincerely,

N. C. Kaufman
President

NCK:RW:bsb
Enclosure

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Model Calibration
Technical Objectives/Technical Approach

DRAFT

The groundwater flow and solute transport model of the Great Miami Aquifer (GMA) prepared for simulating flow and transport in the vicinity of the FEMP will be recalibrated based upon the most recent data sets. The present model, originally constructed and calibrated before 1990, utilizes the Sandia Waste Isolation Flow and Transport (SWIFT) code for simulating flow and transport.

The task to recalibrate the flow and solute transport model is defined in the Groundwater Modeling Evaluation Report and Improvement Plan (MIP), (April 1993). This Technical Objectives/Technical Approach (TO/TA) document describes the model calibration task in more detail than the MIP. Additional procedural details are described in the attachment to this TO/TA.

Technical Objective

The objective of the recalibration task is to create a reasonable and defensible model that is acceptable to the U.S. and Ohio EPA for designated applications at the FEMP. The recalibrated model will be used for:

- Performing CRU5 Remedial Investigation (RI) fate and transport modeling;
- Supporting Feasibility Studies:
- Supporting relevant preliminary design efforts:
- Conducting performance modeling during detailed design; and
- Supporting cleanup operations.

Task Approach

The calibration process will consist of grid expansion, calibration criteria development, flow and solute transport calibration, and quality assurance steps. The approach to the calibration is summarized below.

The model grid for steady-state flow and solute transport will be expanded under another task (see Model Design TO/TA). This grid is to be an expansion of the previous solute transport grid of 78 cells by 102 cells. A band approximately 5250 feet wide will be added along the eastern side and a band approximately 1250 feet wide will be added along the north. The new grid will contain approximately 120 x 112 cells, each 125 feet square. The layering of the model will also be refined. The five layers of the original model will be replaced with six layers to better match existing well screen elevations. This will allow field data to be more accurately depicted and provide better vertical control over contaminant dispersion.

New data sets will be used in the construction and calibration of the model. Table 1 compares the data sets used in the original construction and calibration of the model versus the data sets that will be used in the improved model. In summary, new data sets reflect:

- Monitoring data from the 1990 to 1993 time period;
- Monitoring data from new wells installed since original calibration:
- Results of additional aquifer analysis to define Kd;
- Geostatistical analysis of data sets;
- Results from the South Plume Pumping Test;
- Results from construction and operation of the South Plume Recovery System: and
- Output from additional models (Glacial overburden, Paddys Run) to define hydraulic and solute loading terms.

Calibration criteria will be developed for the transient flow, steady-state flow, and solute transport models. Geostatistical analysis, conducted to understand and correlate the spatial distribution of water level and uranium data from monitoring wells, will be used to determine water level and uranium targets for each block and to identify areas of the site where lower confidence exists in the analyzed data sets. Confidence information will be used to weight the calibration targets. Calibration criteria will include quantitative measures (compare model output to field data), qualitative measures (inspect accuracy of the simulation), and relative measures (compare the accuracy of different calibration simulations). Quantitative criteria will include the definition of both target cell locations and statistical parameters (and acceptable ranges of these parameters) for model calibration. A qualitative evaluation of the correspondence among model simulations and the physical structures of the hydrogeological system will be conducted (i.e., pattern of heads and concentrations). Sum weighted residuals (weighted with the geostatistically determined uncertainty parameter) will be calculated to determine the overall accuracy of the simulation relative to other simulations. The best simulation with the minimum summed weighted residual will be selected.

A transient flow calibration will be performed using the South Plume Pumping Test results. Parameter values for porosity and rock compressibility will be developed from this calibration. Because of the scale and orientation of the pumping test wells, a telescoped grid (25 foot cell size) will be created in the south plume area to effectively simulate the results of the pumping test.

A steady-state flow calibration will be conducted using the expanded and reconstructed steady-state grid. Steady-state heads will be matched to the established criteria. This recalibrated steady-state model will be the primary model used for flow and solute transport simulations.

