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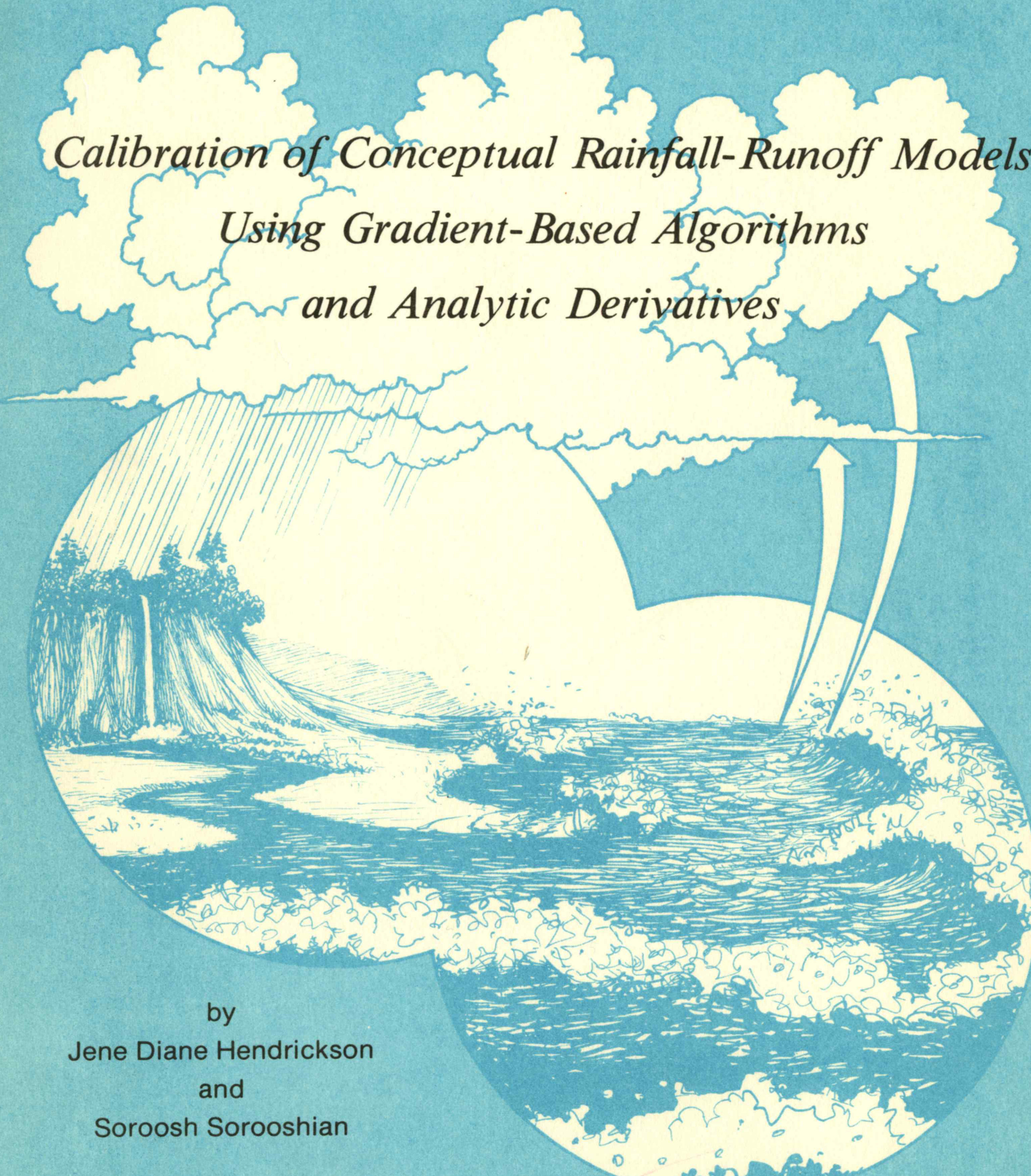
Calibration of Conceptual Rainfall-Runoff Models Using Gradient-Based Algorithms and Analytic Derivatives



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Research Project Report

on

CALIBRATION OF RAINFALL-RUNOFF MODELS USING GRADIENT-BASED ALGORITHMS AND ANALYTIC DERIVATIVES

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ABSTRACT

In the past, derivative-based optimization algorithms have not frequently been used to calibrate conceptual rainfall-runoff (CRR) models, partially due to difficulties associated with obtaining the required derivatives. This research applies a recently-developed technique of analytically computing derivatives of a CRR model to a complex, widely-used CRR model. The resulting least squares response surface was found to contain numerous discontinuities in the surface and derivatives. However, the surface and its derivatives were found to be everywhere finite, permitting the use of derivative-based optimization algorithms. Finite difference numeric derivatives were computed and found to be virtually identical to analytic derivatives.

A comparison was made between gradient (Newton-Raphson) and direct (pattern search) optimization algorithms. The pattern search algorithm was found to be more robust. The lower robustness of the Newton-Raphson algorithm was thought to be due to discontinuities and a rough texture of the response surface.

CHAPTER 1

INTRODUCTION

The content of this report is based on a thesis by Hendrickson (1987).

The use of hydrologic models for scientific study and engineering problem-solving has become so prevalent that hydrologic modeling has become one of the most important tools available for the study and application of hydrology. Typically, the development of a hydrologic model occurs in several steps: problem definition, selection of a suitable type and structure of model, calibration of the model so that it most closely matches the behavior of the natural system, and, ideally, controlled verification of model performance. This thesis deals with the calibration aspect of hydrologic modeling and is concerned with the calibration of conceptual rainfall-runoff (CRR) models using gradient-type optimization algorithms and analytical derivatives. Specifically, this thesis is concerned with the calibration of the widely-used Soil Moisture Accounting model of the U.S. National Weather Service using the Newton-Raphson algorithm.

Gradient-search optimization algorithms require the computation of the derivatives of the estimation criterion with respect to model parameters and direct-search algorithms do not. This thesis was motivated by recent suggestions (Sorooshian and Gupta, 1984) that the use of gradient-type optimization algorithms may be preferable to non-gradient algorithms in the calibration of hydrologic models. In the past, however, gradient-type algorithms have not been a popular choice for the calibration of hydrologic models, possibly because of the difficulty of evaluating the required derivatives, or concern over possible inaccuracies arising from the use of numerical derivatives. Therefore, an important feature of this thesis is the computation of the derivatives of the estimation criterion with respect to model parameters in accordance with the principles of analytical calculus, using a technique developed by Gupta and Sorooshian (1984).

The chief objectives of this thesis are to (a) demonstrate the feasibility of calibrating a complex CRR model using a gradient search algorithm, (b) study the characteristics of the resulting response surface in order to evaluate the potential for calibration problems, and (c) compare the performance of gradient-search algorithms to that of direct-search algorithms.

The organization of this thesis is as follows. Chapter 2 contains background information on the calibration of hydrologic models and specfic calibration techniques. Related research is described in Chapter 3, and Chapter 4 describes the Soil Moisture Accounting model and the techniques currently employed by the National Weather Service to calibrate it. The techniques used to implement analytical derivatives for the Soil Moisture Accounting model are set forth in Chapter 5. Chapters 6, 7, and 8 describe the response surface studies, the calibration studies, and the sensitivity analysis, respectively.

CHAPTER 2

CALIBRATION OF CONCEPTUAL WATERSHED MODELS

A hydrologic model is an idealized representation of selected aspects of the behavior and characteristics of a particular hydrologic system. Hydrologic models may be grouped into four types: physical analogue, boundary value, conceptual, and black box. Resistance capacitance networks are examples of a physical analogue model of an aquifer. Boundary value models utilize the partial differential equations, along with boundary and intitial conditions, believed to describe the relevant hydrologic processes. Conceptual models use simplified representations of the significant physical processes. Black box models, also known as empirical or systems-theoretic models, develop relationships between system inputs and outputs without reference to internal processes. Index-type response functions may be considered to be a type of black box model.

Description of Conceptual Watershed Models

This paper will focus on conceptual watershed models, although many of the topics discussed could apply equally well to other types of models. Conceptual watershed models, also known as conceptual rainfall-runoff models (CRR), are concerned with the conversion of rainfall to streamflow through processes such as Hortonian overland flow, interflow, and groundwater discharge. Frequently, these models view the watershed as a system of water storages at various levels in the soil column, with mathematical equations governing the flow of water between storages.

Numerous CRR models have been developed, each of which views the structure of the watershed and the equations governing the flow of water somewhat differently. However, none of these models may be used to represent a particular watershed until the model's parameters have been determined for that watershed. Some parameters (for example, per cent paved area) may be measured directly, while other parameters must be estimated.

Calibration of Conceptual Watershed Models

Calibration of a CRR model involves finding those parameter values for a particular model and hydrologic system, such that the behavior and characteristics of the model mimic those of the natural system as closely as possible. When calibrating a CRR model, a historical sequence of, say, precipitation and streamflow data must be available for the watershed of interest. The first step in calibration is to provide initial parameter estimates for those parameters that cannot be measured directly. This can be done by the study of historical precipitation and hydrographs. The initial parameter estimates are then refined through manual or automatic calibration or a combination of each. In both manual and automatic calibration, the general procedure is to run the model using historical precipitation, parameter estimates, and initial moisture estimates, thereby producing a sequence of simulated streamflows. The estimation criterion provides a numerical measure of agreement between simulated and historical streamflow.

In manual calibration, the judgement of the hydrologist calibrating the model is used to select what he believes will be a good parameter set. The process of selecting a new set of parameters, running of the model using those parameters, and analysis of results is repeated in a trial and error procedure. Skilled and knowledgeable hydrologists are frequently successful at this task. However, the process is quite tedious, and requires a skilled hydrologist with specific knowledge of the model and watershed. Therefore, automated calibration techniques are often employed.

Insofar as a hydrologic model is an idealized representation of a natural system which is imperfectly understood, it is not surprising that models are imperfect. The failure of a model to perfectly or even crudely mimic the natural system is likely to stem from the following causes: (1) error in the measurement of precipitation, streamflow, evaporation, and so forth, (2) failure of point measurements to represent mean basin processes, (3) inaccurate or oversimplified mathematical model of the system, and (4) non-optimal parameter estimates. Data errors, particularly precipitation errors, can be a large impediment to rainfall-runoff modeling. For example, it is difficult for the model to match rising observed streamflows when the precipitation gauges show no rainfall.

Estimation Criterion

The estimation criterion is a numerical measure of closeness between model output and the observed behavior of the natural system. Ordinary least squares is a commonly-used criterion, consisting of the sum of the squares of the difference between simulated and observed flows. Recall that for a rainfall-runoff model, the simulated flows are themselves a function of historical inputs such as precipitation and evaporation, the model structure, model parameters, and initial moisture content used for the run. For the purpose of model calibration, if there are n parameters, the estimation criterion is defined in n-dimensional parameter space. The surface of the estimation criterion is referred to as the response surface. During calibration, the estimation criterion is sampled repeatedly at different points in parameter space by running the model with those parameter sets.

During model calibration, the objective is to find that parameter set which minimizes (or maximizes) the estimation criterion. This process is called optimization. The model is calibrated, but the estimation criterion is optimized. Several mathematical techniques from the field of optimization theory are available to assist in automated optimization. The response surface derived from a watershed model is often nonlinear with respect to parameters, with an irregular instead of smooth surface, and often contains multiple local optima (minima or maxima). This makes the optimization process much more difficult. The presence of multiple optima is a particularly serious problem, since convergence to a local optima is quite possible.

Mathematical means are available to prove the presence of a local optima, but not the presence of a global optima.

Automatic Calibration

The use of automated calibration techniques can considerably enhance the calibration process. Benefits of these techniques include: substantially less time required to calibrate a model, the potential for improved parameter estimates, and lessened reliance on the skill of the person performing the calibration in order to achieve acceptable results. The NWS has found that a combination of manual and automated calibration procedures is the best strategy, combining the hydrologist's knowledge of physical watershed processes with the speed of the automatic technique (Brazil and Hudlow, 1981).

Automated calibration of CRR models is a nonlinear optimization problem. Numerous algorithms have been developed for the solution of such problems. These algorithms are iterative. Starting from the initial parameter estimates $\underline{\theta}$, the algorithm selects a vector $\underline{V}$ in parameter space and a step size S, then samples the estimation criterion at the new parameter point $\underline{\theta}_2 = \underline{\theta}_1 + S\underline{V}$. The method of selection of the vector and step size differs with individual algorithms and depends on the results of previous steps and information gained when the estimation criterion is sampled. Possible termination criteria for the algorithms include (1) a specified number of steps, (2) the estimation criterion changing less than a specified percentage between successful steps (function convergence), or (3) the parameter values have changed less than a specified percentage between successful steps (parameter convergence). For practical application, these algorithms are encoded on a digital computer.

Parameters of conceptual watershed models are sometimes constrained in order to maintain physical realism. For example, many parameters are constrained to be positive. Nevertheless, algorithms designed for unconstrained optimization have commonly, if not exclusively, been used to calibrate them. Presumably, this is because the value of the estimation criterion in the nonfeasible region is very high, whereas in a typical constrained optimization problem, the global minimum lies within the nonfeasible region.

Unconstrained algorithms may be considered to fall into two major categories: those using derivatives of the estimation criterion (gradient methods), and those which do not (direct-search methods). Some derivative methods use the second partial derivatives of the estimation criterion (with respect to the parameters) or approximations thereof, and some use only first derivatives. Methods which view or approximate the estimation criterion as a quadratic surface are sometimes called least squares methods.

In discussing optimization, Himmelblau (1972) states that:

> "As a general rule in solving unconstrained nonlinear programming problems, gradient and second-derivative methods converge faster than direct search methods. However, in practice, the derivative-type methods have two main barriers to their implementation. First, in problems with a modestly large number of variables, it is laborious or impossible to provide analytical functions for the derivatives needed in a gradient or second-derivative algorithm. Although evaluation of the derivative by difference schemes can be substituted for evaluation of the analytical derivatives, ... , the numerical error introduced, particularly in the

> vicinity of the extremum, can impair the use of such substitutions."

Newton-Raphson Algorithm

The Newton-Raphson algorithm employed in this thesis is a modified Newton method, which may be classified as a least squares gradient method. The search is restricted to the space of dominant eigenvalues to prevent steps in the direction of non-identifiable parameters. Using the supplied values of the first and second derivatives at the current parameter point, it constructs a quadratic surface approximating the estimation criterion, and solves for the minimum of that surface. Complex algorithm logic determines whether to construct a new quadratic surface or to search along the line connecting the old and new parameter points. Further details of the algorithm are given in Sorooshian and Gupta (1984). The code for the algorithm was supplied by Gupta.

CHAPTER 3

RELATED RESEARCH

The work presnted in this thesis is a direct extension of the work of Gupta and Sorooshian (Gupta and Sorooshian, 1985; Sorooshian and Gupta, 1984; Gupta 1984) which dealt with the use of gradient-based calibration of CRR models. Their primary contribution was to introduce a method of analytically computing derivatives of such models, using methods explained in Chapter 5. Analytic derivatives have the advantage of being free of possible inaccuracies associated with the finite difference derivatives. Gradient-based calibration and derivative-based sensitivity and identifiability analyses can therefore be used with greater confidence when using error-free analytic derivatives.

Gupta and Sorooshian (1984) applied the analytic derivative methodology to a simplified version of the Soil Moisture Accounting model: model Sixpar. Synthetic calibration studies then compared the performance of the (direct search) simplex algorithm of Nelder and Mead (1965) with that of a modified Newton-Raphson algorithm (gradient search). Results indicated that both algorithms had similar abilities to find--or not find--optimal parameters, but the Newton-Raphson algorithm used significantly less computer time. The current work extends the work of Gupta and Sorooshian primarily through applying analytic derivative-based calibration and sensitivity and identifiability analyses to the full Soil Moisture Accounting model in a fashion which will be of practical use to the National Weather Service.

Other researchers have also investigated the area of automatic calibration of conceptual watershed models. Johnston and Pilgrim (1976) spent two years of full-time work attempting to find a true set of optimum parameters for one watershed using a conceptual watershed model. They were unsuccessful. They used both the (direct search) simplex optimization algorithm and the gradient-type Davidon method presented by Fletcher and Powell (1963), which is similar to the Newton-Raphson algorithm. They found that "Although both methods were reasonably satisfactory, the simplex method (a direct search method) appeared to be less susceptible to irregularity of the response surface than the Davidon method (a descent method) and was more efficient in the early stages of optimzation."

The work of Ibbitt and O'Donnell (Ibbitt, 1970; Ibbitt and O'Donnell, 1971) is particularly interesting. They investigated the performance of five direct-search algorithms, three gradient-search algorithms, and one stochastic search algorithm using a conceptual watershed model and synthetic data. In selecting the "best" algorithm, they emphasized robustness, or the ability to frequently obtain a correct solution, irregardless of computer cost. They concluded that the direct search "rotating coordinate method of Rosenbrock, after suitable modification for dealing with hydrologic models ..., is the most [robust] of the nine methods used for fitting the model..."

However, the Davidon method, as modified by Fletcher and Powell, was the next most robust. Ibbitt and O'Donnell also noted convergence problems associated with methods which assume a quadratic form of the estimation criterion. Also, they noted that the "peculiar" behavior of the (gradient) least squares algorithm of Marquardt (1965) was probably attributed to violation of its assumption of continuity of objective function derivatives.

Pickup (1976) compared the performance of four optimization algorithms on a CRR model using synthetic data. He found the simplex method (direct search) to be most successful in finding correct parameter values. A gradient method, the Davidon method as modified by Fletcher and Powell, performed poorly due to getting "trapped" on a local minima. It should be noted that the results of Pickup are based on only one calibration run; those of Ibbitt and O'Donnell on six calibration runs. The results of the calibration studies presented in this thesis indicate that many calibration runs with different initial parameter values are needed in order to compare the performance of several algorithms.

A number of researchers have noted the existence of discontinuities (in the criteria or its derivatives) of estimation criteria created by conceptual watershed models (Restrepo-Posada and Bras, 1982; Pickup, 1976; Johnston and Pilgrim, 1976; Ibbitt and O'Donnell, 1971; Gupta and Sorooshian, 1985). Restrepo-Posada and Bras noted the existence of discontinuities in a log likelihood objective function using a simplified version of the Soil Moisture Accounting Model. They attributed the discontinuity to the variable time step integration feature of the model. However, results presented in Chapter 6 of this thesis do not support that view.

CHAPTER 4

THE SOIL MOISTURE ACCOUNTING MODEL

The Soil Moisture Accounting model of the U.S. National Weather Service (NWS) is a CRR model which may be classified as a deterministic, lumped parameter, lumped input, lumped output, continuous time model. The original model was published as a version of the Stanford Watershed Model IV, based on the work of Crawford and Linsley (1966). The present form of the model incorporates the soil moisture accounting system developed by Burnash et al. (1973) at the Sacramento, California River Forecast Center of the NWS, and is sometimes referred to as a modified version of the Sacramento model.

Description of the Soil Moisture Accounting Model

The Soil Moisture Accounting model is a versatile, generalized model. It has been widely applied by the NWS to watersheds across the country and around the world. These watersheds range in size from several acres to several thousand square miles. It can be used for flood forecasting, low flow studies, and streamflow simulation from historical or synthetic precipitation records. The model traces the movement of rainall and snowmelt as it moves through an idealized representation of the soil column and underlying aquifers. The structure of this "pot and pipeline" model is dominated by five underground reservoirs as shown in Figure 4.1. Mathematical

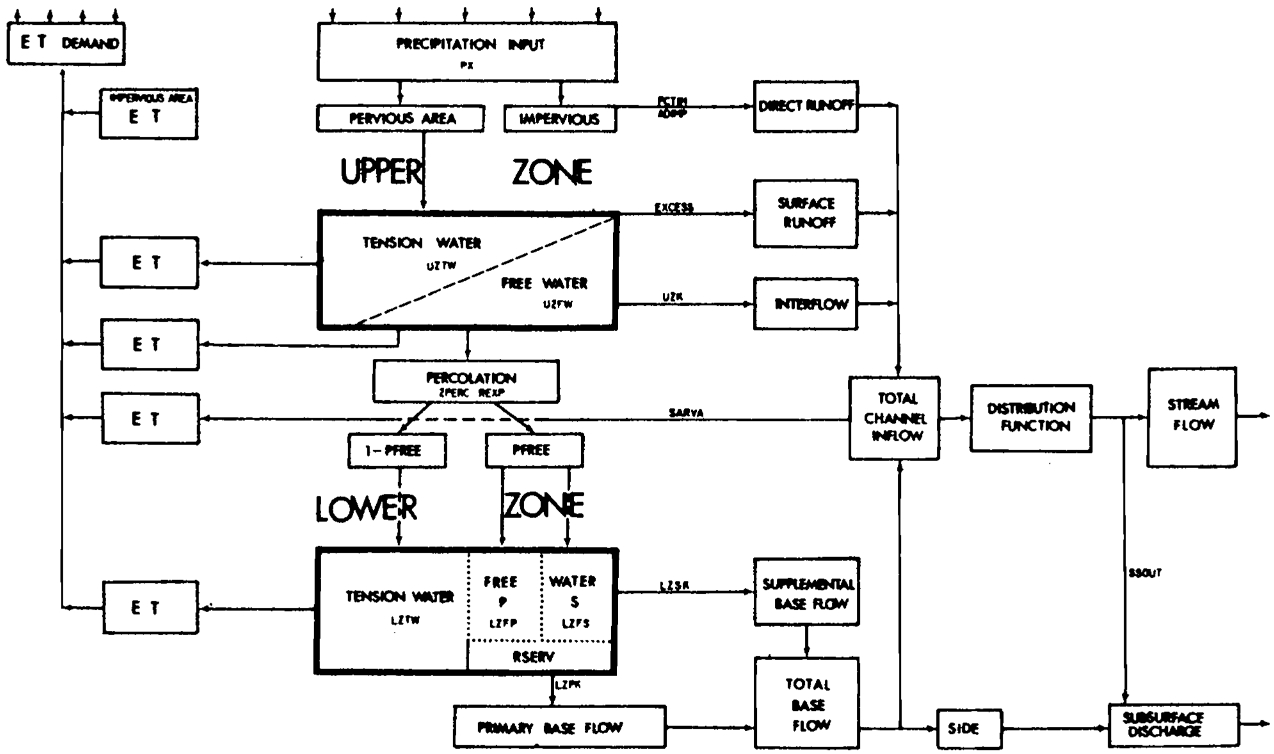

Figure 4.1. Schematic diagram of the Soil Moisture Accounting model.
This diagram from Peck, 1976.

relationships govern the flow of water between reservoirs and evaporation rates. Water tightly bound to soil particles is stored in tension reservoirs, which can only be depleted by evaporation. Water in excess of tension reservoirs is free to drain and is stored in free reservoirs. The porous subsurface is divided into an upper and lower zone. Groundwater discharge occurs from the lower zone and interflow from the upper zone. During each time step, evaporation is subtracted from each moisture store, water percolates from the upper to the lower zone, baseflow is generated, precipitation is added up the upper zone, and runoff is calculated. Complex percolation and evaporation functions are considered to be special features of the model.

The model generates runoff from several mechanisms. Direct runoff occurs from precipitation onto the watershed's impervious area. Surface runoff occurs after the upper zone becomes saturated. Interflow is the lateral drainage of the upper zone free storage. Baseflow is modeled as the combined discharge of the primary and secondary lower zone free storages. The sum of runoff generated by these mechanisms is termed "total channel inflow", which is the basic output of the model. A unit hydrograph is applied to "total channel inflow" to obtain estimated streamflow. The unit of "total channel inflow" is the millimeter, and the output of the unit hydrograph operation has streamflow units.

The data inputs to the model are basin average precipitation and measured or estimated potential evapotranspiration. Model inputs and outputs are sums for a discrete time period, usually six hours.

The model is nonlinear with respect to inputs and parameters. The most significant nonlinearity results from the tension storages. Incoming precipitation must satisfy upper zone tension storage requirements before it is available for runoff or percolation. Percolation to the lower zone must satisfy lower zone tension storage before being available for baseflow generation.

River Forecast System

The National Weather Service River Forecast System (NWSRFS) is a system of hydrologic techniques used by regional NWS River Forecast Centers in carrying out their operational duties. It was first conceived by the NWS in 1971, and is still evolving today as new needs arise and hydrologic techniques are developed (Peck, 1976). The NWSRFS takes the form of a large, sophisticated FORTRAN computer software package.

