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GROUNDWATER MODEL PARAMETER ESTIMATION
USING RESPONSE SURFACE METHODOLOGY

THESIS

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AFIT/GOR/ENS/95M

THESIS APPROVAL

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GROUNDWATER MODEL PARAMETER ESTIMATION USING RESPONSE SURFACE METHODOLOGY

THESIS

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of the Air Force Institute of Technology

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Captain, USAF

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Rick Cotman

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ABSTRACT

This thesis examined the use of response surface methodology (RSM) to estimate the parameters of a finite-element groundwater model. An existing two-dimensional, steady-state flow model of a fractured carbonate groundwater system in southwestern Ohio served as the calibration target data set. A Plackett-Burman screening design showed that only four of the ten hydraulic conductivity zones significantly contributed to the output of the finite-element model. Also, the effective porosity parameter did not significantly affect the model's output. Using only the four significant hydraulic conductivity parameters; four two-level, four-factor designed experiments were conducted to exploit the first-order response surface defined by a residual sum of squares function. Additionally, a central composite design and ridge analysis were used to adjust the four parameters and finally arrive at a calibrated model in a grand total of 146 runs. The final calibrated model, which had an average head elevation of 292 meters, matched the calibration target data set with a mean absolute error of only 7 mm over all 524 nodes of the model. RSM provided an effective calibration technique to estimate groundwater flow parameters.

Groundwater Model Parameter Estimation Using Response Surface Methodology

I. Introduction

Background

Water quality is a topic of concern in the United States and around the world. Fresh water occurs at the surface of the earth in ice, lakes, and rivers and as groundwater in the openings in rocks and soils. While surface sources of water satisfy important irrigation and population needs, the predominant source of fresh water is provided by groundwater systems. To assess the flow and quality of groundwater in a particular region, groundwater hydrologists are often asked to predict the behavior of groundwater systems. Hydrologists use groundwater models to predict how the groundwater will flow in a particular area. These models are often numerical models implemented on computers to simulate groundwater flow.

These simulation models are mathematical descriptions of the groundwater flow in an underground system. They incorporate the relevant physical laws which control the system, as well as specific hydraulic and geologic (hydrogeologic) properties unique to the particular groundwater system of interest. The hydrologist modeling the system must properly adjust the parameters representing the local hydrogeological properties to ensure the model accurately reflects the flow characteristics of the system under study.

The process of adjusting the model's parameters until its output (typically hydraulic heads) conforms to the observed field heads is termed calibration. Mathematically, this process of parameter estimation is known as solving the inverse problem. Methods to solve the inverse problem are numerous, and only a few have been implemented to calibrate groundwater models automatically. In fact, most practitioners still use manual, trial-and-error calibration methods (Anderson and Woessner, 1992:235).

One approach that has not been discussed in the groundwater literature on model calibration is response surface methodology (RSM). RSM incorporates a number of statistical techniques used in the empirical study of the relationships between one or more output responses and a group of input variables. By systematic, simultaneous adjustment of multiple hydrogeological parameters, the RSM technique should yield a calibrated groundwater model with known statistical properties.

Problem Statement

The goal of this research was to demonstrate that RSM could serve as an effective calibration technique to estimate groundwater flow parameters.

Research Objectives

To accomplish the stated goal, the following objectives were established:

1. Obtain a data set of hydraulic heads to serve as a calibration target data set. The data set used by Smith and Ritzi (1993) was chosen as the calibration target.

2. Ensure the calibration target set produces results similar to those obtained by Smith and Ritzi when their simulation model is implemented on the AFIT computer system.

3. Conduct a screening analysis to determine the statistically significant parameters for this groundwater model.

4. Using only those parameters found to be statistically significant, demonstrate that response surface methods can be used to calibrate the groundwater model.

Scope and Limitations

1. This study used the entire stratigraphic section of the selected aquifer to demonstrate the applicability of RSM to calibrating a groundwater model in a realistic situation.

2. A data-rich calibration target data set of 524 nodes was used to evaluate the match between the groundwater model's output and the calibration target set.

3. Only the groundwater flow model was calibrated (i.e. the calibration of heads). The issue of solute transport calibration was deferred to a later study.

II. Literature Review of the Inverse Problem in Groundwater Systems

Introduction

Many groundwater flow models simulate the flow of groundwater by computing the flow of water through relatively small portions (elements) of the groundwater system. The results of the water flow through each of these elements are combined to produce a simulated description of the entire groundwater system. This type of simulation is called a finite-element model. Finite-element models require estimates of the hydrogeologic parameters to compute groundwater flow or to determine contaminant concentrations.

Mathematically, the process of determining the model parameters is known as solving the inverse problem. "The inverse problem has been defined as that of estimating the model parameters from measurements of the output. Therefore, the inverse problem can be equated to parameter estimation" (Carrera, 1987: 551). The difficulty of estimating these parameters lies in the mathematical construction of the model. A well-posed model will have a unique and continuous solution. Groundwater models of the real-world do not contain enough information to make a well-posed mathematical model. Finite-element, groundwater models are thus very difficult to solve due to uncertainties in estimating these parameters. Although the professional literature contains numerous methods on how to solve the inverse problem, Response Surface Methodology (RSM) has not been applied to its solution. The goal of this thesis was to demonstrate the usefulness of RSM in parameter estimation.

This chapter begins with a brief overview of the mathematical concepts associated with ill-posed mathematical models. The solution techniques applied to determining the parameters of groundwater flow models are then reviewed based upon the solution approach -- direct or indirect. Finally, the latest development in the inverse solution of groundwater systems, solving the coupled (simultaneous) flow-contaminant problem, is presented.

The Ill-Posed Inverse Problem

For an inverse problem to be well posed, it must meet the following three conditions: 1) the parameters are identifiable, 2) the solution is unique, and 3) the solution is stable (Carrera and Neuman, 1986b:211). A parameter is said to be identifiable if the model output is sensitive to it. If a parameter is nonidentifiable, then regardless of the value assigned to the parameter, the model will produce the same output. Even if all the parameters are identifiable, the solution to the inverse problem may be nonunique. Nonunique solutions are usually associated with multiple local optima. Unstable solutions have spatially oscillating parameters and depend heavily on the initial parameter settings. If any one of the three conditions is not met, the problem is said to be ill-posed.

Groundwater models are often ill-posed. In groundwater modeling, the known information is limited to the data gathered from a limited sampling of observation wells.

These wells are spread out geographically and the samples are spread out over time. This data also has various uncertainties and errors associated with the data collection process. These limitations in the observed data can result in non-unique or unstable solutions. Additionally, when the hydrologist selects parameters, a thorough sensitivity analysis or screening should be performed to determine which of these parameters are identifiable or significant. However, a screening for significant parameters is often not performed (Carrera and Neuman, 1986b:212-217). Thus, the limitations of the available data, combined with the failure to screen for the significant hydrologic parameters, render many real-world groundwater inverse problems ill-posed.

Parameter Estimation Methods

In an attempt to deal with the difficulties associated with ill-posed models, numerous mathematical methods have been used to solve the inverse problem. These methods may be grouped into "direct" and "indirect" methods (Neuman, 1973:1006). The "direct" methods assume the model parameters are dependent variables of the flow equation (see equation 3-13). The flow equation is a partial differential equation of the model parameters. Thus, the model parameters are found directly by solving a formal inverse boundary problem (Carrera, 1987:559; Yeh, 1986:96). The "indirect" methods seek to improve on the output error by iteratively adjusting the existing parameter estimates until the model produces results "close" to the real system (Neuman, 1973:1006).

Direct Methods. To apply the direct approach, the hydrostatic head information must be known over the entire flow region and the measurement errors must be small. In reality, information is known only at sparsely distributed wells. To properly formulate the inverse problem, additional data must be interpolated to fill in the missing nodal points. With the aid of boundary conditions and flow data, a direct solution of the unknown parameters in the original governing equation may be made. However, when the measured and interpolated hydrostatic head values are entered into the governing equation, an error term will be generated. This term is known as equation error, and is minimized by the proper choice of parameters (Yeh, 1986:96).

Yeh (1986:96) and Carrera (1987:560-561) list a number of investigators that use the direct method to solve the inverse problem. The following listing presents the various techniques, along with the investigator:

Energy dissipation (Nelson, 1968)
Linear programming (Deininger, 1969; Vemuri and Karplus, 1969;
    Kleinecke, 1971)
Flatness criterion (Emsellem and de Marsily, 1971)
Multiple-objective decision process (Neuman, 1973)
Galerkin method (Frind and Pinder, 1973)
Algebraic approach (Sagar and others, 1975)
Inductive method (Nutbrown, 1975)
Linear and quadratic programming (Hefez and others, 1975)
Minimization of a quadratic objective function
    with penalty function (Navarro, 1977)
Matrix inversion with kriging (Yeh and others, 1983)

The above methods are not based on a statistical framework. The variability of the parameters and the error terms are not accounted for in a statistical sense. This lack of a statistical foundation may be the reason why hydrologists generally do not use the above techniques to solve the inverse problem (Carrera, 1987:567). Most current approaches to solve the inverse problem are statistically based and can be categorized as "indirect" methods.

Indirect Methods. The indirect methods are all based on the idea of minimizing the difference between the model's calculated response (typically, hydraulic head) and the actually observed value. This approach is well suited to the real-world situation where observation wells are limited in number. Because the relationship between hydraulic head and model parameters is nonlinear, indirect methods usually require an iterative approach to solve the inverse problem.

Typically, an initial set of parameters is chosen for the groundwater simulation model. The model's output is compared to the field observations and the difference (error) is computed. If the error is too large, one or more parameters are adjusted, and the model is re-run. If this error is within a pre-defined performance criterion, the latest parameters are adopted for the model (Neuman, 1973:1006). There are: 1) a wide variety of ways to compute the error between the modeled and measured observations and 2) numerous methods to adjust the parameters after each iteration. These characteristics of the indirect approach have lead to numerous publications on how to implement the indirect approach to solve the inverse problem.

A manual trial-and-error method is most often used to arrive at estimates of the model parameters. This method is labor intensive (therefore expensive), frustrating (therefore often left incomplete), and subjective (therefore biased) (Carrera and Neuman, 1986a:200).

Yeh (1986:96-98) lists a number of investigators that used indirect methods for parameter estimation. The following review lists the various techniques, along with the investigator:

Quasilinearization and control-oriented techniques (Bellman and Kabala, 1965; Yeh and Tauxe, 1971; DiStefano and Rath, 1975)
Minimax and linear programming (Yeh and Becker, 1973)
Maximum principle (Lin and Yeh, 1974)
Optimal control and gradient procedure (Vermuri and Karplus, 1969)
Optimal control using steepest descent and conjugate gradient method (Chen and others, 1974; Chavent and others, 1975)
Kalman filtering techniques (McLaughlin, 1975; Wilson and others, 1978)
Maximum likelihood estimation and kriging (Kitanidis and Vomvoris, 1983)

Additional inverse problem solution methods have been presented since the publication of Yeh (1986). The papers by Carrera and Neuman (1986a; 1986b; 1986c) advocate using a maximum likelihood method that reaches its solution by means of a penalty criterion based on prior estimates of the model parameters. Xiang and others (1992) use an L1 norm to measure the error between the fitted and actual response in estimating model parameters. Doughty and others (1994) base their method on iterated function systems using fractal theory.

All of these indirect methods primarily deal with solving the inverse problem by calibrating the model for either observed head or contaminant concentration values. Usually, the flow model is calibrated first, and then it is adjusted to properly model the concentration behavior. Recently, the solution to the coupled flow-concentration inverse problem has been presented in the literature (Sun and Yeh, 1990; Wagner, 1992).

Coupled Flow-Contaminant Modeling

The common method of estimating the hydrogeologic parameters independent of the characterization of the contaminant sources requires extra iterations to eventually calibrate the model for both flow and contaminants. To solve for the hydrogeologic parameters, the contaminant sources must be assumed; moreover, to estimate the contaminant sources, the hydrogeologic parameters must be assumed. This situation can lead to numerous trial-and-error runs until both objectives are calibrated.

Wagner (1992) presents a method that solves the inverse model as a non-linear maximum likelihood problem. The method simultaneously estimates the hydrogeologic parameters along with contaminant source characterization. Due to the statistical framework of this maximum likelihood model, statistical estimates of the uncertainties of the parameters may also be made.

The coupled problem may also be applied to the freshwater-saltwater flow problem, and the oil-water two-phase flow problem (Sun and Yeh, 1990:2508). These problems are all concerned with simultaneously estimating the groundwater model parameters that jointly calibrate the model for two types of response.

Summary

The published approaches to calibrating groundwater flow models present numerous alternatives to solving an ill-posed inverse problem. Over the last thirty years, the efficiency and precision of determining the model's parameters have improved. A further step toward efficient calibration of groundwater simulation models is the simultaneous estimation of the parameters for both groundwater flow and contaminant transport. However, the groundwater model calibration literature does not contain an RSM approach to solving the inverse problem. The next chapter presents how the techniques of RSM may be effectively applied to groundwater model calibration.

III. Groundwater Model Calibration

Introduction

This chapter reviews the fundamental principles involved in groundwater model calibration. It first presents the geologic framework and hydrogeological principles of groundwater modelling. These principles are then used to develop the governing differential equation found in most numerical groundwater flow models. Finally, the problem of calibrating the groundwater flow model and how response surface methods may be applied to the calibration effort are discussed.

Groundwater Hydrogeology

Geological Terms. The mathematical model that represents the physical processes of a groundwater system is based upon the geological properties of the rocks and sediments in the modeled area. A basic understanding of these properties and the associated terminology is necessary to develop the governing equation of the groundwater flow model.

The *aquifer* is the geological unit of porous material capable of storing and transmitting appreciable quantities of water to wells (Anderson and Woessner, 1992:12). The aquifer is often composed of several different rock and sediment types which vary spatially. This heterogeneous nature of aquifers is often modeled by dividing the aquifer into zones which posses similar hydraulic properties.

The aquifer itself is composed of solid matter called the solid *matrix* and void spaces between individual grains or in cracks (fractures), which are collectively referred to as the *pore space*. *Fractures* are the separated cracks that exist in many massive rock formations. When the inter-granular pore space has been reduced or eliminated by minerals and cements, fractures may provide the dominant storage space in an aquifer. In fractured aquifers, the frequency and direction of the fractures will control the amount and ease of movement of the water from one area to another.

Hydraulic Properties. There are several properties of aquifers that characterize groundwater systems. The properties of most importance to groundwater modeling are porosity, hydraulic conductivity, and permeability.

Porosity is the ratio of the volume of pore space to the total volume of the aquifer system. This ratio is a dimensionless number less than 1, but most rocks have a porosity below 0.30. Fractured rocks exhibit a wide range of porosity from 0.01 to 0.10 . In the saturated zone of the aquifer, the water resides in this pore space, and the amount of water contained per unit volume is directly measured by the porosity. For groundwater flow systems, only the interconnected pores that permit the flow of water are considered (Smith and Wheatcraft, 1992:6.9). This *effective porosity* determines the amount of water per unit volume that is available for flow and is defined as

$$Effective\ Porosity = \frac{Interconnected\ Void\ Volume}{Total\ Volume} \tag{3-1}$$

Hydraulic conductivity measures the ability of a fluid to move through a porous medium. The hydraulic conductivity (K) is a function of both the medium and the fluid and is defined as

$$K = \frac{k\ \rho\ g}{\mu} \tag{3-2}$$

where k (m^2) is the *permeability,* a property of the medium only that describes how well the medium transmits water; ρ (kg/ m^3) is the fluid density; g (m/min^2) is the acceleration due to gravity; and μ (kg/m·min) is the dynamic viscosity of the fluid, giving K units of m/min (Smith and Wheatcraft, 1992:6.9).

Groundwater Flow

Hydraulic Head. Under the influence of gravity, groundwater flows from regions of high hydraulic head to regions with lower hydraulic head. *Hydraulic head* (h) is measured in meters and is defined as

$$h = z + \frac{p}{\rho\ g} \tag{3-3}$$

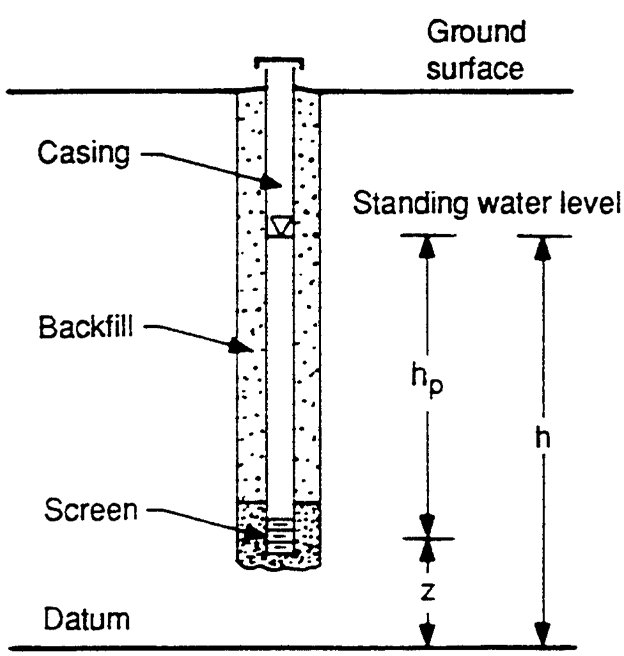
where p (g kg/m^2) is the pressure of the fluid with constant density ρ, and g is the acceleration due to gravity. z is the elevation of the measure point above datum (a level reference height), and is known as the *elevation head*.

The *water table* is defined as the surface on which the *pressure head* (h_p) is equal to zero. The pressure head is expressed in terms of values above atmospheric pressure as

$$h_p = \frac{p}{\rho g} \tag{3-4}$$

The relationship among hydraulic head, pressure head , and elevation head are illustrated in Figure 3.1 (Smith and Wheatcraft, 1992:6.7).

Figure 3.1 Relationship Among Heads



Groundwater Flow Governing Equation. The basic principles of groundwater flow were investigated and reported by Henri Darcy in 1856. His studies established that the flow rate through porous media is proportional to the hydraulic head loss and inversely proportional to the length of the flow path. Darcy's law in three dimensions is

$$q_x = -K_x \frac{\partial h}{\partial x} \qquad q_y = -K_y \frac{\partial h}{\partial y} \qquad q_z = -K_z \frac{\partial h}{\partial z}$$

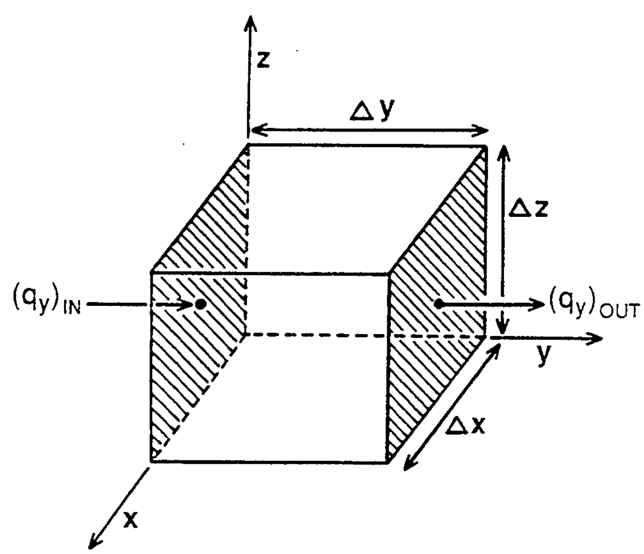
or

$$\boldsymbol{q} = -\boldsymbol{K}\nabla h \tag{3-5}$$

where $\boldsymbol{q}$ is the specific discharge rate (m/min), $\boldsymbol{K}$ is the hydraulic conductivity, and h is the hydraulic head.

To derive the general form of the governing equation of groundwater flow, first consider a representative elementary volume (REV) of the aquifer, as shown in Figure 3.2.

Figure 3.2 Representative Elementary Volume (Anderson and Woessner, 1992:16)



This cube represents a portion of the aquifer large enough to represent the properties of the porous medium, yet small enough that the change in head within this cube is relatively small. The volume of this REV is $\Delta x \Delta y \Delta z$. The flow of water through this volume is expressed in terms of the specific discharge rate $\boldsymbol{q}$, which may be expressed as

$$\boldsymbol{q} = q_x \mathbf{i}_x + q_y \mathbf{i}_y + q_z \mathbf{i}_z \tag{3-6}$$

in terms of the orthogonal unit vectors $\mathbf{i}_x$, $\mathbf{i}_y$, and $\mathbf{i}_z$ along the x, y, and z axes, respectively.

By conservation of mass[1], the rate of change in storage is defined as

$$\text{Outflow rate - Inflow rate} = \text{Rate Of Change in Storage } (ROCS) \tag{3-7}$$

Considering only the flow along the y axis, the change in flow rate through the REV is

$$\frac{\partial q_y}{\partial y}(\Delta x \Delta y \Delta z) \tag{3-8}$$

Similar expressions may be written for the x and z axes. The sum of the change in flow for all three axes, minus a term for the recharge R, is equal to the *ROCS*:

$$\left(\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} - R\right)\Delta x \Delta y \Delta z = ROCS \tag{3-9}$$

The *ROCS* is the ratio of change in volume per unit of time. The change of volume is described by *specific storage* S_s, defined as the volume of water released from storage per unit change in head h, per unit volume of aquifer:

[1] With the assumption of constant density, conservation of volume is also maintained.

$$S_s = -\frac{\Delta V}{\Delta h \Delta x \Delta y \Delta z} \qquad (3\text{-}10)$$

Therefore, the rate of change in storage in the REV is

$$ROCS = \frac{\Delta V}{\Delta t} = -S_s \frac{\Delta h}{\Delta t} \Delta x \Delta y \Delta z \qquad (3\text{-}11)$$

By combining equations 3-9 with 3-11, dividing through by $\Delta x \Delta y \Delta z$, and taking the limit as $\Delta t \to 0$, the final theoretical form of the water balance equation is

$$\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} = -S_s \frac{\partial h}{\partial t} + R \qquad (3\text{-}12)$$

Because the discharge rate ***q*** cannot be measured directly, this equation cannot be applied to field observations. However, Darcy's law (equation 3-5) defines the relation between ***q*** and *h*; and head is a parameter that may be directly measured in the field. This equation may be further simplified for steady-state simulations. Under steady-state conditions, the heads will not change with time, thus $\frac{\partial h}{\partial t}$ equals zero. If we additionally assume that no recharge occurs, then, when the equations of 3-5 are substituted into equation 3-12, the governing equation of groundwater flow under steady-state conditions is

$$\frac{\partial}{\partial x}\left(K_x \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial h}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial h}{\partial z}\right) = 0 \qquad (3\text{-}13)$$

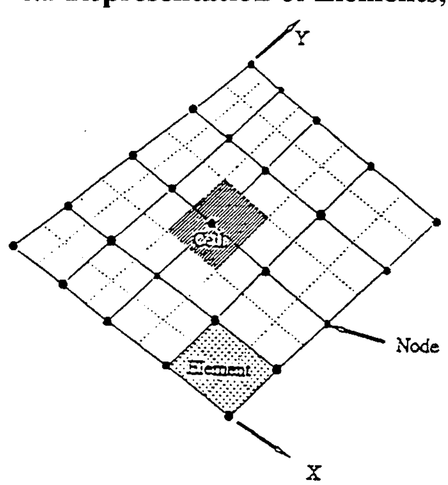
Some form of equation 3-13 is used in all steady-state, numerical, groundwater flow models with no recharge (Anderson and Woessner, 1992:13-18).

Numerical Groundwater Modeling.

The numerical model SUTRA (*S*aturated-*U*nsaturated *TRA*nsport) was used to simulate groundwater flow for this study. SUTRA was developed by the United States Geological Survey for computer modeling of groundwater systems. The version used in this study, V-0690-2D, was released in June of 1990. The program employs a two-dimensional hybrid finite-element and integrated finite-difference method to approximate the governing differential equation presented as equation 3-13 (Voss, 1984:3).

The numerical method used by SUTRA divides the cross-section of the aquifer into a single layer of contiguous blocks, called finite elements. Flow parameters and variables which vary from point to point within the aquifer are approximated at these elements. The corners of the elements are termed nodes, and regions that are centered at nodes are called cells (figure 3.3). This grid of interconnected nodes may be constructed on a cross-sectional view of the aquifer being modeled. The spacing and placement of the nodes will depend on the actual geology of the aquifer and will need to be adjusted by the analyst to accurately reflect the hydrogeological changes of the aquifer.

Figure 3.3 Graphical Representation of Elements, Nodes, and Cells



Each execution of SUTRA requires an input parameter file to specify the hydraulic conductivities and porosity for each element of the grid. Once this parameter file is prepared, SUTRA solves equation 3-13 and provides the steady-state fluid pressures at every node of the grid as its primary output. When SUTRA is run in steady-state mode, the fluid pressures do not vary with time. For convenience, these output pressures can be converted to hydraulic head (h) using equation 3-3. Appendixes B and C contain the FORTRAN code and VAX command files that were developed to streamline the execution of SUTRA for this project. These files allowed for rapid, interactive data entry and automatic reporting of results.