The solute transport model will be recalibrated to determine reasonable values of Kd (for uranium) and dispersivity for a representative source loading. The range of acceptable uranium Kd values will be established by reviewing site data related to Kd and by reviewing sensitivity runs of previously utilized Kd values corresponding to retardation factors of 9 and 12. The recalibrated flow model will be simulated with all of the original transport parameters unchanged to determine which transport parameters need to be adjusted.

The historical source loading terms will be decoupled from the model and monitoring data will be used to define initial conditions of uranium concentrations. Results from the glacial overburden and Paddys Run models will be used to define future loading terms.

Quality assurance/quality control procedures for modeling will be defined to control and confirm the quality of the modeling effort. This procedure will outline the specific steps for controlling quality in the calibration task. In addition, internal procedures will be followed for performing calculations and modeling runs and performing code verification. Independent quality assurance checks of conformance with procedures will be conducted.

Table 1
Comparison of Original and Revised Data
Used for GMA Model Design and Calibration

Parameter	Original Data Set	Projected Data Set in Improved Model
Steady-state groundwater elevations for boundaries and calibration targets	Single measurement event - April 1986	Kriged - average from January 1990 to present, wells installed since 1986 added to data set
Horizontal hydraulic conductivity	Historical studies in the region - refined during calibration	Historical studies in the region updated with South Plume Pumping Test and slug test results
Vertical hydraulic conductivity	Historical studies in the region and literature values	Historical studies in the region, literature values, and South Plume Pumping Test results
Pumping wells locations and rates	Data collected from users and recent studies - refined during calibration	Data collected from users and recent studies
Porosity	Literature	Transient calibration
Rock compressibility	Literature	Transient calibration
Bedrock surface configuration	Seismic study and well logs	Seismic study and well logs updated with recent 4000 series wells
Blue clay configuration and thickness	Well logs	Well logs
River elevations	HEC 2 modeling from Zone of Influence Study	River gaging data from 1990 to present
Uranium loading through glacial overburden	Site operations history - refined during calibration	GMA monitored uranium data defines initial conditions

Uranium concentrations in GMA for calibration targets	Average and confidence interval from compilation of all data from 1985 to 1989	Kriged - average for 1990, 1991, 1992, 1993 - modified to reflect recent trends seen in field, updated with wells installed since 1990
Kd	Results of geochemical study (miscalculated) - refined during calibration	Recalculated results from geochemical study and additional aquifer testing - refined during calibration
Dispersivity	Literature - refined during calibration	Literature - refined during calibration
River leakage	Zone of Influence Study - refined during calibration	Zone of Influence Study - refined during calibration
Paddys Run hydraulic and uranium loading	Historical site operations data - refined during calibration	Paddys Run model output - GMA uranium data defines initial conditions
Recharge	Historical regional studies - refined during calibration	Historical regional studies, HELP* modeling, supplemental model output - refined during calibration

* HELP (Hydrologic Evaluation of Landfill Performance) is a computer modeling code developed by the U.S. Army Corps of Engineers to simulate water movement across, into, through, and out of landfills.

Attachment to the Model Calibration Technical Objectives/Technical Approach

DRAFT

As described in the Model Calibration Task Objective/Technical Approach (TO/TA), the Great Miami Aquifer flow and transport groundwater model for the FEMP is being recalibrated as part of a comprehensive model improvement effort. This document is provided as supporting material for the Model Calibration TO/TA. The model recalibration task consists of flow calibration followed by solute transport calibration.

1.0 Flow Model Calibration

The present FEMP steady-state flow model was calibrated to 1986 water elevation data. Since that time, additional data have been collected, new wells have been installed, and a large scale pumping test (South Plume Pumping Test) has been conducted. The flow model will be recalibrated to incorporate this additional data.

The flow model calibration will consider both transient and steady-state conditions. Transient calibration will by used to further refine hydraulic parameters for steady-state conditions. Calibration to transient conditions is necessary to finalize input values to the SWIFT steady-state model such as porosity, rock compressibility, horizontal and vertical hydraulic conductivity.

Steady-state conditions will be used for most model applications. The steady-state model covers a large domain, and solute transport loadings and parameters will be simulated on the flow field created by the steady-state flow model. Calibration to steady-state and transient conditions will be an iterative process.