Components of the NWSRFS include the soil moisture accounting model, a snow model, a unit hydrograph operation, other channel routing models, parameter estimation procedures, techniques for estimating basin average precipitation from point data, and hydrologic data processing functions (Peck, 1976). Two versions of the NWSRFS exist: the operational version used by the River Forecast Centers, and a research version which is developed by the Hydrologic Research Lab of the NWS in Silver Spring, Maryland. The components of the NWSRFS are shown in Figure 4.2. It should be noted that, for operational use, the Soil Moisture Accounting model does not completely stand on its own,

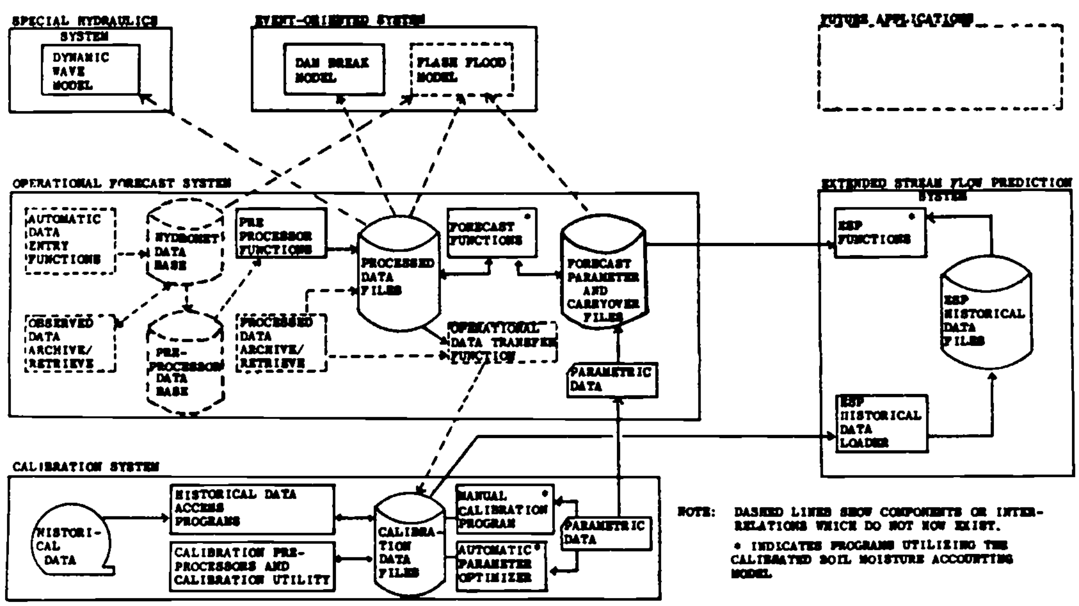

Figure 4.2. Schematic diagram of the components of the NWS River Forecast System.

This diagram from Brazil and Hudlow (1981).

since it depends on various operations available in the NWSRFS for complete implementation.

Calibration of the Soil Moisture Accounting Model

The parameters of the Soil Moisture Accounting model must be estimated for each watershed to which it is applied. The data calibration requirements are a historical sequence of mean basin precipitation (rainfall plus snowmelt), estimated potential evapotranspiration, and streamflows. Additionally, a unit hydrograph for the basin is required before the model can be calibrated. The model is ordinarily run on a six-hour time step, and precipitation must be six hour sums. However, only mean daily streamflows are required. During a NWSRFS run of the Soil Moisture Accounting model, the model ouput (in millimeters) is used as input to the unit hydrograph operation. The output of the unit hydrograph operation is six-hour instantaneous streamflow. These are averaged into mean daily flows by the "MEANQ" operation of the NWSRFS before they may be compared to historical streamflows. In some cases, if the gauging station is far downstream from the watershed of interest, additional routing is used. However, for the purpose of this thesis, it is assumed that no additional routing takes place.

According to Peck (1976), potential evapotranspiration rates may be estimated from either meteorological data or pan observations. Either daily or mid-month values may be used. The NWSRFS contains algorithms for converting these data into six-hour values to be input directly into the model.

The Soil Moisture Accounting model contains 16 parameters, which are listed in Table 4.1. Most of these parameters do not represent physical variables which can be measured in the field or laboratory. However, they generally have physically-intuitive meanings. For example, the maximim capacity of the tension storages represents the amount of water the watershed will absorb before runoff begins. Three additional parameters (PXADJ, PEADJ, and EFC), which are used to adjust precipitation and evaporation inputs, are also listed in Table 4.1. The model has six state variables whose initial values constitute the model's initial state. These variables represent the amount of moisture in each of the reservoirs, and are listed in Table 4.2.

Peck (1976) sets forth valuable information on estimating initial parameter values. Three or four parameters need not be calibrated at all. The value of parameter SARVA may be taken directly from topographic maps. Peck recommends that parameter ADIMP be given a permanent value of 0.01, and SAVED a value of 0.30. Unless it is known that considerable groundwater flow bypasses the streamchannel, parameter SIDE should have a value of 0.0.

Assignment of initial parameter values for remaining parameters is accomplished through study of historical precipitation and hydrographs. Furthermore, parameter values from nearby catchments may be useful in selecting initial parameter values. It is doubtful that model calibration would be successful without rational initial estimates.

Table 4.1. Parameters of the Soil Moisture Accounting model

Parameter	Explanation
UZTWM	Maximum capacity of upper zone tension storage. (mm)
UZFWM	Maximum capacity of upper zone free storage. (mm)
LZTWM	Maximum capacity of lower zone tension storage. (mm)
LZFPM	Maximum capacity of lower zone primary free storage. (mm)
LZFSM	Maximum capacity of lower zone secondary free storage. (mm)
ADIMP	Fraction of basin which becomes impervious as all tension storage is met.
UZK	Lateral drainage rate of upper zone free storage. (fraction per day)
LZPK	Lateral drainage rate of lower zone primary storage. (fraction per day)
LZSK	Lateral drainage rate of lower zone secondary storage. (fraction per day)
ZPERC	Percolation parameter which indicates, when used with other parameters, the maximum possible percolation rate. (Dimensionless)
REXP	Percolation parameter, an exponent, determining the rate of change of the percolation rate as the lower zone moisture varies from full to dry. (Dimensionless)
PCTIM	Fraction of basin which is impervious and contiguous with stream channels.
RIVA	Fraction of basin covered by streams, lakes, and riparian vegetation. (Also known as parameter SARVA).
PFREE	Fraction of percolation water entering free storages, regardless of tension water deficiency.
SIDE	Ratio of groundwater flow entering channel to that bypassing channel.
SAVED	Fraction of lower zone free water unavailable for evapotranspiration. (Also known as parameter RSERV).
PXADJ	Precipitation adjustment factor. (Dimensionless)
PEADJ	Potential evapotranspiration adjustment factor. (Dimensionless)
EFC	Evapotranspiration extrapolation parameter. (Dimensionless)

Table 4.2. State variables of the Soil Moisture Accounting model

Variable	Explanation
UZTWC	Upper zone tension water contents. (mm)
UZFWC	Upper zone free water contents. (mm)
LZTWC	Lower zone tension water contents. (mm)
LZFPC	Lower zone free primary water contents. (mm)
LZFSC	Lower zone free secondary contents. (mm)
ADIMP	Additional impervious area contents. (mm)

Subsequent calibration can be be accomplished by either manual or automatic procedures, as discussed in Chapter 2. The NWS uses the pattern search algorithm of Hooke and Jeeves (1961) as its optimization algorithm. Care must be taken to ensure that parameters remain hydrologically realistic. The experience of the NWS is that manual fitting, followed by automatic fitting once reasonable fit has been achieved, is the best procedure (Peck, 1976).

CHAPTER 5

CALCULATION OF ANALYTICAL DERIVATIVES OF CONCEPTUAL MODELS

The efficiency and reliability of derivative-based optimization algorithms have made them attractive methods for the automatic calibration of CRR models such as the Soil Moisture Accounting model. The use of such methods requires the ability to evaluate or approximate, at any point in parameter space:

(1) the value of the estimation criterion;

(2) the vector of partial first derivatives of the estimation criterion with respect to each parameter being optimized; and

(3) the matrix of second partial derivatives of the estimation criterion with respect to the parameters being optimized.

The numerical accuracy of such methods depends on the accuracy with which the partial derivatives of the estimation criterion with respect to the model parameters can be calculated. The derivatives of interest can be evaluated either numerically or analytically. To evaluate numerical derivatives, the estimation criterion is sampled at two closely-spaced points in parameter space and the difference between the two values of the estimation criterion divided by the incremental change in the parameter of interest. In the past, it was generally believed that accurate analytic derivatives of CRR watershed models could not be obtained or were too difficult to obtain. However, Gupta and Sorooshian (1985) have demonstrated that this can be done. The strength of the procedure is that threshold structures are not replaced by smoothing functions, thereby preserving the conceptual integrity of the model. Sorooshian and Gupta have demonstrated the validity and effectiveness of the methodology developed using a simplified version of the Soil Moisture Accounting model.

Methodology for Exact First Derivatives

Consider a generalized, one-parameter, one-state CRR model and its estimation criterion:

$$X_t(\theta) = f(\theta,\ X_{t-1}(\theta), U_t) \tag{5.1}$$

$$q_t(\theta) = g(\theta,\ X_{t-1}(\theta), U_t) \tag{5.2}$$

$$F = \sum_{t=1}^{ndata} h(q_t(\theta),\ qobs_t) \tag{5.3}$$

where

X_t = model state at time t;

q_t = model flow at time t;

F = estimation criterion;

Θ = model parameter;

U_t = model input at time t;

$qobs_t$ = historical observed flow at time t; and

ndata = number of time steps.

Calculation of the derivatives of the above equations requires the use of the chain rule, which states that if:

$$X_t = f(X_{t-1})$$

$$X_{t-1} = g(\Theta)$$

then:

$$\frac{\partial X_t}{\partial \theta} = \frac{\partial X_t}{\partial X_{t-1}} \cdot \frac{\partial X_{t-1}}{\partial \theta} \tag{5.4}$$

Thus, it can easily be seen that the derivatives of Equations (5.1), (5.2), and (5.3) are given by:

$$\frac{\partial X_t(\theta)}{\partial \theta} = \frac{\partial f(\theta, X_{t-1}(\theta), Ut)}{\partial \theta} + \frac{\partial f(\theta, X_{t-1}(\theta), U_t)}{\partial X_{t-1}(\theta)} \cdot \frac{\partial X_{t-1}(\theta)}{\partial \theta} \tag{5.5}$$

$$\frac{\partial q_t(\theta)}{\partial \theta} = \frac{\partial g(\theta, X_{t-1}(\theta), U_t)}{\partial \theta} + \frac{\partial g(\theta, X_{t-1}(\theta), U_t)}{\partial X_{t-1}(\theta)} \cdot \frac{\partial X_{t-1}(\theta)}{\partial \theta} \tag{5.6}$$

$$\frac{\partial F(\theta)}{\partial \theta} = \sum_{t=1}^{ndata} \frac{\partial h(q_t(\theta),\ qobs_t)}{\partial q_t(\theta)} \cdot \frac{\partial q_t(\theta)}{\partial \theta} \tag{5.7}$$

However, in a typical CRR model, a closed expression for functions $f(\cdot)$, $g(\cdot)$, and (possibly $h(\cdot)$) are not available. In the model, which takes the form of a computer program, states and outputs are assigned new values in an iterative fashion, line of computer code, by line of computer code. The fact that CRR models usually operate in any one of several modes of behavior at any given time step, depending on the values of state variables at that time, further assures that closed forms of $f(\cdot)$ and $g(\cdot)$ are not available. The solution to this dilemma is to compute, after each line of original code, the derivative of the intermediate or final state, output, or estimation criterion which was assigned a new value in that original line of code. The derivative computation is performed analytically, in accordance with the rules of calculus, as demonstrated in Equations (5.5) through (5.7). If the model has n parameters, then n separate derivatives must be computed after each line of code: $\frac{\partial}{\partial \theta_1}, \frac{\partial}{\partial \theta_2}, \ldots \frac{\partial}{\partial \theta_n}$.

To provide an example, if several lines of original model code were given by:

```
If (X .LT.10), then
   X = X + precip
   X = θ*X
END If
    Q = .2*θ*X,                                    (5.8)
```

then the corresponding code for the model and derivatives would be given by:

```
If (X.LT.10), then
      X = X + precip
```

$$\frac{\partial X}{\partial \theta} = \frac{\partial X}{\partial \theta}$$

```
   X = θ*X
```

$$\frac{\partial X}{\partial \theta} = X + \theta \frac{\partial X}{\partial \theta} \qquad (5.9)$$

```
END If
   Q = .2*θ*X
```

$$\frac{\partial Q}{\partial \theta} = .2{*}X + .2{*}\theta{*}\frac{\partial X}{\partial \theta}$$

where X = model state;

Θ = parameter; and

Q = model output.

Similar procedures are employed in subroutines where the estimation criterion is calculated.

It can be seen that the modal behavior of the model poses no problem in the implementation of this technique. In general, derivatives of model states and outputs at any time step are a function of state derivatives at previous time steps. At time = 0, all derivatives are set to zero.

It is important to stress that the above procedure produces exact values of first partial derivatives for particular values of parameters, inputs, and initial states. A closed expression for the derivatives is not available; the values of derivatives must be sampled at discrete points in parameter space.

A comprehensive example of practical implementation of analytical derivatives (exact first derivatives and approximated second derivatives) for a simple CRR model is given in Appendix A.

It should be noted that analytical derivatives referred to the above are called "exact" because they are computed using exact equations. After practical implementation on a digital computer, however, the values of the "exact" derivatives will be affected by computer round-off error.

Methodology for Approximate Second Derivatives

The use of gradient-based calibration or derivative-based sensitivity analysis often requires the computation of the Hessian, defined as:

$$H_{ij} = \frac{\partial^2 F}{\partial \theta_i \partial \theta_j} \qquad i,j = 1,2,\ldots n \qquad (5.10)$$

where

F = estimation criterion;

θ_i = i^{th} parameter; and

n = number of parameters.

At least three methods are available for obtaining the Hessian: (1) numeric, (2) exact analytic, and (3) approximate analytic. Exact analytic second derivatives can be computed as follows. Consider an ordinary Least Squares Estimation Criterion:

$$F = \sum_{t=1}^{n} (q_t - qobs_t)^2 \tag{5.11}$$

where

F = value of ordinary least squares objective function;

t = time period;

n = number of time periods;

qobs = observed streamflow; and

q = model flows.

Applying the chain rule of calculus, an exact analytical expression for the Hessian is given by:

$$H_{ij} = 2* \sum_{t=1}^{n} \left[(q_t - qobs_t) \frac{\partial^2 q_t}{\partial \theta_i \partial \theta_j} + \frac{\partial q_t}{\partial \theta_i} * \frac{\partial q_t}{\partial \theta_j} \right]. \tag{5.12}$$

This equation requires the first and second derivatives of model output with respect to each parameter be available. The first derivatives can be obtained using techniques described in the previous section. The second derivatives can also be obtained through an extension of those techniques. However, for an n-parameter model, this would require that, after each line of original model code, n^2 lines of derivative code be inserted. For many models, this is a prohibitive undertaking, both in terms of programming effort and in computer storage and time. Fortunately, an approximation of the exact analytical expression can be made through omission of higher order terms. Employing this alternative, Equation (5.12) becomes:

$$H_{ij} = \sum_{t=1}^{n} 2 * \frac{\partial q_t}{\partial \theta_i} * \frac{\partial q_t}{\partial \theta_j} \qquad (5.13)$$

Equation (5.13) describes the method used to compute SLS "approximate second derivatives" for the response surface and calibration studies, the sensitivity and identifiability analyses, and the sample program in Appendix A.

The daily root mean square (DRMS) estimation criterion used by the National Weather Service takes the form:

$$\text{DRMS} = \left[\frac{1}{n} \sum_{t=1}^{n} (q_t - qobs_t)^2 \right]^{1/2} \qquad (5.14)$$

where terms are described as in Equation (5.11). DRMS has units of runoff and, therefore, has a physically-intuitive meaning. If an analytical expression for the Hessian is developed, and terms containing second derivatives are omitted, the approximate expression for the DRMS Hessian becomes:

$$H_{ij} = \frac{1}{n\ \mathrm{DRMS}} \sum_{t=1}^{n} \left[\frac{\partial q_t}{\partial \theta_i} \frac{\partial q_t}{\partial \theta_j} \right] - \frac{1}{\mathrm{DRMS}} \frac{\partial\ \mathrm{DRMS}}{\partial \theta_i} \frac{\partial\ \mathrm{DRMS}}{\partial \theta_j} \tag{5.15}$$

where $$\frac{\partial\ \mathrm{DRMS}}{\partial \theta_i} = \frac{1}{n\ \ \mathrm{DRMS}} \sum_{t=1}^{n} (q_t - qobs_t) \frac{\partial q_t}{\partial \theta_i}$$

In addition to convenience, the use of approximate Hessians may have some mathematical advantages. In the Newton-Raphson algorithm, the Hessian is used to determine the direction of the next step in multi-parameter space. Use of the suggested approximation to the Hessian will have the effect of smoothing the estimation criterion. This may prevent the algorithm from taking missteps based on higher order nonlinearities in the estimation criterion.

Implementation of Analytical Derivatives for the Soil Moisture Accounting Model

Exact analytical first derivatives and approximate analytical second derivatives for the Soil Moisture Accounting Model were implemented and tested in two steps. In the first step, the first partial derivatives of the output of the model ("total channel inflow") with respect to 16 model parameters were programmed and tested. These 16 parameters are the first 16 listed in Table 4.1. Derivatives with respect to parameters PEADJ, PXADJ, and EFC were not programmed since these parameters are external to the Soil Moisture Accounting subroutine.

In programming the derivatives, a copy of the model subroutine was first obtained. Each line of code which assigns new values to state or output variables was identified. Immediately after each of these lines, 16 new lines of derivative computations were added--one for each parameter. All derivatives were set to zero previous to beginning the time loop. Derivatives of model output for each parameter at each time step are stored for use in calculation of estimation criterion derivatives. This portion of the programming was performed by Gupta.

To test the resulting subroutine, analytic derivatives were compared with numeric derivatives. Finite difference derivatives were calculated in the following manner. The parameter in question would be perturbed upwards by .05% and model output saved at each time step. Then, the original parameter value would be perturbed downwards by 0.05%. For every time step, the difference between the two perturbed total channel inflows divided by 0.1% of the original parameter value gave the approximate numeric derivative of total channel inflow with respect to that parameter. Using a synthetic precipitation and evapotranspiration sequence, time streams of partial derivatives with respect to each parameter were generated using both analytic and numeric methods. After computer code errors had been detected and corrected, it was found that numeric and analytical derivatives were identical to at least the sixth decimal place. The results were not found to be sensitive to the step size. The computer runs were made on a Cyber 175, which with a 64-bit word, has less round-off error than most machines.

The second step of implementing analytic derivatives for the Soil Moisture Accounting model involved (1) extending derivative computations to the unit-hydrograph and other operations, and (2) integrating the derivative subroutines into the NWS River Forecast System (NWSRFS) software. The Soil Moisture Accounting model does not really stand on its own; a unit hydrograph operation must be added to it. Therefore, derivative computations were added to the unit hydrograph and streamflow averaging subroutines. Practical implementation of gradient techniques within the NWSRFS was one of the major goals of this research. Since the NWS operates their research and development version of the NWSRFS on a Prime mini-computer, a Prime machine was used for the second stage of derivative implementation. This was to assure that the resulting gradient version of the NWSRFS would be as compatible as possible with existing NWS programs and computers.

The research and development version of the NWSRFS was obtained from the Hydrologic Research Laboratory of the NWS in Silver Spring, Maryland. The derivative subroutine for the model was integrated into this system, and derivative computations were carried through the subroutines in which the unit hydrograph, flow averaging, and estimation criterion calculation operation are carried out. Due to the complexity of the NWSRFS software, this was a lengthy task. It was necessary to simplify the calculations so that any derivatives carried over from one month to the next are neglected. This was the result of an NWSRFS data flow structure that processes data one month at a time. For multi-month calibration data sets, this means that the derivatives will contain some error, but it was simply not practical to do otherwise. Testing of derivatives evaluation within the NWSRFS software was also accomplished numerically.

Practical and Theoretical Implications

For most CRR models, a closed-form expression of the model output or estimation criterion is not available. Therefore, in the past, it was generally believed that it was not possible to obtain analytical expressions for derivatives. Gupta and Sorooshian (1985) have shown that this is not the case. Part of the contribution of the research presented here is to demonstrate that analytical derivatives of a complex CRR model can indeed be implemented in a practical, operational setting.

Until now, it has not been possible to evaluate the accuracy of numerical derivatives of CRR models. However, the work presented in this chapter has made it possible to compare numerical and analytical first derivatives. Results showing that the two are identical to at least the sixth decimal place (when using a 64-bit word and 0.1% step size) are interesting and significant. The amount of programming effort required to program analytic derivatives for a complex CRR model is non-trivial. Roughly four or five man-months were required to program and test the derivatives of the Soil Moisture Accounting model (see above). In view of the evidence that analytical derivatives may not be significantly more accurate than numerical derivatives, the effort required to program analytical derivatives may not be justified. For many operational and research applications of gradient-based calibration and sensitivity analyses, the author would recommend numerical derivatives. It should be noted that a disadvantage of analytical derivatives is that any modifications to the model become more difficult because these modifications must be carried through the derivative computations.

If gradient-based calibration is extended to the unit hydrograph and snowmelt operations of the NWSRFS, the author recommends that numerical derivatives be used. The complex internal logic and data flows within the NWSRFS would make the programming effort associated with analytic derivatives unjustifiable. Further, analytical derivatives would make modifications to the NWSRFS subroutines more difficult.

CHAPTER 6

RESPONSE SURFACE STUDIES

This chapter examines the nature of a response surface generated by the Soil Moisture Accounting model. The motivation for doing so is that the nature of the response surface has a significant impact on the calibration process (see Chapter 4). An understanding of the nature of the response surface can provide some insight into the calibration problem for the model which generated the surface, and enhance an understanding of model behavior.

This chapter is organized into three sections: (1) methods, (2) results, and (3) a section which looks at response surface discontinuities in more detail. The results section also discusses how the sensitivity of the model to parameters changes with the mode of model behavior.

Methods

A simple least squares (SLS) estimation criterion was used to generate the response surface. This criterion takes the form:

$$SLS(\underline{\theta}) = \sum_{t=1}^{ndata} (SIMQ_t(\underline{\theta}) - OBSQ_t)^2 \qquad (6.1)$$

where

$SIMQ_t$ ($\underline{\theta}$) = simulated flows at time t;

$OBSQ_t$ = observed flows at time t;

$\underline{\theta}$ = model parameters; and

ndata = number of data points.

The response surface is defined in n-dimensional space, where n is the number of model parameters. Since SLS ($\underline{\theta}$) is not available in closed form, it must be sampled at discrete points in parameter space.

Synthetic data were used to generate the response surface in order to (1) eliminate model and data errors, and (2) ensure that the location of the global optimum is known. Model parameters for Bird Creek near Sperry, Oklahoma, were used. Bird Creek is a 2,344 square kilometer watershed. The Bird Creek parameter estimates were supplied by the National Weather Service.

A 15-day sequence of six-hour precipitation sums was generated using personal judgment as to what constituted a reasonable sequence. Care was taken to ensure that the precipitation activated all modes of the model (such as baseflow only, overland flow, etc.). Using arbitrarily-selected initial states, the Soil Moisture Accounting Model was run on the synthetic storm using "true" Bird Creek parameters to produce "true" synthetic flows. The response surface study was conducted before derivatives were integrated into NWSRFS software. Therefore, the unit hydrograph was not coupled to the model for results presented in this chapter. The synthetic data are plotted in Figure 6.1.

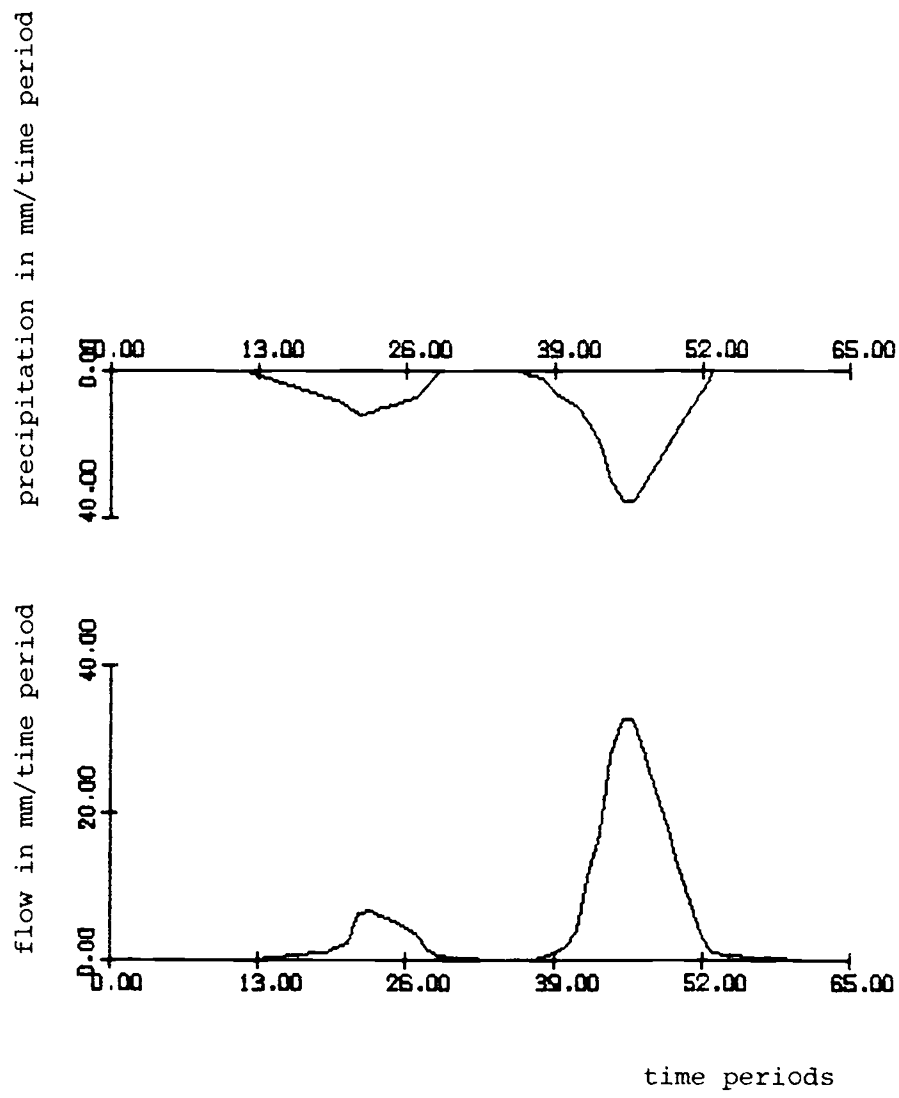

Figure 6.1. Synthetic precipitation and flows used in the Response Surface Study.