Calibration

As mentioned above, SUTRA requires several parameters for each of the elements of the grid to solve the finite-element model of the aquifer. The process of adjusting the model's parameters (e.g. hydraulic conductivity and effective porosity) to obtain a reasonable but nonunique match between the observed site-specific data (calibration target) and the model's estimated values is known as *model calibration* (Walton, 1992:35). The difference between an observed calibration target and the model's estimate of that target is the residual or error in the estimate.

The calibration target dataset for this study was composed of the hydraulic head values (h_m) observed (measured) within an aquifer. By computing the differences between the heads in the calibration target (h_m) with the heads computed from the finite-element model of SUTRA (h_s), the accuracy of the model may be assessed. For this study, four residual statistics were computed for each execution of the SUTRA model, where the number n of elements in the model was 524. The equations for calculating the Sum of Squared Error (SSE), Root Mean Squared Error (RMS), Mean Absolute Error (MAE), and Mean Error (ME) are respectively (Anderson and Woessner, 1992:238-241)

$$SSE = \sum_{i=1}^{n} \left(h_m - h_s\right)_i^2 \tag{3-14}$$

$$RMS = \left[\frac{1}{n} \sum_{i=1}^{n} \left(h_m - h_s\right)_i^2 \right]^{0.5} \tag{3-15}$$

$$MAE = \frac{1}{n} \sum_{i=1}^{n} \left| \left(h_m - h_s\right)_i \right| \tag{3-16}$$

$$ME = \frac{1}{n} \sum_{i=1}^{n} \left(h_m - h_s\right)_i \tag{3-17}$$

During the calibration process, the input parameters to the SUTRA model are adjusted until a suitably small residual statistic is computed using one of the above equations. As discussed in Chapter II, numerous methods have been proposed to analytically determine the optimal choice of input parameters that will provide a calibrated model with a small error. Response Surface Methodology (RSM) provides a means for systematically altering the input parameters to the SUTRA model to achieve a suitably small residual.

Response Surface Methodology

Response surface methodology comprises a group of statistical techniques for empirical model building and exploitation. One primary goal of RSM is to find the best value of the estimated response. The response chosen for this study was SSE (equation 3-14) because SSE was believed to be amenable to local approximation by the low-order polynomials typically used in RSM studies. The goal would be to find the set of parameter values which minimize the SSE, thus yielding calculated hydraulic heads from the finite-element groundwater model that closely match the calibration data set.

Using RSM to calibrate a groundwater model involves three basic phases of investigation. The first phase is a screening process that determines which parameters significantly influence the value of the estimated SSE response. The second phase uses local first-order approximations of the SSE response surface to determine parameter values associated with a smaller SSE. Finally, the third phase employs second-order approximations of the SSE response surface to identify locally optimal parameter settings that minimize the SSE for the calibrated model.

A key feature of the RSM technique is the empirical testing of the response surface. At no time is an attempt made to determine the shape of the entire response surface; rather, through first- and second-order models, pieces of the response surface are approximated and actual tests made in the direction of suggested improvement. This empirical testing leads to an understanding of the underlying SSE response without the need to precisely define it (Box and Draper, 1987:1-19).

I Parameter Screening Phase. The first step in calibrating a groundwater model is to determine which parameters need to be adjusted. Parameters such as porosity and hydraulic conductivity may be adjusted for as many hydrogeologic zones as are deemed necessary to account for the presumed differences in the aquifer. This approach may lead to a dozen or more parameters that need to be set in the groundwater model. Fortunately, only relatively few of these parameters are likely to significantly influence the behavior of the groundwater model. The purpose of the screening experiment is to determine which parameters have a significant effect on the groundwater model's estimate of the hydraulic heads. Thus, the screening phase serves the same purpose as sensitivity analysis in traditional groundwater modeling studies.

The parameter screening phase usually relies on a two-level experimental design. In a two-level design, the parameters are set to high and low levels of their expected range, based on the observed local hydrogeological conditions. For convenience and computational efficiency, these parameter values ξ_k, are often linearly transformed into coded or standardized variables x_k, such that

$$x_k = \frac{\xi_k - \xi_{k0}}{S_k} \tag{3-18}$$

where ξ_{k0} is the center of the region of interest and S_k is the half range of the region. A two-level factorial (2^k) design where each of the k variables occurs at just two levels (± 1 in coded space) may be used to estimate the k main effects in 2^k runs. As an alternative especially suited for parameter screening, Plackett-Burman designs allow for estimation of the k main effects in only $k + 1$ runs (Box and Draper, 1987:162).

Once the experimental runs have been performed, the SSE responses are fit to a first-degree polynomial model in k coded variables (Cornell, 1990:13)

$$Y_u = \beta_0 + \beta_1 x_{u1} + \beta_2 x_{u2} + \cdots + \beta_k x_{uk} + \varepsilon_u \tag{3-19}$$

The β_k coefficients are proportional to the effect the kth variable has on the output of the groundwater model ($\text{Effect}_k = 2\beta_k$). The presumption of the screening phase is that only those parameters with significant first-order effects need to be considered in subsequent experiments. Normally, ANOVA methods would indicate which coefficients are significant, but the relatively few runs in a Plackett-Burman design preclude this approach. In such instances, the significant effects can be identified through use of a normal probability plot.

In a properly fit first-order linear model, the residuals are approximately normally distributed with equal variance. If there are no significant effects, each of the computed effects will represent an observation from a common normal error distribution. A plot on normal probability paper of the empirical cumulative distribution function of these ordered, insignificant effects should roughly form a straight line. However, if some of the plotted points differ noticeably from a straight line either at the top right or bottom left, then the corresponding effects are presumed to be significant.

Standard graph paper may be used to identify the significant effects using the following procedure:

1) Order the effects from smallest to largest and scale the x-axis accordingly.

2) Plot the quantity $\phi^{-1}[(i\text{-}0.5)/k]$, where ϕ^{-1} (p) is the inverse cumulative distribution function of the standard normal distribution and *i* represents the rank of the effect. This function may be approximated by

$$\phi^{-1}(p) = [p^{0.1349} - (1\text{-}p)^{0.1349}]/0.1975 \tag{3-20}$$

From this plot, only those parameters which significantly contribute to the output of the groundwater model are selected for further analysis. In the next two phases, the settings of these parameters are adjusted to reduce the value of the SSE response to within calibration tolerances.

II First-Order Design Phase. Response surface methodology investigates the nature of the SSE response surface by conducting designed experiments centered at particular design points. A two-level, full-factorial (2^k) design, where each of the *k* variables occurs at just two levels (±1 in coded space), can be used to empirically evaluate the SSE response surface. This design requires 2^k runs. Using the responses from the actual process (the SSE responses from individual SUTRA runs), an estimate of the gradient of the SSE response surface in the design region may be made. The estimate of the gradient is determined by fitting a first-order model like equation 3-19 to estimate the SSE responses actually observed as a function of the coded input values. This first-order model of the response surface is analogous to using a truncated Taylor's series to approximate a function.

Once the gradient direction is determined (from the coefficients of the first-order model), further experiments are conducted in the direction of steepest descent. The experiments are conducted away from the center of the starting design region until the response begins to increase (in groundwater model calibration, the goal is to locate a minimum in the SSE response). Once a minimum along a gradient is reached, a new design may be established, a new gradient direction computed, and the gradient search along the steepest descent may be continued.

The first-order designs may be iteratively executed as long as measures to asses the adequacy of fit indicate a first-order design is still appropriate. A first-order model should have good explanatory power. This explanatory power is demonstrated by relatively high R Square and F values of the regression used to determine the coefficients of the first-order model. Also, a reasonable amount of improvement in the response should be realized over the previous design point. Finally, a test for curvature should indicate there is no significant curvature in the fitted first-order model. This test evaluates whether a run performed at the design center falls on a hyperplane running through the 2^k factorial points or if a significant amount of curvature is needed to fit the center point. Evidence of curvature implies significant higher-order terms have been omitted.

Single Degree of Freedom Test for Curvature In order to statistically evaluate the adequacy of the first-order model, the center point run can be used in a Single Degree of Freedom Test for Curvature. A Sum of Squares of Pure Quadratic terms (*SSPQ*) is given by the following "curvature contrast":

$$SSPQ = \frac{n_0 n_f (\bar{y}_{n_f} - \bar{y}_{n_0})^2}{n_0 + n_f} \tag{3-21}$$

where n_0 is the number of center point runs (which equals 1 in the case of a deterministic model like SUTRA), n_f is the number of factorial point runs (which equals 2^k for a full factorial design), $\bar{y}_{n_f}$ is the average of the SSE responses for the factorial points, and $\bar{y}_{n_0}$ is the SSE response observed at the center point run. The Sum of Squares Residual (*SSR*) presented in an ANOVA table is partitioned into Quadratic Terms and Other Terms as follows:

$$\text{Quad. Terms} = SSPQ \tag{3-22}$$

$$\text{Other Terms} = SSR - SSPQ \tag{3-23}$$

These two terms are divided by their respective degrees of freedom forming Mean Square of Quadratic (*MSQ*) and Other Terms (*MSO*). The ratio of *MSQ/MSO* is an F statistic which may be compared to an F-distribution with 1 and 2^k-k-1 degrees of freedom, for a full factorial design, corrected for the mean. A high F-value or the correspondingly low p-value implies significant quadratic effects. Thus, when this test fails, a first-order model (equation 3-19) should probably not be used to approximate the response surface at that design point. In general, if several measures indicate the first-order model is not adequate, the first-order phase should be terminated and the second-order design phase should be pursued.

III Second-Order Design Phase. The primary reason the first-order strategy had to be abandoned was because the first-order polynomial, equation 3-19, was not able to adequately fit the observed responses. In effect, the truncated Taylor's series had been truncated too far. In the second-order design phase, the following second-degree polynomial model is used (Box and Draper, 1987:376):

$$Y = \beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k + \beta_{11} x_{11} + \cdots + \beta_{kk} x_k^2 + \beta_{12} x_1 x_2 + \cdots + \beta_{k-1,k} x_{k-1} x_k \qquad (3\text{-}24)$$

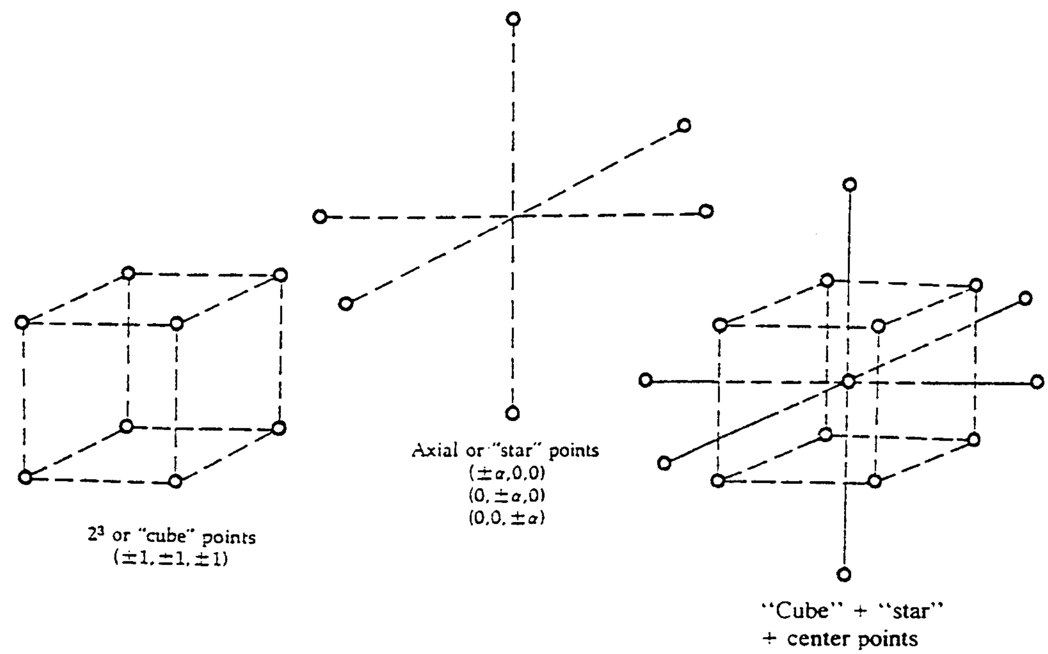
The two-level, full-factorial (2^k) design used in the first-order phase is not able to provide enough information to estimate the quadratic terms of equation 3-24. To build a quadratic model, a central composite design (CCD) may be used. A central composite design consists of the following three parts

i) the 2^k vertices (for a full factorial design) of a k-dimensional cube where the factor levels are coded so that the design center is at (0, 0, . . . ,0). The values of the coded variables in this factorial portion are (±1, ±1, . . . , ±1);

ii) the center point, n_0=(0, 0, . . . , 0) and;

iii) the $2k$ vertices (±α, 0, 0, . . . , 0), (0, ±α, 0, . . . , 0), . . . (0, 0, . . . , 0, ±α) of a k-dimensional "star" (Cornell, 1990:52). Figure 3.4 shows a central composite design for three variables (k = 3).

Figure 3.4 CCD for *k* = 3 (Cornell, 1990:53)



A desirable, but not necessary feature often incorporated into a CCD is rotatability. In a rotatable design, the accuracy of prediction of the response depends only on its distance from the center of the design, producing a variance function that is nearly spherical. Rotatability is achieved by assigning appropriate α values to the "star" points of the CCD. A general formula used to achieve rotatability in a full factorial design is:

$$\alpha = \left(2^{k}\right)^{\frac{1}{4}} \quad (3\text{-}25)$$

where k is the number of factors (Cornell, 1990:52). For a more general formula, see Box and Draper (1987:488).

One of the advantages of the central composite design is that the factorial points in (i) above are the same points used in the last two-level, full-factorial (2^k) design from the first-order phase. In most cases, the center point response would already have been determined from either the single degree of freedom test for curvature or the steepest descent gradient search conducted from the center of the last first-order design. Thus, to begin the second-order design phase, only the star points are run to obtain the additional responses needed to estimate the β coefficients of equation 3-24.

Once this second-order model has been fit to the data, the method of steepest descent applied to second-order surfaces needs to be performed to identify potential design points to use in experimenting beyond the design region. This second-order surface method of steepest descent is known as *ridge analysis*.

Ridge Analysis. The method of ridge analysis locates the minimum estimated response on the fitted model, equation 3-24, that is a distance R from the design center. Ridge analysis may be summarized as the following constrained optimization problem:

$$\textit{Minimize} \qquad Y = \beta_0 + \mathbf{x}'\boldsymbol{\beta} + \mathbf{x}'\boldsymbol{\beta}\mathbf{x}$$

$$\textit{Subject to} \qquad \sum_i x_i^2 - R^2 = 0$$

This optimization problem can be solved using the SAS statistical package to automatically exploit a ridge system. By conducting a ridge analysis for each of several distances R from the design center, SAS provides a set of promising points to use in establishing the location of improved responses. Ridge analysis does not conduct a search along the specified path; it only identifies potential design points to use in experimenting beyond the design region (Box and Draper, 1987:375-380). By actually conducting experiments along the identified path, the responses will typically improve (decrease) and then become worse (increase) as the second-order model diverges from the true underlying response surface. If the lowest response found provides a groundwater model which is calibrated within tolerances, the hydrologist is finished. If further improvement is sought, another CCD may be established at the lowest response, and the second-order design phase repeated.

The iterative use of response surface methods will identify, within error tolerances, a local minimum of the response surface. The parameters of the groundwater model used at this minimum have calibrated the finite-element model. Although several first- and second-order experimental designs may be needed to locate this minimum, a suitably calibrated model could possibly be achieved before this local minimum is found. In this case, the hydrologist may elect to discontinue the iterative procedure once the desired degree of tolerance is achieved.

IV. Results and Analysis

Introduction

The primary objective of this project was to determine if the techniques of Response Surface Methodology (RSM) could be used to calibrate a groundwater flow model. First, a set of steady-state hydraulic head values was established to validate the proper functioning of the finite-element code being used (SUTRA, *S*aturated-*U*nsaturated *TRA*nsport). These steady-state hydraulic head values also served as the calibration target data set to compare against the flow model's output. Next, a screening experiment was conducted to determine which parameters had a significant effect on the flow model's outcome. Finally, the RSM approach was used to calibrate this two-dimensional, steady-state flow model by adjusting the significant parameters until a local, if not global, optimum was obtained.

Calibration Target Data Set Preparation / Validation

In choosing an example to validate the RSM approach, a previously calibrated groundwater model was used as a calibration target rather than calibrating a new model using field observations. Using a previously calibrated model also had the advantage of eliminating uncertainties due to field measurement errors. This approach effectively provided observational head data at each computational node in the calibration target data set. While such resolution is unrealistic for field applications, it nonetheless provided an excellent platform for testing the RSM procedure. This validation approach is commonly seen in the literature (Xiang and others, 1993; Willis and Yeh, 1987; Carrera and Neuman, 1986c).

Smith and Ritzi (1993) used a two-dimensional, finite-element model in cross-section mode to simulate groundwater flow and nitrate transport on the Sycamore Farm research facility of Wright State University, Ohio. A complete hydrogeologic description of the Sycamore Farm area is provided in Smith (1991:55-56). The Smith-Ritzi model served as the calibration target data set for this thesis effort. As the input parameters were adjusted in the SUTRA model using the principles of RSM, the output was compared to the Smith-Ritzi model to determine how closely the SUTRA model was being calibrated.

The Smith-Ritzi model contains ten hydraulic conductivity zones. The values used for these ten hydraulic conductivity zones are presented in table 4.1.

Table 4.1 Hydraulic Conductivity Zones

Hydraulic Conductivity Zone	Geological Formation	Hydraulic Conductivity (m/min)
Unit 1	Dayton Dolomite	2.0×10^{-3}
Unit 2	Upper Brassfield	1.0×10^{-3}
Unit 3	Upper Brassfield	1.0×10^{-4}
Unit 4	Upper Brassfield	3.0×10^{-5}
Unit 5	Upper Brassfield	2.0×10^{-3}
Unit 6	Gray Clayey Shale	3.0×10^{-4}
Unit 7	Middle Brassfield	6.0×10^{-4}
Unit 8	Middle Brassfield	6.0×10^{-6}
Unit 9	Lower Brassfield	4.0×10^{-6}
Unit 10	Lower Brassfield	1.0×10^{-5}

The hydraulic conductivities listed above and a single effective porosity of 11% were used as the parameters for the SUTRA program to produce a calibration target set of heads. This raw output contained the horizontal (X) and vertical (Y) grid coordinates as well as the hydraulic pressure for each of the 524 nodes in the finite-element grid. Figure 4.1 shows the finite-element grid used by SUTRA to compute the hydraulic pressures at the 524 nodes. The aquifer being modeled consists of nine stratigraphic units, divided into ten hydrologic units, each with its own hydraulic conductivity. The spacing and arrangement of these nodes was determined by the local geology of the groundwater system and reflects the hydraulic conductivity zonation shown in figure 4.2.

The raw output from the SUTRA run was not in units that were directly useful. The vertical coordinates (Y) were given in meters above a horizontal datum fixed at 274.35 meters above mean sea level (AMSL). These vertical coordinates were transformed to heights AMSL (Y_{AMSL}) by simply adding 274.35 m to all 524 vertical coordinates. The hydraulic pressures computed by SUTRA at each node were transformed to steady-state hydraulic heads via the following function:

$$Head_{AMSL} = Pressure/9800 + Y_{AMSL} \tag{4-1}$$

where the pressure is given in units of $kg/m \cdot s^2$ and heights AMSL in terms of m.

Figure 4.1 Cross-Sectional Finite-Element Grid (Smith, 1991:28)