1.1 Calibration of Transient Flow Model

Transient flow calibration of the SWIFT model will consist of four main steps:

- Develop a new model grid for transient flow calibration:
- Develop a steady-state input file for SWIFT model;
- Process pumping test results into a format which can be used for calibration; and
- Perform pumping test simulations and compare the modeled and measured pumping test results.

These steps and the assumptions inherent in these steps are described below.

Pumping Test Model Grid Development

A telescoped model grid covering the pumping test area will be developed for the transient flow calibration. The telescoped grid will have smaller cell dimensions and a different overall orientation than current model grids. Pumping test piezometers were spaced at intervals as small as 25 feet, and the orientation of the pumping wells and piezometers was based upon local groundwater flow direction and not model orientation: therefore, a new grid oriented orthogonal to the axis of the pumping test network and with a 25 foot cell size is needed to provide the appropriate resolution for the transient flow analysis. It is anticipated that this model grid will contain over 10,000 cells (100 x 100 cells) covering an area approximately 2875' by 2875'.

The layering of the new grid will be a simplified to reflect aquifer conditions in the pumping test area. Layers will correspond to 2000 series well screens, the pumping well screen, and selected piezometers (used in the analysis) with 5 foot screens. Intervening layers are also necessary to appropriately represent the vertical dimensions of the aquifer.

Steady-State SWIFT Input File Development

Development of the new SWIFT steady-state input file will include the following steps:

- Determine the initial groundwater head distribution for the model domain based on measurements taken just prior to the constant rate pumping test:

- Estimate boundary conditions for SWIFT from the initial head distribution:

- Execute the SWIFT code and compare the modeled steady-state head results with the initial groundwater heads: and

- If the modeled water table is within 1 foot of the field measured water table, continue to the transient calibration. If they do not agree, investigate the boundary conditions again and other model parameters and rerun the SWIFT code until agreement is reached.

Processing Pumping Test Data

Processing of pumping test data will be completed as follows:

- Wells will be selected from the pumping test to be used for model simulations;

- An appropriate number of data points will be chosen to adequately represent the drawdown and recovery portions of the pumping test; and

- Summary tables and figures of the selected pumping test results will be prepared.

Wells in the pumping test area will be selected so that the anisotropy and homogeneity of the aquifer can be investigated. Pumping test data will be used for calibration.

Approximately 20 drawdown data points for each well will be selected from the pumping test data. Ten data points will be selected from the pumping portion of the test and 10 from the recovery portion of the test.

Comparison of Simulated Versus Measured Results

The following steps will be performed:

- Modify SWIFT steady-state input file so that transient simulations can be performed and so that model output will be obtained at the appropriate times:

- Perform model simulations and obtain output at the desired times:

- Estimate the drawdown (difference between steady-state heads and modeled heads);

- Compare the modeled drawdown with the measured drawdown at each well;

- If the difference in drawdowns is not within the transient calibration criteria outlined in Table 3-1, then modify influential model parameters, such as, porosity, vertical and horizontal hydraulic conductivity, rock compressibility, and layer allocation factors to minimize the difference between the measured and modeled results; and

- Continue the above steps until an acceptable match is obtained for all wells.

Assumptions

The transient flow calibration is based upon the following assumptions:

- Results/model parameters from a telescoped transient flow model grid can be incorporated into the steady-state/solute transport model grid.

- Surface infiltration through the ground surface and Paddys Run will be assumed to be zero for the transient simulations based upon the insignificant infiltration that occurred during the pumping test.

1.2 Calibration of the Steady-state Flow Model

The procedure for steady-state flow calibration of the SWIFT model can be divided into three main steps:

- Develop a new expanded grid;
- Define initial and boundary conditions: and
- Perform simulations using the SWIFT code and compare the model results with target heads (the calibration) until a successful match is achieved.

These steps and the assumptions inherent in these steps are described below.