Since the response surface is defined in multi-parameter space, it was necessary to examine the surface by taking one-dimensional cross-sections along each of the parameter axes. To generate a cross-sectional plot of the surface, the estimation criterion was sampled at 100 closely-spaced points along the parameter axis of interest. Analytic derivatives were computed at the same time, using the methodology presented in Chapter 5. Results of each run were plotted on three plots, with parameter value along the X axis. The SLS value, the first partial derivative of SLS with respect to the parameter of interest, $\frac{\partial SLS}{\partial \theta_j}$, and the second partial derivative, $\frac{\partial^2 SLS}{\partial \theta_j^2}$, are plotted along the Y axis of the three plots.

Results

While running the Soil Moisture Accounting model with the synthetic storm, the model changes from one mode of behavior to another. For example, during periods of no precipitation, baseflow may be the only model process generating streamflow, while during intense rains, interflow and overland flow may also be runoff-generating process. Various model parameters are more active in certain modes than in others. For example, parameters describing the amount of soil tension storage will have little effect during a long dry spell.

In order to learn something about the sensitivity of various parameters in different modes, time plots of the derivatives of model output with respect to parameters were made. Figures 6.2 through 6.4 are plots of the derivative of model output (total channel inflow) with

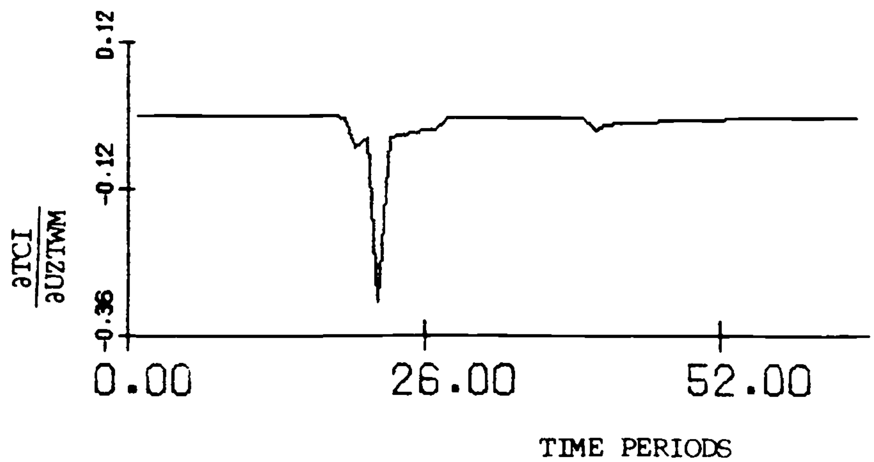

Figure 6.2. Derivative of model output with respect to parameter UZTWM (upper zone tension reservoir maximum) versus time for the synthetic storm.

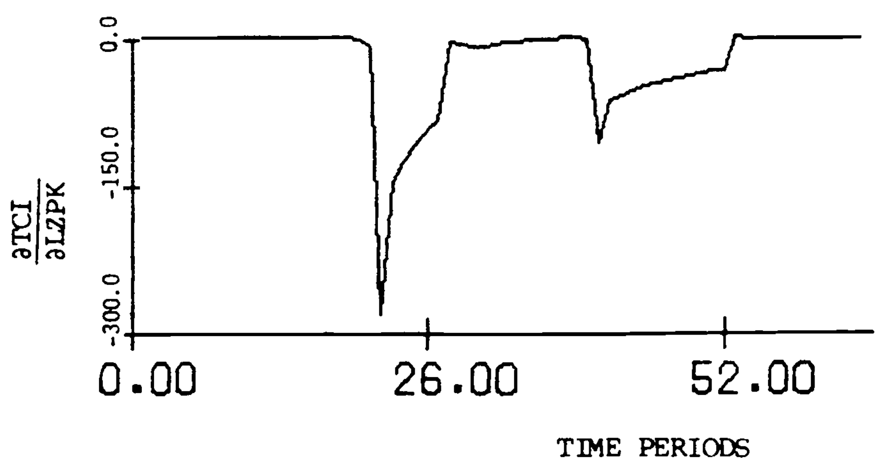

Figure 6.3. First derivative of model output with respect to parameter LZPK (lower zone primary recession constant) versus time for the synthetic storm.

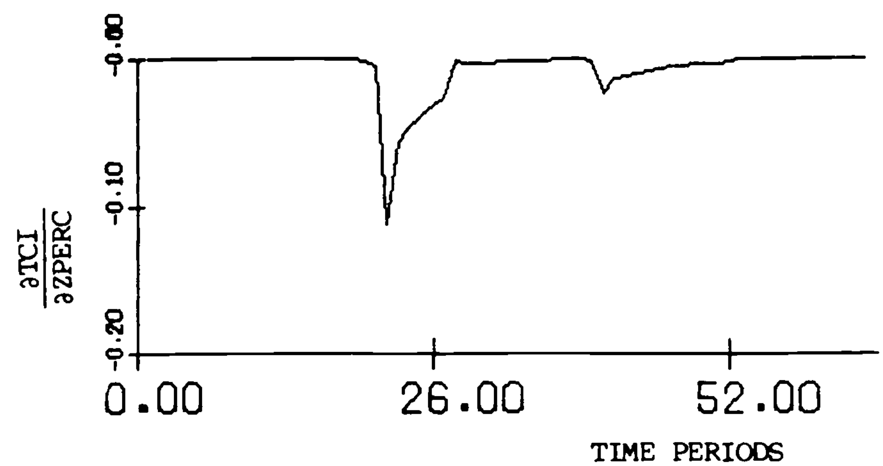

Figure 6.4. First derivative of model output with respect to parameter ZPERC (percolation parameter) versus time for the synthetic storm.

respect to parameters UZTWM, LZPK, and ZPERC, respectively, versus time for the synthetic storm. These plots show that in certain time periods (very dry), the model is completely insensitive to parameter UZTWM (Upper Zone Tension Water Maximum). They also show that each of the three parameters have the most influence during an intense rainstorm. Such observations highlight the desirability of using calibration data which activate all the modes of the model. It is also important to note that the figures indicate the model is approximately three orders of magnitude more sensitive to LZPK (Lower Zone Recession Coefficient) than to UZTWM or ZPERC (Percolation Parameter). Perhaps more attention should be given to estimating LZPK than to UZTWM and ZPERC.

One-dimensional response surface cross-sections for each of the 16 parameters are plotted in Figures 6.5 through 6.20. In each figure, the bottom plot is the SLS cross-section, the middle plot is of first derivatives, $\frac{\partial SLS}{\partial \theta_j}$, and the bottom plot is of second derivatives, $\frac{\partial^2 SLS}{\partial \theta_j^2}$. In each case, parameter value is represented along the x axis. In each figure, the "true" parameter value is denoted by an asterisk. Due to computer roundoff error, the minimum value of the estimation criterion is not zero for several of the less sensitive parameters (ADIMP, RIVA, PFREE, and SIDE). Also, due to roundoff error, the minimum function value is not at the "true" parameter value for ADIMP, PFREE, and SIDE. An interesting and important result is that the estimation criterion is completely insensitive to parameter SAVED (Figure 6.20). Obviously, there is nothing to be gained by

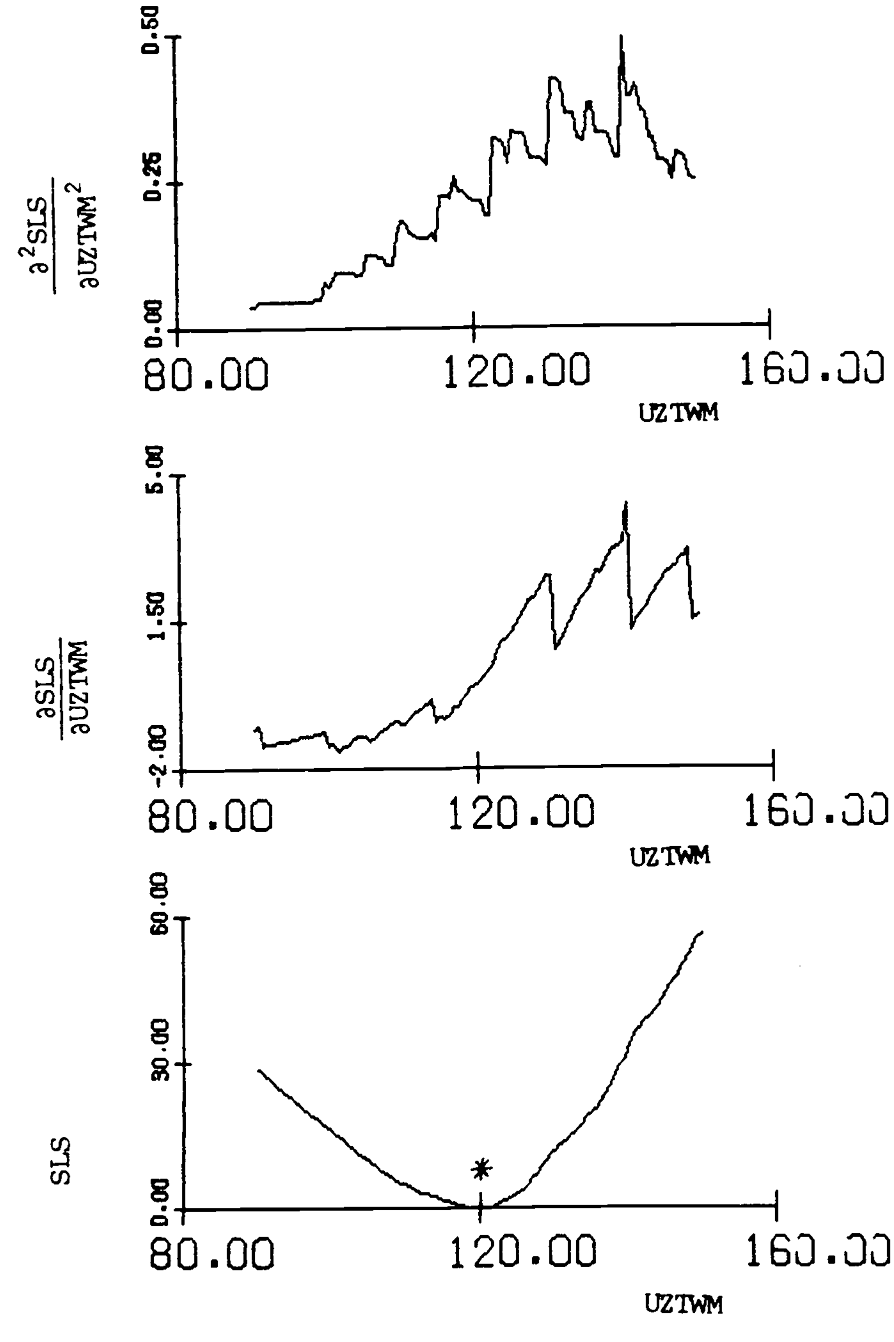

Figure 6.5. Cross-section and derivatives of SLS function along axis of parameter UZTWM.

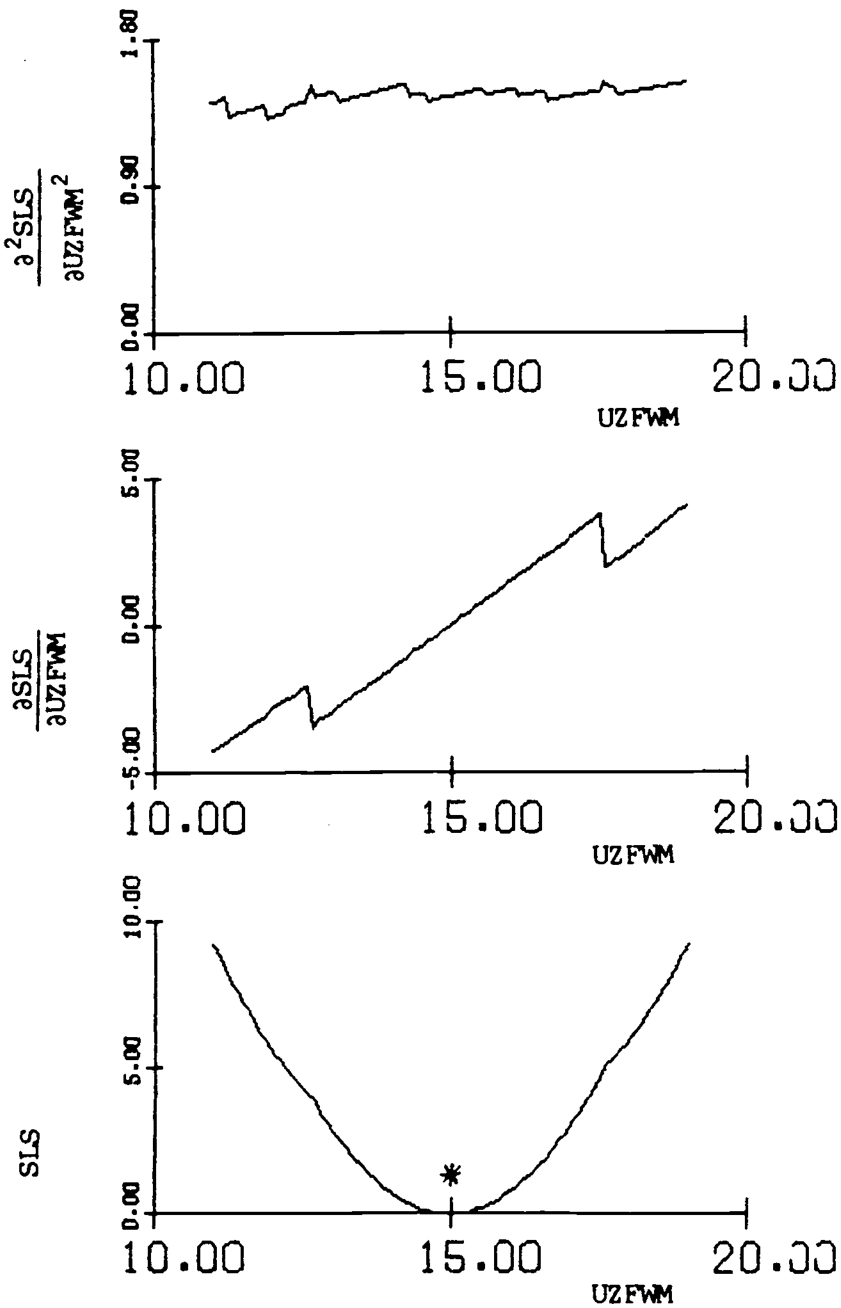

Figure 6.6. Cross-section and derivatives of SLS function along axis of parameter UZFWM.

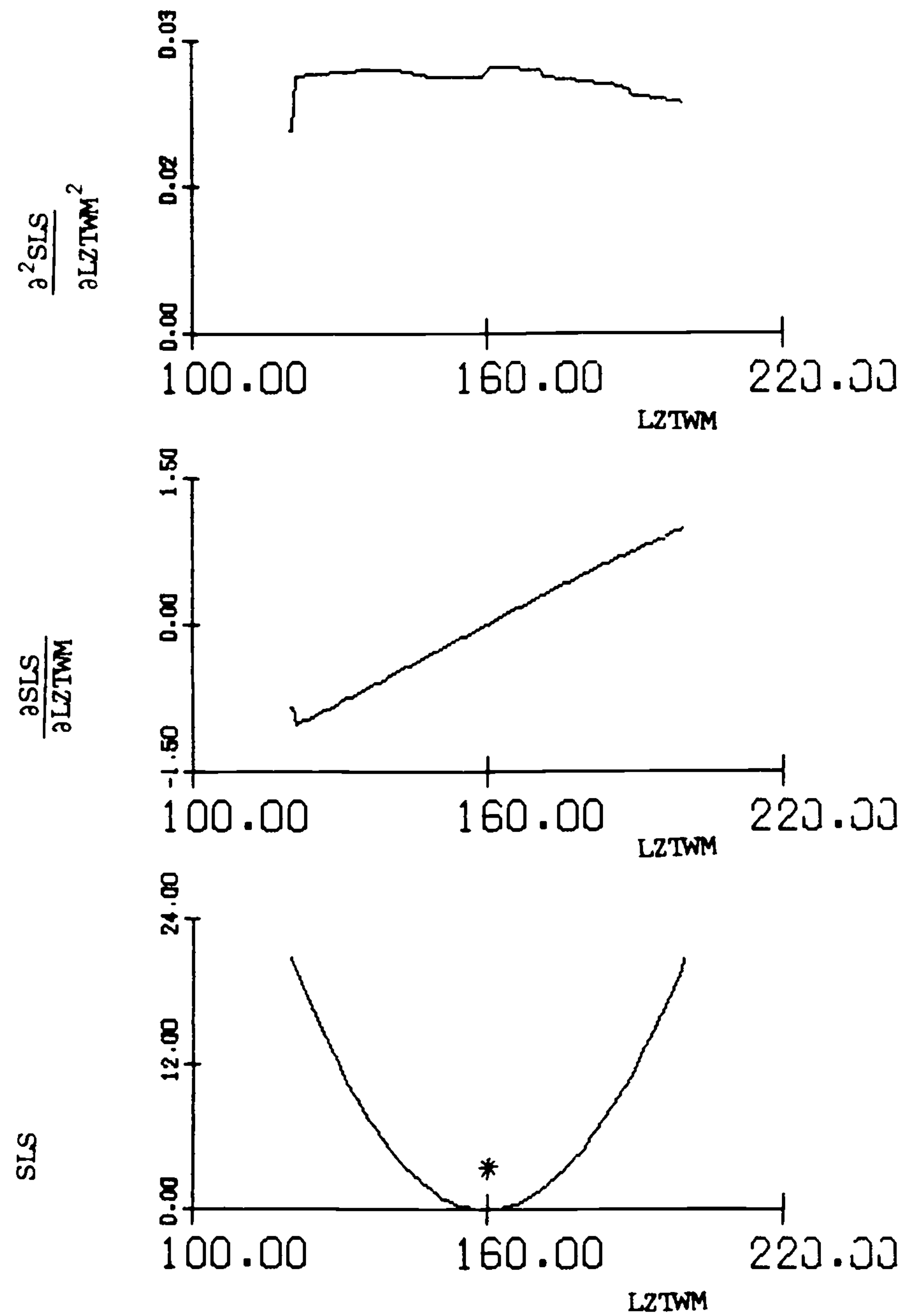

Figure 6.7. Cross-section and derivatives of SLS function along axis of parameter LZTWM.

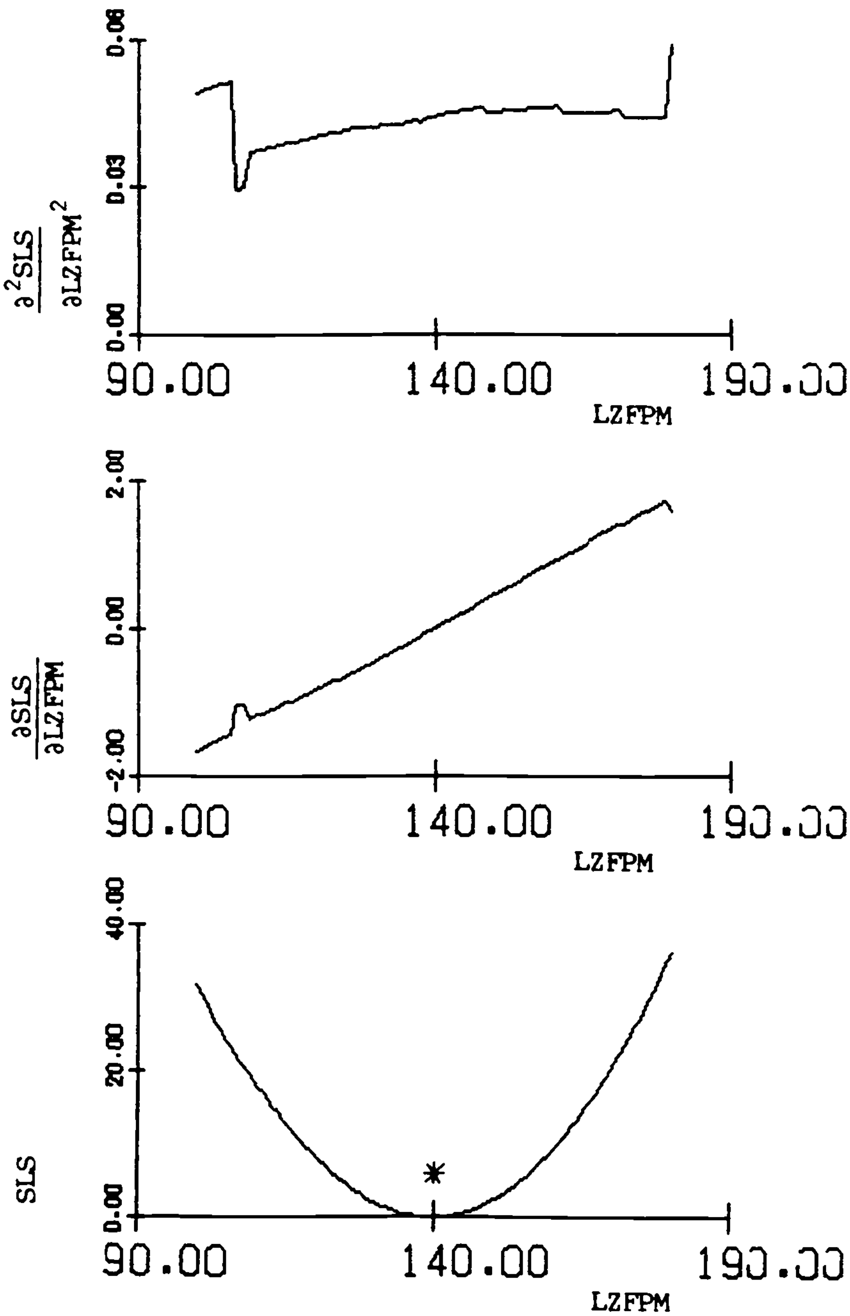

Figure 6.8. Cross-section and derivatives of SLS function along axis of parameter LZFPM.

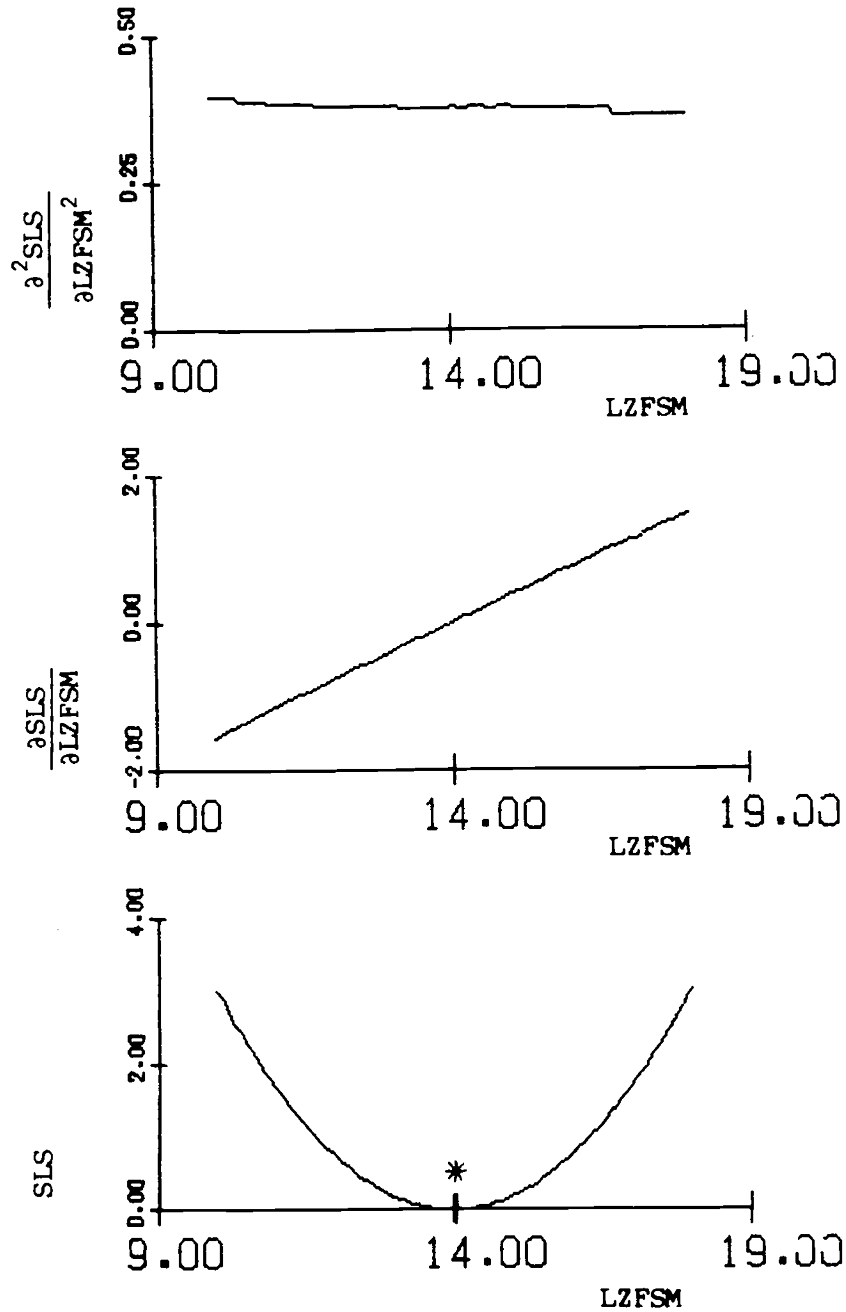

Figure 6.9. Cross-section and derivatives of SLS function along axis of parameter LZFSM.