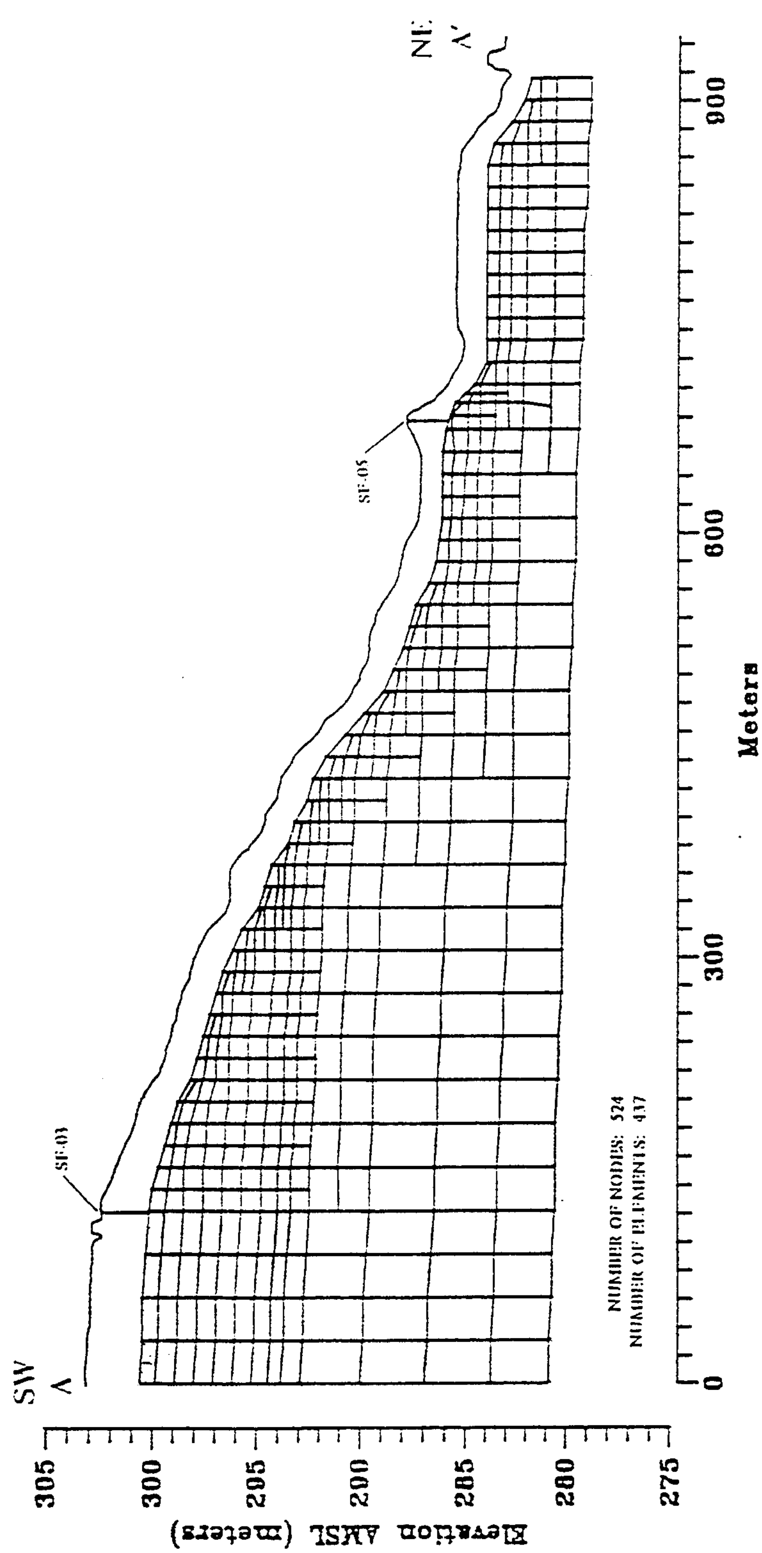
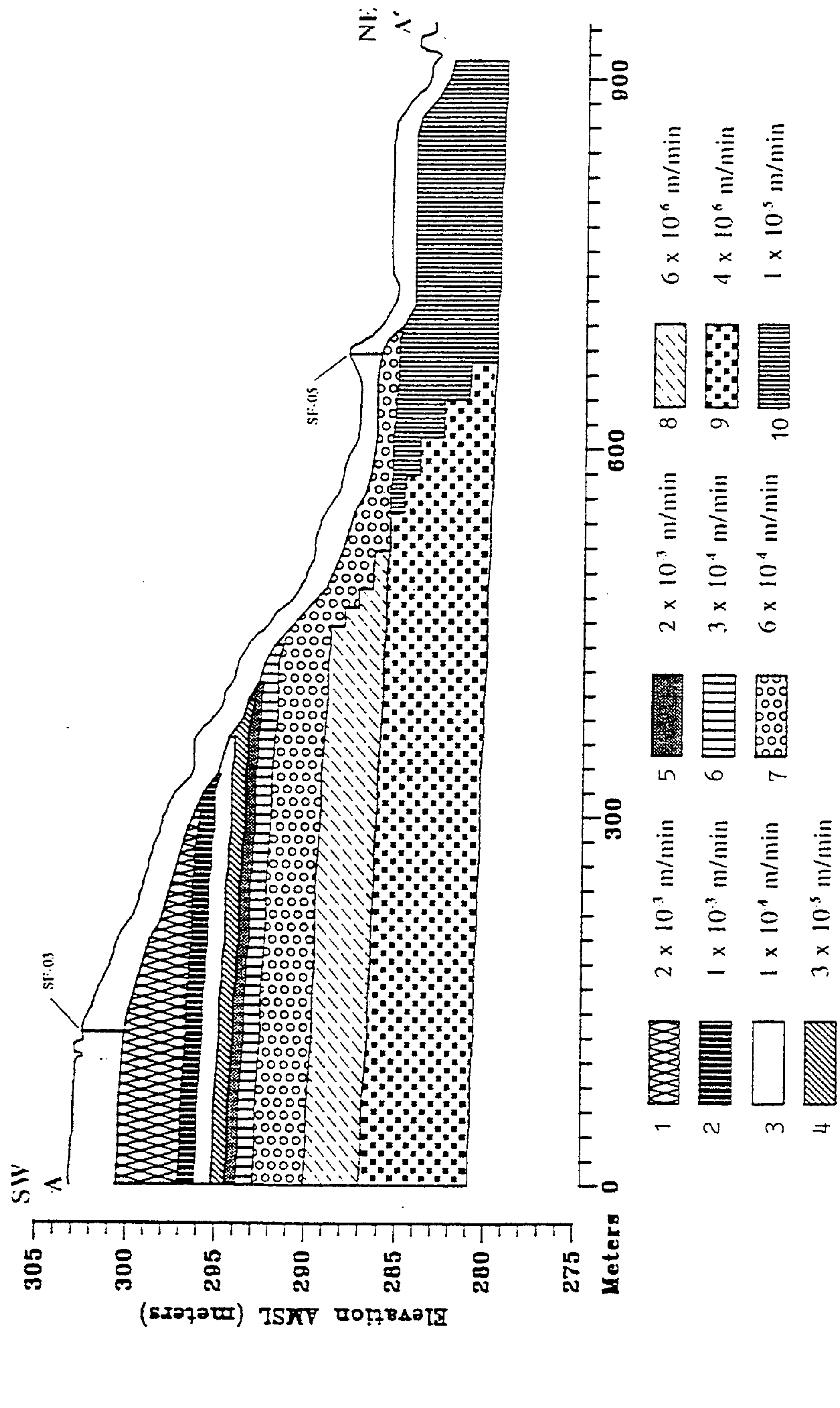
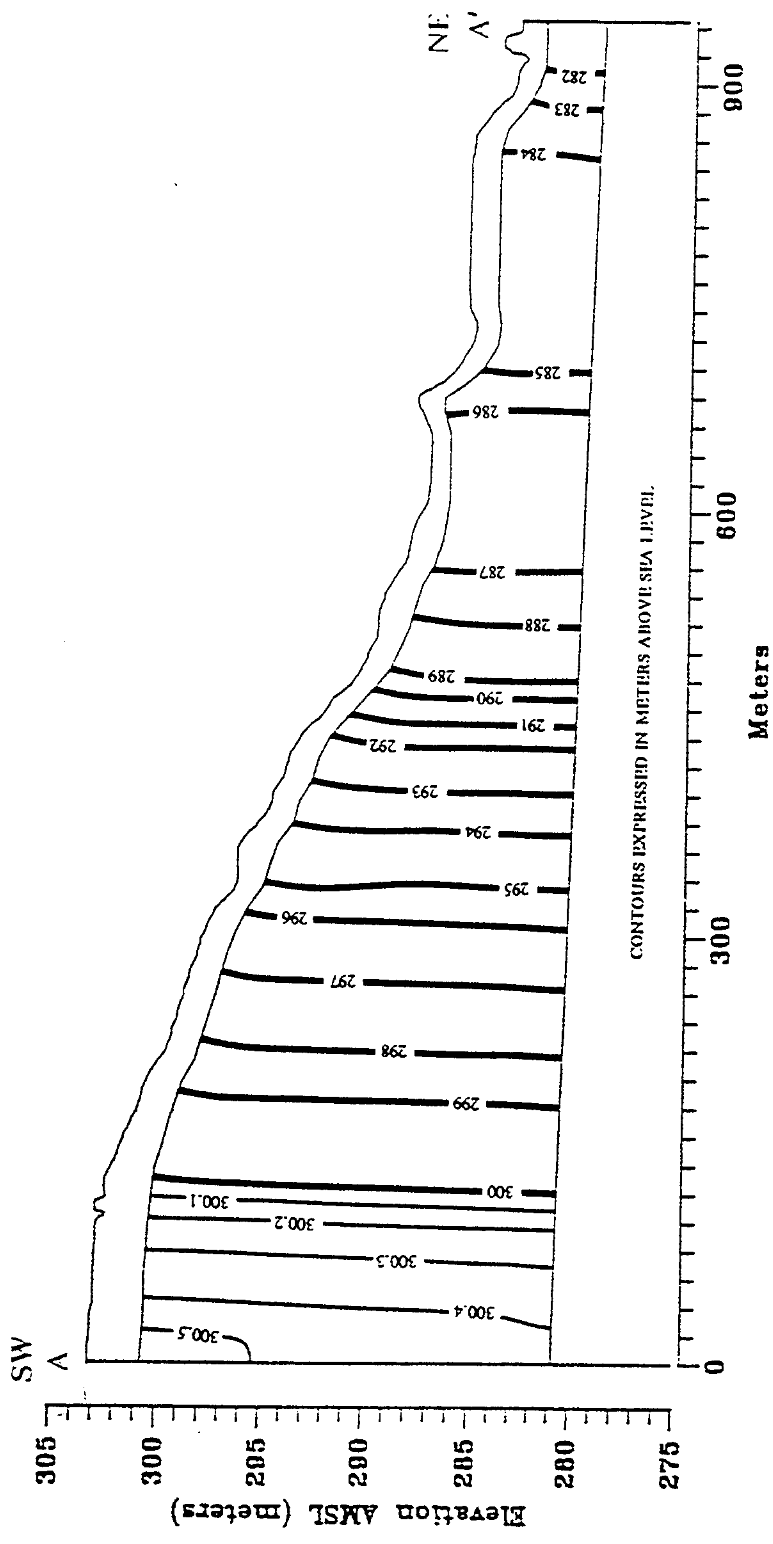


Figure 4.2 Hydraulic Conductivity Zones Within Finite-Element Grid (Smith, 1991:29)



After completing the above calculations, a calibration target data set consisting of the steady-state hydraulic heads at all 524 nodes was ready. It contained the X and Y_{AMSL} coordinates in meters from the lower left (southwest) corner of the cross section, along with their accompanying steady-state hydraulic head values ($Head_{AMSL}$), also measured in meters AMSL. This calibration target data set of hydraulic heads was in perfect agreement with the hydraulic heads presented by Smith (1991:35) (see figure 4.3). By computing a set of heads that matched the heads of the calibrated Smith-Ritzi model, the calibration target set was validated for use in the following calibration study. All subsequent outputs from the SUTRA model were compared to this calibration target set to determine the progress of the calibration.

Figure 4.3 Computed Steady-state Hydraulic Head Distribution (Smith, 1991:35)



Screening Experiments / Sensitivity Analysis

The aquifer being modeled contained ten hydraulic conductivity zones, and an overall effective porosity. Thus, eleven possible parameters may be adjusted to try and match the output of the SUTRA model with the calibration target set of hydraulic heads. Before attempting to adjust 11 parameters to calibrate the model, a screening experiment or sensitivity analysis was conducted to determine which parameters significantly contributed to the model's output.

A screening experiment, based on a two-level Plackett-Burman design (Box and Draper, 1987:162), was established to evaluate the significance of the 11 parameters. Table 4.2 presents the settings used for the 12 runs of this screening experiment. The complete results are listed in Appendix A.

Table 4.2 Plackett-Burman Experimental Values

Run	Unit 1	Unit 2	Unit 3	Unit 4	Unit 5	Unit 6	Unit 7	Unit 8	Unit 9	Unit 10	Porosity
1	1.0E-02	1.0E-07	1.0E-02	1.0E-07	1.0E-07	1.0E-07	1.0E-02	1.0E-02	1.0E-02	1.0E-07	20
2	1.0E-02	1.0E-02	1.0E-07	1.0E-02	1.0E-07	1.0E-07	1.0E-07	1.0E-02	1.0E-02	1.0E-02	1
3	1.0E-07	1.0E-02	1.0E-02	1.0E-07	1.0E-02	1.0E-07	1.0E-07	1.0E-07	1.0E-02	1.0E-02	20
4	1.0E-02	1.0E-07	1.0E-02	1.0E-02	1.0E-07	1.0E-02	1.0E-07	1.0E-07	1.0E-07	1.0E-02	20
5	1.0E-02	1.0E-02	1.0E-07	1.0E-02	1.0E-02	1.0E-07	1.0E-02	1.0E-07	1.0E-07	1.0E-07	20
6	1.0E-02	1.0E-02	1.0E-02	1.0E-07	1.0E-02	1.0E-02	1.0E-07	1.0E-02	1.0E-07	1.0E-07	1
7	1.0E-07	1.0E-02	1.0E-02	1.0E-02	1.0E-07	1.0E-02	1.0E-02	1.0E-07	1.0E-02	1.0E-07	1
8	1.0E-07	1.0E-07	1.0E-02	1.0E-02	1.0E-02	1.0E-07	1.0E-02	1.0E-02	1.0E-07	1.0E-02	1
9	1.0E-07	1.0E-07	1.0E-07	1.0E-02	1.0E-02	1.0E-02	1.0E-07	1.0E-02	1.0E-02	1.0E-07	20
10	1.0E-02	1.0E-07	1.0E-07	1.0E-07	1.0E-02	1.0E-02	1.0E-02	1.0E-07	1.0E-02	1.0E-02	1
11	1.0E-07	1.0E-02	1.0E-07	1.0E-07	1.0E-07	1.0E-02	1.0E-02	1.0E-02	1.0E-07	1.0E-02	20
12	1.0E-07	1.0E-07	1.0E-07	1.0E-07	1.0E-07	1.0E-07	1.0E-07	1.0E-07	1.0E-07	1.0E-07	1

The choice of the high and low levels was based upon regional values for massive Paleozoic limestone rocks as presented by Beck and others (1988: 336-337). The approach taken was to use as wide a range of values as was deemed reasonable for the type of rocks comprising this aquifer. No effort was made to limit the values of the hydraulic conductivities of each zone to any particular range, although such delineation may be made, if desired. The single porosity value used represented the effective porosity for this entire fractured carbonate system.

The 12 individual experiments were run through SUTRA, and the sum of the squared differences (SSE) between the hydraulic head pressures for the 524 nodes of the run and the calibration target set was computed. To determine which parameters had a significant effect on the output response (SSE) of the model, a normal probability plot (Figure 4.4) was made (Box and Draper, 1987:128-134). Using this method, those factors which do not significantly contribute will fall toward the center of the plot and lie along a line, thus indicating they do not appear to stand above the normal noise of the data. In figure 4.4, Units 2, 9, 10, and possibly 6 appear to fall off of the line near its ends; indicating only these four parameters had a significant effect on the model.

In addition to this graphical technique, a step-wise linear regression was performed on the data. Using an alpha of 0.075 to enter and exit the linear model, the step-wise regression procedure also selected Units 2, 6, 9, and 10 to enter into the model.

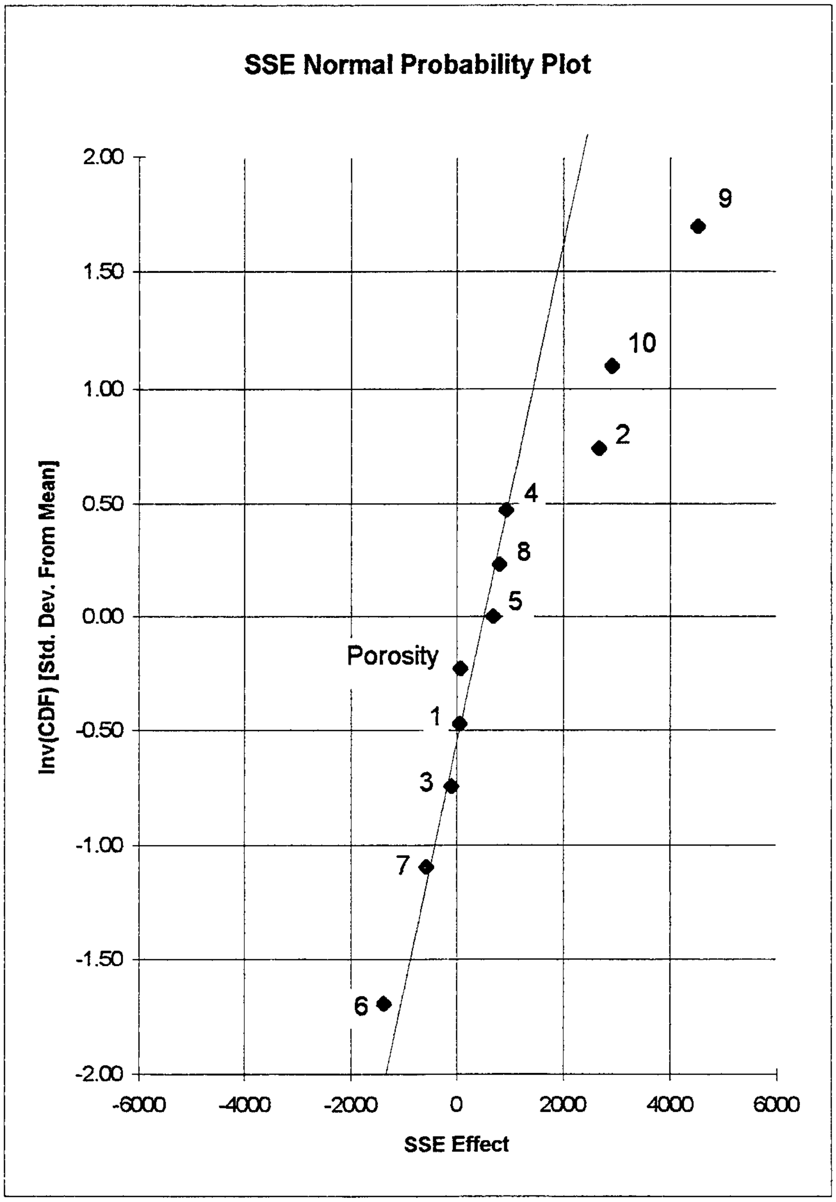
This screening experiment determined that only four parameters needed to be varied to calibrate the finite-element model. Efforts to adjust any of the other parameters would have minimal effect, as their contribution is no greater than the noise contained within the data. Therefore, in applying the RSM to the calibration, only the hydraulic conductivities for Units 2, 6, 9, and 10 were adjusted. The settings for all the other parameters were fixed to values at the center of the Plackett-Burman design. Porosity was fixed at 10% and the hydraulic conductivities for Units 1, 3, 4, 5, 7, and 8 were fixed at 5.0×10^{-3} m/min. It should be emphasized, however, that this analysis has shown that the settings for these units are not significant, so they may be set to any value in the parameter range.

In closing this discussion, a risk associated with screening designs should be highlighted. Screening designs generally provide the ability to estimate only *linear* effects and may not identify certain types of *higher order* effects. For example, a factor that imparts a significant quadratic effect on the response could potentially be included in the set of factors having no appreciable effect on it. If the observed responses at the high and low levels of this factor were approximately equal, the estimated linear effect would be negligible. The important quadratic effect would have been overlooked, as a design with only two levels cannot estimate a quadratic effect. Thus, it is possible that a screening experiment may unknowingly delete one or more variables with significant higher order effects from further consideration.

If response surface methods are not able to calibrate the finite-element model sufficiently well, the investigator may need to reexamine or reaccomplish the screening experiment to determine if significant factors were inadvertently omitted. In this study, it is believed that no influential factors were incorrectly screened from the calibration effort. Thus, by adjusting only the four hydraulic conductivities for Units 2, 6, 9, and 10; a calibrated model should be achieved.

Figure 4.4 SSE Normal Probability Plot

FACTOR	Coeff.	EFFECT	RANK	CDF	Inv(CDF)
Unit 9	2256.23	4512.46	11	0.9545	1.69
Unit 10	1452.46	2904.93	10	0.8636	1.09
Unit 2	1333.31	2666.63	9	0.7727	0.74
Unit 4	467.28	934.56	8	0.6818	0.47
Unit 8	403.56	807.13	7	0.5909	0.23
Unit 5	344.10	688.19	6	0.5000	0.00
Porosity	35.18	70.36	5	0.4091	-0.23
Unit 1	28.08	56.16	4	0.3182	-0.47
Unit 3	-49.85	-99.71	3	0.2273	-0.74
Unit 7	-286.32	-572.64	2	0.1364	-1.09
Unit 6	-690.07	-1380.14	1	0.0455	-1.69



First-Order Designs

Once the significant parameters were determined, first-order designed experiments were used to provide local approximations of the response surface. Four designs (A, B, C, and D) were used to fully exploit the first-order strategy.

Based upon the screening experiments, only four hydraulic conductivity parameters needed adjusting (the other six hydraulic conductivities were fixed at 5.0×10^{-3} m/min and effective porosity at 10%). Thus a 2^4 (two-level, four factor) factorial design was used throughout the first-order phase. This design required 16 runs and generated the SSE responses that were regressed to estimate the gradient at each design region. Tables of the specific settings used for each of the four 2^4 factorial designs and their subsequent steepest descent trials are contained in Appendix A.

Design A The starting point for the first first-order design was based upon the approximate center point of the Plackett-Burman design. The starting point could have used the settings from the best run found during the Plackett-Burman screening experiment (Run 12, SSE = 0.14596). This run gave a rather small SSE and provided a good starting point for calibrating the finite-element model. However, the intent of this study was to demonstrate the general applicability of the RSM technique. The discovery of "good" parameter settings was not exploited in order to demonstrate the methodology in the absence of such fortuitous results.

Although the Plackett-Burman design used the same settings for all the hydraulic conductivities, the deeper units were assigned smaller values in Design A since the hydraulic conductivities usually decrease with depth. The high and low settings for these experimental runs were based on ± 80% of the center point's value. Table 4.3 presents the four hydraulic conductivity values used for Design A. Table 4.4 presents the results of regressing the 16 SSE responses using the Regression Analysis Tool from *Microsoft Excel*. The Residual statistic was partitioned into Quadratic and Other Terms as presented in Chapter 3, "Single Degree of Freedom Test For Curvature."

This first-order model had high explanatory power as indicated by the high R Square (0.9287) and F value (39.06). However, quadratic terms seemed to be significant (as seen in the high F statistic for the single degree test for curvature). Because of the high explanatory power of this first-order model, further exploration was warranted down the path of steepest descent in spite of the evidence of curvature suggested by the single degree of freedom test for curvature. The steepest descent gradient was determined from the negative of the regression coefficients and normalized in the units of the design (Box and Draper, 1987:187). Experiments were conducted along this gradient until the SSE response failed to become smaller. Figure 4.5 illustrates the behavior of the SSE response along this gradient determined from the Design A experiments (Note the curve is interpolated by the graphics package; only the points represent actual data). The lowest SSE response occurred at 14 unit vector lengths from the center of Design A. The SSE response was reduced from a value of 0.1573 to 0.1439. The point 14 unit vector lengths from the center of Design A served as the center of the next design, Design B.

Table 4.3 Design A Experimental Values

Hydraulic Conductivity Zone	Low (m/min)	Center (m/min)	High (m/min)
Unit 2	1.0000×10^{-3}	5.0000×10^{-3}	9.0000×10^{-3}
Unit 6	1.0000×10^{-4}	5.0000×10^{-4}	9.0000×10^{-4}
Unit 9	1.0000×10^{-6}	5.0000×10^{-6}	9.0000×10^{-6}
Unit 10	1.0000×10^{-6}	5.0000×10^{-6}	9.0000×10^{-6}

Table 4.4 Design A Regression Analysis

SUMMARY OUTPUT

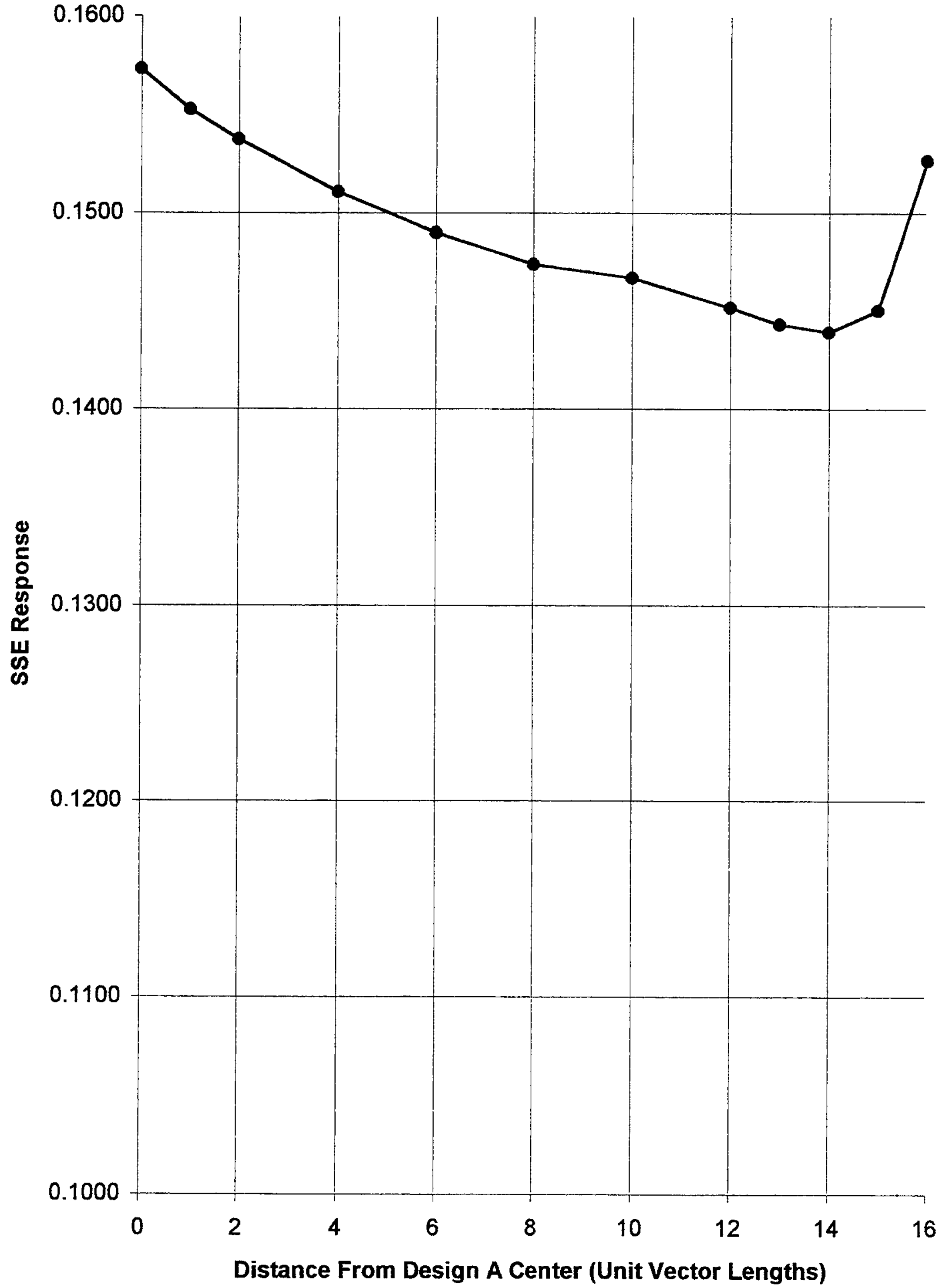
Regression Statistics	
Multiple R	0.9637
R Square	0.9287
Adjusted R Square	0.9049
Standard Error	1.347E-02
Observations	17

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	4	2.836E-02	7.090E-03	39.06459	0.00000
Residual	12	2.178E-03	1.815E-04		
Quad. Terms	1	1.532E-03	1.532E-03	26.08723	0.00034
Other Terms	11	6.460E-04	5.873E-05		
Total	16	3.054E-02			

	Coefficients	*Standard Error*	*t Stat*	*P-value*
Intercept	1.953E-01	3.267E-03	5.977E+01	3.182E-16
Unit 2	2.919E-03	3.368E-03	8.668E-01	4.031E-01
Unit 6	-4.141E-02	3.368E-03	-1.229E+01	3.691E-08
Unit 9	4.992E-03	3.368E-03	1.482E+00	1.641E-01
Unit 10	-4.959E-03	3.368E-03	-1.472E+00	1.666E-01

Figure 4.5 SSE Response Along Steepest Descent From Design A



Designs B, C, & D For the second, third, and fourth, first-order designs, the high and low settings were fixed at ± 50% of the center point's value in an attempt to reduce the amount of curvature in the resulting empirical models. Tables 4.5 - 4.7 present the hydraulic conductivity values used for Designs B, C, & D. Each design was centered on the lowest SSE response observed during the steepest descent search away from the previous design.