Develop Expanded Grid

The grid will be expanded under another task (see model design TO/TA). This grid is to be an expansion of the previous solute transport grid (78 x 102 cells) with a band approximately 5250 feet added along the eastern side and a band approximately 1250 feet added along the north. The new grid will contain approximately 120 x 112 cells with a square grid of 125 feet.

The layering of the model will also be refined. The five layers of the original model will be replaced with six layers to better match existing well screen elevations.

The final step in the model design is the creation of a new SWIFT input file corresponding to the new structure of the model.

Define Initial and Boundary Conditions for New SWIFT Input File

Development of initial and boundary conditions for the SWIFT input file, for the new model grid, will consist of the following steps:

- Extract boundary heads from geostatistical analysis (performed under another task) and create SWIFT input for these heads;

- Define initial values of horizontal and vertical hydraulic conductivities and porosity from the pumping test results and the previously calibrated model;

- Define the most recent pumping rates of significant wells within the model domain;

- Define initial river leakage values and surface recharge based upon previous model values in the steady-state regional and local models and other site data. The regional model is used because the domain has been increased beyond the existing solute transport model; and

- Test run the completed SWIFT file and compare patterns of head output to previous model runs to confirm file accuracy.

Perform Calibration

The steady-state flow calibration will include the following steps:

- Post processing routines are created which will aid in the data comparisons;

- Target heads are set for selected cells based upon geostatistical analysis (see calibration criteria Table 3-3);

- Modeled heads are compared to field data;

- If the difference in heads is not within the established calibration criteria outlined in Table 3-3, then model parameters are adjusted to minimize the difference. Zonation of parameters will be maintained on a reasonable basis that is consistent with understanding of the geologic system as defined in the calibration criteria;

- The previous two steps are continued until an acceptable match is obtained between modeled and target heads; and

- Once steady-state flow calibration criteria have been satisfied, all of the calibration criteria are formally checked versus model results. This more detailed check may lead to further refinement of model parameters.

Initially runs will be screened by inspection of residual head contour plots. Statistical measures (see Section 3) will be calculated and compared to the established criteria.

Assumptions

The following assumptions pertain to the steady-state calibration:

- Parameters will not be varied outside reasonable ranges of possible physical values based on field data and as defined in the calibration criteria: and
- Model layer thicknesses will be established based on the known stratigraphy and will not be varied.

1.3 Flow Model Validation

A transient flow model prediction will be performed, after the overall flow calibration is completed, by simulating the step-drawdown portion of the pumping test or operation of the recovery well system. The only model parameter that will be changed for this simulation is the pumping rate. Therefore, this simulation can be used as to validate the calibrated flow model and to further characterize the accuracy of the calibrated flow model.

The transient flow grid described in Section 1.1 will be used for this validation exercise. In general, the same process as the transient flow calibration will be followed in performing this validation.

2.0 Solute Transport Model Calibration

The solute transport model needs to be recalibrated because additional data have been collected and new monitoring wells have been installed and sampled. These data show the southern extent of the south plume does not extend as far south as was believed during the original calibration. Also, the uncertainty involving Kd is not acceptable.

The original calibration, using an estimated retardation factor of 9, resulted in a reasonable match to the monitoring data (except for the southern extent of the South Plume as described above) with most of the contamination in the shallower model layers. Based on the results of a geochemical study (DOE 1993, Appendix A), the retardation factor was revised upward to 12. The calibration using the retardation of 12 resulted in more uranium modeled at depth (which does not match new monitoring data) and a much larger historical mass loading to the aquifer. The geochemical study miscalculated the retardation factor by using a grain density instead of a bulk density in the retardation equation. In fact, geochemical studies indicate a range of retardation factors from approximately 8 to 33, indicating that the original calibration with a retardation factor equal to 9 was within the range. Further calibration efforts need to consider these factors.

2.1 Calibration of the Solute Transport Model

The solute transport calibration will consist of the following steps:

- Review geochemical parameters:
- Recalibrate solute transport model, and
- Decouple initial source loading.