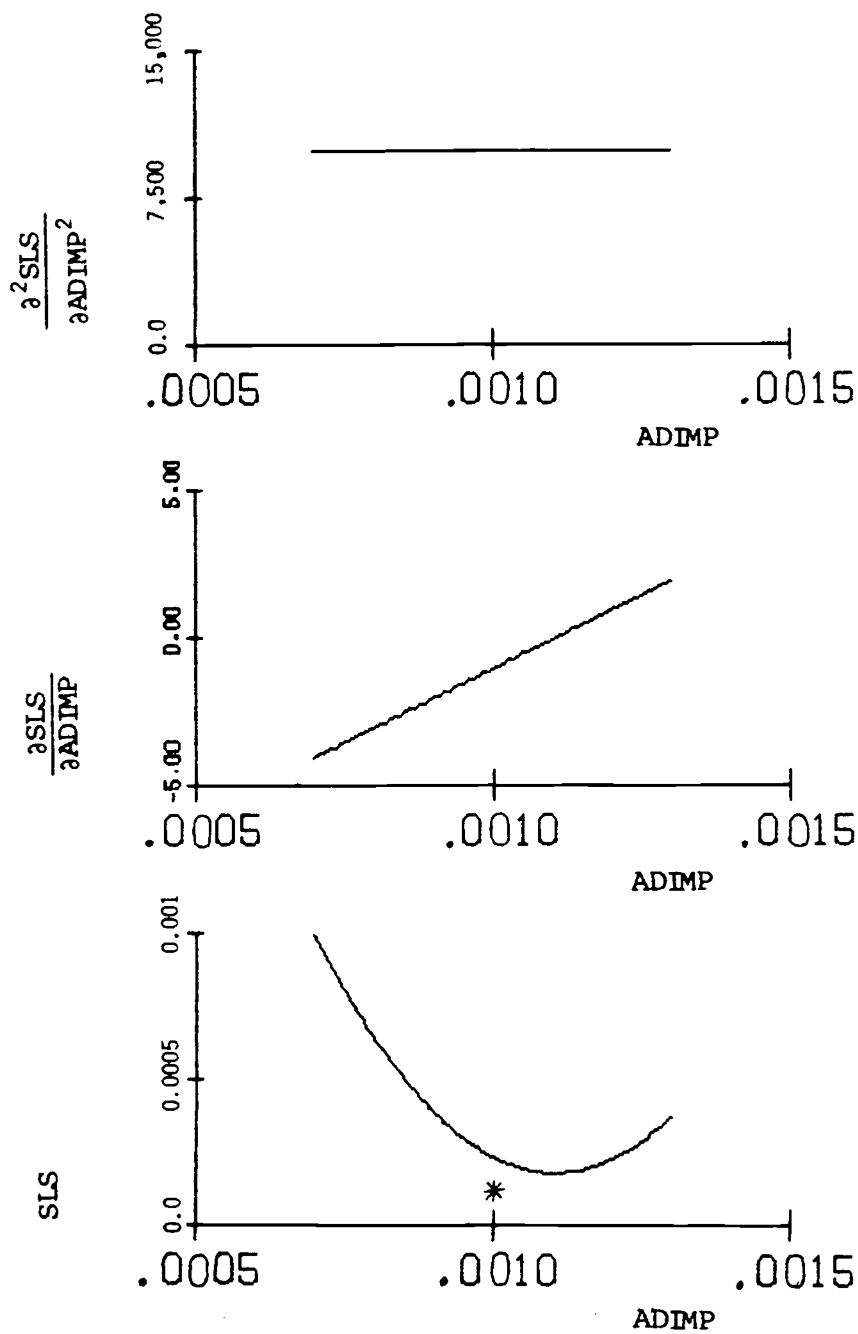

Figure 6.10. Cross-section and derivatives of SLS function along axis of parameter ADIMP.

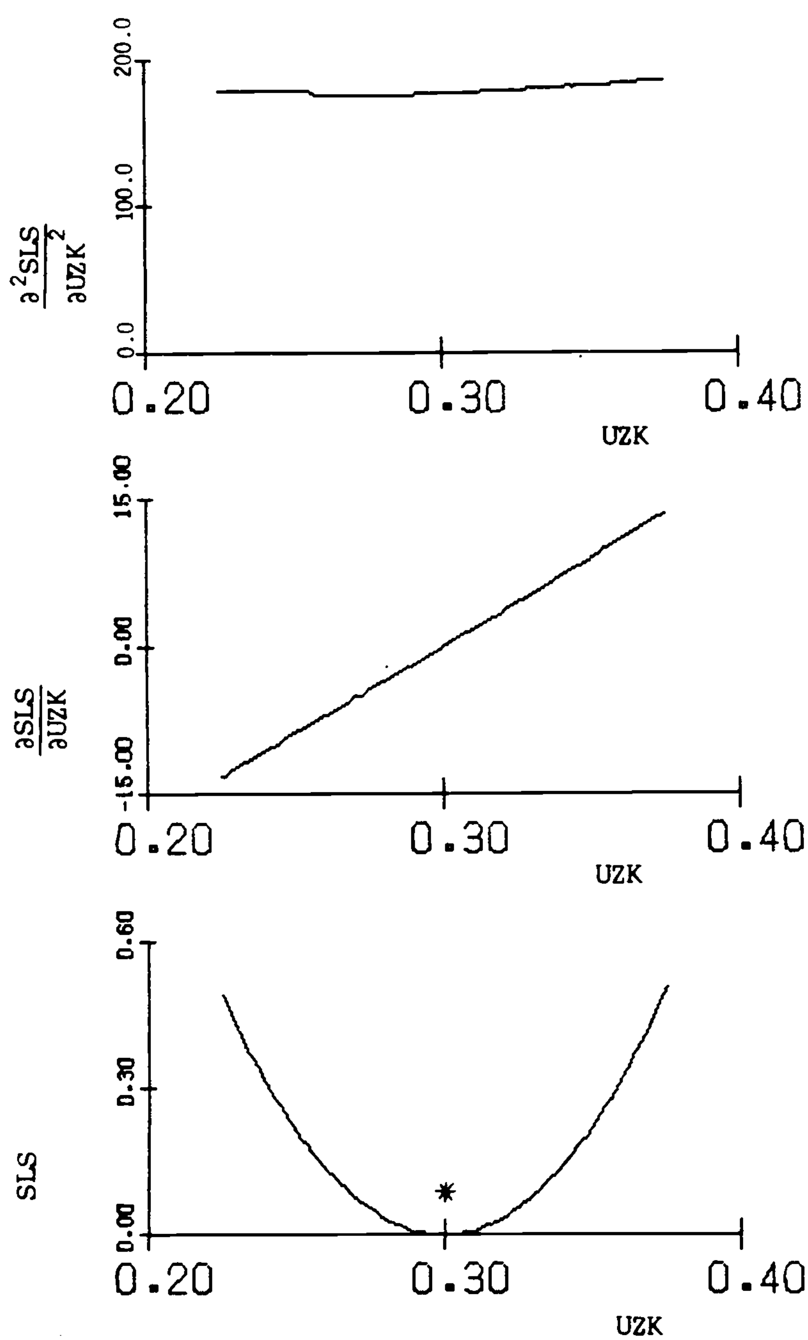

Figure 6.11. Cross-section and derivatives of SLS function along axis of parameter UZK.

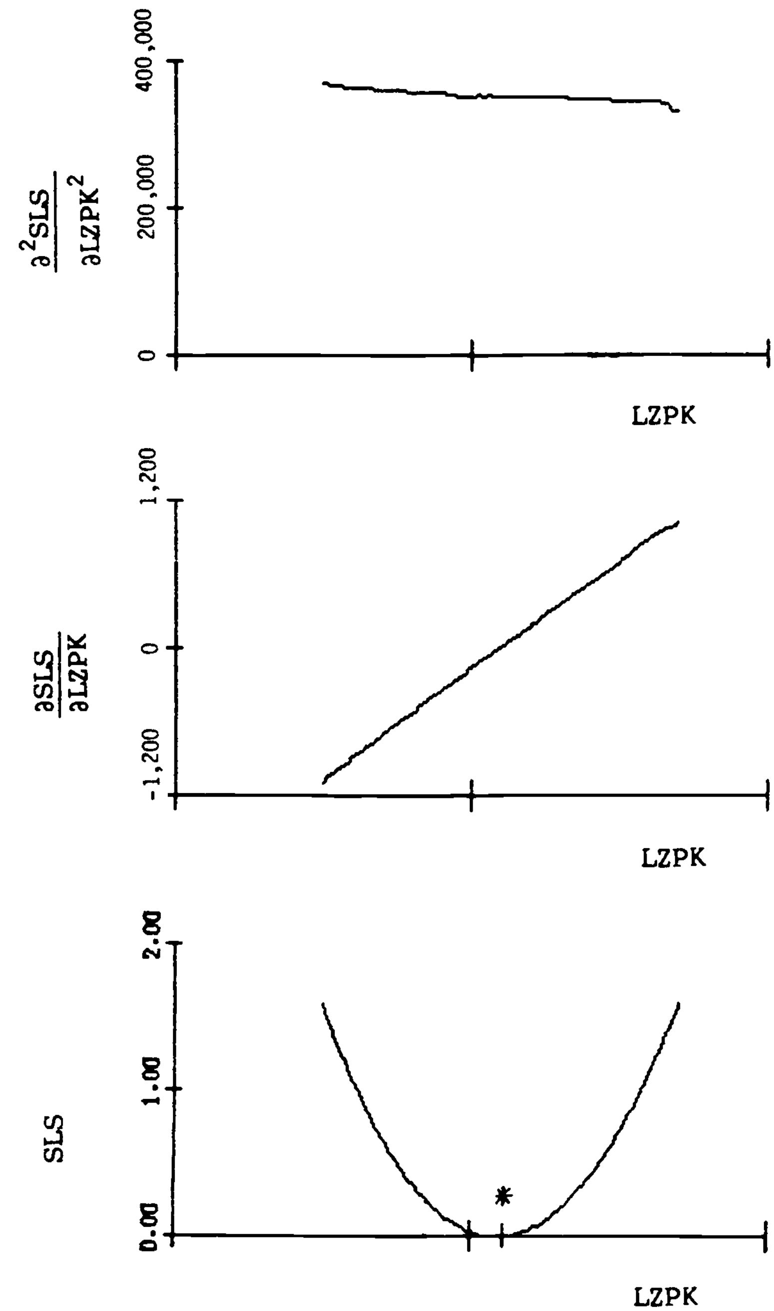

Figure 6.12. Cross-section and derivatives of SLS function along axis of parameter LZPK.

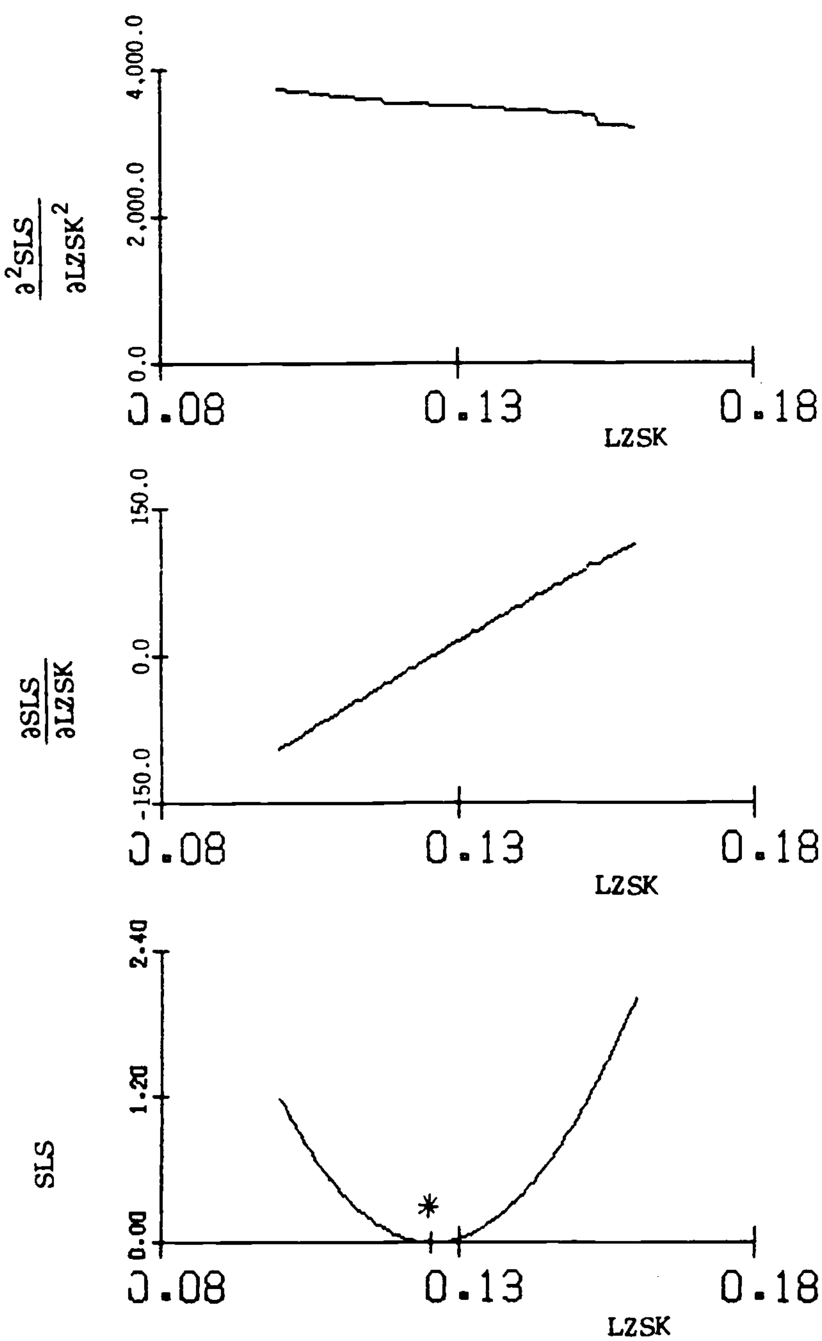

Figure 6.13. Cross-section and derivatives of SLS function along axis of parameter LZSK.

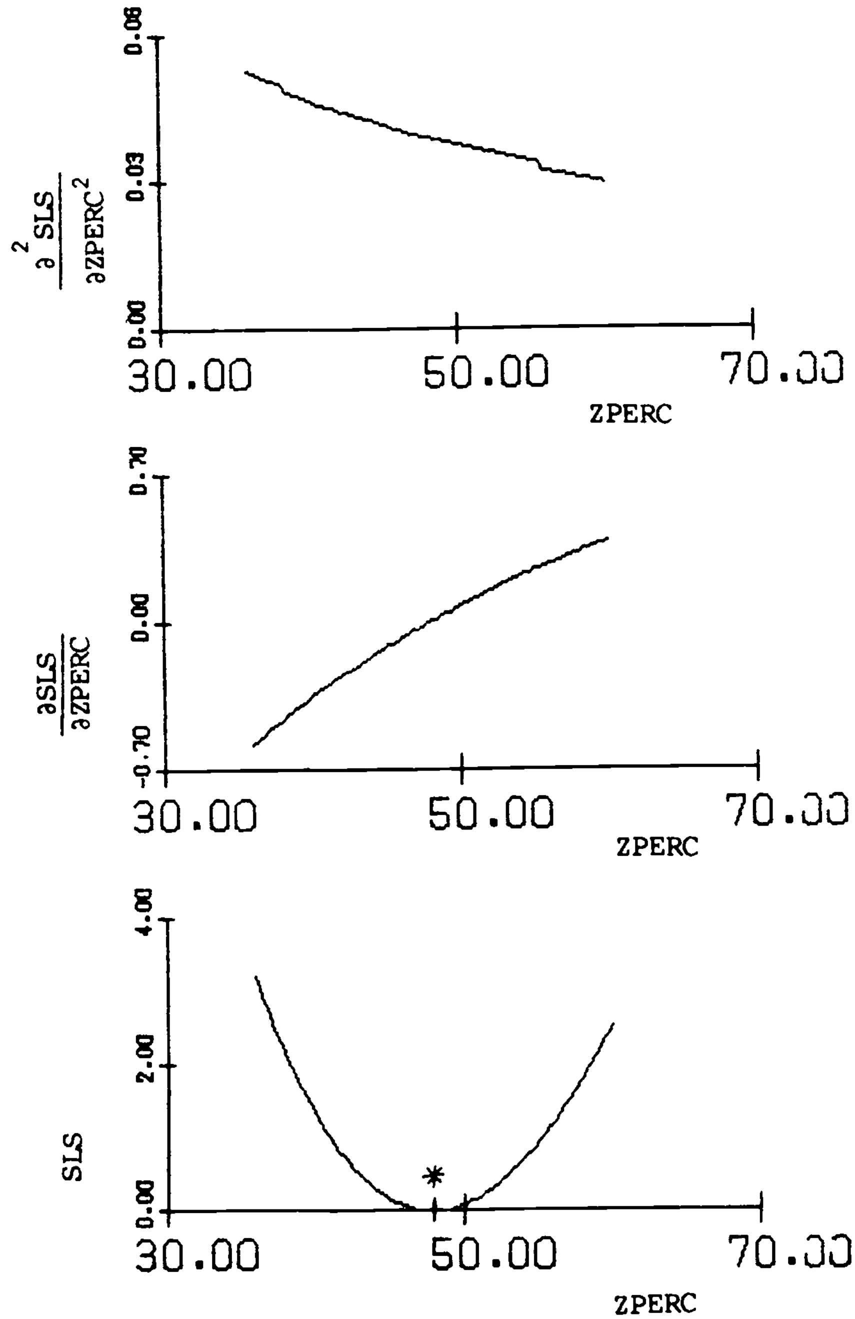

Figure 6.14. Cross-section and derivatives of SLS function along axis of parameter ZPERC.

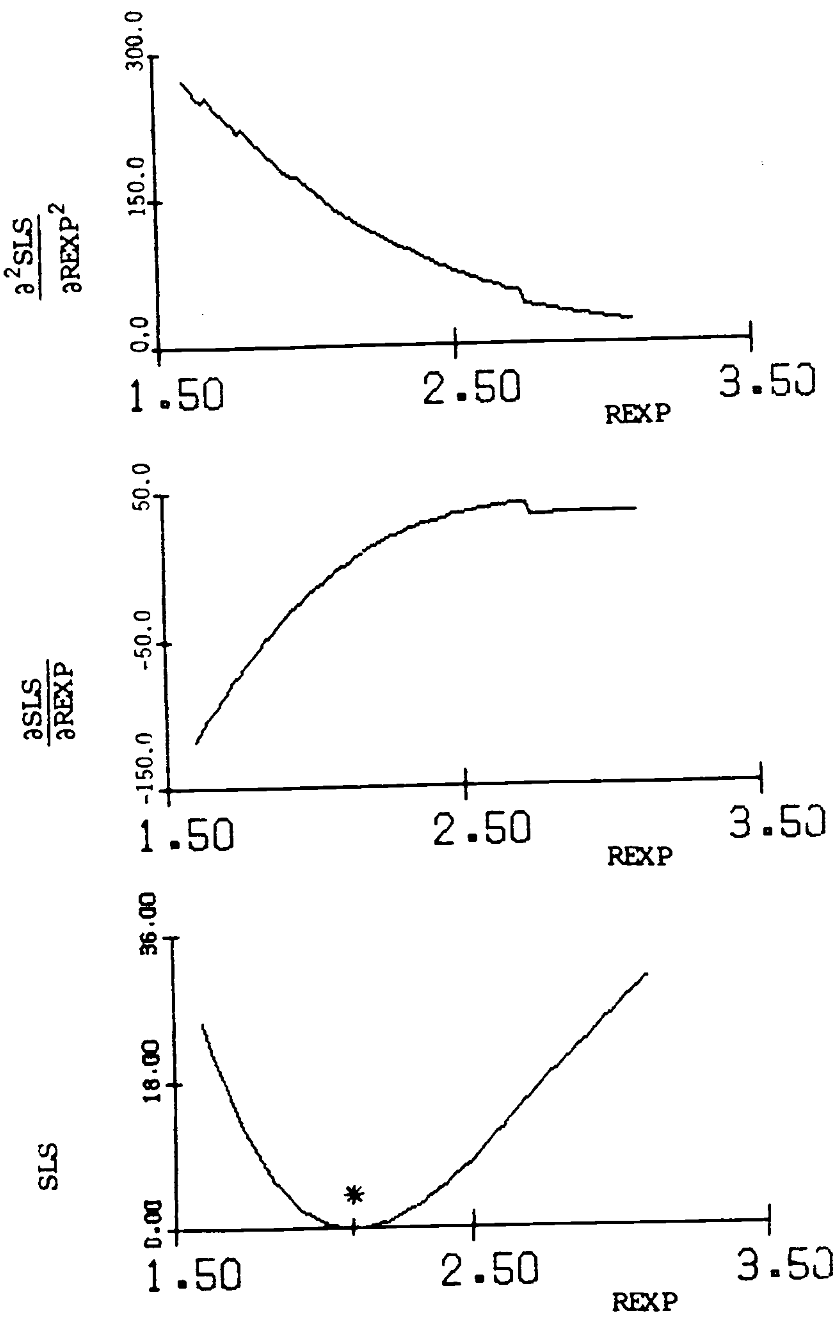

Figure 6.15. Cross-section and derivatives of SLS function along axis of parameter REXP.

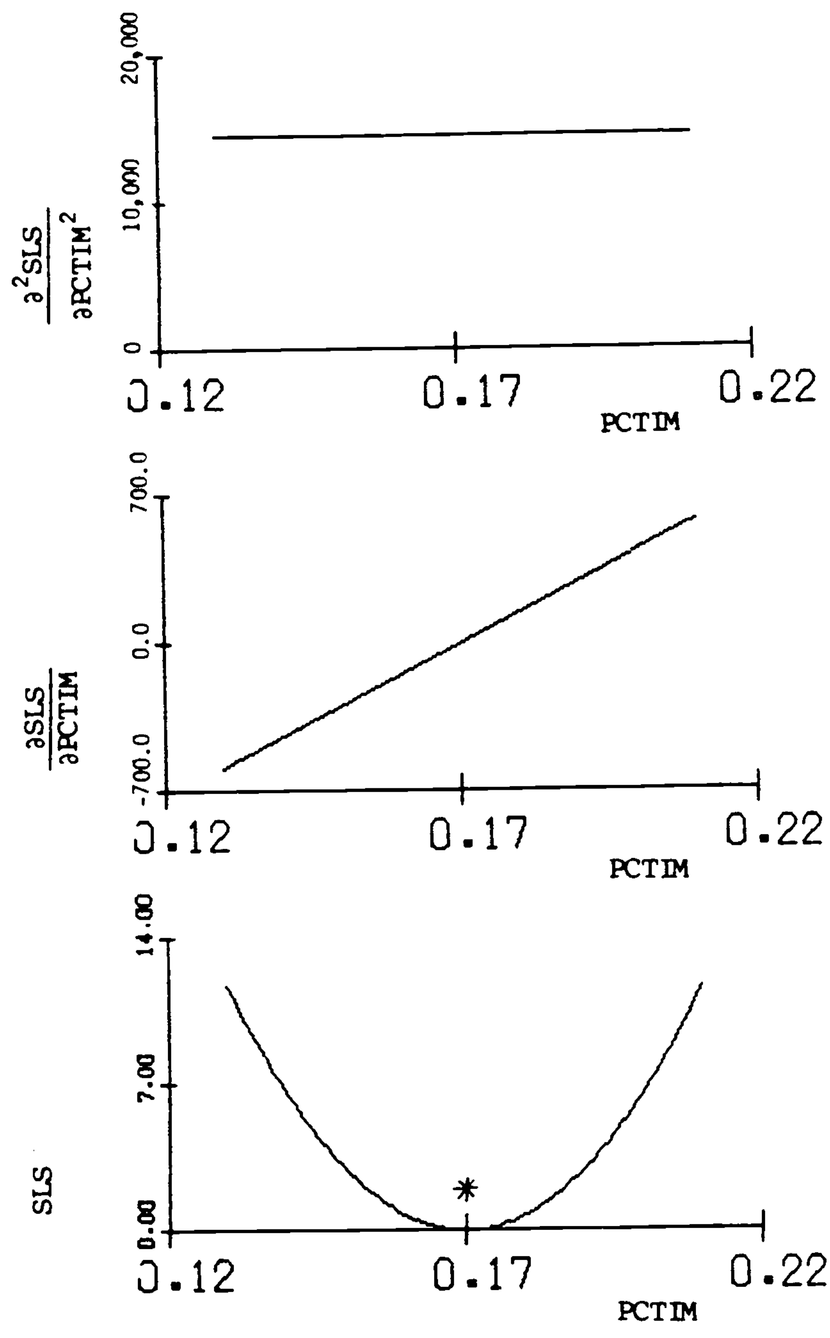

Figure 6.16. Cross-section and derivatives of SLS function along axis of parameter PCTIM.