Table 4.5 Design B Experimental Values

Hydraulic Conductivity Zone	Low (m/min)	Center (m/min)	High (m/min)
Unit 2	5.5845×10^{-4}	1.1169×10^{-3}	1.6754×10^{-3}
Unit 6	3.0038×10^{-3}	6.0076×10^{-3}	9.0114×10^{-3}
Unit 9	5.0000×10^{-8}	1.0000×10^{-7}	1.5000×10^{-7}
Unit 10	5.7985×10^{-6}	1.1597×10^{-5}	1.7396×10^{-5}

Table 4.6 Design C Experimental Values

Hydraulic Conductivity Zone	Low (m/min)	Center (m/min)	High (m/min)
Unit 2	2.2201×10^{-2}	4.4402×10^{-2}	6.6603×10^{-2}
Unit 6	3.1991×10^{-2}	6.3982×10^{-2}	9.5973×10^{-2}
Unit 9	1.2884×10^{-7}	2.5767×10^{-7}	3.8650×10^{-7}
Unit 10	5.0000×10^{-8}	1.0000×10^{-7}	1.5000×10^{-7}

Table 4.7 Design D Experimental Values

Hydraulic Conductivity Zone	Low (m/min)	Center (m/min)	High (m/min)
Unit 2	9.2195×10^{-3}	1.8439×10^{-2}	2.7658×10^{-2}
Unit 6	6.2300×10^{-2}	1.2460×10^{-1}	1.8690×10^{-1}
Unit 9	7.7060×10^{-8}	1.5412×10^{-7}	2.3118×10^{-7}
Unit 10	7.0100×10^{-8}	1.4020×10^{-7}	2.1030×10^{-7}

For each design, the SSE responses were regressed on the coded parameters, the steepest descent gradient was determined, and experiments were run along this gradient until the SSE response failed to become smaller. Figures 4.6 - 4.8 illustrate the behavior of the SSE response out along the gradients determined from Designs B, C, & D. Both Designs B and C demonstrated significant improvement (lowering of the SSE response), and the single degree test for curvature indicated only a minor amount of curvature. Table 4.8 summarizes the results from all of the first-order designs.

Table 4.8 Summary of First-Order Designs

Design	R Square	Quadratic F-value	Quadratic p-value	Distance From Design Center	Lowest SSE Response Along Gradient
A	0.9287	26.087	0.00034	14	0.14394
B	0.8070	4.127	0.06707	80	0.11730
C	0.9216	4.152	0.06637	2.25	0.10318
D	0.8675	94.156	0.00000	0.50	0.10099

Design D did not show significant improvement over Design C, the R Square of the fitted first-order model fell, a very significant amount of curvature existed, and the local minimum is found well within the design region. These observations indicated the first-order approach had reached its limits of applicability and a second-order design appeared justified to further evaluate the response surface.

The first-order strategy yielded very good results; improving the SSE response from 0.15732 (at the center of Design A) to 0.10099 (after following the gradient from Design D). The calibrated model 0.50 units from the center of Design D had a mean absolute error (MAE) of only 7.1505 mm at each of the 524 nodes. In fact, the calibrated model obtained after searching down the gradient from Design C would probably have been good enough, in most cases, to use in groundwater simulation studies without further fine-tuning of the input parameters. However, to fully demonstrate the RSM technique, a second-order model was evaluated to calibrate the SUTRA model even closer to the calibration target data set.

Figure 4.6 SSE Response Along Steepest Descent From Design B

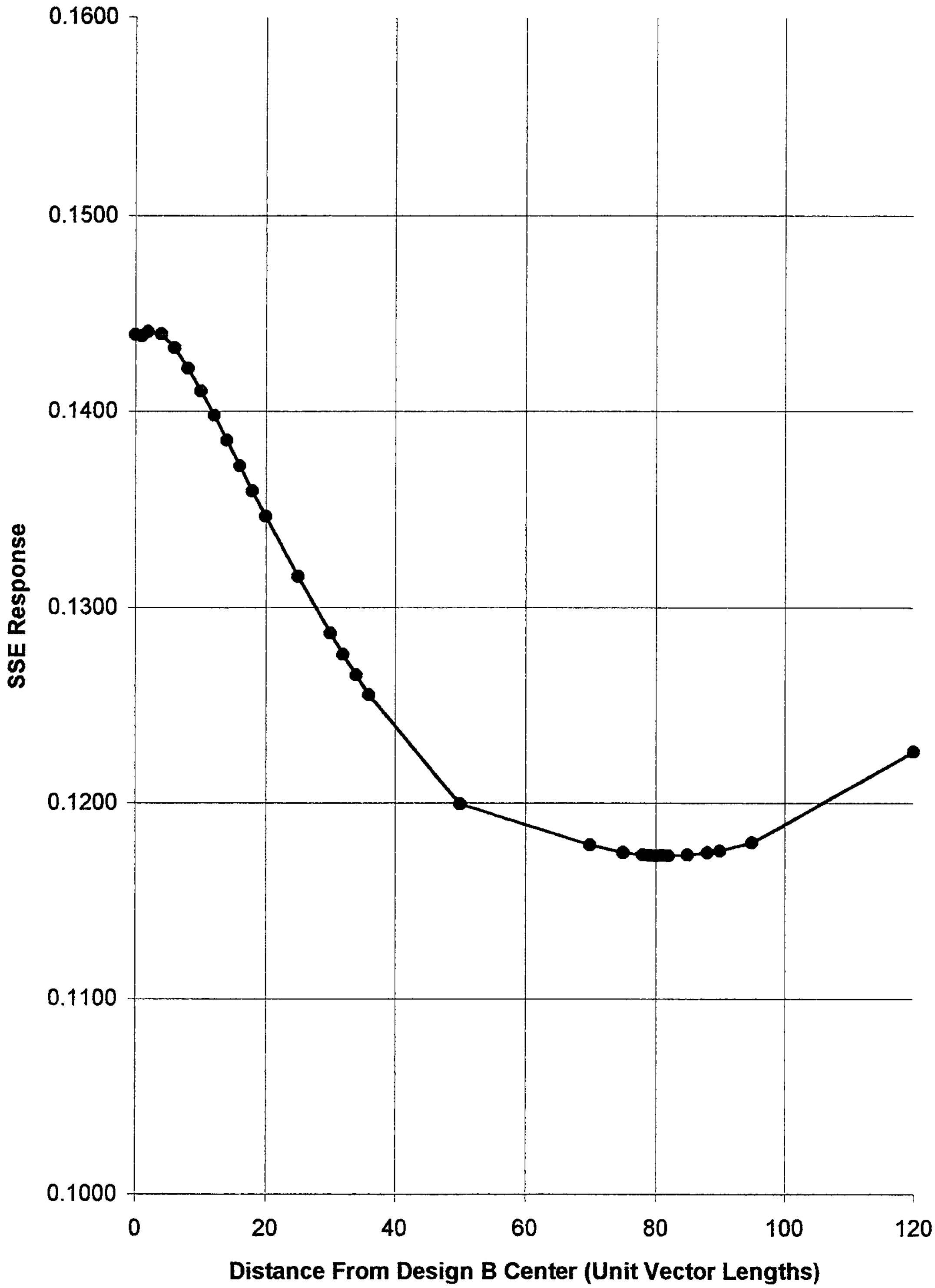


Figure 4.7 SSE Response Along Steepest Descent From Design C

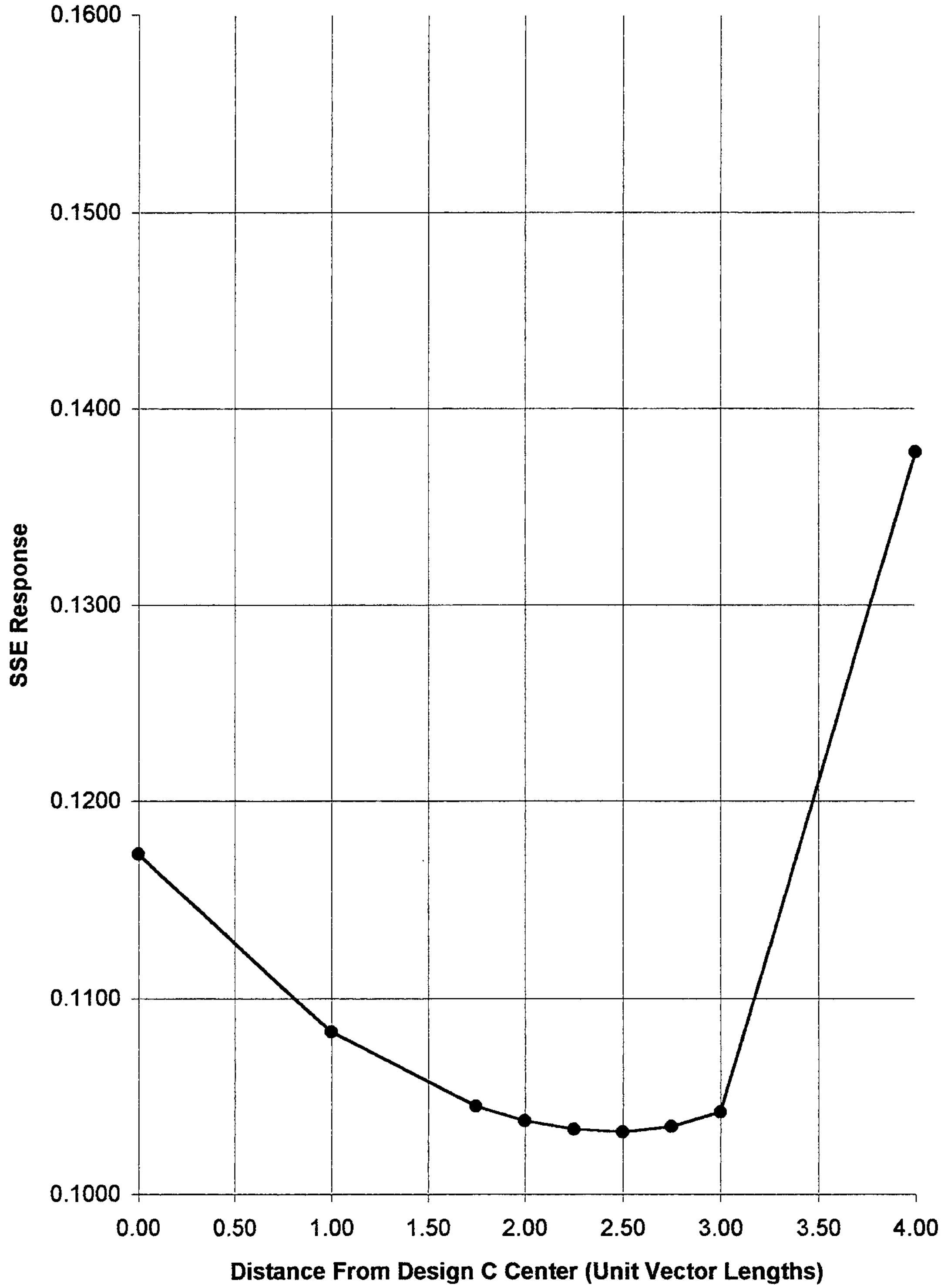
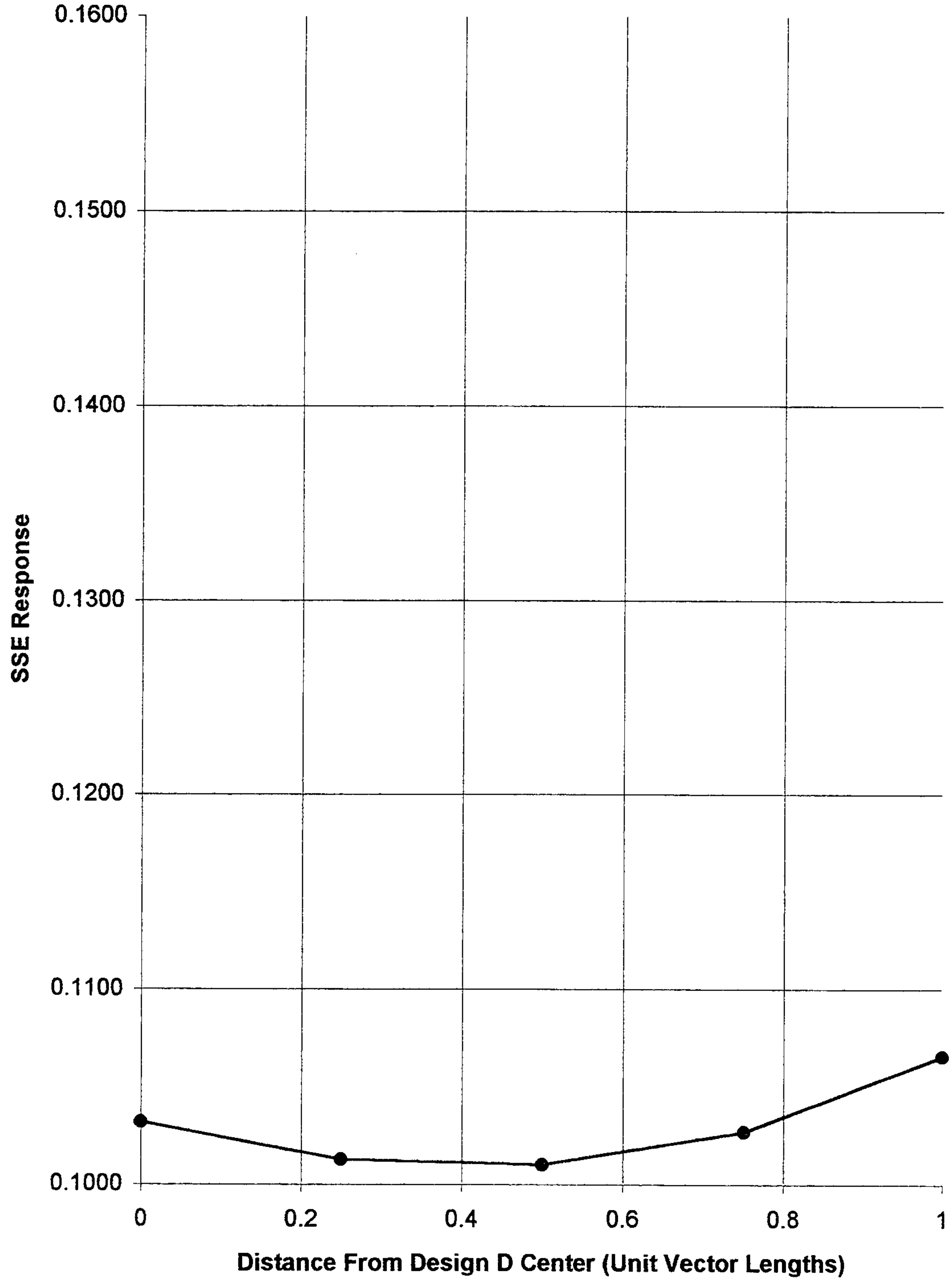


Figure 4.8 SSE Response Along Steepest Descent From Design D



Second-Order Designs

To evaluate the SSE response surface further, a second-order model was fit to the data. The 2^4 factorial design, used in Design D, was augmented with 8 axial points and a center point, to form a central composite design (CCD) experiment. The axial length (α) for these points should be equal to 2 in order to have a rotatable CCD. However, when $\alpha = 2$, the actual parameter values became zero. To avoid this problem, an α of 1.99 was used in the first CCD, named CCD A. Other settings of α were used to investigate the effect this setting had on the results of the CCD experiment. Although in this study three different values of α were used, only CCD C was really necessary. Once the additional axial points were run through SUTRA, the SSE responses were regressed to a second-order model using the SAS statistical analysis computer package. SAS also presented a ridge analysis of the fitted surface, suggesting a path of lowest responses. Table 4.9 summarizes the results of the three CCDs.

Table 4.9 Summary of Second-Order Designs

CCD Name	α Value	R Square	Lowest Min. Ridge SSE Response
CCD A	1.99	0.4730	0.10171
CCD B	1.50	0.9806	0.09918
CCD C	1.00	0.9988	0.09820

CCD C, with $\alpha = 1.00$, had the best fit of the second-order surfaces with an R Square of 0.9988. By following the suggested minimum ridge away from the center of CCD C (based upon the fitted second-order surface), the lowest SSE response in this study was found, 0.0982. Figures 4.9 - 4.11 show the SSE responses as the ridge minimum is followed away from each CCD.

Figure 4.9 CCD A Minimum Ridge Analysis

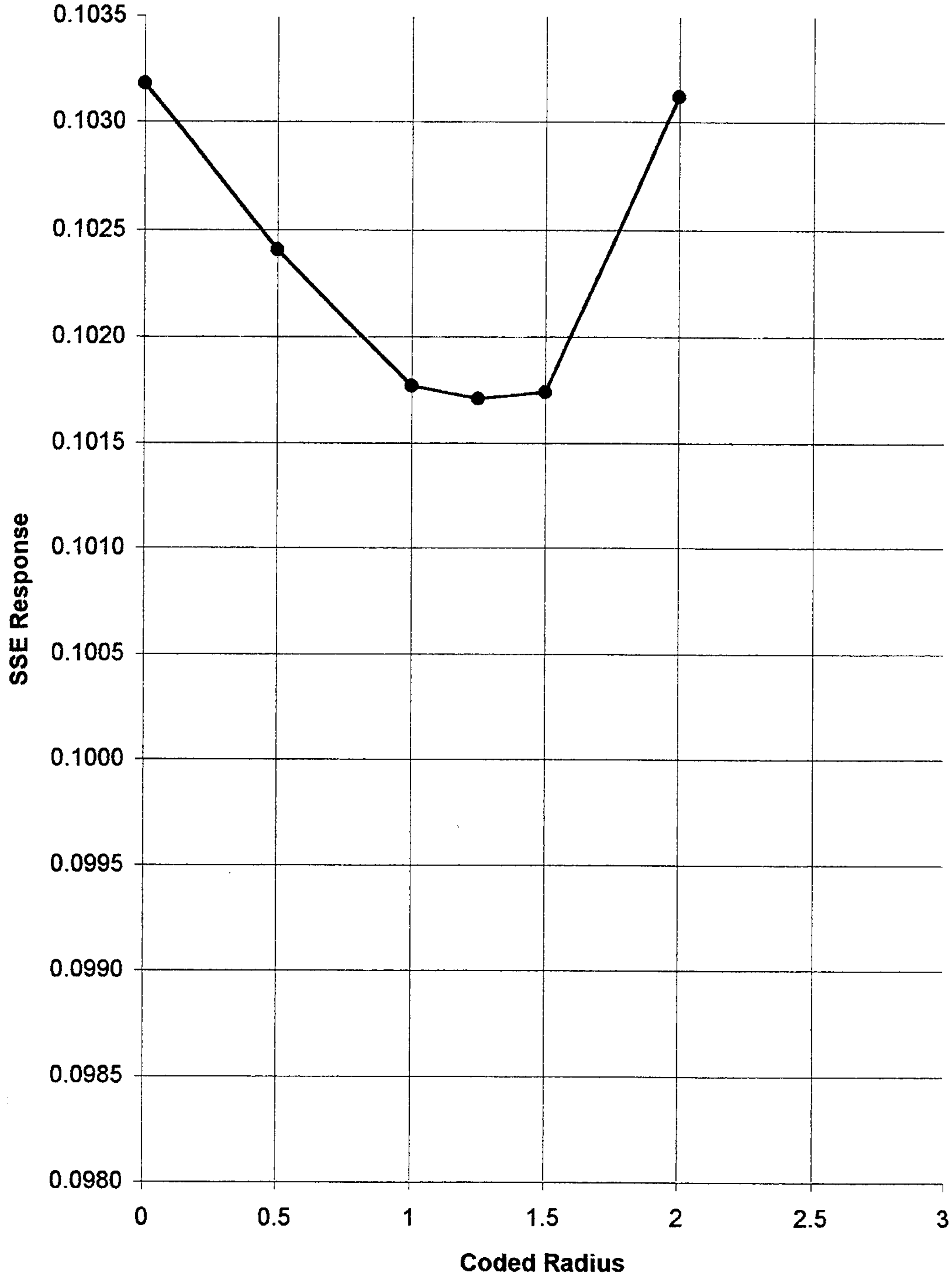


Figure 4.10 CCD B Minimum Ridge Analysis

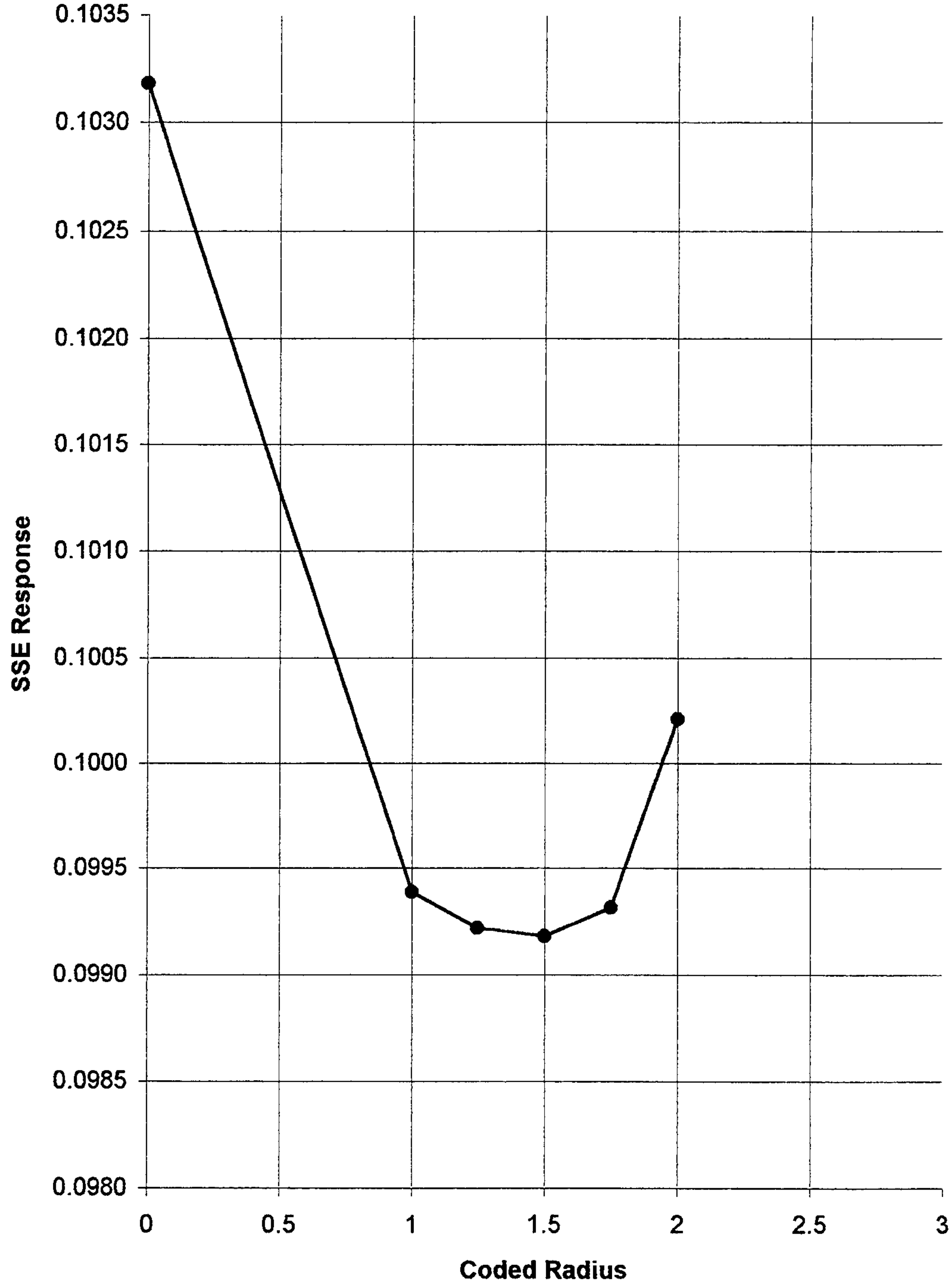
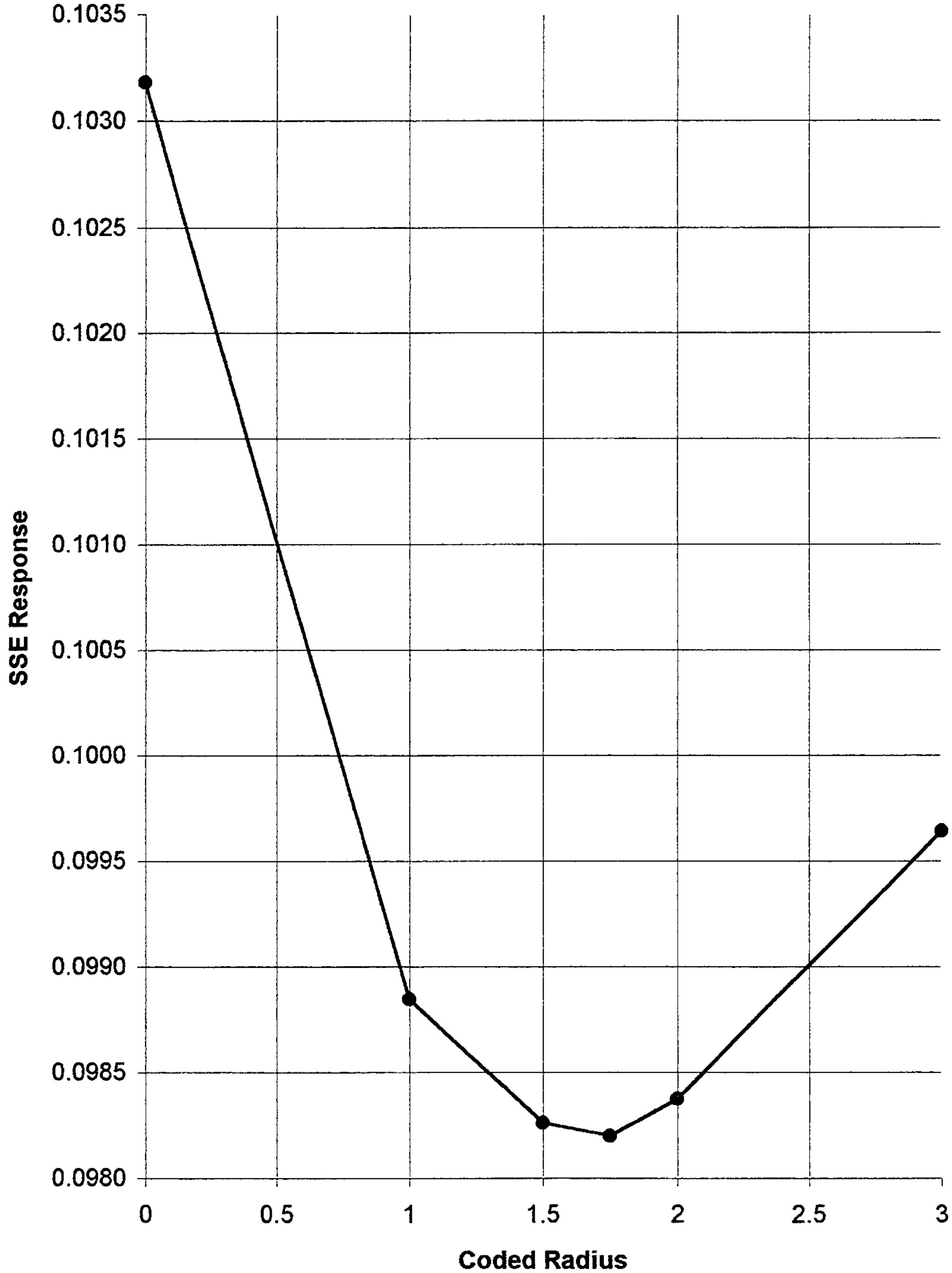


Figure 4.11 CCD C Minimum Ridge Analysis



Summary and Calibration Precision

Figure 4.12 presents the lowest SSE responses observed from (1) the Plackett-Burman screening experiment; (2) each gradient search for each of the four first-order models; (3) the ridge analysis of the second-order model, CCD C. This figure demonstrates the improvement in the calibration of the SUTRA model with each new designed set of experiments. Table 4.10 summarizes the number of experimental runs expended to achieve the various levels of calibration. As discussed earlier, Design A intentionally was not set at the best response observed in the screening design. Selecting the center of the screening design, with its correspondingly higher SSE, provided a greater opportunity to evaluate the appropriateness of both the SSE response and the RSM technique for calibrating a groundwater flow model. Depending on the level of precision desired, the calibration effort could have required as little as 12 runs or as many as 146.