Review Geochemical Parameters and Existing Solute Transport Calibrations

The derivation of the distribution factor (Kd) for uranium will be assessed to select the most appropriate Kd for the solute transport model. Available data related to Kd will be compiled and reviewed. These data will be analyzed to determine the range and spatial distribution of Kd. Results of all pertinent solute transport calibration runs (especially the two final calibrations with retardation factors of 9 and 12) will be reevaluated by using the updated calibration criteria. A range of acceptable Kd will then be determined based on the review of geochemical data and the existing calibration runs. If necessary, as determined by the data, multiple zones may be created for Kd in the updated solute transport model.

Recalibrate Solute Transport Model

After the flow model is successfully recalibrated, its impact on the solute transport model will be evaluated. This evaluation will be performed for all previously accepted solute transport calibration runs. Calibration criteria shown in Table 3-4 will be used to determine if recalibration is needed. Uranium concentration residuals will be calculated and analyzed during the calibration. Mass balances will be calculated based on uranium predicted to be present in the aquifer (both dissolved and adsorbed states) versus the required source loading.

The solute transport calibration will include the following steps:

- Post processing routines will be used to compare data;
- Target uranium concentrations will be set for selected cells based upon geostatistical analysis of field data (see calibration criteria Table 3-4);
- The current model will be run and the modeled uranium concentrations in each cell will be compared with the target concentration distributions;

- If the difference in concentrations is not within the established calibration criteria, model parameters will be adjusted to minimize the difference between modeled and target concentrations;

- Continue the previous two steps until an acceptable match is obtained between modeled and target concentrations; and

- Once a successful match is made between model and target concentrations, all of the calibration criteria will be formally checked versus model results. This more detailed check may lead to further refinement of model parameters.

Decoupling Initial Source Loading

Once recalibrated, historical source loading terms will be decoupled from the model. Results from the Glacial Overburden/Upper Great Miami Aquifer model and Paddys Run model will be inserted as future source terms. Also, monitoring data will be contoured and directly inserted as initial concentrations in future model applications. By decoupling the historical source term and using the monitoring data directly as initial conditions, the model will be more modular and flexible.

3.0 Calibration Criteria

Calibration criteria are defined below for the transient flow, steady-state flow, and solute transport models. Geostatistical analysis of the spatial distribution of water level and uranium data from monitoring wells will be used to determine water level and uranium targets for each block and to identify areas of the site where lower confidence exists in the analyzed data sets. These calibration criteria consist of quantitative measures to compare cells with wells, qualitative measures for overall inspection of the simulation, and relative measures to compare the accuracy of different calibration runs.

3.1 Transient Flow Calibration Criteria

A summary of the transient flow calibration criteria is presented in Table 3-1. Several highlights of the table are listed below:

- Each modeled drawdown and recovery curve should match the corrected measured curve along its entire length by approximately +/- 10% (comparison of residuals);

- The average error of the twenty modeled and measured points for an individual well will not exceed 10% (average of residuals);

- Other statistical tests which may be performed during calibration include maximum residual, variance of residual, and spatial correlation of residuals (i.e., residual contour plots); and

- Influential parameters will be varied within specific ranges during the calibration. The parameter ranges will be based on field measurements or typical literature values.

Table 3-1
Summary of Transient Flow Calibration Criteria

Calibration Parameter	Criteria
Maximum Residual of Individual Drawdown or Recovery Modeled Data Point Versus Measured Data Point	< +/- 15% of Measured Data Point
Average Residual for Modeled Individual Well (Approx. 20 total points of comparison)	< +/-10% of Measured Data
Average Residual for All Wells (Approx. 9 Wells)	< +/-10% of Measured Data
Variance of Residuals for All Wells (Approx. 9 Wells)	0.20 ft^2
Modeled Drawdown and Recovery Curves	Time of Change in Curvature Matches Measured within 10%
Horizontal Hydraulic Conductivity	Within 292 to 678 ft/day
Vertical Hydraulic Conductivity	Within 20 to 115 ft/day
Porosity	0.2 to 0.4
Rock Compressibility/Storativity	Within Typical Range of Literature Values

3.2 Steady-state Flow Calibration Criteria

Table 3-2 summarizes the model parameters that may be adjusted during the steady-state calibration and the projected range over which the parameter will be adjusted. As shown on this table, several of these parameters may be further refined based upon the transient flow calibration. Results from the pumping test, defining hydraulic conductivity and results of the transient flow calibration, will be incorporated as initial values for hydraulic parameters in the model at the beginning of the steady-state flow calibration effort. It is expected that constant head boundary conditions will be used; however, other types of boundary conditions (e.g., constant flux condition) will also be considered based on the results during calibration and available data.