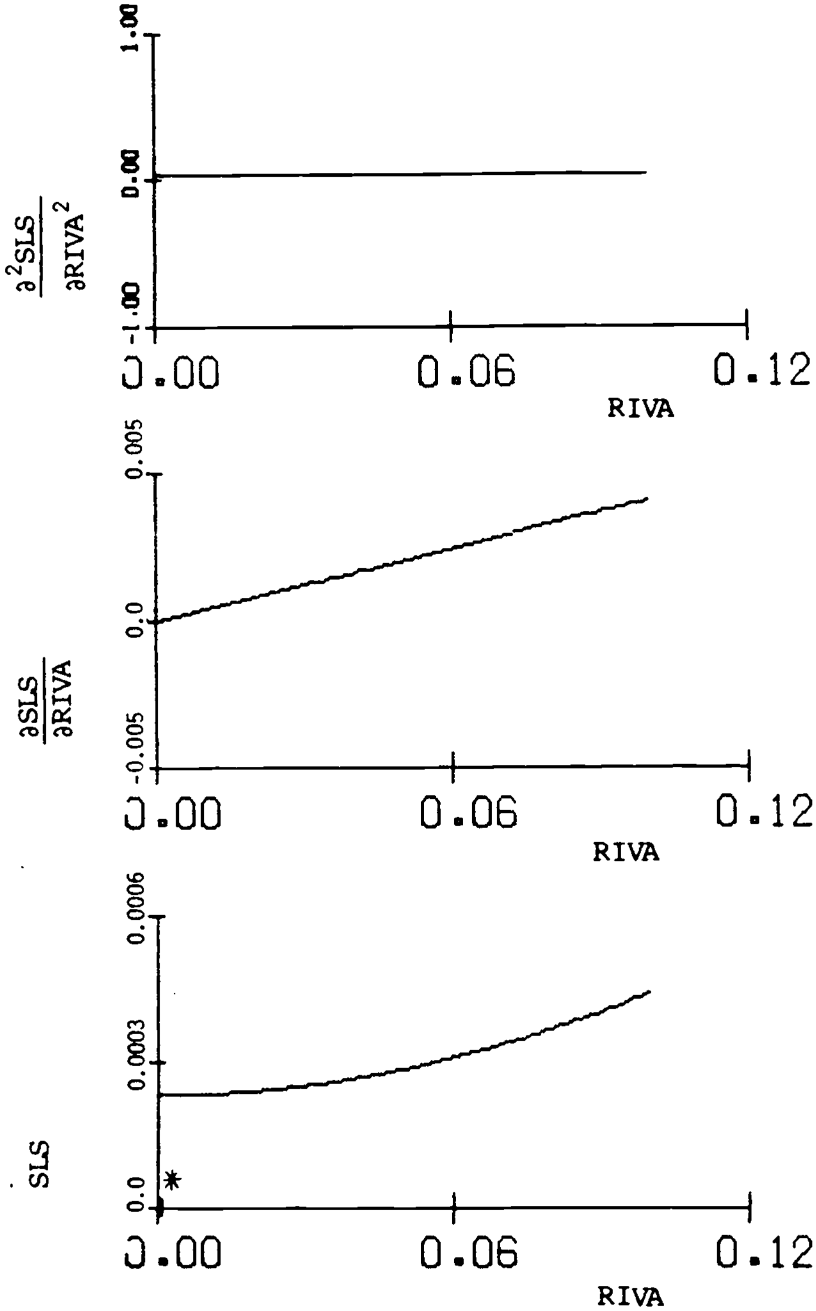

Figure 6.17. Cross-section and derivatives of SLS function along axis of parameter RIVA.

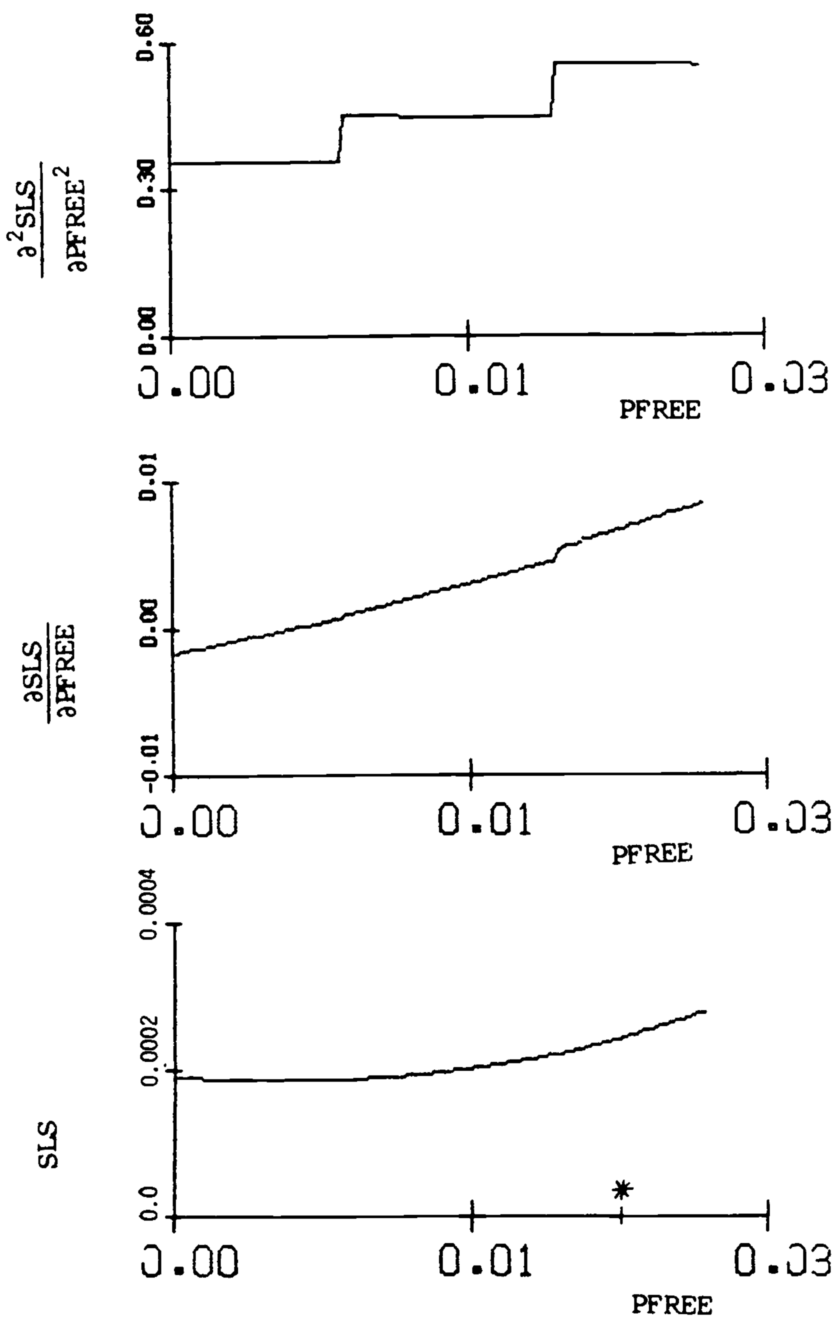

Figure 6.18. Cross-section and derivatives of SLS function along axis of parameter PFREE.

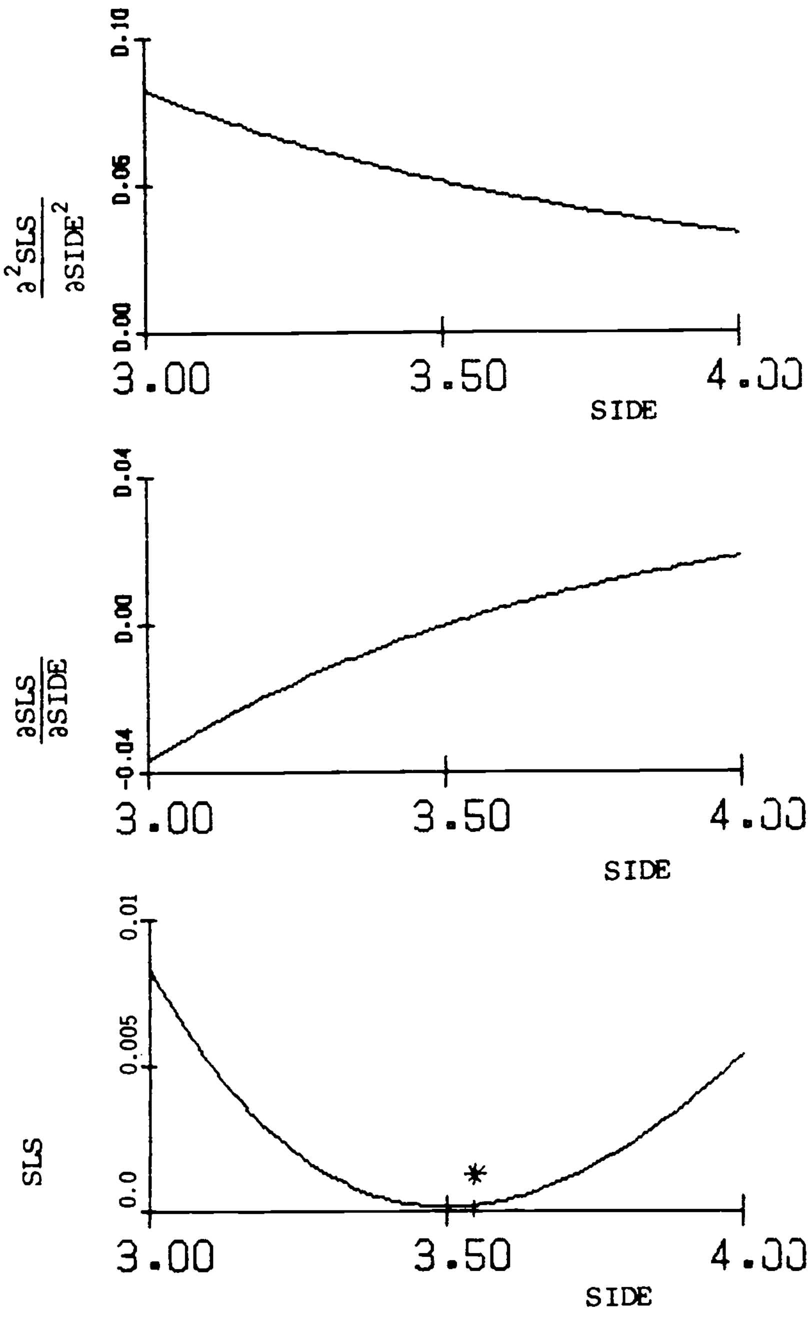

Figure 6.19. Cross-section and derivatives of SLS function along axis of parameter SIDE.

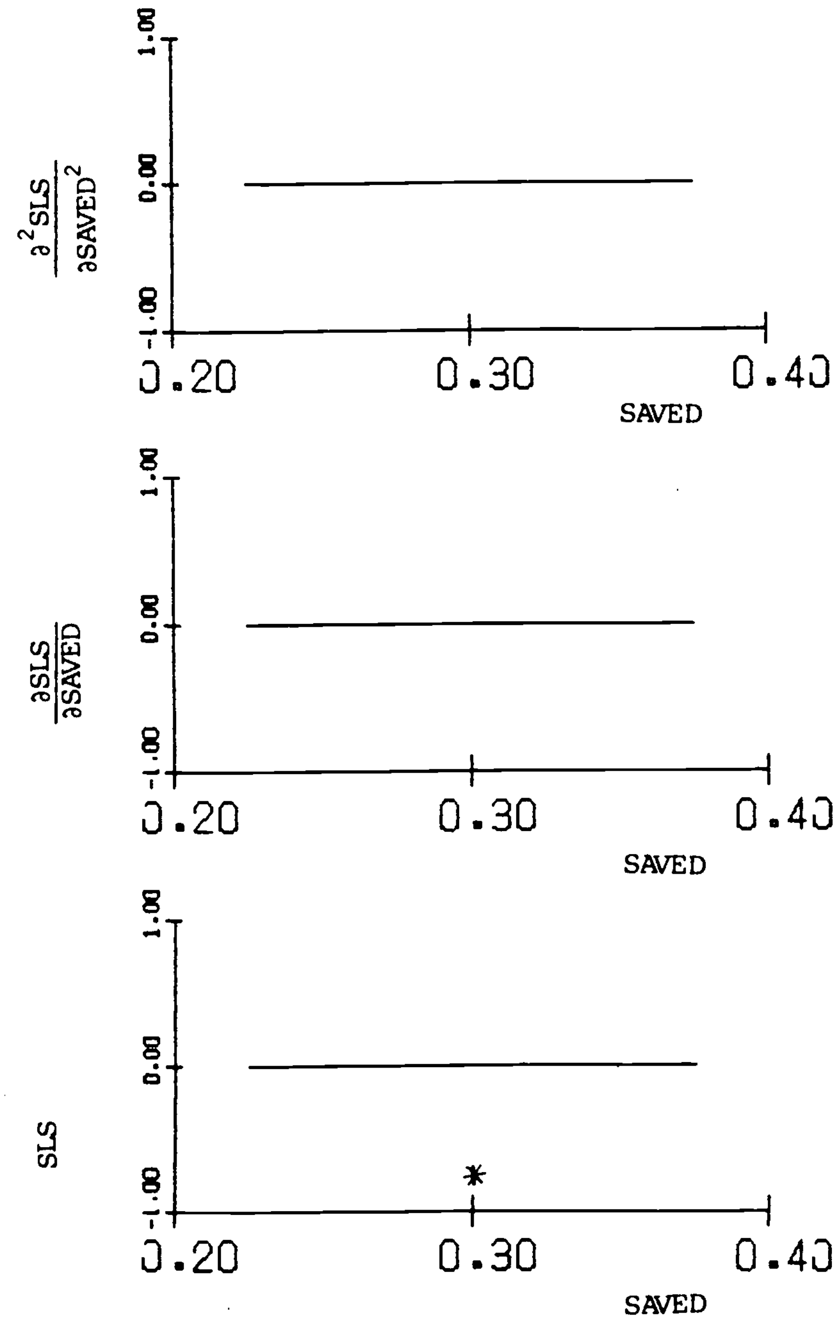

Figure 6.20. Cross-section and derivatives of SLS function along axis of parameter SAVED.

attempting to estimate SAVED except unnecessarily complicating the parameter estimation process.

Two aspects of the response surface are of special interest here.

(1) Is the surface convex in the region of the global optimum?

(2) Are the surface and its derivatives smooth and continuous?

If the response surface is convex along each of the parameter axes near the global optimum, then it is convex in multi-parameter space. A convex response surface is highly desirable for successful model calibration. Fortunately, the response surface plots show that the generated surface is convex near the "true" parameter values, for each parameter.

As will be discussed in the next section, CRR models such as the Soil Moisture Accounting model appear to have neither continuous estimation criteria nor continuous derivatives. If a gradient algorithm sampled the estimation criterion at a discontinuity at which the derivatives blow up, the algorithm would also blow up. However, extensive sampling of the Soil Moisture Accounting model's estimation criterion has always yielded finite values of derivatives. Therefore, it appears that both the criterion and its first and second derivatives are piecewise continuous, and everywhere finite. It is to be expected that these discontinuities will adversely affect a gradient algorithm. They do not, however, prevent its use.

The behavior of the first and second derivatives of the estimation criterion is important because these derivatives control the step direction during optimization with a derivative-based algorithm. Smooth, continuous derivatives will improve the efficiency and reliability of calibration.

In this study, the derivatives with respect to most parameters were relatively smooth and well-behaved, but the derivatives with respect to most of the reservoir storage parameters were poorly-behaved. Derivatives with respect to parameter UZPK, shown in Figure 6.12, are typical of well-behaved derivatives. Derivatives with respect to parameter UZTWM, shown in Figure 6.5, were the most poorly-behaved. The lack of smoothness in the derivatives of the objective function is a matter of concern, because they may make the use of a derivative-based optimization algorithm less efficient.

Discontinuity Investigation

Close examination of the SLS estimation criterion, whose generation is discussed in the previous section, reveals the existence of discontinuities in the function and its derivatives. This discovery posed three questions: What is the cause of the discontinuities? To what extent will they affect the parameter estimation process? Is there any way to eliminate them? Attention is given here to the first question.

A discontinuity in the first and second derivatives but not the function itself was the most common type of discontinuity observed. Figure 6.21 shows a closeup of this phenomenon. Discovering a discon-

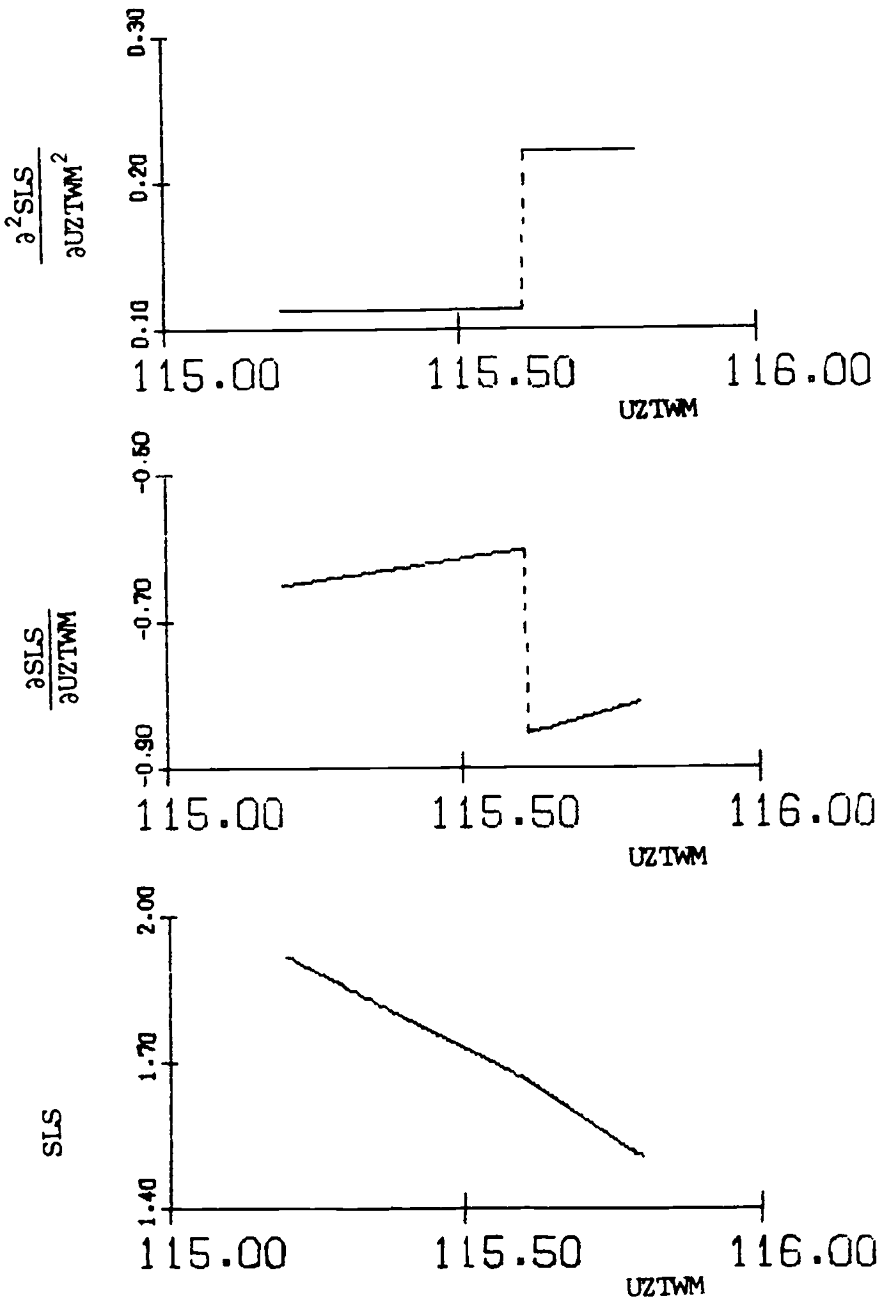

Figure 6.21. Example of a discontinuity in the derivatives of an estimation criterion.

tinuity is not always straightforward. The function can only be sampled at discrete points, and if the discontinuity is small relative to the distance between sampling points, it could be overlooked. For example, the discontinuity in the function shown in Figure 6.22 was not visible at the larger scale of Figure 6.23. Please note that the dotted lines in Figures 6.21 and 6.22 have been drafted by hand to indicate a discontinuity. In all other response surface plots, the automatic plotter drew a solid line between sampled points; the presence of a discontinuity must be inferred from abrupt changes in value.

Restrepo-Posada and Bras (1982) found discontinuities in a log likelihood function generated by the Soil Moisture Accounting model. They believed that the cause of the discontinuities was the variable time step employed by the model. The variable NINC represents the number of times the model passes through an inner calculation loop. When more water is processed through the model, NINC increases, and the model integrates over time more effectively with more accurate results. For example, if at time t NINC equals, say, 5 for a certain parameter set. It can be argued that if the parameter set is changed slightly, NINC may then equal, say, 4 and the model will be less accurate and the objective function will increase, leading to a discontinuity (Restrepo-Posada and Bras, 1982).

Another possible cause of discontinuities is the existence of thresholds in the structure of the Soil Moisture Accounting model. For example, overland flow will not occur until the upper zone free reservoir fills and overflows. Discontinuities could occur because overflow

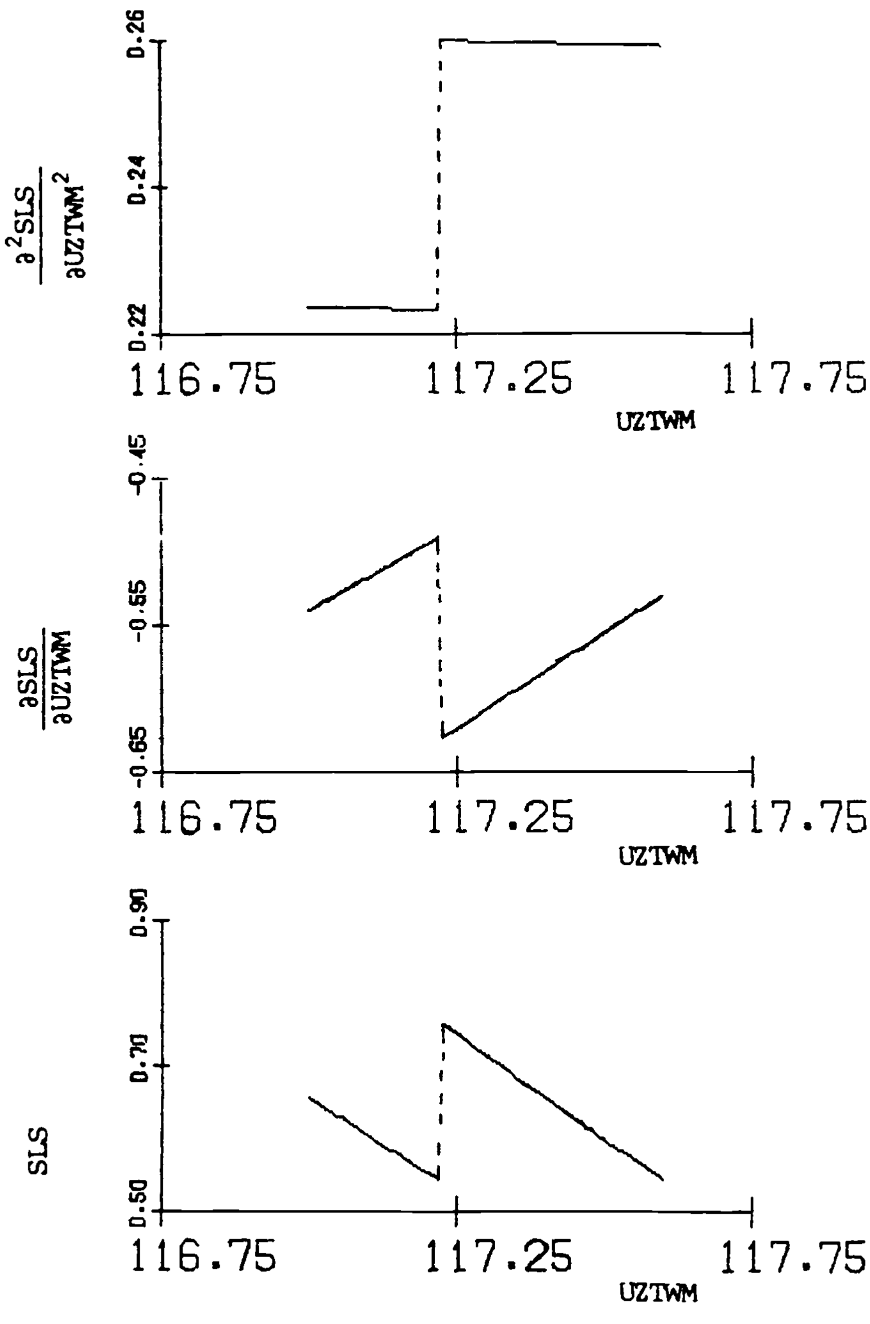

Figure 6.22. Example of a discontinuity in an estimation criterion and its derivatives.

This figure is a closeup of Figure 6.23.