Table 4.10 Number of Experimental Runs

Experimental Design	Number of Runs
Screening Design:	
Plackett-Burman Design	12
First-Order Designs:	
Design A	16
Gradient Search	12
Design B	16
Gradient Search	30
Design C	16
Gradient Search	9
Design D	16
Gradient Search	5
Second-Order Design:	
CCD C	8
Min. Ridge Run	6
TOTAL RUNS	146

Figure 4.13 plots the best computed hydraulic heads (based on the minimum ridge run 1.75 units away from CCD C) versus the calibration target set of heads that were being matched. The data plot along a 45° line, indicating the excellent calibration of the SUTRA model. Table 4.11 lists other measures of the error between the best SUTRA run and the calibration target set, indicating the close match achieved.

Table 4.11 Measures of Calibration Precision

Measure of Error	Value (units)
Sum of Squared Error (SSE)	0.09819 m^2
Root Mean Squared Error (RMS)	0.01369 m
Mean Absolute Error (MAE)	0.00698 m
Mean Error (ME)	0.00148 m
Maximum AE	0.07573 m
Median AE	0.00197 m
Minimum AE	0.00000 m

Figures 4.14 and 4.15 plot the error between the heads computed at the 524 nodes and the horizontal and vertical positions of the nodes. These plots show the errors are symmetrically distributed over almost all of the nodes, indicating the SUTRA model has been evenly calibrated, without concentrating its errors in any particular area of the aquifer. By empirically testing the SUTRA model and systematically evaluating the response surface using the response surface methodology, a finely calibrated groundwater model was achieved.

Although the RSM technique produced a very well calibrated model, the final values of the hydraulic conductivities found do not match the values used in the Smith-Ritzi model very closely. Table 4.12 compares the settings of the parameters used in the

Smith-Ritzi model with the values used to produce the calibrated model of this thesis. Recall that as a result of the screening experiment, only the hydraulic conductivities of Units 2, 6, 9, and 10 were adjusted using RSM. The remaining parameters were fixed at notional values. The differences between the target and calibrated parameter settings illustrate the nonuniqueness property typical of many inverse problems. However, the goal of this investigation was to calibrate a groundwater model so that its computed hydraulic heads closely matched the calibration target data set, not necessarily the true parameters of the groundwater model. Clearly, the RSM technique has located a local optimum on the SSE surface that results in a finely calibrated groundwater model without having matched the parameters used in the calibration target data set.

Table 4.12 Parameter Settings: Smith-Ritzi Model vs Calibrated Model

SUTRA Groundwater Model Parameter	Value in Smith-Ritzi Model	Value in Calibrated Model
Porosity	11%	10%
Hydraulic Conductivity Unit 1	2.000×10^{-3} m/min	5.000×10^{-3} m/min
Hydraulic Conductivity Unit 2	1.000×10^{-3} m/min	9.843×10^{-3} m/min
Hydraulic Conductivity Unit 3	1.000×10^{-4} m/min	5.000×10^{-3} m/min
Hydraulic Conductivity Unit 4	3.000×10^{-5} m/min	5.000×10^{-3} m/min
Hydraulic Conductivity Unit 5	2.000×10^{-3} m/min	5.000×10^{-3} m/min
Hydraulic Conductivity Unit 6	3.000×10^{-4} m/min	1.009×10^{-1} m/min
Hydraulic Conductivity Unit 7	6.000×10^{-4} m/min	5.000×10^{-3} m/min
Hydraulic Conductivity Unit 8	6.000×10^{-6} m/min	5.000×10^{-3} m/min
Hydraulic Conductivity Unit 9	4.000×10^{-6} m/min	4.385×10^{-8} m/min
Hydraulic Conductivity Unit 10	1.000×10^{-5} m/min	1.400×10^{-7} m/min

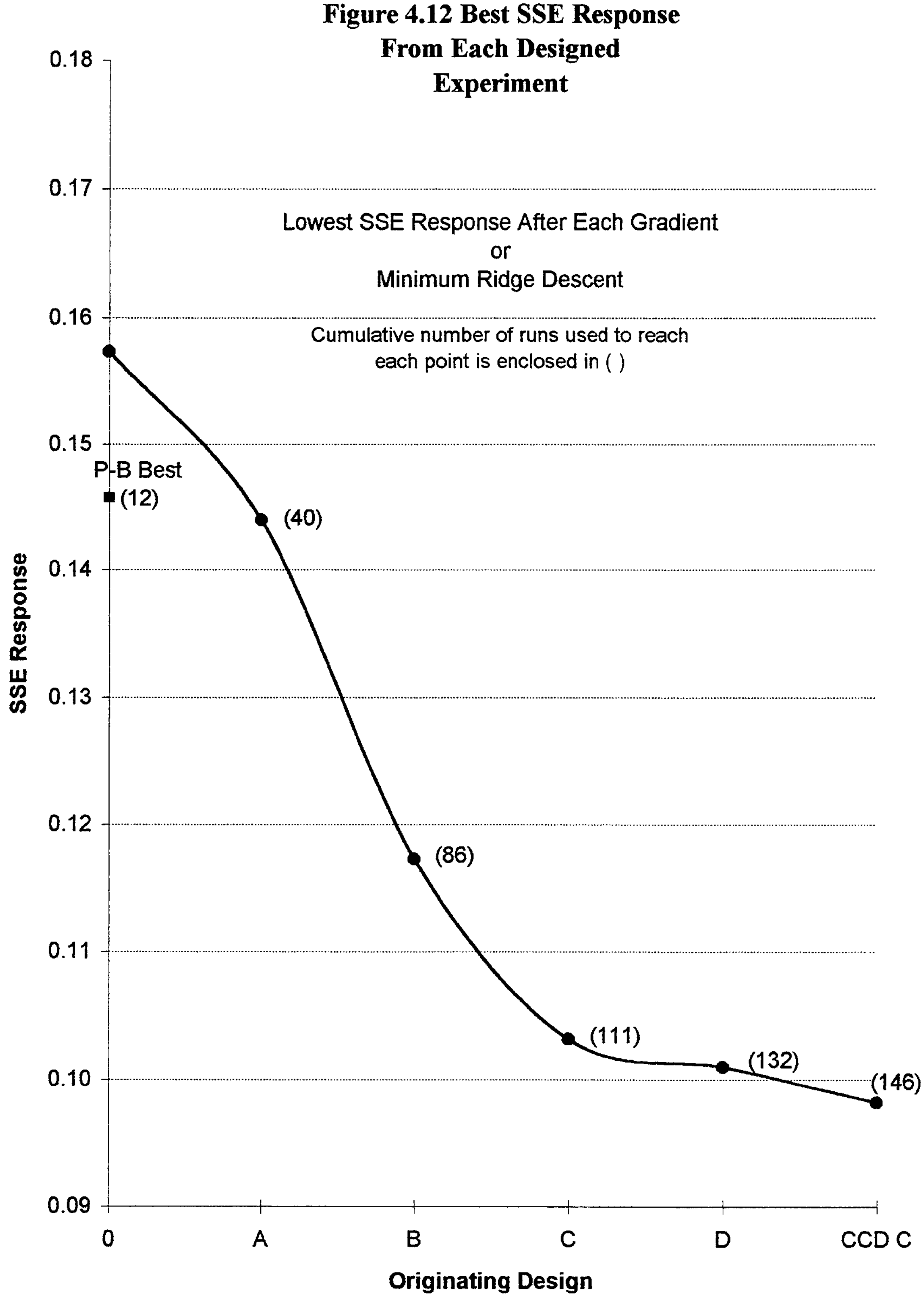


Figure 4.12 Best SSE Response
From Each Designed
Experiment
Lowest SSE Response After Each Gradient
or
Minimum Ridge Descent
Cumulative number of runs used to reach
each point is enclosed in ( )
P-B Best
(12)
(40)
(86)
(111)
(132)
(146)
SSE Response
0.18
0.17
0.16
0.15
0.14
0.13
0.12
0.11
0.10
0.09
0
A
B
C
D
CCD C
Originating Design

Figure 4.13 Computed vs Calibration Target Heads

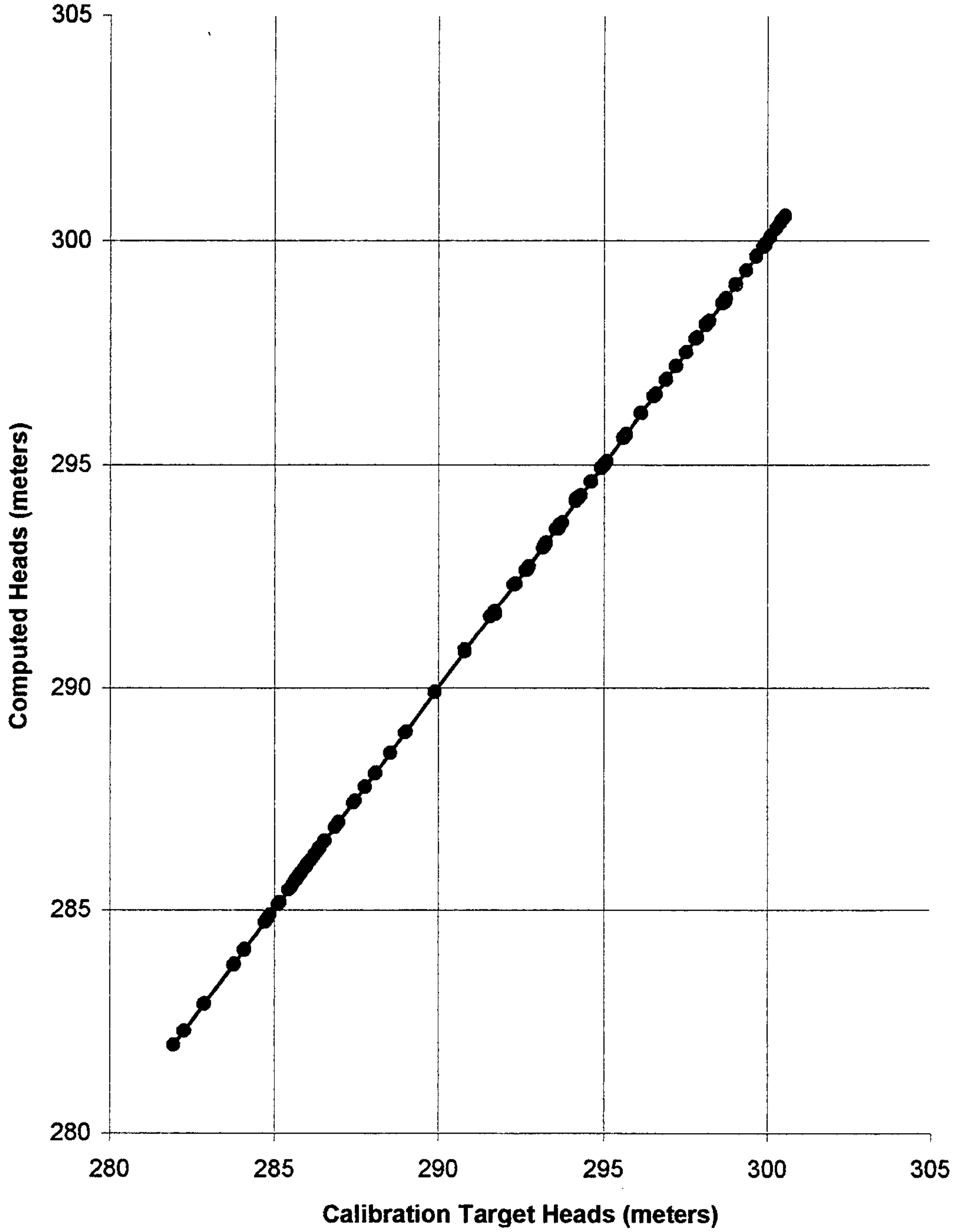


Figure 4.14 Error vs Horizontal Position

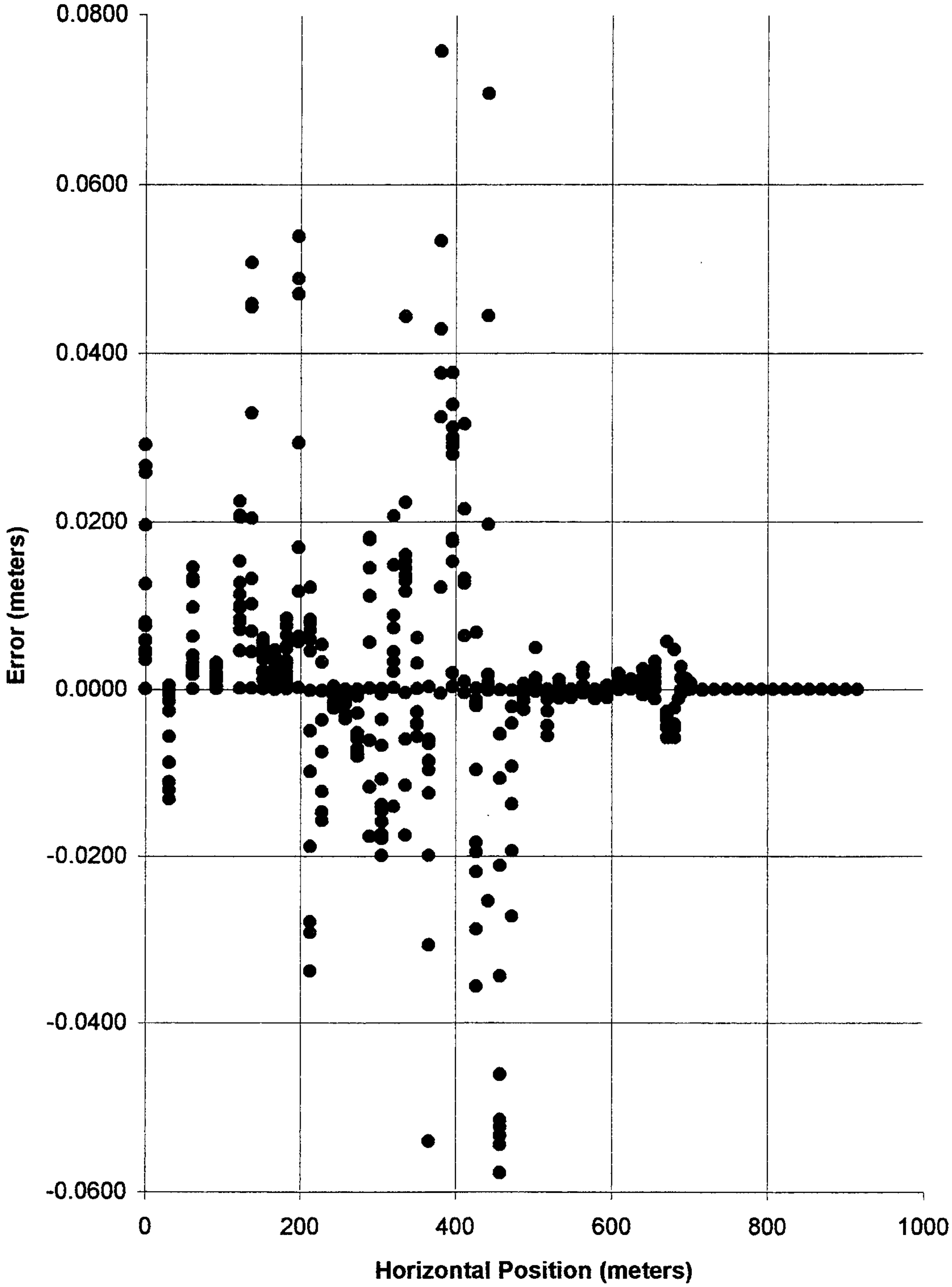
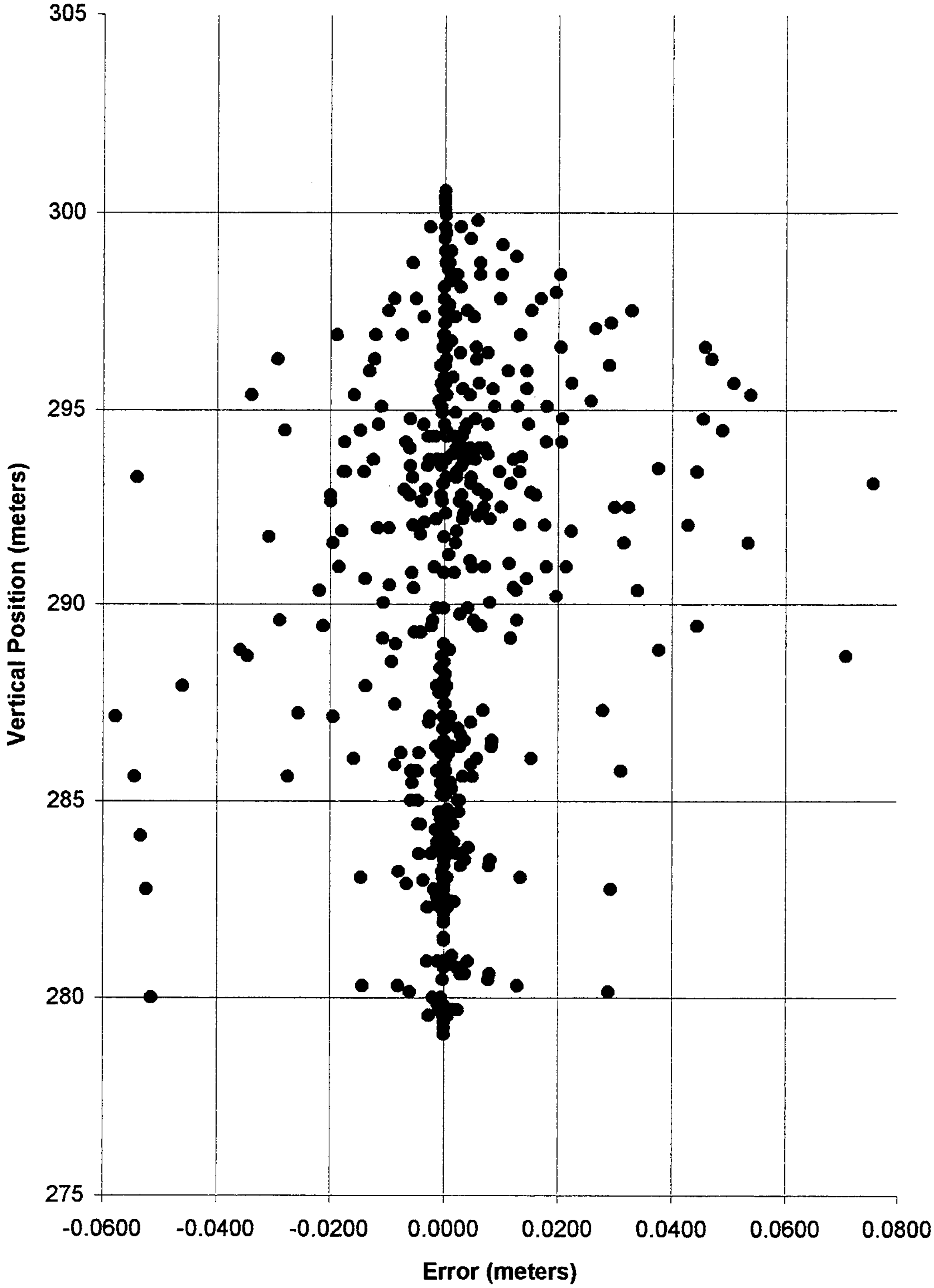


Figure 4.15 Error vs Vertical Position



V. Conclusions and Recommendations

Conclusions

Response surface methodology (RSM) can be used to estimate groundwater model flow parameters. RSM provides an efficient and effective process to determine those parameters which have a significant effect on the groundwater model. RSM also provides the systematic methods to adjust these parameters to quickly arrive at a calibrated model.

An existing two-dimensional, steady-state, saturated flow model was calibrated using RSM. A screening experiment, based upon a Plackett-Burman design, provided an efficient method to determine the most important groundwater model parameters to adjust. This screening experiment gave information that is usually obtained through sensitivity analysis in traditional calibration studies. By the use of the normal probability plot, a direct indication of the statistically significant parameters was made apparent. Once the significant parameters were determined, the calibration of the groundwater model was made by adjusting these chosen parameters.

Response surface methods provided an effective means to adjust the parameter values to calibrate the groundwater model to the calibration target data set. First-order models were exploited to rapidly adjust the parameters to produce a well calibrated finite-element model. A second-order model was applied to further calibrate the finite-element model even closer to the calibration target data set.

The SSE proved to be a suitable response for the RSM calibration technique. However, the fairly significant single degree of freedom tests for curvature indicated that the SSE response surface is at least quadratic, even at distances somewhat removed from a local optimum. Due to the quadratic properties exhibited by the SSE surface, the design regions for the first-order designs should be sufficiently "small" to ensure adequate first-order models. As an alternative measure, the root mean square (RMS) or square root of SSE would probably produce a "flatter" response surface. With a flatter response surface, the first-order designs may converge more efficiently and may preclude the need to develop any second-order models, at all.

This investigation was conducted with a minimum of assumptions regarding the initial values of the hydrogeologic parameters to use in the groundwater model. In this manner, RSM was being tested to see if its methods would calibrate a groundwater model in a realistic setting. The groundwater model calibrated with RSM may be used to estimate contaminate transport or evaluate flow patterns, now that the hydraulic heads are calibrated.

Response surface methods provide a systematic technique to model calibration versus manual trial-and-error methods. RSM enables the hydrologist to adjust all the parameters simultaneously to arrive at the calibration settings. By adjusting the parameters simultaneously, possible interaction effects of one parameter upon another are taken into account as they are mutually adjusted. Manual trial-and-error methods that only adjust one parameter at a time are likely to miss interaction effects (Montgomery, 1991:487).

RSM also provides a good alternative to the automated techniques that attempt to solve the inverse problem by deriving the shape of the response surface. RSM does not need any special computer code to explicitly derive the response surface. Using any readily available spreadsheet program, the local nature of the response surface may be elucidated through first-order linear models. Second-order models are handled most conveniently with the SAS statistical package, but may not be required since, in some cases, the groundwater model may be adequately calibrated using only first-order designs.

In summary, RSM has been demonstrated to be a viable method of calibrating groundwater flow models. Its methods can be readily applied in the calibration process to both choose the relevant parameters to adjust and to determine at what level they should be set to achieve a calibrated model.