It is expected that the primary parameters adjusted during the calibration will include the horizontal and vertical hydraulic conductivity, the recharge rate, and the river leakage factor. Overall, an approach of keeping the model simple without over complicating the zonation of parameters will be followed during the calibration. The lower GMA (new layers 5 and 6) will have a higher hydraulic conductivity than the upper GMA (new layers 1, 2 and 3) based upon earlier stratigraphic correlations and the south plume pumping test. New layer 4 represents the blue clay layer (when present) and thus has a much lower hydraulic conductivity value than the other layers. In general, a single value for hydraulic conductivity for the upper and lower portions of the aquifer will be used. Recharge values will be zoned in a similar manner as the present model with less recharge occurring through the till than the alluvium or surface exposed GMA. It is not intended to zone porosity.

Constant head boundary conditions and head calibration targets will be set based upon geostatistical analysis of water elevations. Geostatistical analysis will also identify areas of the site where lower confidence exists in the analyzed water level data sets. This confidence determination will be used to weight the heads determined during the model calibration thus allowing qualitative comparison of the heads predicted at locations not supported by field data.

Table 3-2
Ranges of Steady-state Flow Calibration Parameters

Calibration Parameter	Projected Range During Calibration
Horizontal Hydraulic Conductivity	Within 292 to 678 ft/day or tighter range as determined with Transient Flow Calibration
Vertical Hydraulic Conductivity	Within 20 to 115 ft/day or tighter range as determined with Transient Flow Calibration
Porosity	As determined with Transient Flow Calibration
Rock Compressibility	As determined with Transient Flow Calibration
Boundary Conditions	Constant heads determined with geostatistical analysis. Maintain within kriged confidence interval. Other type boundary conditions possible if determined during calibration.
Recharge	0 to 16 inches/year based upon HELP* runs, surface features and interim results from the Glacial Overburden/Upper Great Miami Aquifer Model and calibration. 20 to 40 inches/year from Paddys Run based upon Paddys Run Model and calibration.
Great Miami River Leakage	Set based on latest data
Pumping Wells	Set based on latest data.

* HELP (Hydrologic Evaluation of Landfill Performance) is a computer modeling code developed by the U.S. Army Corps of Engineers to simulate water movement across, into, through, and out of landfills.

Table 3-3 shows the measures that will be used to quantitatively assess the calibration. Quantitative criteria for the flow model will include measures of mean residual, mean of absolute residuals, maximum residual, regression coefficient, and water mass balances. These measures will only be applied at blocks which contain field data and will compare the target value (determined at the block centroid with geostatistical analysis) and the model simulation results. In general, the criteria used for the original model have been followed, with the following exceptions:

- A maximum residual measure has been added. This measure uses block by block confidence intervals generated by geostatistical analysis at control points within the model domain;
- The water balance criteria has been reduced from 20 percent to 5 percent; and
- The spatial correlation of residuals measure has been replaced with a similar qualitative measure of inspecting plots for clustered residuals. Because of the new approach of using the kriged uncertainty values on a block by block basis, the original measure is no longer applicable on a quantitative basis.

The calibration will also be evaluated with qualitative measures. These measures include:

- Contours of head will be plotted, inspected, and compared to target contour plots to identify trends of differences in the model output versus targets. This measure will determine if there is any clustering of residuals;
- Model velocity vector output will be evaluated and compared to observed and postulated conditions; and
- Results in the vicinity of the SOWC collector wells will be evaluated since there are large gradients in this area.