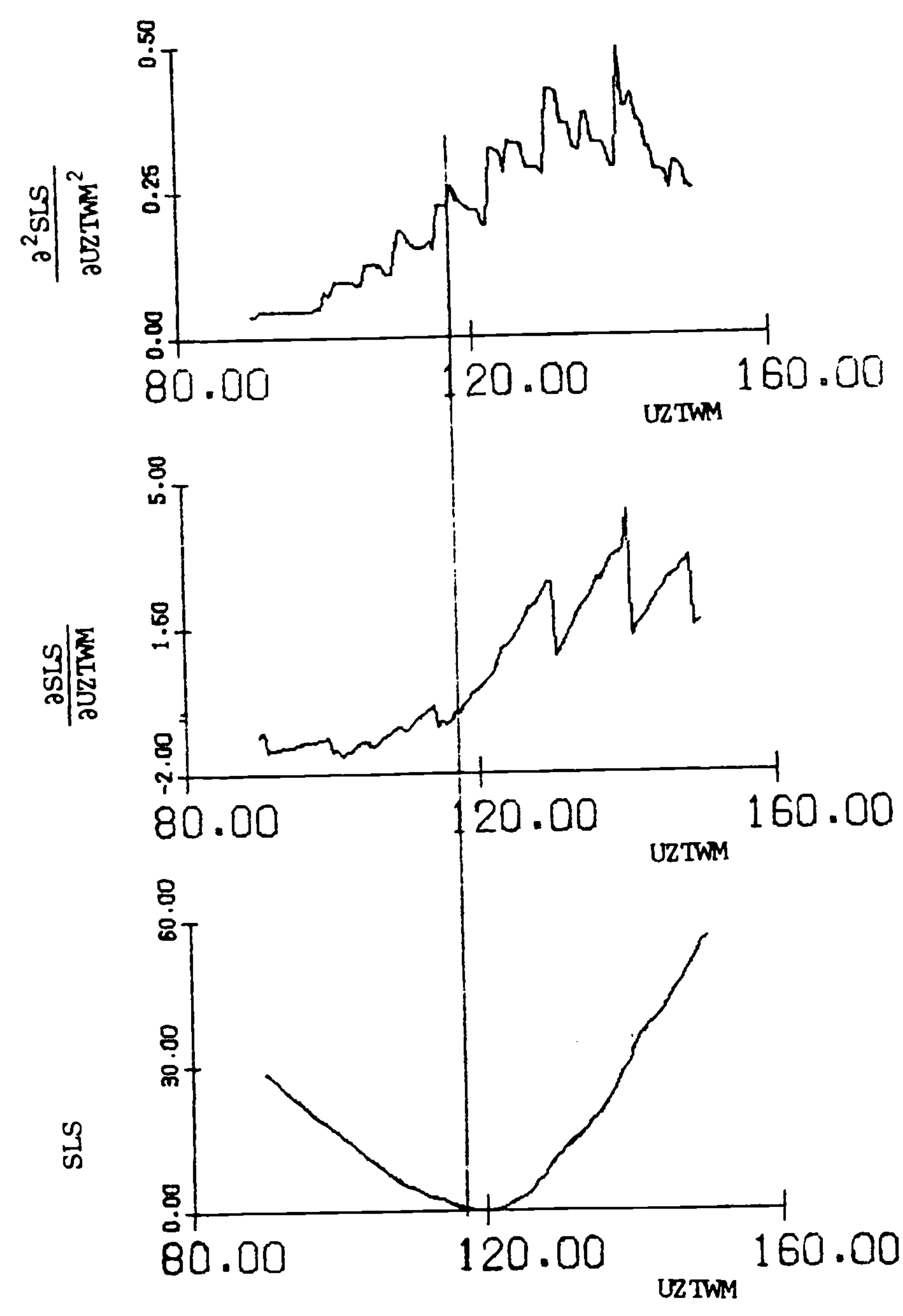

Figure 6.23. Discontinuity of Figure 6.22 on a larger scale.

The long vertical line marks the location of the discontinuity shown in Figure 6.22.

occurs for a certain value of parameter UZFWM (upper zone free water maximum) and not for a slightly larger value of UZFWM. It should be noted that Figures 6.5 through 6.20 indicate that discontinuities are most often associated with parameters which describe a threshold. The worst discontinuities were associated with the paramater UZTWM (upper zone tension water maximum) which describes the most significant threshold in the model.

The following exercise tested the hypothesis that the inner calculation loop is the cause of the discontinuities. Four versions of the Soil Moisture Accounting model were prepared: the original model, one with the inner calculation loop automatically set to one pass, and two intermediate versions. Cross sections of the repsonse surfaces of these models were generated along the axis of parameter UZTWM. The methodology for doing this is the same as for the response surface studies described earlier in this chapter. The four methods of determining the value of NINC were:

$$NINC = 1 + [x(t) + PAV(t)] / 5 \qquad \text{(original model)}$$

$$NINC = 1$$

$$NINC = 5$$

$$NINC = 1 + PAV(t) / 5$$

where

x(t) = upper zone free water contents at time step t; and

PAV(t) = precipitation in excess of tension storage requirements at time step t.

It was expected that removing the inner loop would eliminate or reduce the discontinuities. However, as can be seen in Figures 6.24 through 6.26, the alternate methods failed to definitively improve the properties of the reponse surface.

Proving the cause of the discontinuities associated with the Soil Moisture Accounting model is a difficult task due to the high degree of model complexity and nonlinearity. Therefore, an analysis was carried out with two simple models, each of which contains a significant feature of the Soil Moisture Accounting model. Model BOX, shown in Figure 6.27, generates streamflow only when cumulative rainfall minus evaporation exceeds the threshold and the reservoir overflows. The streamflow generated by model HOLE (Figure 6.28) is the product of reservoir contents and a recession constant. Model HOLE has an inner calculation loop identical to the one found in the Soil Moisture Accounting model. The important feature of model BOX is its threshold, and the important feature of model HOLE is its inner loop. Neither model has both features.

Response surface studies were carried out on model BOX and model HOLE using a precipitation sequence in which rainfall is constant in all time periods. A third run was done with model BOX and a precipitation sequence which caused the model to overflow three times (instead of once with the first precipitation sequence). A fourth run was done with a modified version of model HOLE in which the inner calculation loop was removed. Results are shown in Figures 6.29 through 6.32.

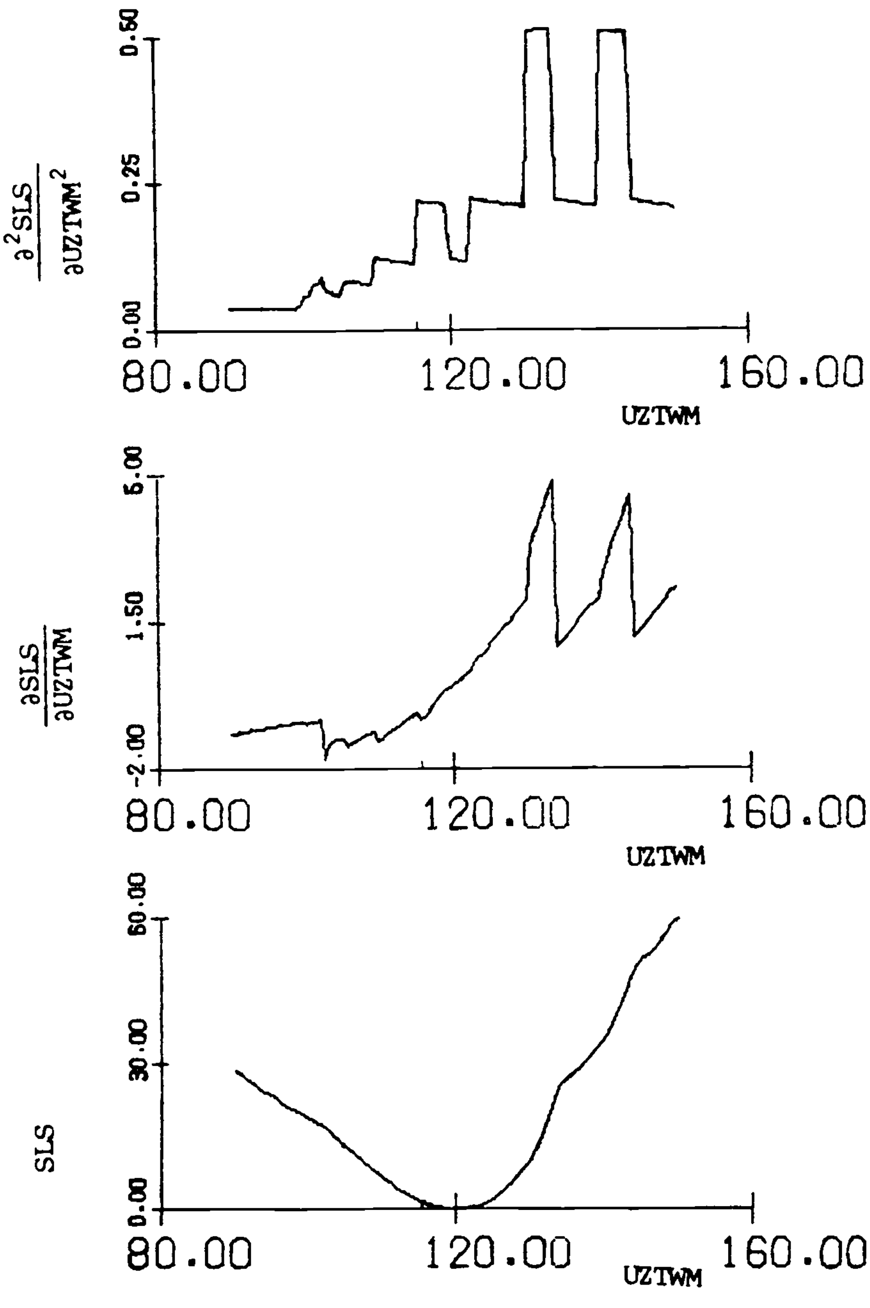

Figure 6.24. Response surface cross-section along UZTWM axis for model without inner loop calculation (NINC = 1).

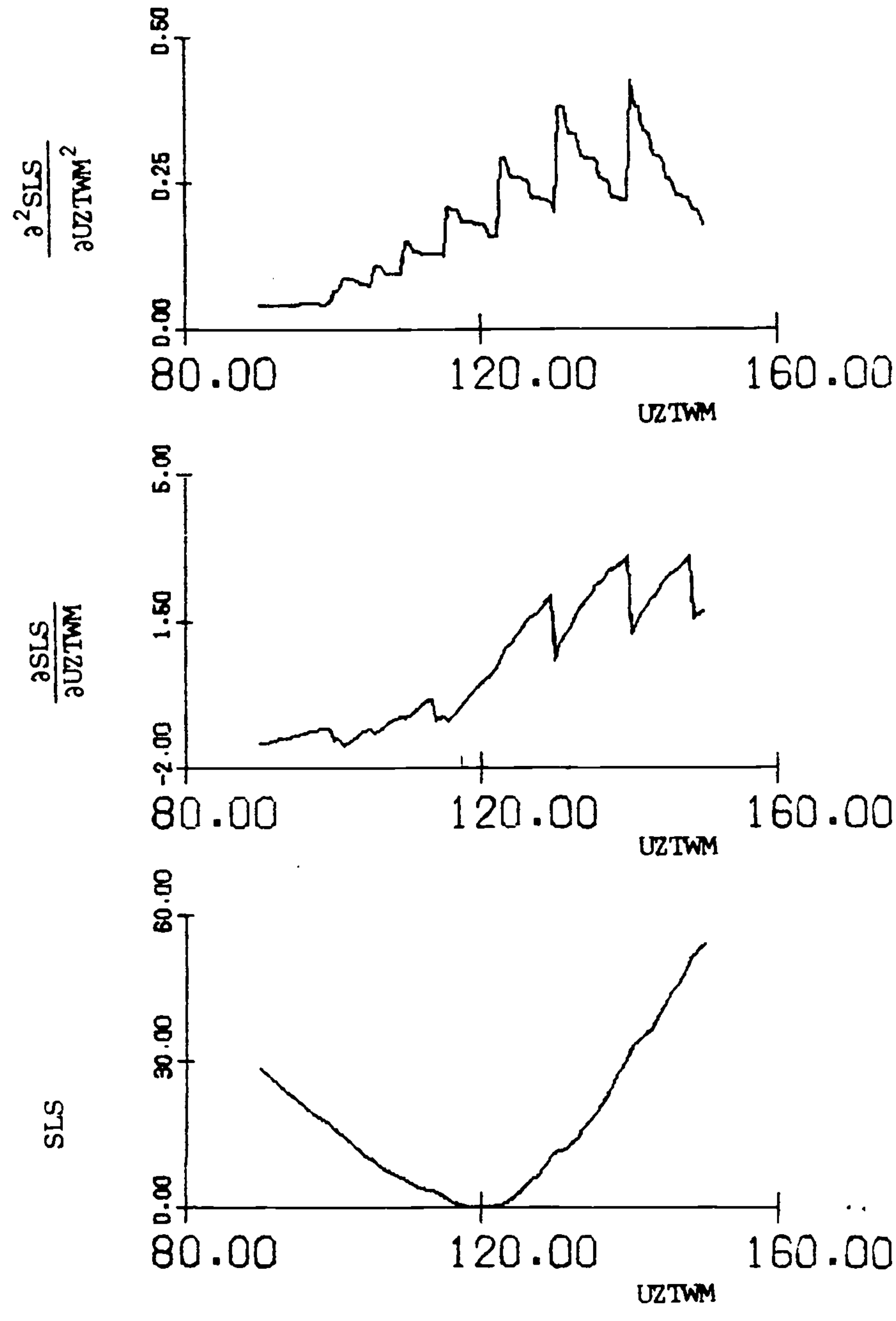

Figure 6.25. Response surface cross-section along UZTWM axis for model where NINC = 5.

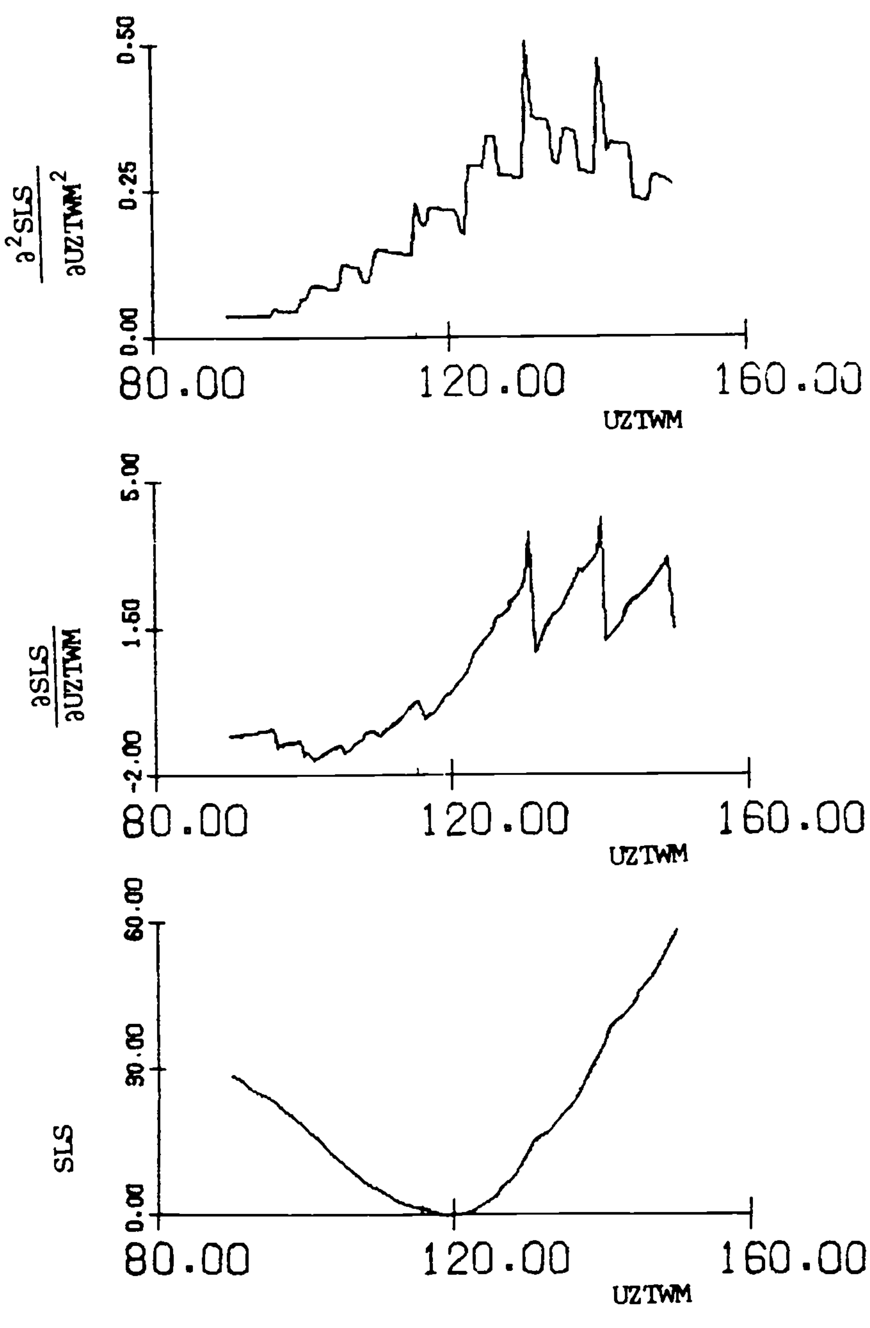

Figure 6.26. Response surface cross-section along UZTWM axis for model where inner loop is a function of precipitation only.

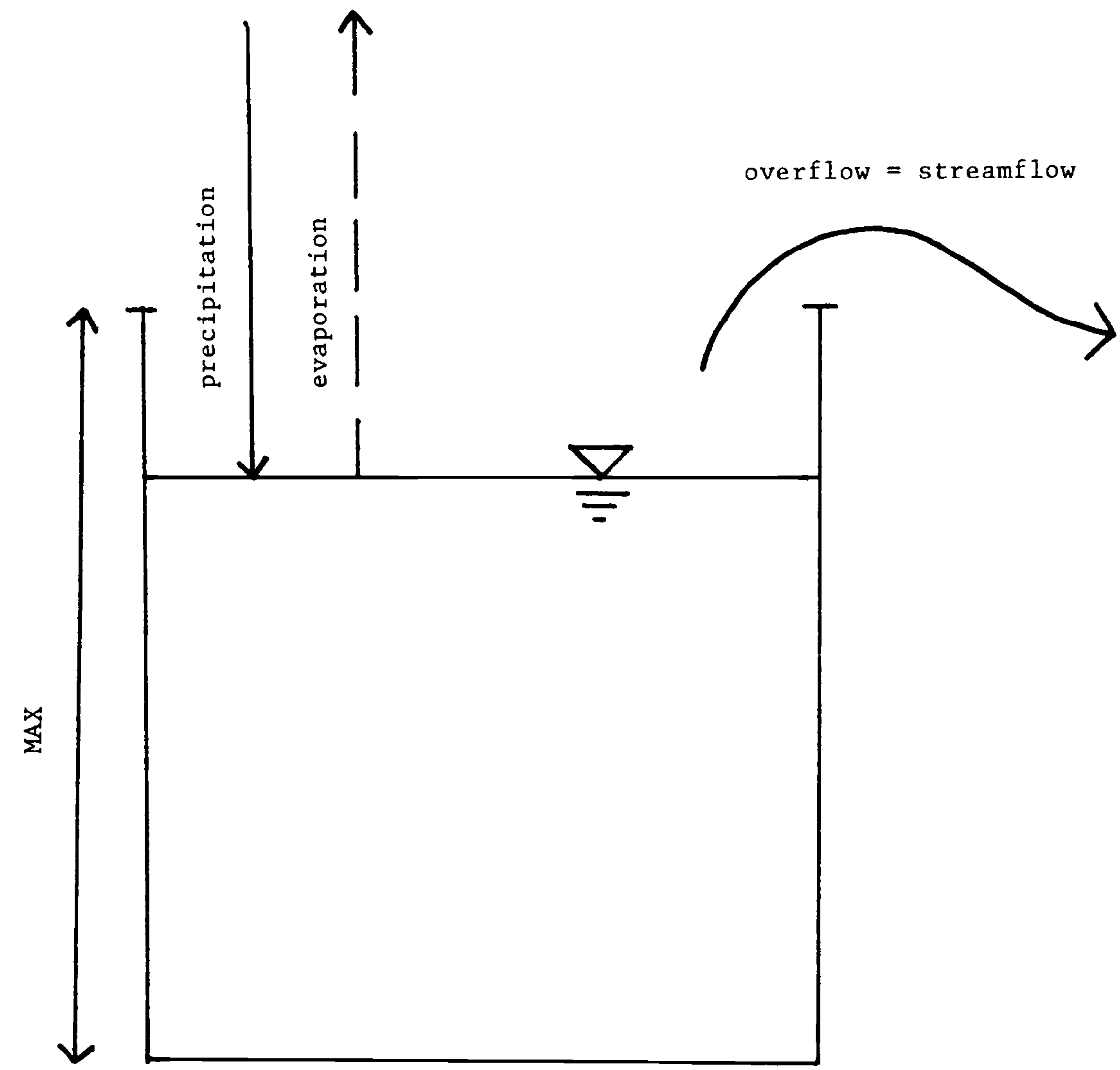

Figure 6.27. Model BOX

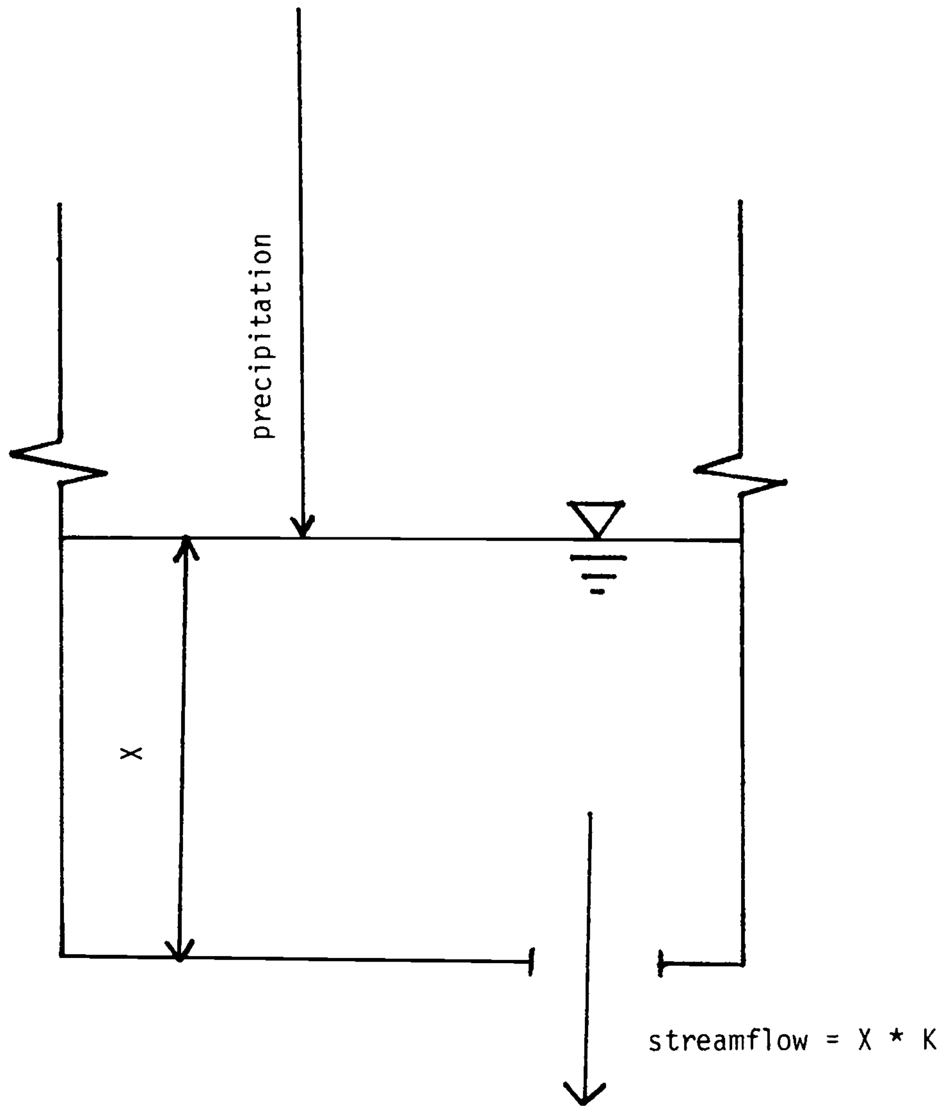

Figure 6.28. Model HOLE

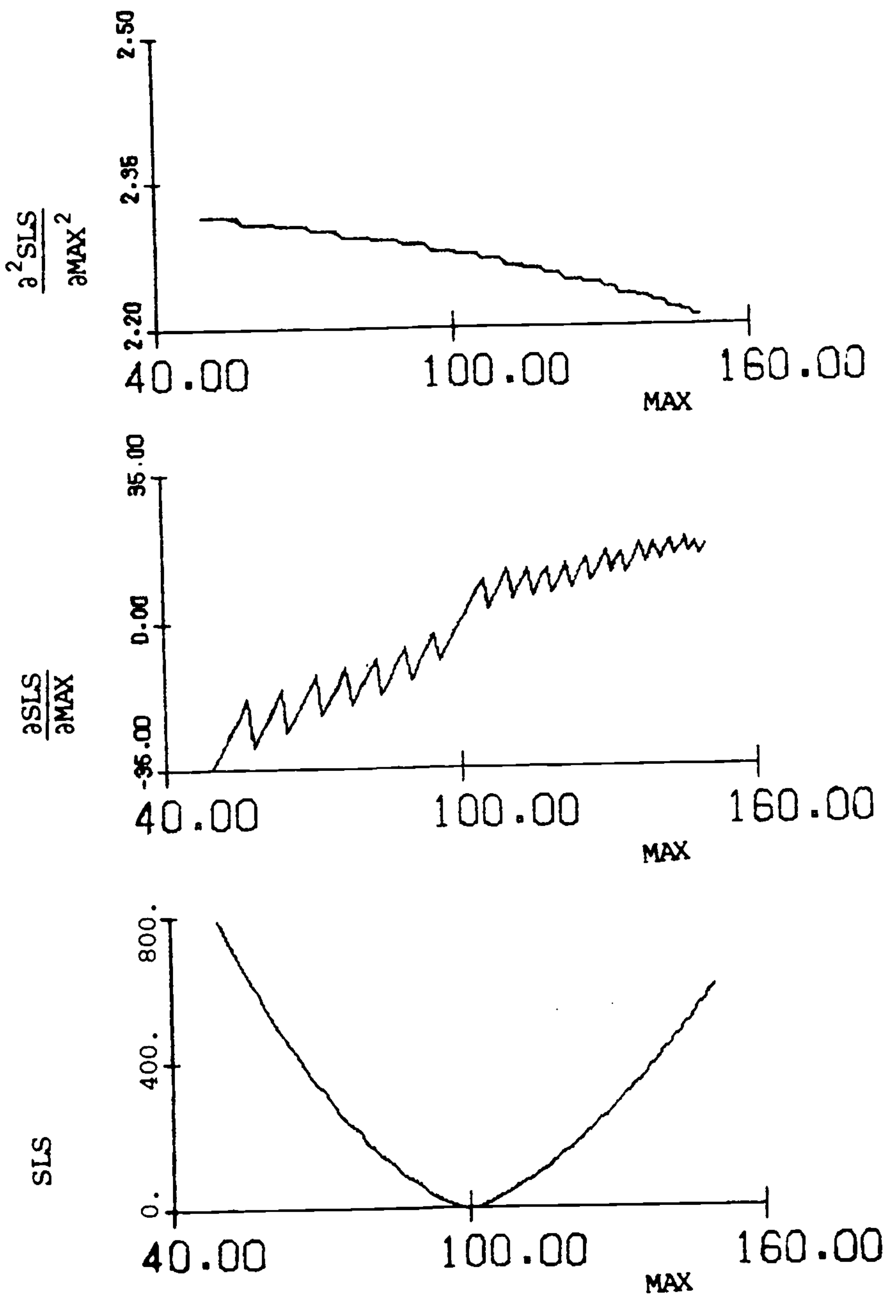

Figure 6.29. Response surface cross-section along MAX axis for model BOX and precipitation causing one reservoir overflow.