Recommendations

The following are some recommendations for extending this research:

1. Investigate how well the calibration proceeds in a data-poor situation. Rather than using a calibration target data set of 524 nodes, a calibration target data set with about 12-18 observation points (wells), or less, would be more representative of a "typical" water well field (Carrera and Neuman, 1986c). Kriging techniques may also be investigated to enrich the limited data.

2. The initial starting values of the groundwater model's parameters will determine how closely the groundwater model may be calibrated to the calibration target data set. The inverse problem is solved using RSM to locate a local minimum. The influence of different starting values on the minimum actually found should be evaluated.

3. Instead of using the SSE response surface, a possibly "flatter" surface may be realized by using RMS or the square root of SSE. If this surface is flatter, first-order strategies may be exploited with even greater efficiency.

4. If the groundwater flow model is to be used in contaminant transport studies, it should be calibrated for solute transport, too. Joint optimization can be handled by RSM techniques and should be investigated for a groundwater modelling problem with simultaneous flow/transport calibration requirements.

Appendix A

Experimental Design Settings and Responses

This appendix contains the *Microsoft Excel* worksheets used to record the parameter settings for the experimental runs. The experimental settings and the responses for each run are listed for the Plackett-Burman, four first-order, and three second-order designs. Also included are the gradient or ridge analysis searches away from the designed regions.

	Plackett-Burman Design for N = 12, k = 11					Experimental Values					
Run	Unit 1	Unit 2	Unit 3	Unit 4	Unit 5	Unit 6	Unit 7	Unit 8	Unit 9	Unit 10	Porosity
1	1.0000E-02	1.0000E-07	1.0000E-02	1.0000E-07	1.0000E-07	1.0000E-07	1.0000E-02	1.0000E-02	1.0000E-02	1.0000E-07	20
2	1.0000E-02	1.0000E-02	1.0000E-07	1.0000E-02	1.0000E-07	1.0000E-07	1.0000E-07	1.0000E-02	1.0000E-02	1.0000E-02	1
3	1.0000E-07	1.0000E-02	1.0000E-02	1.0000E-07	1.0000E-02	1.0000E-07	1.0000E-07	1.0000E-07	1.0000E-02	1.0000E-02	20
4	1.0000E-02	1.0000E-07	1.0000E-02	1.0000E-02	1.0000E-07	1.0000E-02	1.0000E-07	1.0000E-07	1.0000E-07	1.0000E-02	20
5	1.0000E-02	1.0000E-02	1.0000E-07	1.0000E-02	1.0000E-02	1.0000E-07	1.0000E-02	1.0000E-07	1.0000E-07	1.0000E-07	20
6	1.0000E-02	1.0000E-02	1.0000E-02	1.0000E-07	1.0000E-02	1.0000E-02	1.0000E-07	1.0000E-02	1.0000E-07	1.0000E-07	1
7	1.0000E-07	1.0000E-02	1.0000E-02	1.0000E-02	1.0000E-07	1.0000E-02	1.0000E-02	1.0000E-07	1.0000E-02	1.0000E-07	1
8	1.0000E-07	1.0000E-07	1.0000E-02	1.0000E-02	1.0000E-02	1.0000E-07	1.0000E-02	1.0000E-02	1.0000E-07	1.0000E-02	1
9	1.0000E-07	1.0000E-07	1.0000E-07	1.0000E-02	1.0000E-02	1.0000E-02	1.0000E-07	1.0000E-02	1.0000E-02	1.0000E-07	20
10	1.0000E-02	1.0000E-07	1.0000E-07	1.0000E-07	1.0000E-02	1.0000E-02	1.0000E-02	1.0000E-07	1.0000E-02	1.0000E-02	1
11	1.0000E-07	1.0000E-02	1.0000E-07	1.0000E-07	1.0000E-07	1.0000E-02	1.0000E-02	1.0000E-02	1.0000E-07	1.0000E-02	20
12	1.0000E-07	1.0000E-07	1.0000E-07	1.0000E-07	1.0000E-07	1.0000E-07	1.0000E-07	1.0000E-07	1.0000E-07	1.0000E-07	1

	Plackett-Burman Design for N = 12, k Coded Factor Levels											Error Response Values			
Run	Unit 1	Unit 2	Unit 3	Unit 4	Unit 5	Unit 6	Unit 7	Unit 8	Unit 9	Unit 10	Porosity	SSE	RMS	MAE	ME
1	1	-1	1	-1	-1	-1	1	1	1	-1	1	4.7739E+03	3.0183E+00	1.6282E+00	1.5183E+00
2	1	1	-1	1	-1	-1	-1	1	1	1	-1	1.1882E+04	4.7619E+00	2.6381E+00	2.6370E+00
3	-1	1	1	-1	1	-1	-1	-1	1	1	1	1.0743E+04	4.5278E+00	2.6795E+00	2.6786E+00
4	1	-1	1	1	-1	1	-1	-1	-1	1	1	2.4863E+03	2.1783E+00	1.2155E+00	1.2015E+00
5	1	1	-1	1	1	-1	1	-1	-1	-1	1	3.8434E+03	2.7083E+00	1.3418E+00	1.3400E+00
6	1	1	1	-1	1	1	-1	1	-1	-1	-1	2.7384E+03	2.2860E+00	1.1894E+00	6.6944E-01
7	-1	1	1	1	-1	1	1	-1	1	-1	-1	6.0613E+03	3.4011E+00	1.8760E+00	1.7681E+00
8	-1	-1	1	1	1	-1	1	1	-1	1	-1	4.6626E+03	2.9830E+00	1.6999E+00	1.6947E+00
9	-1	-1	-1	1	1	1	-1	1	1	-1	1	5.6327E+03	3.2786E+00	2.1929E+00	1.1613E+00
10	1	-1	-1	-1	1	1	1	-1	1	1	-1	6.2091E+03	3.4423E+00	1.7554E+00	1.7527E+00
11	-1	1	-1	-1	-1	1	1	1	-1	1	1	4.4964E+03	2.9293E+00	1.6617E+00	1.6566E+00
12	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	1.4596E-01	1.6690E-02	9.1907E-03	6.8513E-04

	Design A						Experimental Values			
Run	Porosity	Unit 1	Unit 2	Unit 3	Unit 4	Unit 5	Unit 6	Unit 7	Unit 8	Unit 9	Unit 10
1	10	5.0000E-03	1.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.0000E-04	5.0000E-03	5.0000E-03	1.0000E-06	1.0000E-06
2	10	5.0000E-03	9.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.0000E-04	5.0000E-03	5.0000E-03	1.0000E-06	1.0000E-06
3	10	5.0000E-03	1.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	9.0000E-04	5.0000E-03	5.0000E-03	1.0000E-06	1.0000E-06
4	10	5.0000E-03	9.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	9.0000E-04	5.0000E-03	5.0000E-03	1.0000E-06	1.0000E-06
5	10	5.0000E-03	1.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.0000E-04	5.0000E-03	5.0000E-03	9.0000E-06	1.0000E-06
6	10	5.0000E-03	9.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.0000E-04	5.0000E-03	5.0000E-03	9.0000E-06	1.0000E-06
7	10	5.0000E-03	1.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	9.0000E-04	5.0000E-03	5.0000E-03	9.0000E-06	1.0000E-06
8	10	5.0000E-03	9.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	9.0000E-04	5.0000E-03	5.0000E-03	9.0000E-06	1.0000E-06
9	10	5.0000E-03	1.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.0000E-04	5.0000E-03	5.0000E-03	1.0000E-06	9.0000E-06
10	10	5.0000E-03	9.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.0000E-04	5.0000E-03	5.0000E-03	1.0000E-06	9.0000E-06
11	10	5.0000E-03	1.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	9.0000E-04	5.0000E-03	5.0000E-03	1.0000E-06	9.0000E-06
12	10	5.0000E-03	9.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	9.0000E-04	5.0000E-03	5.0000E-03	1.0000E-06	9.0000E-06
13	10	5.0000E-03	1.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.0000E-04	5.0000E-03	5.0000E-03	9.0000E-06	9.0000E-06
14	10	5.0000E-03	9.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.0000E-04	5.0000E-03	5.0000E-03	9.0000E-06	9.0000E-06
15	10	5.0000E-03	1.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	9.0000E-04	5.0000E-03	5.0000E-03	9.0000E-06	9.0000E-06
16	10	5.0000E-03	9.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	9.0000E-04	5.0000E-03	5.0000E-03	9.0000E-06	9.0000E-06
Center	10	5.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	5.0000E-04	5.0000E-03	5.0000E-03	5.0000E-06	5.0000E-06

	Coded Values				Design A		Responses	
Run	Unit 2	Unit 6	Unit 9	Unit 10	SSE	RMS	MAE	ME
1	-1	-1	-1	-1	2.3518E-01	2.1185E-02	1.0419E-02	2.2981E-03
2	1	-1	-1	-1	2.3295E-01	2.1085E-02	1.0176E-02	1.3501E-03
3	-1	1	-1	-1	1.4443E-01	1.6602E-02	7.5482E-03	3.9894E-05
4	1	1	-1	-1	1.5838E-01	1.7385E-02	8.4279E-03	-1.0993E-03
5	-1	-1	1	-1	2.5514E-01	2.2066E-02	1.1489E-02	1.5230E-03
6	1	-1	1	-1	2.5286E-01	2.1967E-02	1.1246E-02	5.7360E-04
7	-1	1	1	-1	1.6407E-01	1.7695E-02	8.6050E-03	-7.4127E-04
8	1	1	1	-1	1.7799E-01	1.8430E-02	9.4854E-03	-1.8821E-03
9	-1	-1	-1	1	2.3506E-01	2.1180E-02	1.0410E-02	2.3851E-03
10	1	-1	-1	1	2.3283E-01	2.1079E-02	1.0168E-02	1.4372E-03
11	-1	1	-1	1	1.4431E-01	1.6595E-02	7.5391E-03	1.2685E-04
12	1	1	-1	1	1.5825E-01	1.7379E-02	8.4189E-03	-1.0124E-03
13	-1	-1	1	1	2.3542E-01	2.1196E-02	1.0424E-02	2.3067E-03
14	1	-1	1	1	2.3314E-01	2.1093E-02	1.0181E-02	1.3573E-03
15	-1	1	1	1	1.4436E-01	1.6598E-02	7.5415E-03	4.2457E-05
16	1	1	1	1	1.5828E-01	1.7380E-02	8.4218E-03	-1.0984E-03
Center	0	0	0	0	1.5732E-01	1.7327E-02	7.5808E-03	-7.7721E-04

Steepest Descent Along Gradient Defined by Design A

Coded Conditions:

X2	X6	X9	X10	Unit Vector Lengths	SSE Response
0	0	0	0	0	1.5732E-01
-6.9341E-02	9.8349E-01	-1.1857E-01	1.1779E-01	1	1.5524E-01
-1.3868E-01	1.9670E+00	-2.3713E-01	2.3559E-01	2	1.5371E-01
-2.7736E-01	3.9340E+00	-4.7427E-01	4.7118E-01	4	1.5107E-01
-4.1604E-01	5.9010E+00	-7.1140E-01	7.0677E-01	6	1.4900E-01
-5.5473E-01	7.8679E+00	-9.4853E-01	9.4236E-01	8	1.4742E-01
-6.9341E-01	9.8349E+00	-1.1857E+00	1.1779E+00	10	1.4671E-01
-8.3209E-01	1.1802E+01	-1.4228E+00	1.4135E+00	12	1.4520E-01
-9.0143E-01	1.2785E+01	-1.5414E+00	1.5313E+00	13	1.4435E-01
-9.7077E-01	1.3769E+01	-1.6599E+00	1.6491E+00	14	1.4394E-01
-1.0401E+00	1.4752E+01	-1.7785E+00	1.7669E+00	15	1.4505E-01
-1.1095E+00	1.5736E+01	-1.8971E+00	1.8847E+00	16	1.5263E-01

Unit Vector	Experimental Settings										
Lengths	Porosity	Unit 1	Unit 2	Unit 3	Unit 4	Unit 5	Unit 6	Unit 7	Unit 8	Unit 9	Unit 10
0	10	5.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	5.0000E-03	5.0000E-04	5.0000E-03	5.0000E-03	5.0000E-06	5.0000E-06
1	10	5.0000E-03	4.7226E-03	5.0000E-03	5.0000E-03	5.0000E-03	8.9340E-04	5.0000E-03	5.0000E-03	4.5257E-06	5.4712E-06
2	10	5.0000E-03	4.4453E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.2868E-03	5.0000E-03	5.0000E-03	4.0515E-06	5.9424E-06
4	10	5.0000E-03	3.8905E-03	5.0000E-03	5.0000E-03	5.0000E-03	2.0736E-03	5.0000E-03	5.0000E-03	3.1029E-06	6.8847E-06
6	10	5.0000E-03	3.3358E-03	5.0000E-03	5.0000E-03	5.0000E-03	2.8604E-03	5.0000E-03	5.0000E-03	2.1544E-06	7.8271E-06
8	10	5.0000E-03	2.7811E-03	5.0000E-03	5.0000E-03	5.0000E-03	3.6472E-03	5.0000E-03	5.0000E-03	1.2059E-06	8.7694E-06
10	10	5.0000E-03	2.2264E-03	5.0000E-03	5.0000E-03	5.0000E-03	4.4340E-03	5.0000E-03	5.0000E-03	2.5733E-07	9.7118E-06
12	10	5.0000E-03	1.6716E-03	5.0000E-03	5.0000E-03	5.0000E-03	5.2208E-03	5.0000E-03	5.0000E-03	1.0000E-07	1.0654E-05
13	10	5.0000E-03	1.3943E-03	5.0000E-03	5.0000E-03	5.0000E-03	5.6142E-03	5.0000E-03	5.0000E-03	1.0000E-07	1.1125E-05
14	10	5.0000E-03	1.1169E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.0076E-03	5.0000E-03	5.0000E-03	1.0000E-07	1.1597E-05
15	10	5.0000E-03	8.3955E-04	5.0000E-03	5.0000E-03	5.0000E-03	6.4010E-03	5.0000E-03	5.0000E-03	1.0000E-07	1.2068E-05
16	10	5.0000E-03	5.6219E-04	5.0000E-03	5.0000E-03	5.0000E-03	6.7944E-03	5.0000E-03	5.0000E-03	1.0000E-07	1.2539E-05

	Design B (Centered on Run AIE14)						Experimental Values				
Run	Porosity	Unit 1	Unit 2	Unit 3	Unit 4	Unit 5	Unit 6	Unit 7	Unit 8	Unit 9	Unit 10
1	10	5.0000E-03	5.5845E-04	5.0000E-03	5.0000E-03	5.0000E-03	3.0038E-03	5.0000E-03	5.0000E-03	5.0000E-08	5.7985E-06
2	10	5.0000E-03	1.6754E-03	5.0000E-03	5.0000E-03	5.0000E-03	3.0038E-03	5.0000E-03	5.0000E-03	5.0000E-08	5.7985E-06
3	10	5.0000E-03	5.5845E-04	5.0000E-03	5.0000E-03	5.0000E-03	9.0114E-03	5.0000E-03	5.0000E-03	5.0000E-08	5.7985E-06
4	10	5.0000E-03	1.6754E-03	5.0000E-03	5.0000E-03	5.0000E-03	9.0114E-03	5.0000E-03	5.0000E-03	5.0000E-08	5.7985E-06
5	10	5.0000E-03	5.5845E-04	5.0000E-03	5.0000E-03	5.0000E-03	3.0038E-03	5.0000E-03	5.0000E-03	1.5000E-07	5.7985E-06
6	10	5.0000E-03	1.6754E-03	5.0000E-03	5.0000E-03	5.0000E-03	3.0038E-03	5.0000E-03	5.0000E-03	1.5000E-07	5.7985E-06
7	10	5.0000E-03	5.5845E-04	5.0000E-03	5.0000E-03	5.0000E-03	9.0114E-03	5.0000E-03	5.0000E-03	1.5000E-07	5.7985E-06
8	10	5.0000E-03	1.6754E-03	5.0000E-03	5.0000E-03	5.0000E-03	9.0114E-03	5.0000E-03	5.0000E-03	1.5000E-07	5.7985E-06
9	10	5.0000E-03	5.5845E-04	5.0000E-03	5.0000E-03	5.0000E-03	3.0038E-03	5.0000E-03	5.0000E-03	5.0000E-08	1.7396E-05
10	10	5.0000E-03	1.6754E-03	5.0000E-03	5.0000E-03	5.0000E-03	3.0038E-03	5.0000E-03	5.0000E-03	5.0000E-08	1.7396E-05
11	10	5.0000E-03	5.5845E-04	5.0000E-03	5.0000E-03	5.0000E-03	9.0114E-03	5.0000E-03	5.0000E-03	5.0000E-08	1.7396E-05
12	10	5.0000E-03	1.6754E-03	5.0000E-03	5.0000E-03	5.0000E-03	9.0114E-03	5.0000E-03	5.0000E-03	5.0000E-08	1.7396E-05
13	10	5.0000E-03	5.5845E-04	5.0000E-03	5.0000E-03	5.0000E-03	3.0038E-03	5.0000E-03	5.0000E-03	1.5000E-07	1.7396E-05
14	10	5.0000E-03	1.6754E-03	5.0000E-03	5.0000E-03	5.0000E-03	3.0038E-03	5.0000E-03	5.0000E-03	1.5000E-07	1.7396E-05
15	10	5.0000E-03	5.5845E-04	5.0000E-03	5.0000E-03	5.0000E-03	9.0114E-03	5.0000E-03	5.0000E-03	1.5000E-07	1.7396E-05
16	10	5.0000E-03	1.6754E-03	5.0000E-03	5.0000E-03	5.0000E-03	9.0114E-03	5.0000E-03	5.0000E-03	1.5000E-07	1.7396E-05

	Coded Values				Design B		Responses	
Run	Unit 2	Unit 6	Unit 9	Unit 10	SSE	RMS	MAE	ME
1	-1	-1	-1	-1	1.5153E-01	1.7005E-02	7.6775E-03	1.2498E-03
2	1	-1	-1	-1	1.4703E-01	1.6751E-02	8.8063E-03	-5.5351E-04
3	-1	1	-1	-1	1.5296E-01	1.7085E-02	7.7394E-03	1.7358E-03
4	1	1	-1	-1	1.4167E-01	1.6443E-02	8.7544E-03	-2.9114E-04
5	-1	-1	1	-1	1.5108E-01	1.6980E-02	7.6327E-03	1.2588E-03
6	1	-1	1	-1	1.4658E-01	1.6725E-02	8.7614E-03	-5.4448E-04
7	-1	1	1	-1	1.5251E-01	1.7060E-02	7.6945E-03	1.7449E-03
8	1	1	1	-1	1.4121E-01	1.6416E-02	8.7094E-03	-2.8194E-04
9	-1	-1	-1	1	1.5172E-01	1.7016E-02	7.6928E-03	1.2433E-03
10	1	-1	-1	1	1.4722E-01	1.6762E-02	8.8216E-03	-5.6009E-04
11	-1	1	-1	1	1.5315E-01	1.7096E-02	7.7547E-03	1.7290E-03
12	1	1	-1	1	1.4186E-01	1.6454E-02	8.7698E-03	-2.9790E-04
13	-1	-1	1	1	1.5153E-01	1.7005E-02	7.6764E-03	1.2470E-03
14	1	-1	1	1	1.4703E-01	1.6751E-02	8.8051E-03	-5.5636E-04
15	-1	1	1	1	1.5296E-01	1.7085E-02	7.7381E-03	1.7327E-03
16	1	1	1	1	1.4167E-01	1.6443E-02	8.7531E-03	-2.9405E-04
Center	0	0	0	0	1.4394E-01	1.6574E-02	8.4871E-03	7.3498E-05

Steepest Descent Along Gradient Defined by Design B (Part 1 of 2)					
Coded Conditions:				**Unit Vector**	**SSE**
X2	X6	X9	X10	**Lengths**	**Response**
0	0	0	0	0	0.14394
9.6886E-01	2.4126E-01	3.9417E-02	-3.9417E-02	1	0.14384
1.9377E+00	4.8251E-01	7.8834E-02	-7.8834E-02	2	0.14409
3.8754E+00	9.6502E-01	1.5767E-01	-1.5767E-01	4	0.14398
5.8132E+00	1.4475E+00	2.3650E-01	-2.3650E-01	6	0.14326
7.7509E+00	1.9300E+00	3.1534E-01	-3.1534E-01	8	0.14221
9.6886E+00	2.4126E+00	3.9417E-01	-3.9417E-01	10	0.14102
1.1626E+01	2.8951E+00	4.7300E-01	-4.7300E-01	12	0.13977
1.3564E+01	3.3776E+00	5.5184E-01	-5.5184E-01	14	0.13848
1.5502E+01	3.8601E+00	6.3067E-01	-6.3067E-01	16	0.13717
1.7439E+01	4.3426E+00	7.0950E-01	-7.0950E-01	18	0.13589
1.9377E+01	4.8251E+00	7.8834E-01	-7.8834E-01	20	0.13462
2.4221E+01	6.0314E+00	9.8542E-01	-9.8542E-01	25	0.13156
2.9066E+01	7.2377E+00	1.1825E+00	-1.1825E+00	30	0.12868
3.1003E+01	7.7202E+00	1.2613E+00	-1.2613E+00	32	0.12760
3.2941E+01	8.2027E+00	1.3402E+00	-1.3402E+00	34	0.12653
3.4879E+01	8.6852E+00	1.4190E+00	-1.4190E+00	36	0.12550
4.8443E+01	1.2063E+01	1.9708E+00	-1.9708E+00	50	0.11994
6.7820E+01	1.6888E+01	2.7592E+00	-2.7592E+00	70	0.11785
7.2664E+01	1.8094E+01	2.9563E+00	-2.9563E+00	75	0.11747
7.5571E+01	1.8818E+01	3.0745E+00	-3.0745E+00	78	0.11736
7.6540E+01	1.9059E+01	3.1139E+00	-3.1139E+00	79	0.11733
7.7509E+01	1.9300E+01	3.1534E+00	-3.1534E+00	80	0.11730
7.8478E+01	1.9542E+01	3.1928E+00	-3.1928E+00	81	0.11731
7.9446E+01	1.9783E+01	3.2322E+00	-3.2322E+00	82	0.11730
8.2353E+01	2.0507E+01	3.3504E+00	-3.3504E+00	85	0.11734
8.5260E+01	2.1231E+01	3.4687E+00	-3.4687E+00	88	0.11745
8.7197E+01	2.1713E+01	3.5475E+00	-3.5475E+00	90	0.11756
9.2042E+01	2.2919E+01	3.7446E+00	-3.7446E+00	95	0.11797
1.1626E+02	2.8951E+01	4.7300E+00	-4.7300E+00	120	0.12260