Finally, a relative measure will be used to compare the accuracy of different calibration simulations. The relative measure will sum weighted residuals at every active model block (weighted with the geostatistically determined uncertainty parameters) to determine the overall "accuracy" of a particular simulation for comparison with other simulations. With these results, it is intended to select the "best simulation", i.e., with the minimum summed weighted residual.

Table 3-3
Steady-state Flow Calibration Analysis Parameters
for Blocks with Well Control

Calibration Parameter	Criteria
Mean Residual Head	< +/- 0.5 feet
Mean of the Absolute Residuals of Head	< +/- 2 feet
Standard Deviation of Differences of Head	< +/- 3 feet
Regression Coefficient Between Measured and Computed Values of Head	0.95
Maximum Residual	Within the kriged confidence interval for the defined block
Water Balance	Within 5 percent

3.3 Solute Transport Calibration Criteria

For the solute transport model, quantitative and qualitative criteria are established for matching model results to target concentrations. Quantitative criteria include the definition of both target locations and statistical parameters (and acceptable ranges of these parameters) for calibration of the transport models. In addition, qualitative comparisons between monitoring data and model predictions are defined. Both quantitative and qualitative assessments of the calibration will be performed; nevertheless, solute transport calibration is a more qualitative process because of the complexities of multiple sources and spatially varying transport parameters. Therefore, quantitative measures are less rigorous than for the flow calibration. In general, an attempt will be made to balance two primary calibration targets: (1) concentrations at particular blocks representing locations of measured data, and (2) total mass of contaminant in the aquifer.

Since additional data have become available through monitoring and additional well installation, data from 1990 to the present will be compiled and evaluated to redefine the solute transport calibration targets for uranium. Geostatistical analysis of the spatial distribution of uranium analytical data from the 2000, 3000, and 4000 series monitoring wells will provide these targets. Geostatistical calculations will include the sample semi-variogram, and kriging and co-kriging estimators, along with their estimation variance. This analysis will be used to determine uranium targets for each block and to identify areas of the site where lower confidence exists in the analyzed data sets.

Averaged annual uranium data sets from years 1990, 1991 and 1992 will be used in this analysis to provide kriged plume depictions for each of these three years. Based upon these depictions and the most recent analytical data, an idealized plume will be selected as representative for the calibration effort. Data mean and confidence interval of mean will be defined for each block with well control and will serve as the calibration target.

Table 3-4 defines the quantitative criteria for the solute transport calibration. These measures will only be applied at blocks which contain wells and will compare the target value (determined at the block centroid with geostatistical analysis) and the model simulation results. The calibration will attempt to meet these criteria; however, if in isolated instances the criteria can not be met, appropriate explanation will be provided in the summary report.

The calibration will also be evaluated with qualitative measures. These measures include:

- Contours of modeled concentrations and contours of modeled and measured concentration differences will be plotted, inspected, and compared to target contour plots at representative model layers to identify trends of differences in the model output versus targets. This measure will determine if there is any clustering of residuals.

- Results in the vicinity of the south plume will be evaluated since a large percentage of the uranium mass in the GMA is in this area. Cross sections through the centerline of plumes will also be evaluated to determine the accuracy of the vertical definition of the plume.

Finally, a relative measure will be used to compare the accuracy of different calibration simulations. The relative measure will sum weighted residuals at every active model block (weighted with the geostatistically determined uncertainty parameters) to determine the relative accuracy of a particular simulation for comparison with other simulations. With these results. it is intended to select the "best" simulation, the one with the minimum summed weighted residual.

Table 3-4
Solute Transport Calibration Analysis Goals
for Blocks with Well Control

Calibration Parameter	Criteria
Mean Residual Concentration	< +/- 5.0 ppb
Mean of the Absolute Residuals of Concentration	< +/- 10.0 ppb
Standard Deviation of Differences of Concentration	< +/- 10.0 ppb
Regression Coefficient Between Measured and Computed Values of Concentrations	0.90
Maximum Residual	Within the kriged confidence interval for the defined block
Total Mass	Within 5 percent of mass determined through operations

4.0 References

1) "Groundwater Modeling Report - Summary of Model Development", prepared for the U.S. Department of Energy by IT Corporation. (DOE. April 1993).