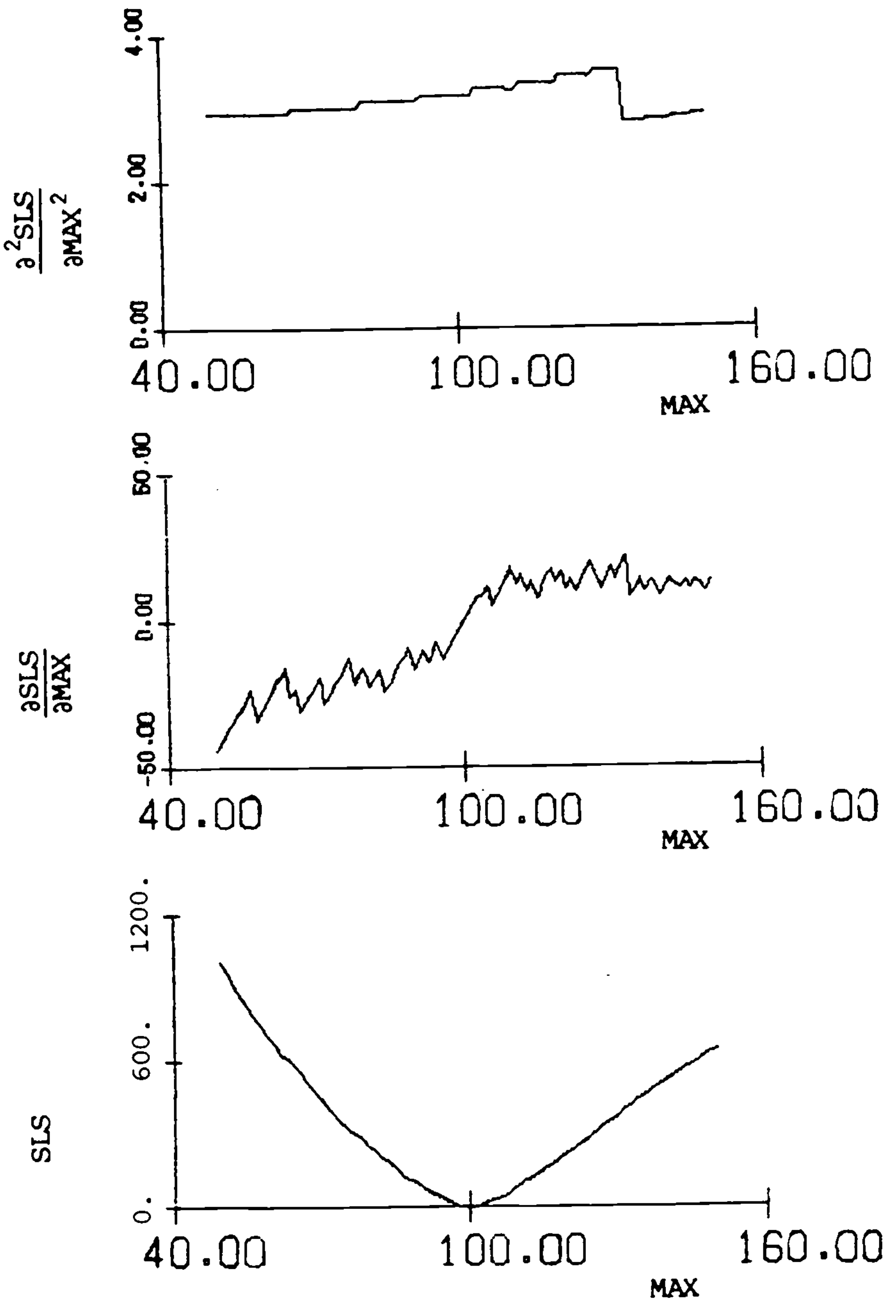

Figure 6.30. Response surface cross-section along MAX axis for model BOX and precipitation causing three reservoir overflows.

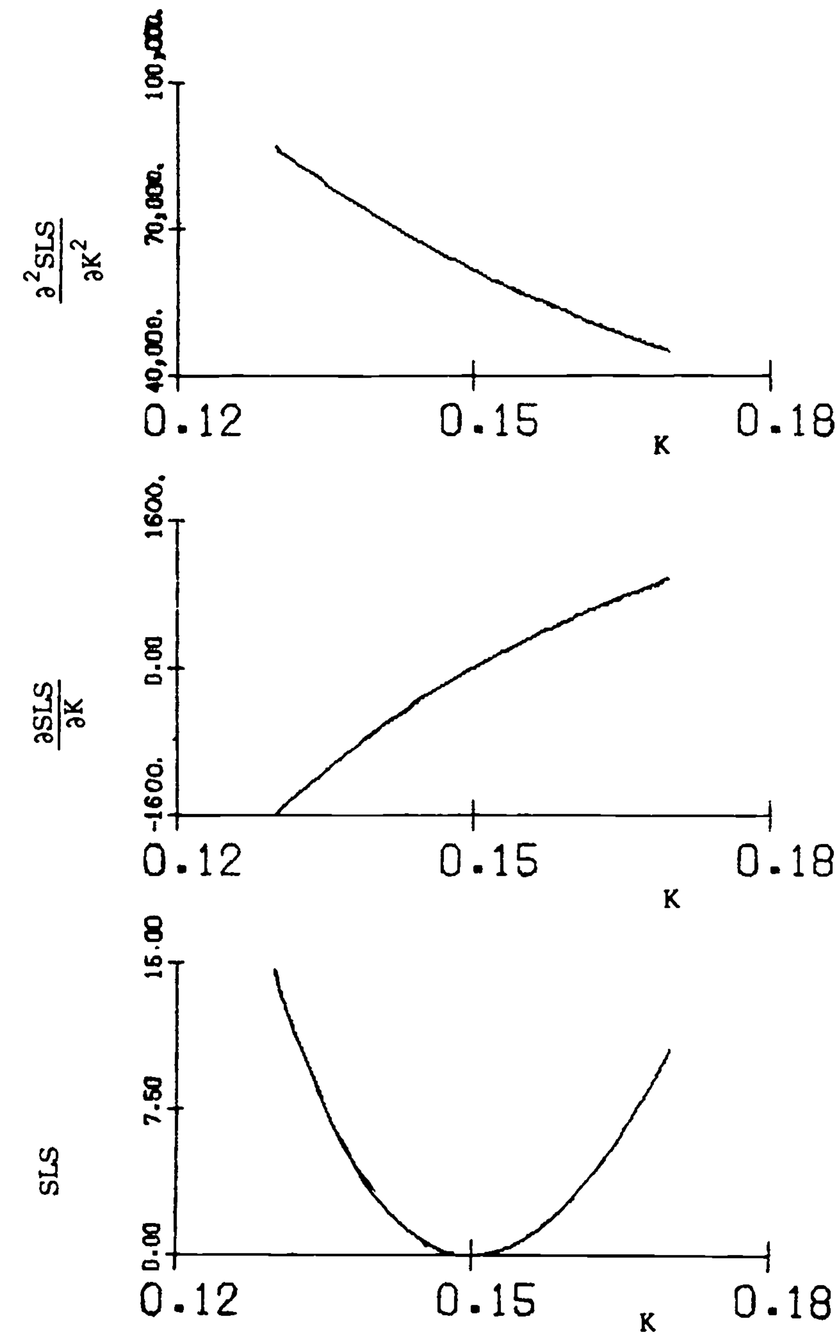

Figure 6.31. Response surface cross-section along K axis for model HOLE with inner loop.

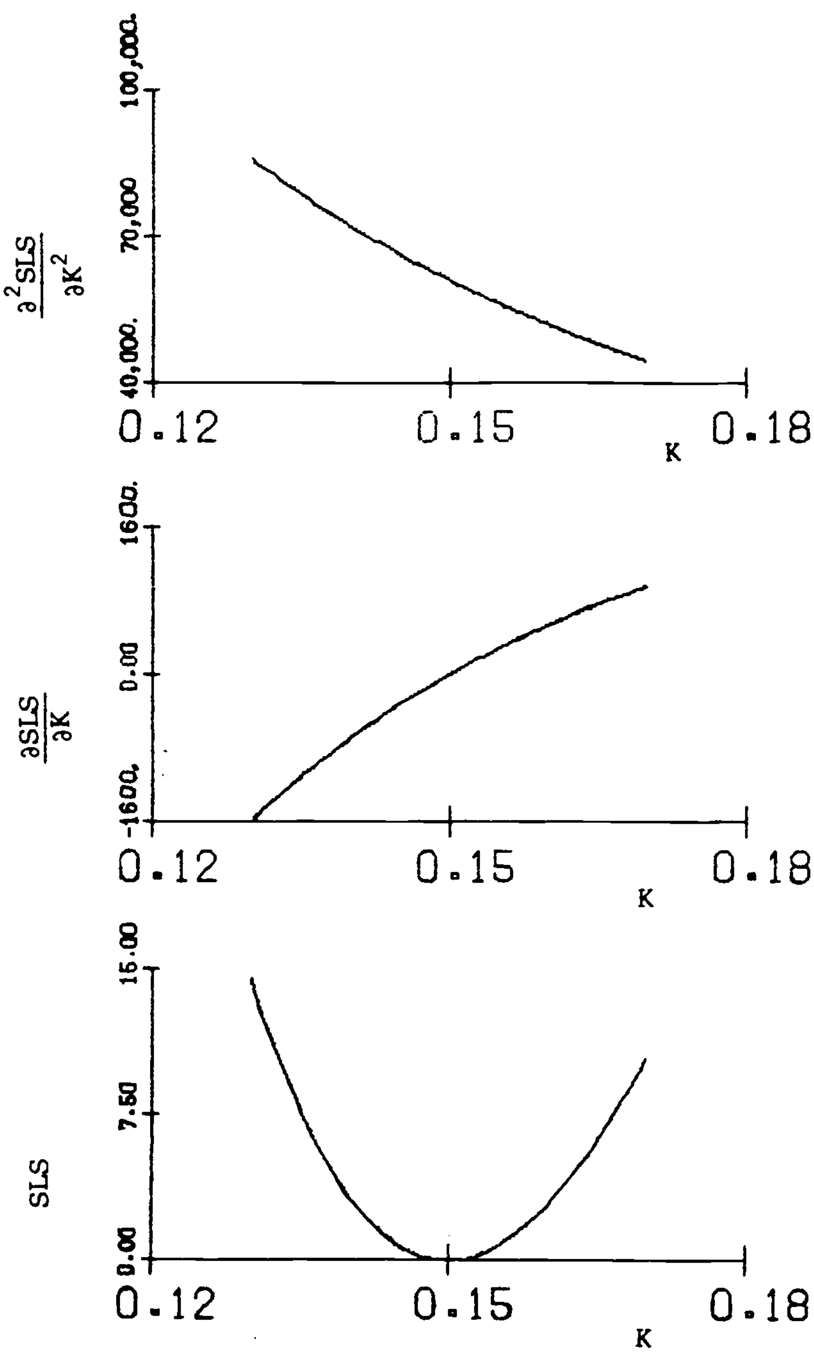

Figure 6.32. Response surface cross-section along K axis for model HOLE without inner loop.

was done with a modified version of model HOLE in which the inner calculation loop was removed. Results are shown in Figures 6.29 through 6.32.

If the inner calculation loop causes discontinuities, it would be expected that model HOLE would produce a discontinuous response surface when the inner loop was employed, and that the discontinuities would disappear when the loop was removed. However, this was not the case, as no discontinuities were associated with model HOLE, either with or without the inner calculation loop. If model thresholds were a cause of discontinuities, it would be expected that the model BOX would have a discontinuous response surface. This was indeed the case, and the natures of the discontinuities changed with the nature of the data, as expected. Based on these results, it seems reasonable to conclude that model thresholds in conjunction with a discrete time step are the cause of objective function discontinuities, and that the inner calculation loop associated with NINC is not a cause of discontinuities.

Gupta and Sorooshian (1985) have shown that for a model similar to model BOX, the identifiability of the threshold parameter (MAX) improves as the number of overflow events increases. However, it appears that the number of discontinuities may also worsen somewhat with increasing overflows. The benefit of an increase in identifiability probably overshadows the problem of increased discontinuities, however.

Since thresholds and discrete time steps are inherent features of CRR models, it appears that a discontinuous objective function and derivatives are also inherent features of any CRR model such as the Soil Moisture Accounting model. Since natural watersheds do indeed exhibit threshold behavior, removing thresholds from CRR models does not appear to be the solution.

CHAPTER 7

CALIBRATION STUDIES

Calibration studies were undertaken in order to compare the performance of direct-search and gradient algorithms in calibrating the Soil Moisture Accounting model. The pattern search algorithm of Hook and Jeeves (1961) was selected as a direct-search algorithm because it is currently used by the NWS. The Newton-Raphson algorithm, which is described in Chapter 2, was selected as the gradient algorithm. The bulk of the calibration studies were performed using synthetic data, but historical data from Bird Creek, Oklahoma were also used. Synthetic data were used so that the results of the study could be more easily interpreted, since neither data error nor model error are present.

The calibration study was broken down into the following steps:

(1) Creation of the synthetic data;

(2) Sensitivity and identifiability analysis;

(3) Calibration with synthetic data;

 (a) single parameter

 (b) multi-parameter; and

(4) Calibration with historical data.

Methods

In designing the calibration study, care was taken to make the the study as similar as possible to those performed by NWS personnel. For this reason, the study used six-hour precipitation totals and mean daily flows.

Initially, the daily root mean square (DRMS) estimation criterion discussed in Chapter 5 was used, since the NWS usually uses that criterion. However, it was found that the Newton-Raphson algorithm performed extremely poor using a DRMS criterion, but performed much better when using a simple least squares (SLS) criterion. The performance of the pattern search algorithm was unaffected by the choice of estimation criterion. It appears that the Newton-Raphson assumption of a quadratic response surface is met by the SLS surface, but not by the DRMS surface. Therefore, a SLS estimation criterion was used for the calibration studies presented here.

Synthetic Data

The synthetic data used in the calibration study differ from the synthetic data used in the response surface studies. One month of six-hour mean basin precipitation totals was generated by the author, using personal judgement as to what constituted a realistic precipitation sequence. Also, care was taken to ensure that all modes of the model were activated by the synthetic precipitation. To generate synthetic streamflows, the synthetic precipitation was input into the Soil Moisture Accounting model, the unit hydrograph subroutine, and the daily averaging subroutine, which averages six-hour flows into mean daily flows. The NWS parameter estimates for the Soil Moisture Accounting model and unit hydrograph were used, along with arbritarily selected initial states, in generating the synthetic flows. The synthetic data set is plotted in Figure 7.1.

Historical Data

The historical data used were from the Bird Creek catchment near Sperry, Oklahoma. The Bird Creek catchment has an area of 2344 square kilometers. Seven years of six-hour mean basin precipitation, mean daily flows, and estimated potential evapotranspiration were provided by the NWS for this study.

The period October 1955 through August 1956 was used to determine the initial contents for the calibration runs. The month of September 1956 was used as a buffer period preceeding the calibration period, which ran from October 1957 through September 1959. The split-sample verification period was from October 1959 to September 1962, preceeded by a six-month buffer period. The same initial contents were used for both the calibrations and verification runs. Buffer periods were used to minimize errors associated with initial contents. Flows during the buffer period are excluded from calculation of the estimation criterion.

Sensitivity and Identifiability Analyses

In order to obtain insight into the properties of the estimation criterion, a parameter sensitivity and identifiability analysis was performed using Bird Creek parameters. A discussion of methods and results is found in Chapter 8. During the calibration study, the

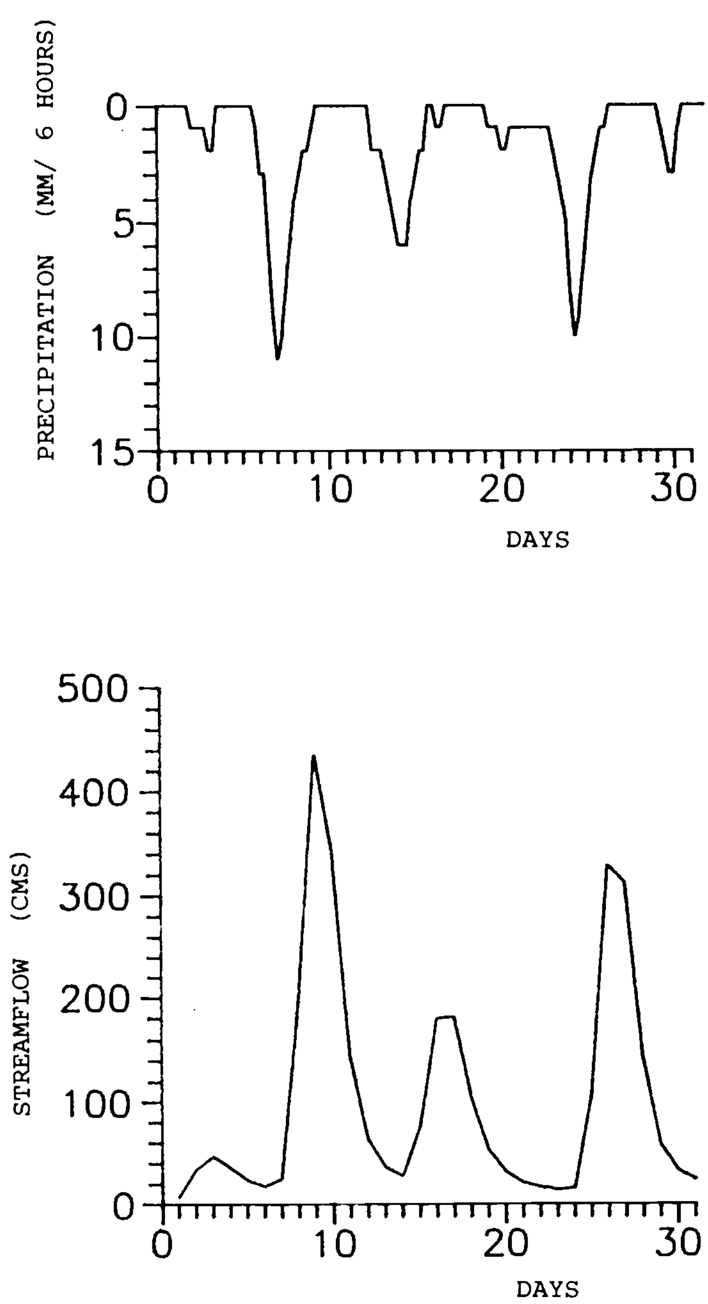

Figure 7.1. Plot of synthetic data used for the calibration study.

sensitivity and identifiability analyses were primarily useful in determining the relative degree of interaction between specific parameters and in determining the most sensitive parameters. In selecting parameter sets for calibration runs, sensitive parameters with an important conceptual role in the model were chosen. In most cases, parameter sets were chosen to reduce parameter interaction.

Synthetic Calibrations

Using synthetic calibration data, the value of the estimation criteria is zero at the true parameter set. Official NWS parameter estimates used to create the synthetic flows were used as the true parameters. Therefore, a successful calibration is easily defined as one which terminates at the true parameter set. In conducting the synthetic calibration study, the basic approach was to perturb selected parameters from their true values and use the perturbed parameters as initial parameter values of a calibration run using either the pattern search or Newton-Raphson optimization algorithms. The parameters to be optimized in any run were always specified to be the parameters which had been perturbed. The algorithm would search the multi-parameter space for a minima until one of several termination criteria were satisfied.

Three types of runs were performed: single-parameter, two-parameter and four-parameter. Single-parameter optimization is a relatively easy problem, and any optimization algorithm should be successful in the simplified case of synthetic data. However, multi-parameter optimization is a more difficult problem due to parameter interaction. The two-parameter runs were conducted to study the effect of the relatively straightforward two-parameter interaction on the calibration problem. Four-parameter runs dealt with more complex parameter interaction.

Parameters were perturbed 15, 35, or 50 percent for different runs. Since lower initial values may be more likely to produce successful calibration than high initial values due to certain response surface properties, the parameters were perturbed downward where possible. However, in some instances, it was not possible to perturb downward in order to maintain positive initial reservoir contents values, or to avoid initial values of zero. Also, since the NWSRFS software allows only a specified number of columns for inputting the value of each parameter, some parameters are not perturbed exactly 35 percent due to rounding.

During calibration runs, the NWSRFS software automatically adjusts some initial storage values as certain parameter values are changed. For example, if the value of parameter UZTWM (upper zone tension water maximum) is increased one millimeter by the optimization routine, the initial contents of the upper zone tension water reservoir are increased by one millimter so that the intiial moisture deficit in that reservoir remains the same.

Where possible, the calibration runs used the same initial contents used to create the synthetic flows. Exceptions were made when automatic adjustment of initial contents accompanied changes in certain parameters. In these cases, the values of initial contents were designed so that when the true parameter value was reached, the "true" initial contents were also reached, and the estimation criteria may then have a value of zero.

Care was taken to ensure that similar termination criteria were used for both optimization algorithms. However, due to the differing structure of each algorithm, it was not possible to make termination criteria for each algorithm identical. Specific termination criteria are set forth in Table 7.1. To prevent excessive searching in the immediate vicinity of the minima at the true parameter set, an additional termination criterion was added to both algorithms: termination if the SLS estimation criterion falls below 0.05. The Newton-Raphson algorithm was allowed a fewer number of maximum iterations than the pattern search algorithm since the Newton-Raphson algorithm obtains more information at each iteration and should converge faster. During the study, function convergence due to the estimation criterion changing less than a specified amount in an iteration was the most common type of termination.

Results

In interpreting the results of the calibration runs, it was useful to establish an index describing the overall success of individual runs. An overall performance index was devised which considered the closeness of the estimation criteria to zero, and percent closeness of final parameters to true parameters. This index emphasized robustness, or the ability to obtain correct solutions, and did not consider efficiency of computer run time. This was done because the ability to obtain optimal and unique parameter estimates for CRR seems to be a

Table 7.1. Convergence criteria for calibration study

	Pattern Search	Newton-Raphson
Maximum # of Iterations		
Single-parameter	60	25
Two-parameter	120	50
Four-parameter	240	100
Minimum Estimation Criterion (SLS)	.05	.05
Function changes less than certain per cent in each		
Iteration	N/A	1.0%
Pattern	1.0%	N/A
Parameters change less than certain per cent in each iteration/pattern	Unsure[1]	Disabled

[1] This was not well-documented in the program. However, this termination criterion caused termination only a few times.

more serious problem than inadequate computer resources, particularly in light of recent advances in computers. The possible values of the index are very poor, poor, fair, good, and excellent.

Synthetic Studies

One-parameter calibration runs were performed for each Soil Moisture parameter which is normally optimized (all parameters except RIVA and SAVED). For each run, the parameter of interest was perturbed 35 percent. Ending parameter values for all one-parameter runs are set forth in Table 7.2. The pattern search algorithm was successful for all but one of 14 parameters in obtaining the correct parameter value, while the Newton-Raphson algorithm failed for five of 14 parameters. Examination of the algorithm output revealed that the cause of the failure may have been misleading derivatives at the initial parameter value. As is shown in Figure 7.2, an irregularity in the estimation criterion can cause the algorithm to search in the wrong direction, a problem from which it sometimes never recovered.

Four sets of two parameters each were selected for the two-parameter calibrations and are shown in Table 7.3. The ending parameter values of the two-parameter calibration runs are listed in Table 7.4. Table 7.5 sets forth the overall performance index, ending estimation criterion value, and CPUs for each run. A 35 percent perturbation was used for the two-parameter calibrations.