Steepest Descent Along Gradient Defined by Design B (Part 2 of 2)											
Unit Vector	Experimental Settings										
Lengths	Porosity	Unit 1	Unit 2	Unit 3	Unit 4	Unit 5	Unit 6	Unit 7	Unit 8	Unit 9	Unit 10
0	10	5.0000E-03	1.1169E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.0076E-03	5.0000E-03	5.0000E-03	1.0000E-07	1.1597E-05
1	10	5.0000E-03	1.6580E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.7323E-03	5.0000E-03	5.0000E-03	1.0197E-07	1.1368E-05
2	10	5.0000E-03	2.1990E-03	5.0000E-03	5.0000E-03	5.0000E-03	7.4570E-03	5.0000E-03	5.0000E-03	1.0394E-07	1.1140E-05
4	10	5.0000E-03	3.2811E-03	5.0000E-03	5.0000E-03	5.0000E-03	8.9063E-03	5.0000E-03	5.0000E-03	1.0788E-07	1.0683E-05
6	10	5.0000E-03	4.3633E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.0356E-02	5.0000E-03	5.0000E-03	1.1183E-07	1.0226E-05
8	10	5.0000E-03	5.4454E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.1805E-02	5.0000E-03	5.0000E-03	1.1577E-07	9.7685E-06
10	10	5.0000E-03	6.5275E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.3254E-02	5.0000E-03	5.0000E-03	1.1971E-07	9.3114E-06
12	10	5.0000E-03	7.6096E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.4704E-02	5.0000E-03	5.0000E-03	1.2365E-07	8.8543E-06
14	10	5.0000E-03	8.6917E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.6153E-02	5.0000E-03	5.0000E-03	1.2759E-07	8.3972E-06
16	10	5.0000E-03	9.7739E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.7603E-02	5.0000E-03	5.0000E-03	1.3153E-07	7.9401E-06
18	10	5.0000E-03	1.0856E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.9052E-02	5.0000E-03	5.0000E-03	1.3548E-07	7.4829E-06
20	10	5.0000E-03	1.1938E-02	5.0000E-03	5.0000E-03	5.0000E-03	2.0501E-02	5.0000E-03	5.0000E-03	1.3942E-07	7.0258E-06
25	10	5.0000E-03	1.4643E-02	5.0000E-03	5.0000E-03	5.0000E-03	2.4125E-02	5.0000E-03	5.0000E-03	1.4927E-07	5.8830E-06
30	10	5.0000E-03	1.7349E-02	5.0000E-03	5.0000E-03	5.0000E-03	2.7748E-02	5.0000E-03	5.0000E-03	1.5913E-07	4.7402E-06
32	10	5.0000E-03	1.8431E-02	5.0000E-03	5.0000E-03	5.0000E-03	2.9198E-02	5.0000E-03	5.0000E-03	1.6307E-07	4.2831E-06
34	10	5.0000E-03	1.9513E-02	5.0000E-03	5.0000E-03	5.0000E-03	3.0647E-02	5.0000E-03	5.0000E-03	1.6701E-07	3.8260E-06
36	10	5.0000E-03	2.0595E-02	5.0000E-03	5.0000E-03	5.0000E-03	3.2096E-02	5.0000E-03	5.0000E-03	1.7095E-07	3.3689E-06
50	10	5.0000E-03	2.8170E-02	5.0000E-03	5.0000E-03	5.0000E-03	4.2242E-02	5.0000E-03	5.0000E-03	1.9854E-07	1.6904E-07
70	10	5.0000E-03	3.8991E-02	5.0000E-03	5.0000E-03	5.0000E-03	5.6736E-02	5.0000E-03	5.0000E-03	2.3796E-07	-4.4021E-06
75	10	5.0000E-03	4.1696E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.0359E-02	5.0000E-03	5.0000E-03	2.4781E-07	-5.5449E-06
78	10	5.0000E-03	4.3320E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2533E-02	5.0000E-03	5.0000E-03	2.5373E-07	-6.2306E-06
79	10	5.0000E-03	4.3861E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.3258E-02	5.0000E-03	5.0000E-03	2.5570E-07	-6.4592E-06
80	10	5.0000E-03	4.4402E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.3982E-02	5.0000E-03	5.0000E-03	2.5767E-07	-6.6877E-06
81	10	5.0000E-03	4.4943E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.4707E-02	5.0000E-03	5.0000E-03	2.5964E-07	-6.9163E-06
82	10	5.0000E-03	4.5484E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.5432E-02	5.0000E-03	5.0000E-03	2.6161E-07	-7.1448E-06
85	10	5.0000E-03	4.7107E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.7606E-02	5.0000E-03	5.0000E-03	2.6752E-07	-7.8305E-06
88	10	5.0000E-03	4.8730E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.9780E-02	5.0000E-03	5.0000E-03	2.7343E-07	-8.5162E-06
90	10	5.0000E-03	4.9812E-02	5.0000E-03	5.0000E-03	5.0000E-03	7.1229E-02	5.0000E-03	5.0000E-03	2.7738E-07	-8.9733E-06
95	10	5.0000E-03	5.2518E-02	5.0000E-03	5.0000E-03	5.0000E-03	7.4853E-02	5.0000E-03	5.0000E-03	2.8723E-07	-1.0116E-05
120	10	5.0000E-03	6.6044E-02	5.0000E-03	5.0000E-03	5.0000E-03	9.2970E-02	5.0000E-03	5.0000E-03	3.3650E-07	-1.5830E-05

	Design C (Centered on Run BE80)					Experimental Values					
Run	Porosity	Unit 1	Unit 2	Unit 3	Unit 4	Unit 5	Unit 6	Unit 7	Unit 8	Unit 9	Unit 10
1	10	5.0000E-03	2.2201E-02	5.0000E-03	5.0000E-03	5.0000E-03	3.1991E-02	5.0000E-03	5.0000E-03	1.2884E-07	5.0000E-08
2	10	5.0000E-03	6.6603E-02	5.0000E-03	5.0000E-03	5.0000E-03	3.1991E-02	5.0000E-03	5.0000E-03	1.2884E-07	5.0000E-08
3	10	5.0000E-03	2.2201E-02	5.0000E-03	5.0000E-03	5.0000E-03	9.5973E-02	5.0000E-03	5.0000E-03	1.2884E-07	5.0000E-08
4	10	5.0000E-03	6.6603E-02	5.0000E-03	5.0000E-03	5.0000E-03	9.5973E-02	5.0000E-03	5.0000E-03	1.2884E-07	5.0000E-08
5	10	5.0000E-03	2.2201E-02	5.0000E-03	5.0000E-03	5.0000E-03	3.1991E-02	5.0000E-03	5.0000E-03	3.8650E-07	5.0000E-08
6	10	5.0000E-03	6.6603E-02	5.0000E-03	5.0000E-03	5.0000E-03	3.1991E-02	5.0000E-03	5.0000E-03	3.8650E-07	5.0000E-08
7	10	5.0000E-03	2.2201E-02	5.0000E-03	5.0000E-03	5.0000E-03	9.5973E-02	5.0000E-03	5.0000E-03	3.8650E-07	5.0000E-08
8	10	5.0000E-03	6.6603E-02	5.0000E-03	5.0000E-03	5.0000E-03	9.5973E-02	5.0000E-03	5.0000E-03	3.8650E-07	5.0000E-08
9	10	5.0000E-03	2.2201E-02	5.0000E-03	5.0000E-03	5.0000E-03	3.1991E-02	5.0000E-03	5.0000E-03	1.2884E-07	1.5000E-07
10	10	5.0000E-03	6.6603E-02	5.0000E-03	5.0000E-03	5.0000E-03	3.1991E-02	5.0000E-03	5.0000E-03	1.2884E-07	1.5000E-07
11	10	5.0000E-03	2.2201E-02	5.0000E-03	5.0000E-03	5.0000E-03	9.5973E-02	5.0000E-03	5.0000E-03	1.2884E-07	1.5000E-07
12	10	5.0000E-03	6.6603E-02	5.0000E-03	5.0000E-03	5.0000E-03	9.5973E-02	5.0000E-03	5.0000E-03	1.2884E-07	1.5000E-07
13	10	5.0000E-03	2.2201E-02	5.0000E-03	5.0000E-03	5.0000E-03	3.1991E-02	5.0000E-03	5.0000E-03	3.8650E-07	1.5000E-07
14	10	5.0000E-03	6.6603E-02	5.0000E-03	5.0000E-03	5.0000E-03	3.1991E-02	5.0000E-03	5.0000E-03	3.8650E-07	1.5000E-07
15	10	5.0000E-03	2.2201E-02	5.0000E-03	5.0000E-03	5.0000E-03	9.5973E-02	5.0000E-03	5.0000E-03	3.8650E-07	1.5000E-07
16	10	5.0000E-03	6.6603E-02	5.0000E-03	5.0000E-03	5.0000E-03	9.5973E-02	5.0000E-03	5.0000E-03	3.8650E-07	1.5000E-07

	Coded Values				Design C		Responses	
Run	Unit 2	Unit 6	Unit 9	Unit 10	SSE	RMS	MAE	ME
1	-1	-1	-1	-1	0.12847	0.01566	0.00857	-0.00055
2	1	-1	-1	-1	0.13623	0.01612	0.00846	0.00016
3	-1	1	-1	-1	0.10540	0.01418	0.00752	0.00109
4	1	1	-1	-1	0.12118	0.01521	0.00836	0.00173
5	-1	-1	1	-1	0.14136	0.01643	0.00918	-0.00105
6	1	-1	1	-1	0.14912	0.01687	0.00908	-0.00033
7	-1	1	1	-1	0.11828	0.01502	0.00814	0.00059
8	1	1	1	-1	0.13406	0.01600	0.00898	0.00124
9	-1	-1	-1	1	0.12518	0.01546	0.00824	-0.00035
10	1	-1	-1	1	0.13294	0.01593	0.00814	0.00036
11	-1	1	-1	1	0.10211	0.01396	0.00720	0.00129
12	1	1	-1	1	0.11788	0.01500	0.00804	0.00193
13	-1	-1	1	1	0.12847	0.01566	0.00857	-0.00055
14	1	-1	1	1	0.13623	0.01612	0.00846	0.00016
15	-1	1	1	1	0.10540	0.01418	0.00752	0.00109
16	1	1	1	1	0.12117	0.01521	0.00836	0.00173
Center	0	0	0	0	0.11730	0.01496	0.00779	0.00059

Steepest Descent Along Gradient Defined by Design C

Coded Conditions:

X2	X6	X9	X10	Unit Vector Lengths	SSE Response
0	0	0	0	0.00	0.11730
-4.6779E-01	7.5788E-01	-3.2150E-01	3.2160E-01	1.00	0.10827
-8.1863E-01	1.3263E+00	-5.6262E-01	5.6280E-01	1.75	0.10448
-9.3558E-01	1.5158E+00	-6.4300E-01	6.4320E-01	2.00	0.10374
-1.0525E+00	1.7052E+00	-7.2337E-01	7.2360E-01	2.25	0.10331
-1.1695E+00	1.8947E+00	-8.0375E-01	8.0400E-01	2.50	0.10318
-1.2864E+00	2.0842E+00	-8.8412E-01	8.8440E-01	2.75	0.10346
-1.4034E+00	2.2736E+00	-9.6450E-01	9.6480E-01	3.00	0.10420
-1.8712E+00	3.0315E+00	-1.2860E+00	1.2864E+00	4.00	0.13780

Unit Vector	Experimental Settings										
Lengths	Porosity	Unit 1	Unit 2	Unit 3	Unit 4	Unit 5	Unit 6	Unit 7	Unit 8	Unit 9	Unit 10
0.00	10	5.0000E-03	4.4402E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.3982E-02	5.0000E-03	5.0000E-03	2.5767E-07	1.0000E-07
1.00	10	5.0000E-03	3.4017E-02	5.0000E-03	5.0000E-03	5.0000E-03	8.8227E-02	5.0000E-03	5.0000E-03	2.1625E-07	1.1608E-07
1.75	10	5.0000E-03	2.6228E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.0641E-01	5.0000E-03	5.0000E-03	1.8518E-07	1.2814E-07
2.00	10	5.0000E-03	2.3631E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.1247E-01	5.0000E-03	5.0000E-03	1.7483E-07	1.3216E-07
2.25	10	5.0000E-03	2.1035E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.1853E-01	5.0000E-03	5.0000E-03	1.6447E-07	1.3618E-07
2.50	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07
2.75	10	5.0000E-03	1.5842E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.3066E-01	5.0000E-03	5.0000E-03	1.4376E-07	1.4422E-07
3.00	10	5.0000E-03	1.3246E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.3672E-01	5.0000E-03	5.0000E-03	1.3340E-07	1.4824E-07
4.00	10	5.0000E-03	2.8605E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.6096E-01	5.0000E-03	5.0000E-03	9.1982E-08	1.6432E-07

	Design D (Centered on Run CE250) Experimental Values										
Run	Porosity	Unit 1	Unit 2	Unit 3	Unit 4	Unit 5	Unit 6	Unit 7	Unit 8	Unit 9	Unit 10
1	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	7.7060E-08	7.0100E-08
2	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	7.7060E-08	7.0100E-08
3	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	7.7060E-08	7.0100E-08
4	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	7.7060E-08	7.0100E-08
5	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	2.3118E-07	7.0100E-08
6	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	2.3118E-07	7.0100E-08
7	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	2.3118E-07	7.0100E-08
8	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	2.3118E-07	7.0100E-08
9	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	7.7060E-08	2.1030E-07
10	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	7.7060E-08	2.1030E-07
11	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	7.7060E-08	2.1030E-07
12	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	7.7060E-08	2.1030E-07
13	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	2.3118E-07	2.1030E-07
14	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	2.3118E-07	2.1030E-07
15	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	2.3118E-07	2.1030E-07
16	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	2.3118E-07	2.1030E-07

	Coded Values				Design D		Responses	
Run	Unit 2	Unit 6	Unit 9	Unit 10	SSE	RMS	MAE	ME
1	-1	-1	-1	-1	0.10526	0.01417	0.00727	0.00035
2	1	-1	-1	-1	0.11042	0.01452	0.00740	0.00047
3	-1	1	-1	-1	0.12640	0.01553	0.00876	0.00370
4	1	1	-1	-1	0.12812	0.01564	0.00867	0.00358
5	-1	-1	1	-1	0.10978	0.01447	0.00763	0.00011
6	1	-1	1	-1	0.11494	0.01481	0.00776	0.00022
7	-1	1	1	-1	0.13092	0.01581	0.00912	0.00346
8	1	1	1	-1	0.13263	0.01591	0.00903	0.00333
9	-1	-1	-1	1	0.10447	0.01412	0.00707	0.00044
10	1	-1	-1	1	0.10963	0.01446	0.00720	0.00056
11	-1	1	-1	1	0.12561	0.01548	0.00856	0.00379
12	1	1	-1	1	0.12732	0.01559	0.00847	0.00367
13	-1	-1	1	1	0.10526	0.01417	0.00727	0.00035
14	1	-1	1	1	0.11042	0.01452	0.00740	0.00047
15	-1	1	1	1	0.12640	0.01553	0.00876	0.00370
16	1	1	1	1	0.12812	0.01564	0.00867	0.00358
Center	0	0	0	0	0.10318	0.01403	0.00754	0.00196

Steepest Descent Along Gradient Defined by Design D

Coded Conditions:

X2	X6	X9	X10	Unit Vector Lengths	SSE Response
0	0	0	0	0	0.10318
-4.2811E-02	-2.4183E-01	-3.3066E-02	3.3066E-02	0.25	0.10125
-8.5622E-02	-4.8366E-01	-6.6131E-02	6.6131E-02	0.5	0.10099
-1.2843E-01	-7.2548E-01	-9.9197E-02	9.9197E-02	0.75	0.10269
-1.7124E-01	-9.6731E-01	-1.3226E-01	1.3226E-01	1	0.10657
-3.4249E-01	-1.9346E+00	-2.6453E-01	2.6453E-01	2	0.15199

Unit Vector	Experimental Settings										
Lengths	Porosity	Unit 1	Unit 2	Unit 3	Unit 4	Unit 5	Unit 6	Unit 7	Unit 8	Unit 9	Unit 10
0	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07
0.25	10	5.0000E-03	1.8044E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.0953E-01	5.0000E-03	5.0000E-03	1.5157E-07	1.4252E-07
0.5	10	5.0000E-03	1.7650E-02	5.0000E-03	5.0000E-03	5.0000E-03	9.4468E-02	5.0000E-03	5.0000E-03	1.4902E-07	1.4484E-07
0.75	10	5.0000E-03	1.7255E-02	5.0000E-03	5.0000E-03	5.0000E-03	7.9402E-02	5.0000E-03	5.0000E-03	1.4648E-07	1.4715E-07
1	10	5.0000E-03	1.6860E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.4337E-02	5.0000E-03	5.0000E-03	1.4393E-07	1.4947E-07
2	10	5.0000E-03	1.5281E-02	5.0000E-03	5.0000E-03	5.0000E-03	4.0732E-03	5.0000E-03	5.0000E-03	1.3374E-07	1.5874E-07

	CCD A			Second Order Design		(Centered on Run CE250)			Experimental Values		
Run	Porosity	Unit 1	Unit 2	Unit 3	Unit 4	Unit 5	Unit 6	Unit 7	Unit 8	Unit 9	Unit 10
1	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	7.7060E-08	7.0100E-08
2	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	7.7060E-08	7.0100E-08
3	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	7.7060E-08	7.0100E-08
4	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	7.7060E-08	7.0100E-08
5	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	2.3118E-07	7.0100E-08
6	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	2.3118E-07	7.0100E-08
7	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	2.3118E-07	7.0100E-08
8	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	2.3118E-07	7.0100E-08
9	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	7.7060E-08	2.1030E-07
10	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	7.7060E-08	2.1030E-07
11	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	7.7060E-08	2.1030E-07
12	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	7.7060E-08	2.1030E-07
13	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	2.3118E-07	2.1030E-07
14	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	2.3118E-07	2.1030E-07
15	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	2.3118E-07	2.1030E-07
16	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	2.3118E-07	2.1030E-07
17	10	5.0000E-03	3.6786E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07
18	10	5.0000E-03	9.2195E-05	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07
19	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	2.4858E-01	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07
20	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-04	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07
21	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	3.0747E-07	1.4020E-07
22	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	7.7060E-10	1.4020E-07
23	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	2.7970E-07
24	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	7.0100E-10
Center	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07

Note: Alpha set at +/- 1.99 for values of axial points.

CCD A	Coded Values				Second Order Design Responses			
Run	Unit 2	Unit 6	Unit 9	Unit 10	SSE	RMS	MAE	ME
1	-1	-1	-1	-1	0.10526	0.01417	0.00727	0.00035
2	1	-1	-1	-1	0.11042	0.01452	0.00740	0.00047
3	-1	1	-1	-1	0.12640	0.01553	0.00876	0.00370
4	1	1	-1	-1	0.12812	0.01564	0.00867	0.00358
5	-1	-1	1	-1	0.10978	0.01447	0.00763	0.00011
6	1	-1	1	-1	0.11494	0.01481	0.00776	0.00022
7	-1	1	1	-1	0.13092	0.01581	0.00912	0.00346
8	1	1	1	-1	0.13263	0.01591	0.00903	0.00333
9	-1	-1	-1	1	0.10447	0.01412	0.00707	0.00044
10	1	-1	-1	1	0.10963	0.01446	0.00720	0.00056
11	-1	1	-1	1	0.12561	0.01548	0.00856	0.00379
12	1	1	-1	1	0.12732	0.01559	0.00847	0.00367
13	-1	-1	1	1	0.10526	0.01417	0.00727	0.00035
14	1	-1	1	1	0.11042	0.01452	0.00740	0.00047
15	-1	1	1	1	0.12640	0.01553	0.00876	0.00370
16	1	1	1	1	0.12812	0.01564	0.00867	0.00358
17	1.99	0	0	0	0.10993	0.01448	0.00786	0.00216
18	-1.99	0	0	0	3.90270	0.08630	0.04552	0.04153
19	0	1.99	0	0	0.16437	0.01771	0.01037	0.00506
20	0	-1.99	0	0	0.16081	0.01752	0.00811	-0.00086
21	0	0	1.99	0	0.10528	0.01418	0.00775	0.00183
22	0	0	-1.99	0	0.10448	0.01412	0.00771	0.00203
23	0	0	0	1.99	0.10246	0.01398	0.00739	0.00202
24	0	0	0	-1.99	1.95840	0.06114	0.02106	-0.01065
Center	0	0	0	0	0.10318	0.01403	0.00754	0.00196

Responses Along Path Defined by SAS Minimum Ridge Analysis From CCD A

Coded Conditions:				Unit Vector	SSE
X2	X6	X9	X10	**Lengths**	**Response**
0.447696	0.027984	0.001023	0.741526	Crit. Val.	0.10440
0	0	0	0	0	0.10318
0.324585	-0.176188	-0.083301	0.326594	0.5	0.10241
0.32693	-0.217684	-0.858399	0.329972	1	0.10177
0.326992	-0.219043	-1.139736	0.329544	1.25	0.10171
0.327028	-0.219844	-1.409406	0.329083	1.5	0.10174
0.327069	-0.220768	-1.933034	0.328128	2	0.10312

Note: Alpha set at +/- 1.99 for values of axial points.

Unit Vector	Experimental Settings										
Lengths	Porosity	Unit 1	Unit 2	Unit 3	Unit 4	Unit 5	Unit 6	Unit 7	Unit 8	Unit 9	Unit 10
Crit. Val.	10	5.0000E-03	2.2567E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2634E-01	5.0000E-03	5.0000E-03	1.5420E-07	1.9218E-07
0	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07
0.5	10	5.0000E-03	2.1432E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.1362E-01	5.0000E-03	5.0000E-03	1.4770E-07	1.6309E-07
1	10	5.0000E-03	2.1453E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.1104E-01	5.0000E-03	5.0000E-03	8.7972E-08	1.6333E-07
1.25	10	5.0000E-03	2.1454E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.1095E-01	5.0000E-03	5.0000E-03	6.6292E-08	1.6330E-07
1.5	10	5.0000E-03	2.1454E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.1090E-01	5.0000E-03	5.0000E-03	4.5511E-08	1.6327E-07
2	10	5.0000E-03	2.1454E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.1085E-01	5.0000E-03	5.0000E-03	5.1604E-09	1.6320E-07

	CCD B			Second Order Design	(Centered on Run CE250)				Experimental Values		
Run	Porosity	Unit 1	Unit 2	Unit 3	Unit 4	Unit 5	Unit 6	Unit 7	Unit 8	Unit 9	Unit 10
1	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	7.7060E-08	7.0100E-08
2	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	7.7060E-08	7.0100E-08
3	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	7.7060E-08	7.0100E-08
4	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	7.7060E-08	7.0100E-08
5	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	2.3118E-07	7.0100E-08
6	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	2.3118E-07	7.0100E-08
7	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	2.3118E-07	7.0100E-08
8	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	2.3118E-07	7.0100E-08
9	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	7.7060E-08	2.1030E-07
10	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	7.7060E-08	2.1030E-07
11	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	7.7060E-08	2.1030E-07
12	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	7.7060E-08	2.1030E-07
13	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	2.3118E-07	2.1030E-07
14	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	2.3118E-07	2.1030E-07
15	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	2.3118E-07	2.1030E-07
16	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	2.3118E-07	2.1030E-07
17	10	5.0000E-03	3.2268E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07
18	10	5.0000E-03	4.6098E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07
19	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	2.1805E-01	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07
20	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	3.1150E-02	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07
21	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	2.6971E-07	1.4020E-07
22	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	3.8530E-08	1.4020E-07
23	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	2.4535E-07
24	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	3.5050E-08
Center	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07

Note: Alpha set at +/- 1.50 for values of axial points.

CCD B	Coded Values				Second Order Design Responses			
Run	Unit 2	Unit 6	Unit 9	Unit 10	SSE	RMS	MAE	ME
1	-1	-1	-1	-1	0.10526	0.01417	0.00727	0.00035
2	1	-1	-1	-1	0.11042	0.01452	0.00740	0.00047
3	-1	1	-1	-1	0.12640	0.01553	0.00876	0.00370
4	1	1	-1	-1	0.12812	0.01564	0.00867	0.00358
5	-1	-1	1	-1	0.10978	0.01447	0.00763	0.00011
6	1	-1	1	-1	0.11494	0.01481	0.00776	0.00022
7	-1	1	1	-1	0.13092	0.01581	0.00912	0.00346
8	1	1	1	-1	0.13263	0.01591	0.00903	0.00333
9	-1	-1	-1	1	0.10447	0.01412	0.00707	0.00044
10	1	-1	-1	1	0.10963	0.01446	0.00720	0.00056
11	-1	1	-1	1	0.12561	0.01548	0.00856	0.00379
12	1	1	-1	1	0.12732	0.01559	0.00847	0.00367
13	-1	-1	1	1	0.10526	0.01417	0.00727	0.00035
14	1	-1	1	1	0.11042	0.01452	0.00740	0.00047
15	-1	1	1	1	0.12640	0.01553	0.00876	0.00370
16	1	1	1	1	0.12812	0.01564	0.00867	0.00358
17	1.5	0	0	0	0.10814	0.01437	0.00778	0.00210
18	-1.5	0	0	0	0.10591	0.01422	0.00769	0.00249
19	0	1.5	0	0	0.14303	0.01652	0.00945	0.00430
20	0	-1.5	0	0	0.12554	0.01548	0.00833	-0.00045
21	0	0	1.5	0	0.10473	0.01414	0.00771	0.00186
22	0	0	-1.5	0	0.10243	0.01398	0.00738	0.00205
23	0	0	0	1.5	0.10253	0.01399	0.00742	0.00201
24	0	0	0	-1.5	0.11028	0.01451	0.00803	0.00160
Center	0	0	0	0	0.10318	0.01403	0.00754	0.00196

Responses Along Path Defined by SAS Minimum Ridge Analysis From CCD B

Coded Conditions:				**Unit Vector**	**SSE**
X2	X6	X9	X10	**Lengths**	**Response**
-0.972655	-0.371359	0.042003	1.239791	Crit. Val.	0.09837
0	0	0	0	0	0.10318
-0.416969	-0.3233	-0.818966	0.22563	1	0.09939
-0.445523	-0.327221	-1.108932	0.164941	1.25	0.09922
-0.462312	-0.329385	-1.385229	0.094413	1.50	0.09918
-0.473412	-0.330763	-1.651839	0.020098	1.75	0.09931
-0.481345	-0.331724	-1.911841	-0.055939	2	0.10021

Note: Alpha set at +/- 1.50 for values of axial points.

Unit Vector	Experimental Settings										
Lengths	Porosity	Unit 1	Unit 2	Unit 3	Unit 4	Unit 5	Unit 6	Unit 7	Unit 8	Unit 9	Unit 10
Crit. Val.	10	5.0000E-03	9.4716E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.0146E-01	5.0000E-03	5.0000E-03	1.5736E-07	2.2711E-07
0	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07
1	10	5.0000E-03	1.4595E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.0446E-01	5.0000E-03	5.0000E-03	9.1010E-08	1.5602E-07
1.25	10	5.0000E-03	1.4332E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.0421E-01	5.0000E-03	5.0000E-03	6.8666E-08	1.5176E-07
1.50	10	5.0000E-03	1.4177E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.0408E-01	5.0000E-03	5.0000E-03	4.7374E-08	1.4682E-07
1.75	10	5.0000E-03	1.4074E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.0399E-01	5.0000E-03	5.0000E-03	2.6829E-08	1.4161E-07
2	10	5.0000E-03	1.4001E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.0393E-01	5.0000E-03	5.0000E-03	6.7935E-09	1.3628E-07

	CCD C			Second Order Design (Centered on Run CE250)					Experimental Values		
Run	Porosity	Unit 1	Unit 2	Unit 3	Unit 4	Unit 5	Unit 6	Unit 7	Unit 8	Unit 9	Unit 10
1	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	7.7060E-08	7.0100E-08
2	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	7.7060E-08	7.0100E-08
3	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	7.7060E-08	7.0100E-08
4	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	7.7060E-08	7.0100E-08
5	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	2.3118E-07	7.0100E-08
6	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	2.3118E-07	7.0100E-08
7	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	2.3118E-07	7.0100E-08
8	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	2.3118E-07	7.0100E-08
9	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	7.7060E-08	2.1030E-07
10	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	7.7060E-08	2.1030E-07
11	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	7.7060E-08	2.1030E-07
12	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	7.7060E-08	2.1030E-07
13	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	2.3118E-07	2.1030E-07
14	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	2.3118E-07	2.1030E-07
15	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	2.3118E-07	2.1030E-07
16	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	2.3118E-07	2.1030E-07
17	10	5.0000E-03	2.7658E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07
18	10	5.0000E-03	9.2195E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07
19	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.8690E-01	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07
20	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	6.2300E-02	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07
21	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	2.3118E-07	1.4020E-07
22	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	7.7060E-08	1.4020E-07
23	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	2.1030E-07
24	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	7.0100E-08
Center	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07

Note: Alpha set at +/- 1.00 for values of axial points.

CCD C	Coded Values				Second Order Design Responses			
Run	Unit 2	Unit 6	Unit 9	Unit 10	SSE	RMS	MAE	ME
1	-1	-1	-1	-1	0.10526	0.01417	0.00727	0.00035
2	1	-1	-1	-1	0.11042	0.01452	0.00740	0.00047
3	-1	1	-1	-1	0.12640	0.01553	0.00876	0.00370
4	1	1	-1	-1	0.12812	0.01564	0.00867	0.00358
5	-1	-1	1	-1	0.10978	0.01447	0.00763	0.00011
6	1	-1	1	-1	0.11494	0.01481	0.00776	0.00022
7	-1	1	1	-1	0.13092	0.01581	0.00912	0.00346
8	1	1	1	-1	0.13263	0.01591	0.00903	0.00333
9	-1	-1	-1	1	0.10447	0.01412	0.00707	0.00044
10	1	-1	-1	1	0.10963	0.01446	0.00720	0.00056
11	-1	1	-1	1	0.12561	0.01548	0.00856	0.00379
12	1	1	-1	1	0.12732	0.01559	0.00847	0.00367
13	-1	-1	1	1	0.10526	0.01417	0.00727	0.00035
14	1	-1	1	1	0.11042	0.01452	0.00740	0.00047
15	-1	1	1	1	0.12640	0.01553	0.00876	0.00370
16	1	1	1	1	0.12812	0.01564	0.00867	0.00358
17	1	0	0	0	0.10638	0.01425	0.00769	0.00204
18	-1	0	0	0	0.10164	0.01393	0.00748	0.00205
19	0	1	0	0	0.12503	0.01545	0.00859	0.00353
20	0	-1	0	0	0.10795	0.01435	0.00736	0.00036
21	0	0	1	0	0.10418	0.01410	0.00766	0.00189
22	0	0	-1	0	0.10246	0.01398	0.00739	0.00202
23	0	0	0	1	0.10265	0.01400	0.00745	0.00200
24	0	0	0	-1	0.10529	0.01418	0.00775	0.00183
Center	0	0	0	0	0.10318	0.01403	0.00754	0.00196

Responses Along Path Defined by SAS Minimum Ridge Analysis From CCD C

Coded Conditions:

X2	X6	X9	X10	Unit Vector Lengths	SSE Response
0.447696	0.027984	0.001023	0.741526	Crit. Val.	0.10440
0	0	0	0	0	0.10318
-0.672027	-0.361629	-0.594383	0.2536	1	0.09885
-0.881486	-0.377838	-1.148	0.110979	1.5	0.09826
-0.932387	-0.381223	-1.431019	-0.002722	1.75	0.09820
-0.966109	-0.38338	-1.70426	-0.123091	2	0.09838
-1.03266	-0.387461	-2.722159	-0.611012	3	0.09964

Note: Alpha set at +/- 1.00 for values of axial points.

Unit Vector	Experimental Settings										
Lengths	Porosity	Unit 1	Unit 2	Unit 3	Unit 4	Unit 5	Unit 6	Unit 7	Unit 8	Unit 9	Unit 10
Crit. Val.	10	5.0000E-03	2.2567E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2634E-01	5.0000E-03	5.0000E-03	1.5420E-07	1.9218E-07
0	10	5.0000E-03	1.8439E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.2460E-01	5.0000E-03	5.0000E-03	1.5412E-07	1.4020E-07
1	10	5.0000E-03	1.2243E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.0207E-01	5.0000E-03	5.0000E-03	1.0832E-07	1.5798E-07
1.5	10	5.0000E-03	1.0312E-02	5.0000E-03	5.0000E-03	5.0000E-03	1.0106E-01	5.0000E-03	5.0000E-03	6.5655E-08	1.4798E-07
1.75	10	5.0000E-03	9.8429E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.0085E-01	5.0000E-03	5.0000E-03	4.3846E-08	1.4001E-07
2	10	5.0000E-03	9.5320E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.0072E-01	5.0000E-03	5.0000E-03	2.2790E-08	1.3157E-07
3	10	5.0000E-03	8.9184E-03	5.0000E-03	5.0000E-03	5.0000E-03	1.0046E-01	5.0000E-03	5.0000E-03	2.4430E-09	9.7368E-08

Appendix B

SUTRA FORTRAN Post-Processor File

This appendix contains the FORTRAN source code used to automatically compute the error statistics that measured the differences between the SUTRA output and the Smith-Ritzi calibration target data set. This code, named POST.FOR, was automatically called by the VAX command file in Appendix C to produce the SUTRA output report after each model execution.

```
      PROGRAM POST
C
C        THIS PROGRAM PERFORMS POST PROCESSING OF THE SUTRA OUTPUT
C        TO DETERMINE VARIOUS ERROR STATISTICS.
C
      DIMENSION HBASE(600),HNEW(600)
      REAL SSE,RMS,MAE,ME
      OPEN(8, FILE='HBASE.dat',STATUS='UNKNOWN',FORM='FORMATTED')
      OPEN(9, FILE='node83.dat',STATUS='UNKNOWN',FORM='FORMATTED')
      OPEN(10, FILE='input.dat',STATUS='UNKNOWN',FORM='FORMATTED')
      OPEN(11, FILE='final.rpt',STATUS='UNKNOWN',FORM='FORMATTED')
C
      WRITE(11,90) '**************************************************
     1******************'
      WRITE(11,90) ' '
      WRITE(11,90) '                 SSSS   UU  UU  TTTTTT  RRRRR    AA'
      WRITE(11,90) '                SS   S  UU  UU  T TT T  RR  RR  AAAA'
      WRITE(11,90) '                SSSS    UU  UU    TT    RRRRR  AA  AA'
      WRITE(11,90) '                   SS   UU  UU    TT    RR R   AAAAAA'
      WRITE(11,90) '                SS  SS  UU  UU    TT    RR RR  AA  AA'
      WRITE(11,90) '                 SSSS    UUUU     TT    RR  RR AA  AA'
      WRITE(11,90) ' '
      WRITE(11,90) '**************************************************
     1******************'
      WRITE(11,90) ' '
      WRITE(11,90) '                   SUBSURFACE FLOW SIMULATION MODEL'
      WRITE(11,90) ' '
      WRITE(11,90) 'Output report for R. M. Cotman''s MS thesis.  Error
     1measurements are'
      WRITE(11,90) 'compared to the steady state heads presented in R. J
     1. Smith''s thesis.'
      WRITE(11,90) ' '
      WRITE(11,90) '--------------------------------------------------
     1------------------'
      WRITE(11,90) '                              INPUT'
      WRITE(11,90) '--------------------------------------------------
     1------------------'
      WRITE(11,90) ' '
      WRITE(11,90) 'Input SUTRA data file:  filename.D5'
   90    FORMAT(1X,A)
      WRITE(11,90) ' '

         READ(10,*) ITEMP
         WRITE(11,110) ITEMP
  110    FORMAT(1X,'Porosity (Percent): ',I3)
         WRITE(11,90) ' '
      DO 30 I=1,10
         READ(10,*)TEMP
         WRITE(11,100)I,TEMP
 100     FORMAT(1X,'Hydraulic conductivity for Unit',I3,' (m/min): ',E10
     1.4)
         WRITE(11,90) ' '
  30     CONTINUE
      DO 10 I=1,524
         READ(8,*)X,Y,HBASE(I)
         READ(9,*)X,Y,HNEW(I)
 10   CONTINUE
```

```
C
      WRITE(11,90) ' '
      WRITE(11,90) '--------------------------------------------------
     1----------------'
      WRITE(11,90) '                                        OUTPUT'
      WRITE(11,90) '--------------------------------------------------
     1----------------'
      WRITE(11,90) ' '
C     --------------- Sum of Squared Error (SSE) Computation -----------
      SSE=0.0
      DO 20 I=1,524
         SSE=SSE+(HBASE(I)-HNEW(I))**2
 20   CONTINUE
      WRITE(11,120)SSE
 120  FORMAT(1X,'Sum of Squared Error (SSE):    ',E15.5)
      WRITE(11,90) ' '
C     ------------ Root Mean Squared Error (RMS) Computation -----------
      RMS=0.0
      RMS=SQRT(SSE/524)
      WRITE(11,122)RMS
 122  FORMAT(1X,'Root Mean Squared Error (RMS):',E15.5)
      WRITE(11,90) ' '
C     -------------- Mean Absolute Error (MAE) Computation -------------
      MAE=0.0
      DO 40 I=1,524
         MAE=MAE+ABS(HBASE(I)-HNEW(I))
 40   CONTINUE
         MAE=MAE/524
      WRITE(11,124)MAE
 124  FORMAT(1X,'Mean Absolute Error (MAE):     ',E15.5)
      WRITE(11,90) ' '
C     -------------------- Mean Error (MAE) Computation ----------------
      ME=0.0
      DO 50 I=1,524
         ME=ME+(HBASE(I)-HNEW(I))
 50   CONTINUE
         ME=ME/524
      WRITE(11,126)ME
 126  FORMAT(1X,'Mean Error (ME):               ',E15.5)
      WRITE(11,90) ' '

      STOP
      END
```

Appendix C

VAX Command File

This appendix contains the VAX command file used to simplify the execution of the SUTRA model. The command file, named SUTRA.COM, served as an interactive interface to the SUTRA program. To invoke the command file, the user simply entered "@SUTRA" at the VAX command prompt. Upon execution, the command file would prompt the user for the porosity value and the settings of the ten hydraulic conductivities. Once these parameters were entered, the SUTRA input parameter file was automatically created, the SUTRA program was executed, and the error statistics were computed using the POST.FOR program contained in Appendix B, which also created an output report. This output report was saved as a file in the current directory and displayed to the screen for immediate review. A sample output report is presented as the last page of this appendix. It presents the results from the run using the parameters which produced the minimum *SSE* response.

```
$write sys$output "**************************************"
$write sys$output "* SUTRA Interactive Data Input Program *"
$write sys$output "*   For Capt R. Cotman's MS Thesis     *"
$write sys$output "* Answer every question in the units   *"
$write sys$output "* shown in the ( ), using the format   *"
$write sys$output "* shown by the [ ].                    *"
$write sys$output "**************************************"
$inquire p1  "Filename of the input file you're creating [No
extension]:"
$input_file = p1
$inquire p1  "Value for Porosity (percent) [xx]"
$porosity    = p1
$cnt = 0
$      open /write file unit.tmp
$      open /write file1 input.dat
$      write file "$edit template.d5"
$      write file "^Z"
$      write file "sub/po/''porosity'/w"
$      write file1 "''porosity'"
$loop:
$cnt = cnt + 1
$inquire p1  "Hydraulic Conductivity for unit''cnt' (m/min)  [x.xxxxE-
xx]"
$if p1 .eqs. "" then goto finish
$string  = p1
$      write file1 "''string'"
$      write file "sub/     unit''cnt'/''string'/w"
$if cnt .eqs. 10 then write file "sub/    unit''cnt'/''string'/w"
$if cnt .eqs. 10 then write file1 "''string'"
$if cnt .eqs. 10 then goto finish
$goto loop
$finish:
$        write file "exit"
$close file
$close file1
$@unit.tmp
$rename template.d5 'input_file.D5
$      open /write file unit.tmp
$      write file "$edit sutemp.fil"
$      write file "^Z"
$      write file "sub/INPUT/''input_file'/w"
$      write file "exit"
$close file
$@unit.tmp
$rename sutemp.fil SUTRA.FIL
$cls
$cls
$write sys$output "Please wait about 15 seconds, while"
$write sys$output "the SUTRA model runs."
$run main
$run post
$      open /write file final.tmp
$      write file "$edit final.rpt"
$      write file "^Z"
$      write file "sub/filename/''input_file'/w"
$      write file "exit"
```

```
$close file
$@final.tmp
$rename final.rpt 'input_file.RPT
$del/noconfirm input.dat;*
$del/noconfirm unit.tmp;*
$del/noconfirm final.rpt;*
$del/noconfirm final.tmp;*
$pu sutra.fil
$ty 'input_file.RPT
$write sys$output "You're SUTRA model has run.  The "
$write sys$output "output report is in the file named:"
$write sys$output "''input_file'.RPT"
$exit
```

```
**********************************************************************

              SSSS    UU   UU   TTTTTT   RRRRR      AA
             SS    S  UU   UU   T TT T   RR   RR   AAAA
             SSSS     UU   UU     TT     RRRRR    AA  AA
                 SS   UU   UU     TT     RR R     AAAAAA
             SS   SS  UU   UU     TT     RR RR    AA  AA
              SSSS     UUUU       TT     RR   RR  AA  AA

**********************************************************************
```

SUBSURFACE FLOW SIMULATION MODEL

Output report for R. M. Cotman's MS thesis. Error measurements are compared to the steady state heads presented in R. J. Smith's thesis.

INPUT

Input SUTRA data file: VB175.D5

Porosity (Percent): 10

Hydraulic conductivity for Unit 1 (m/min): 0.5000E-02

Hydraulic conductivity for Unit 2 (m/min): 0.9843E-02

Hydraulic conductivity for Unit 3 (m/min): 0.5000E-02

Hydraulic conductivity for Unit 4 (m/min): 0.5000E-02

Hydraulic conductivity for Unit 5 (m/min): 0.5000E-02

Hydraulic conductivity for Unit 6 (m/min): 0.1009E+00

Hydraulic conductivity for Unit 7 (m/min): 0.5000E-02

Hydraulic conductivity for Unit 8 (m/min): 0.5000E-02

Hydraulic conductivity for Unit 9 (m/min): 0.4385E-07

Hydraulic conductivity for Unit 10 (m/min): 0.1400E-06

OUTPUT

Sum of Squared Error (SSE): 0.98201E-01

Root Mean Squared Error (RMS): 0.13690E-01

Mean Absolute Error (MAE): 0.69783E-02

Mean Error (ME): 0.14810E-02

Bibliography

Back, W., J. S. Rosenshein, and P. R. Seaber, eds. (1988). *Hydrogeology.* Geological Society of America, The Geology of North America, vol. O-2, Boulder: CO.

Bellman, R. and Kabala, R. (1965). *Quasilinearization and nonlinear boundary-value problems.* New York, NY: Elsevier.

Box, G. E. P. and Draper, N. R. (1987). *Empirical Model-Building and Response Surfaces.* New York, NY: John Wiley & Sons.

Carrera, J. and Neuman, S. P. (1986a). Estimation of aquifer parameters under transient and steady state conditions: 1. Maximum likelihood method incorporating prior information. *Water Resour. Res.,* **22,** 199-210.

Carrera, J. and Neuman, S. P. (1986b). Estimation of aquifer parameters under transient and steady state conditions: 2. Uniqueness, stability, and solution algorithms. *Water Resour. Res.,* **22,** 211-227.

Carrera, J. and Neuman, S. P. (1986c). Estimation of aquifer parameters under transient and steady state conditions: 3. Application to synthetic and field data. *Water Resour. Res.,* **22**, 228-242.

Carrera, J. (1987). State of the art of the inverse problem applied to the flow and solute transport equations. In *Groundwater Flow and Quality Modelling, Proc. NATO Advanced Research Workshop on Advances in Analytical and Numerical Groundwater Flow and Quality Modelling, 1987, Lisbon,* eds. E. Custodio, A. Gurgui and J.P. Lobo Ferreira, 549-583. Boston, MA: Reidel.

Chavent, G., Dupuy, M. and Lemonnier, P. (1975). History matching by use of optimal control theory. *Soc. Pet. Eng. J.*, **15**, 74-86.

Chen, W. H., Gavalas, G. R., Seinfeld, J. H. and Wasserman, M. L. (1974). A new algorithm for automatic historic matching. *Soc. Pet. Eng. J.*, **14**, 593-608.

Cornell, J. A. (1990). *How to Apply Response Surface Methodology.* Milwaukee, WI: American Society for Quality Control.

Deinenger, R. A. (1969). Linear programming for hydrologic analyses. *Water Resour. Res.,* **5**, 1105-1109.

DiStefano, N. and Rath, A. (1975). An identification approach to subsurface hydrological systems. *Water Resour. Res.*, **11**, 1005-1012.

Doughty, C., Long, J. C. S., Hestir, K. and Benson S. M. (1994) Hydrologic characterization of heterogeneous geologic media with an inverse method based on iterated function systems. *Water Resour. Res.*, **30**, 1721-1745.

Emsellem, Y. and de Marsily, G. (1971). An automatic solution for the inverse problem. *Water Resour. Res.*, **7**, 1264-1283.

Frind, E. O. and Pinder, G. F. (1973). Galerkin solution of the inverse problem for aquifer transmissivity. *Water Resour. Res.*, **9**, 1397-1410.

Hefez, E., Shamir, V. and Bear, J. (1975). Identifying the parameters of an aquifer cell model. *Water Resour. Res.*, **11**, 993-1004.

Kitanidis, P. K. and Vomvoris, E. G. (1983). A geostatistical approach to the inverse problem in groundwater modeling (steady state) and one-dimensional simulations. *Water Resour. Res.*, **19**, 677-690.

Kleinecke, D. (1971). Use of linear programming for estimating geohydrologic parameters of groundwater basins. *Water Resour. Res.*, **8**, 367-375.

Lin, A. C. and Yeh, W. W-G. (1974). Identification of parameters in an inhomogeneous aquifer by use of the maximum principle of optimal control and quasilinearization. *Water Resour. Res.*, **10**, 829-838.

McLaughlin, D. B. (1975). *Investigation of alternative procedures for estimating groundwater basin parameters.* report prepared for the Office of Water Research and Technology, U.S. Dep. Int., Water Resour. Eng., Walnut Creek, CA.

Montgomery, D. C. (1991). *Introduction To Statistical Quality Control.* New York, NY: John Wiley & Sons.

Navarro, A. (1977). A modified optimization method of estimating aquifer parameters. *Water Resour Res.*, **13**, 935-939.

Nelson, R. W. (1968). In-place determination of permeability distribution for heterogeneous porous media through analysis of energy dissipation. *Soc. Pet. Eng. J.*, **8**, 33-42.

Neuman, S. P. (1973). Calibration of distributed parameter groundwater flow models viewed as a multiple-objective decision process under uncertainty. *Water Resour. Res.*, **9**, 1006-1021.

Nutbrown, D. A. (1975). Identification of parameters in a linear equation of groundwater flow. *Water Resour. Res.*, **11**, 581-588.

Sagar, B., Yakowitz, S. and Duckstein, L. (1975). A direct method for the identification of the parameters of dynamic nonhomogeneous aquifers. *Water Resour. Res.*, **11**, 563-570.

Smith, R. T. (1991). *Use of Multilevel Slug Testing and Mass Transport Modeling to Evaluate Impacts of Heterogeneity on Nitrate Transport in Fractured Carbonate Rocks.* MS thesis. Wright State University, Dayton, OH.

Smith, R. T. and Ritzi, R. W., Jr. (1993). Designing a Nitrate Monitoring Program in a Heterogeneous, Carbonate Aquifer. *Ground Water,* **31,** 576-584.

Smith, L. and Wheatcraft, S. W. (1993). Groundwater Flow. In *Handbook of Hydrology,* ed. D. R. Maidment, 6.1-6.58. New York, NY: McGraw-Hill, Inc.

Sun, N.-Z. and Yeh, W. W-G. (1990). Coupled inverse problems in groundwater modeling 1. Sensitivity analysis and parameter identification. *Water Resour. Res.*, **26**, 2507-2525.

Vemuri, V. and Karplus, W. J. (1969). Identification of nonlinear parameters of groundwater basin by hybrid computation. *Water Resour. Res.*, **5**, 172-185.

Voss, Clifford I. (1984). *A Finite-Element Simulation Model for Saturated-Unsaturated Fluid-Density-Dependent Ground-Water-Flow with Energy Transport or Chemically-Reactive Single-Species Solute Transport.* USGS Water Resources Investigation Report 84-4369.

Wagner, B. J. (1992). Simultaneous parameter estimation and contaminant source characterization for coupled groundwater flow and contaminant transport modelling. *J. Hydrol.*, **135**, 275-303.

Walton, W. C. (1992). *Groundwater Modeling Utilities.* Chelsea, MI: Lewis Publishers, Inc.

Wilson, J., Kitanidis, P. and Dettinger, M. (1979). *State and parameter estimation in groundwater models.* paper presented at the Chapman Conference on Application of Kalman Filter to Hydrology, Hydraulics, and Water Resources, AGU, Pittsburgh, PA.

Xiang, Y., Sykes, J. F. and Thomson, N. R. (1992). A composite L1 parameter estimator for model fitting in groundwater flow and solute transport simulation. *Water Resour. Res.*, **29**, 1661-1673.

Yeh, W. W-G. (1986). Review of parameter identification procedures in groundwater hydrology: The inverse problem. *Water Resour. Res.*, **22**, 95-108.

Yeh, W. W-G. and Becker, L. (1973). Linear programming and channel flow identification. *J. Hydraul. Div. Am. Soc. Civ. Eng.*, **99**, 2013-2021.

Yeh, W. W-G. and Tauxe, G. W. (1971). Quasilinearization and the identification of aquifer parameters. *Water Resour. Res.*, **7**, 375-381.

Yeh, W. W-G., Yoon, Y. S. and Lee K. S. (1983). Aquifer parameter identification with kriging and optimum parameterization. *Water Resour. Res.*, **19**, 225-233.

Vita

Captain Richard M. Cotman was born on 16 April 1957 in Cleveland, Ohio. He was graduated from Euclid Senior High School in Euclid, Ohio in 1975 and attended Case Western Reserve University in Cleveland, Ohio, majoring in Earth Sciences (geology). He was graduated with a Bachelor of Science in May 1979 and a Master of Science in August 1979, both in Earth Sciences, through a joint BS/MS program. After graduation, he was a professional geologist and petrophysicist for the Standard Oil Production Company (SOHIO) in Houston, Texas. While at SOHIO, he performed reservoir modeling and statistical analyses to determine the potential productive extent of hydrocarbon reservoirs. In March 1987, he attended Officer's Training School and was commissioned in the USAF as a Second Lieutenant. His first tour of duty was at Griffiss AFB, New York where he served as a Weapons Maintenance Officer and the Wing Weapons Safety Officer. In 1991, he became the Chief of the Weapons Safety Branch at Headquarters Eighth Air Force at Barksdale AFB, Louisiana. While at Eighth Air Force he managed the explosives, missile, and nuclear surety programs for nine Air Force bases, and developed software to plan the safe storage of explosives. He entered the School of Engineering, Department of Operational Sciences, Air Force Institute of Technology (AFIT), in August 1993. His follow-on assignment after AFIT was to Headquarters, Human Systems Center, Brooks AFB, Texas.

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This thesis examined the use of response surface methodology (RSM) to estimate the parameters of a finite-element groundwater model. An existing two-dimensional, steady-state flow model of a fractured carbonate groundwater system in southwestern Ohio served as the calibration target data set. A Plackett-Burman screening design showed that only four of the ten hydraulic conductivity zones significantly contributed to the output of the finite-element model. Also, the effective porosity parameter did not significantly affect the model's output. Using only the four significant hydraulic conductivity parameters; four two-level, four-factor designed experiments were conducted to exploit the first-order response surface defined by a residual sum of squares function. Additionally, a central composite design and ridge analysis were used to adjust the four parameters and finally arrive at a calibrated model in a grand total of 146 runs. The final calibrated model, which had an average head elevation of 292 meters, matched the calibration target data set with a mean absolute error of only 7 mm over all 524 nodes of the model. RSM provided an effective calibration technique to estimate groundwater flow parameters.

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