A single parameter set--ADIMP, UZK, LZPK, and REXP--was used for the four-parameter calibrations. These parameters were all perturbed 15, 35, and 50 percent in separate runs. The ending param-

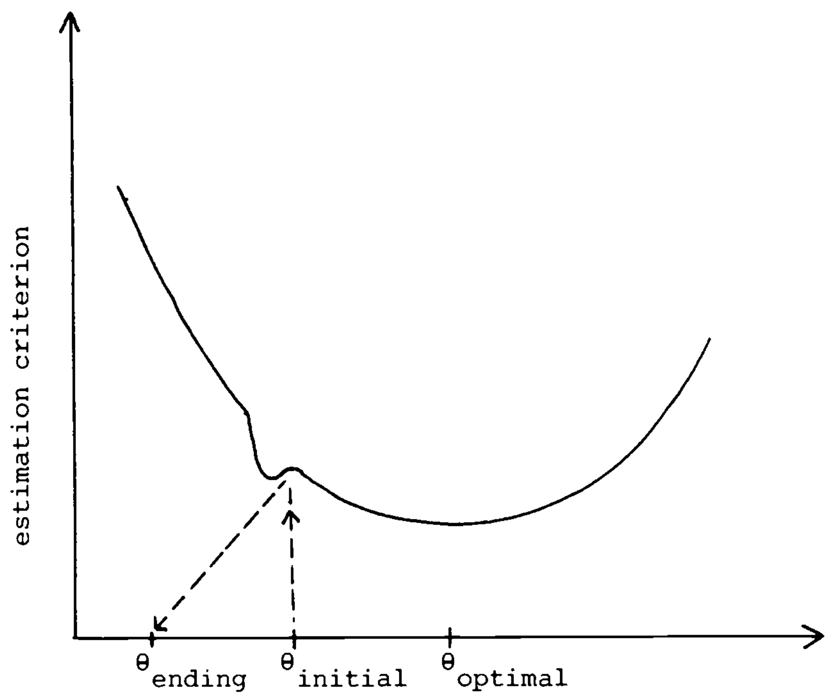

Figure 7.2. Estimation criteria property which contributed to failure of Newton-Raphson algorithm.

The derivatives at the initial point at which the estimation criteria are sampled pointed the algorithm in the wrong direction.

Table 7.2. Ending values for one-parameter synthetic calibrations. Ending values marked with an asterisk were deemed unsuccessful runs; all other runs were deemed successful.

Parameter	Initial Value	True Value	N-R Ending Value	Pattern Ending Value
UZTWM	52.0	80.0	60.6*	80.8
UZFWM	10.0	15.0	15.0	15.0
LZTWM	107.0	160.0	107.0*	159.6
LZFPM	189.0	140.0	140.0	139.9
LZFSM	19.0	14.0	14.0	14.0
ADIMP	0.11	0.17	0.17	0.17
UZK	0.20	0.30	0.30	0.30
LZPK	0.018	0.013	0.013	0.013
LZSK	0.170	0.126	0.126	0.126
ZPERC	31.0	48.0	48.0	47.9
REXP	1.37	2.10	2.39*	2.10
PCTIM	0.002	0.001	0.001	0.001
PFREE	0.027	0.020	0.811*	0.026*
SIDE	2.31	3.55	2.31*	3.55

Average Newton-Raphson CPU's = 25.2 per run

Average Pattern Search CPU's = 45.6 per run

Table 7.3. Two-parameter sets used for calibration study

Parameter Set	Parameters	Correlation Between Parameters
1	ADIMP PCTIM	-.88
2	UZK LZPK	-.80
3	ADIMP UZK	-.06
4	LZPK PCTIM	.27

Table 7.4. Ending parameter values for two-parameter synthetic calibration runs

Parameter	Initial Value	True Value	N-R Ending Value	Pattern Ending Value
		Set #1		
ADIMP	.11	.17	.125	.167
PCTIM	.002	.001	.000	.003
		Set #2		
UZK	.200	.300	.344	.300
LZPK	.018	.013	.013	.013
		Set #3		
ADIMP	.11	.17	.174	.170
UZK	.20	.30	.323	.300
		Set #4		
LZPK	.018	.013	.013	.013
PCTIM	.002	.001	.000	.002

Table 7.5. Statistics for two-parameter synthetic calibration runs

Parameter Set	Overall Performance Index	Estimation Criterion SLS	CPU's
1 (Newton)	Very poor	752.	25
2 (Newton)	Poor	190.	27
3 (Newton)	Fair	92.4	33
4 (Newton)	Very poor	169.	29
1 (pattern)	Poor	.26	64
2 (pattern)	Excellent	.03	124
3 (pattern)	Excellent	.00	174
4 (pattern)	Fair	.33	257

eter values for the four-parameter runs are contained in Tables 7.6 through 7.8. Each run's overall performance index, ending estimation criterion value, and CPUs are found in Table 7.9.

The results of the above calibration runs indicate that the pattern search algorithm is more robust than the Newton-Raphson algorithm when calibrating the Soil Moisture Accounting model. To summarize, the overall performance indices of the two parameter Newton-Raphson runs were very poor, poor, fair, and very poor. Those of the pattern search runs were poor, excellent, excellent, and fair. All of the four-parameter runs had indices of either fair or good, except for the 15% pattern search run, which had an index of excellent. For each of the two-parameter sets, the pattern search algorithm performed better than the Newton-Raphson algorithm. The two algorithms gave comparable results for the 35% and 50% four-parameter sets, but the pattern search results were better than the Newton-Raphson results for the 15% four-parameter case. It is significant that for nearly half of the parameter sets, neither algorithm was successful in estimating the correct parameters, even under the ideal conditions of error-free synthetic data. Clearly, parameter estimation for the Soil Moisture Accounting model is not a trivial task.

Two of the two-parameter sets were composed of parameters with a relatively high degree of interaction (as evidenced by high-parameter correlation), and the other two two-parameter sets had a relatively low degree of interaction. Table 7.3 gives the correlation between parameters in each set, as evaluated at the true parameter set. The purpose of selecting highly- and lowly-correlated parameter sets was to

Table 7.6. Ending parameter values for four-parameter synthetic calibrations with 15% initial perturbation

Parameter	Initial Value	True Value	N-R Ending Value	Pattern Ending Value
ADIMP	0.140	0.170	0.170	0.170
UZK	0.260	0.300	0.299	0.300
LZSK	0.150	0.126	0.150	0.129
REXP	1.79	2.10	2.255	2.119

Table 7.7. Ending parameter values for four-parameter synthetic calibrations with 35% initial perturbation

Parameter	Initial Value	True Value	N-R Ending Value	Pattern Ending Value
ADIMP	0.110	0.170	0.169	0.169
UZK	0.200	0.300	0.300	0.300
LZSK	0.170	0.126	0.101	0.109
REXP	1.370	2.100	1.924	1.985

Table 7.8. Ending parameter values for four-parameter synthetic calibrations with 50% initial perturbation

Parameter	Initial Value	True Value	N-R Ending Value	Pattern Ending Value
ADIMP	0.090	0.170	0.170	0.166
UZK	0.150	0.300	0.301	0.298
LZSK	0.190	0.126	0.176	0.084
REXP	1.050	2.100	2.489	1.830

Table 7.9. Statistics of four-parameter synthetic calibration runs

Algorithm	Overall Performance Index	Estimation Criterion SLS	CPU's
Perturb 15%			
Newton	Fair	6.46	27
Pattern	Excellent	0.13	171
Perturb 35%			
Newton	Good	.35	27
Pattern	Good	.59	142
Perturb 50%			
Newton	Fair	11.9	30
Pattern	Fair	6.11	73

test the hypothesis that a high degree of parameter interaction hinders the parameter estimation process. Results weakly supported the hypothesis, since the calibration runs with poorly-correlated parameter sets obtained slightly better results than those runs with highly-correlated parameter sets. The overall performance indices for the calibration runs with highly-correlated parameter sets were very poor, poor, poor, and excellent; those of the poorly-correlated parameter sets were very poor, fair, fair, and excellent.

The pattern search calibration runs used slightly more than two and one-half (2 1/2) times as much total computer run time than did the Newton-Raphson calibration runs. This is probably due to the Newton-Raphson algorithm obtaining more information at each iteration and therefore requiring fewer iterations. Apparently, the additional computer run time required to compute the derivatives is more than offset by the savings associated with fewer iterations.

Other researchers (Johnston and Pilgrim, 1976) have suggested that the sequential use of several optimization algorithms may produce better results than using one algorithm alone. Therefore, on unsuccessful two- and four-parameter Newton-Raphson runs, the pattern search algorithm was used with initial parameter values equal to the final Newton-Raphson values. The reverse was done for unsuccessful pattern search runs. This procedure was used on 11 unsuccessful runs. In six cases, the pattern search routine improved Newton-Raphson estimates significantly. In one case, the Newton-Raphson routine improved pattern search estimates, and in four cases, there was no effect. For two of the seven multi-parameter sets, sequential use of algorithms gave better results than either algorithm alone. These results seem to indicate that there is potential for improved parameter estimates through sequential use of several algorithms. It is possible that an apparent local minimum which causes one algorithm to converge can be more readily escaped by another algorithm. In two cases, using the Newton routine on unsuccessful Newton estimates improved the final estimates significantly, suggesting that the implementation of the termination criteria for that algorithm can be improved. Overall performance indices for sequential runs can be found in Tables 7.10.

Historical Studies

Four parameters--ADIMP, UZK, LZPK, AND REXP--were chosen for perturbation and estimation using historical Bird Creek data. These parameters were perturbed 35% from NWS estimated values and calibrated using three years of calibration data using both algorithms.

It was interesting to note that although the final estimation criteria were similar (340,608 for pattern search and 303,752 for Newton-Raphson), the two algorithms converged to completely different parameter values (Table 7.11). This result highlights the considerable influence of parameter compensation and interaction. Since the pattern search algorithm was used to estimate the NWS parameter estimates, it is not suprising that it terminated at a point closer to the NWS estimates than did the Newton algorithm. The Newton routine used 169 CPUs, and the pattern search routine used 292 CPUs. See Table 7.12 for a summary of estimation criteria values and CPU time.

Table 7.10. Overall performance indices for synthetic calibration runs using both algorithms sequentially

Parameter Set	Newton	Pattern	Newton-Pattern	Pattern-Newton	Newton-Newton
2-param. #1	Very poor	Poor	Fair	Excellent	Very poor
2-param. #2	Poor	Excellent	Excellent	a	Excellent
2-param. #3	Fair	Excellent	Excellent	a	Excellent
2-param. #4	Very poor	Fair	Poor	Fair	Fair
4-param.(15%)	Fair	Excellent	Good	a	Fair
4-param.(35%)	Good	Good	Good	Good	Good
4-param.(50%)	Fair	Fair	Excellent	Fair	Fair
Average CPU's	28	144	154	158	50

[a] Calibration was not performed because initial calibration with first algorithm produced excellent results.

Table 7.11. Ending parameter values for historical calibration runs

Parameter	Initial Value	Official Value	Final Pattern Value	Final Newton-Raphson Value
ADIMP	.110	.170	.163	.256
UZK	.200	.300	.274	.127
LZPK	.018	.013	.012	.004
REXP	1.37	2.10	1.87	1.05

Table 7.12. Statistics for historical calibration runs

	Initial Estimation Criterion	Ending Estimation Criterion	CPU's
Calibration			
Newton-Raphson	556,665	303,752	169
Pattern search	556,665	340,608	292
Verification			
Newton-Raphson	809,099	---	---
Pattern search	749,450	---	---

A split-sample verification run gave an estimation criterion value of 809,099 for the pattern search parameters, and 749,450 for the Newton parameters. Visual inspection of plots of simulated versus observed flows for the verification period did not reveal one set of parameters to be clearly superior to the other.

Conclusions

Desirable performance objectives of an optimization algorithm include robustness, which describes the ability to consistently obtain correct solutions under a variety of conditions, and a small amount of computer run time. Ease of implementation may also be a consideration. The results of the studies presented here indicate that for the Soil Moisture Accounting model, the pattern search algorithm is more robust than the Newton-Raphson algorithm. However, the Newton-Raphson algorithm requires significantly less computer run time, a characteristic which NWS personnel have indicated is important for their River Forecast System.

If the response surface was smooth, continuous, and quadratic, or nearly so, there is little question that least squares gradient methods such as Newton-Raphson would be more robust than direct-search methods. However, it appears that poor conditioning of the Soil Moisture Accounting model response surface is responsible for the poor performance of the Newton-Raphson algorithm. It is expected that the result would be similar for any CRR model. Aspects of poor conditioning include discontinuities and surface "roughness" or irregularities. Figure 7.2 demonstrates how roughness of the response surface can adversely affect gradient algorithms. Also, recall that gradient algorithms require that the estimation criterion and its derivatives be continuous. Since that requirement is violated for CRR models, it is to be expected that gradient algorithms will not reach their full potential with CRR models. The conclusion of poor performance of gradient algorithms with CRR models is supported by the results of several other researchers, as discussed in Chapter 3.

The robustness of gradient algorithms would be enhanced by any technique which would result in better conditioning of the response surface, such as the use of maximum likelihood estimators. Since the study presented here used error-free synthetic data, however, use of a maximum likelihood estimator would not have affected results.

It appears that for the Soil Moisture Accounting model, the SLS estimator is approximately quadratic, while the DRMS estimator is not. Since the Newton-Raphson and other gradient algorithms assume that the response surface is quadratic, SLS or other least squares estimators should be the choice for gradient calibration, and possibly direct search calibration as well. If desired, the DRMS value, which has a physically-intuitive meaning, can be evaluated at the final parameter values of a calibration run.

With respect to the NWS River Forecast System (NWSRFS), it is clear that the Newton-Raphson algorithm is not a "better" algorithm which can replace the currently-used pattern search algorithm. However, it seems that the NWS would benefit from adding the Newton-Raphson algorithm to their operational version of the NWSRFS. Due to the superior robustness of the pattern search algorithm, the author recommends that the NWS rely primarily on the pattern search algorithm. The Newton-Raphson algorithm would be useful in the following three situations:

(1) It can be used to reduce the amount of calibration computer time, particularly in the latter stages of model "fine-tuning".

(2) The algorithm can assist in finding new search directions when the pattern search algorithm is stuck in an apparent minima. Use of both algorithms, rather than just one alone, can improve parameter estimates in some cases.

(3) It provides derivatives which can be quite useful for sensitivity and identifiability analysis, both during and after calibration.

The author recommends that when implementing the Newton-Raphson algorithm in the operational version of NWSRFS, finite difference numerical derivatives be used. The reasons for this are discussed in Chapter 6.

In general, due to poor robustness, the author would not recommend the use of gradient algorithms for the calibration of CRR models. However, since it appears that the use of several algorithms is better than one, researchers may wish to consider the use of a gradient algorithm to supplement use of a direct-search algorithm as discussed above. For ease of implementation, numerical derivatives are recommended.

The results of the calibration study indicated that the outcome of any calibration run was highly-dependent on characteristics of the response surface in the vicinity of the initial parameter point, and other factors. It appears that a large number of calibration runs using different parameters and different initial parameter points are necessary before comparison between optimization algorithms become meaningful.

CHAPTER 8

SENSITIVITY AND IDENTIFIABILITY ANALYSIS

This chapter briefly introduces several types of parameter sensitivity and identifiability (S/I) analyses which may be applied to CRR models. The chapter also presents the results of applying these techniques to the Soil Moisture Accounting model.

Parameter sensitivity and identifiability analyses can be quite useful for investigating a model's potential for obtaining unique parameter estimates, conducting post-calibration identifiability studies, and as an aid during the parameter estimation process. Such analyses hope to pinpoint the characteristics of parameter sensitivity and interaction, both of which arise as a consequence of model structure.

Methods

The S/I methods applied here are methods developed by Gupta (1984), Sorooshian and Gupta (1985), Sorooshian and Arfi (1982), Nathanson and Saidel (1982), and others. In carrying out the actual analysis, a computer program written by Gupta was used.

An important feature of these techniques is that they use derivative information which is automatically generated during gradient optimization and therefore are far less tedious than the graphical response surface methods first initiated by Plinston (1972). In fact, a definite advantage of the use of gradient optimization is the subsequent ease of application of these S/I techniques.

The S/I measures discussed here are the Parameter Sensitivity and Conditional Parameter Sensitivity measures, Sensitivity Ratio, indices of concentricity and interaction, measure of Multi-Parameter Interaction, and parameter correlation matrix. These methods do not explicitly consider stochastic data errors. They are based on the information contained in the structural identifiability matrix, which is the Hessian of a simple least squares function (see Chapter 5). Many of the above measures are based on the notion of an indifference region, a hyperelliptical surface in multi-parameter space (centered at ($\underline{\theta}$). Parameter points within this region produce virtually indistinguishable sequences of model outputs. An indifference region in two-parameter space is shown in Figure 8.1.

The Parameter Sensitivity (PS) measure is the amount (plus or minus) that a parameter can vary and remain within the indifference region while other parameters are allowed to vary and compensate for that parameter. The Conditional Parameter Sensitivity (CPS) measure is the amount that a parameter can vary and remain within the indifference region while the other parameters remain fixed. Both sensitivities can be considered to be confidence intervals around $\underline{\theta}$, and are a function of a 95% Chi-square statistic. Both measures are illustrated in Figure 8.1. The Sensitivity Ratio proposed by Sorooshian and Gupta (1985) is the ratio of the two, and is useful for isolating parameters which are poorly identifiable due to a high degree of interactions with other parameters. A large Sensitivity Ratio associated with a particular parameter indicates that parameter is highly influenced by interactions.

Consider a two-parameter elliptical indifference region such as shown in Figure 8.1. Two measures of parameter interaction can be derived from this ellipse: the indices of concentricity and interaction. Concentricity measures the deviation of the ellipse from a circle and is given by the ratio of the minor to major axes. A value of unity indicates a perfect circle (no parameter interaction) and a value of zero indicates extreme interaction. Interaction measures the orientation of the major axis of the ellipse with respect to the parameter axes. An angle of 45 degrees is considered least desirable.

The correlation matrix provides information about the relative degree of two-parameter interdependence. It is produced by normalizing the inverse of the structural identifiability matrix. The determinant of this matrix was introduced by Nathanson and Saidel (1982) as the measure of Multi-Parameter Interaction (MPI). The measure varies between zero and unity. A model without parameter interaction would produce a MPI measure of unity.

The partial derivatives of the objective function with respect to parameters also gives very useful information on the relative sensitivity of the model to each parameter.

It is important to note that the results of a S/I analysis are only valid for the parameter values and data used to produce the structural identifiability matrix. Results may change, perhaps significantly, if different parameter values or different precipitation/observed flow data are used.

Application to the Soil Moisture Accounting Model

In order to obtain insight into the structural identifiability of the Soil Moisture Accounting model and to obtain information to assist in the calibration study, the sensitivity and identifiability techniques discussed above were applied to the model using the synthetic calibration data and NWS parameter estimates for Bird Creek. The Soil Moisture Accounting model has been found to be completely insensitive to parameter SAVED. Therefore, it was not possible to perform a S/I analysis for SAVED, since inclusion of SAVED would lead to a singular structural identifiability matrix.

The resulting Parameter Sensitivity measures and Sensitivity Ratio are given in Table 8.1, the correlation matrix is given in Table 8.2, and the concentricity and interaction matrixes are presented in Tables 8.3 and 8.4, respectively. The MPI measure had a value of 6.6×10^{-21}.

Table 8.5 sets forth the first derivatives of a simple least squares criterion using synthetic calibration data and parameters which are perturbed slightly from true parameters. (At the true parameter set, first derivatives are zero). It can be seen that ADIMP, LZPK, LZSK, and PCTIM are extremely sensitive parameters, and LZTWM, LZFPM, ZPERC, RIVA, and PFREE are extremely insensitive. Perhaps very little effort should be spent on estimating the very insensitive parameters.

The Conditional Parameter Sensitivities show that, for the synthetic data and true parameters, most parameters have reasonably small, but not tight, confidence intervals when not considering parameter compensation. Parameters PCTIM, RIVA, and PFREE are notable exceptions; they have ridiculously large confidence intervals. The Sensitivity Ratio ranges in value from 4.6 to 14.1 for all parameters, highlighting the considerable influence of parameter compensation within the model. When considering the effect of parameter compensation, parameters ZPERC and SIDE also have ridiculously large confidence intervals. Obviously, even under ideal conditions, it is difficult, if not impossible, to obtain unique and "correct" parameter estimates for the Soil Moisture Accounting model.

From Tables 8.2 through 8.4, it can be seen that there is a great deal of interaction among model parameters. This interaction can hamper the model calibration process considerably.

During the calibration study described in Chapter 7, the sensitivity and identifiability analyses were primarily useful in determining the relative degree of interaction between specific parameters. First derivatives of the estimation criterion were used to determine which parameters the model was most sensitive to, and these parameters were singled out for calibration.

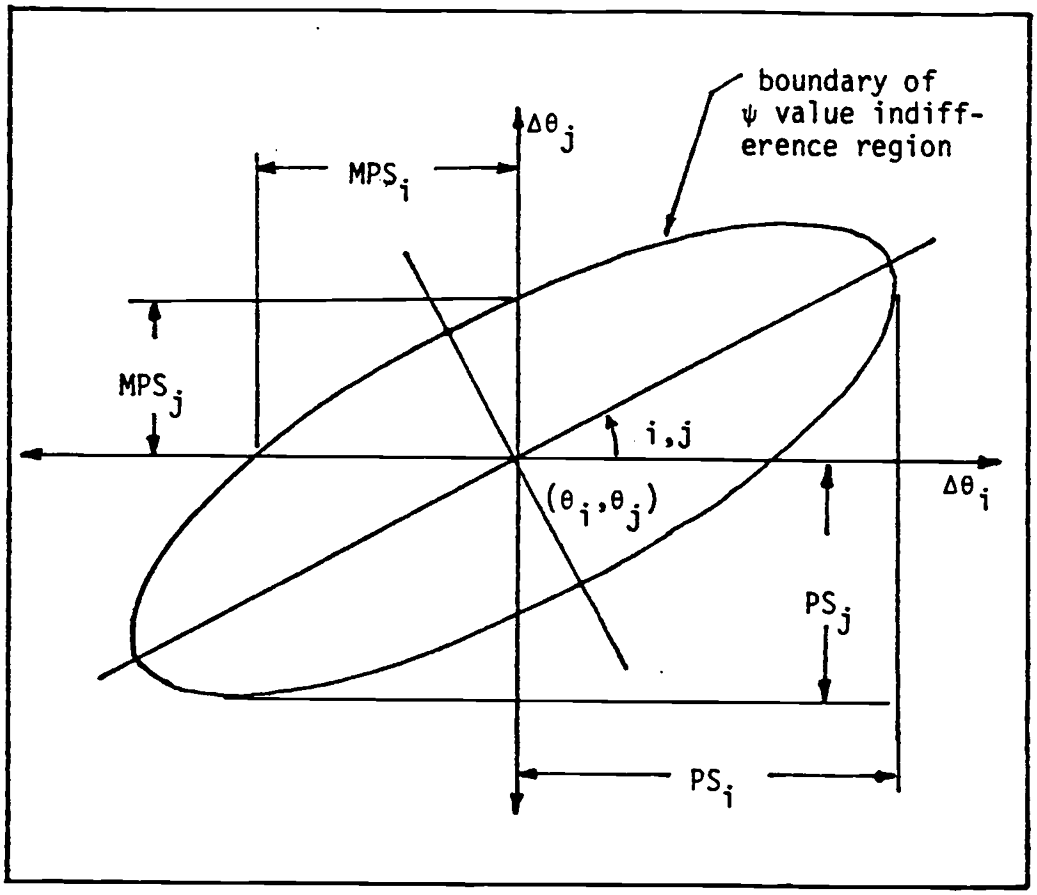

Figure 8.1. Two-parameter example of an indifference region.

Table 8.1. Parameter sensitivity, conditional parameter sensitivity measures, and sensitivity ratio for synthetic data at the true parameter set.

The first two measures are equivalent to 95% confidence intervals (plus or minus).

Parameter	Value	Conditional Parameter Sensitivity	Parameter Sensitivity	Sensitivity Ratio
UZFWM	80.0	0.6	4.4	6.7
UZTWM	15.0	.4	3.6	9.2
LZTWM	160.0	2.9	13.4	4.6
LZFPM	140.0	2.3	20.9	8.9
LZFSM	14.0	.9	4.3	4.9
ADIMP	.170	.006	.032	5.1
UZK	.300	.019	.149	7.9
LZPK	.0130	.0008	.0049	6.1
LZSK	.126	.009	.044	4.6
ZPERC	48.0	5.8	82.1	14.1
REXP	2.10	.06	.70	11.8
PCTIM	.001	.005	.024	4.6
RIVA	.000	1.9	22.9	12.0
PFREE	.020	2.1	16.1	7.6
SIDE	3.55	.56	3.52	6.3

Table 8.2. Parameter correlation matrix for synthetic data at true parameter set

	UZTWM	UZFWM	LZTWM	LZFPM	LZFSM	ADIMP	UZK	LZPK	LZSK	ZPERC	REXP	PCTIM	RIVA	PFREE	SIDE
UZTWM	1.00														
UZFWM	-.61	1.00													
LZTWM	-.75	.92	1.00												
LZFPM	.10	-.26	-.23	1.00											
LZFSM	.87	-.67	-.74	.40	1.00										
ADIMP	.31	.16	-.06	-.16	.20	1.00									
UZK	.66	-.85	-.79	.07	.74	-.06	1.00								
LZPK	-.79	.90	.98	-.16	-.78	-.12	-.80	1.00							
LZSK	.72	-.67	-.78	.25	.71	.17	.45	-.83	1.00						
ZPERC	-.01	.03	.05	.93	.31	-.03	-.15	.10	.09	1.00					
REXP	.15	-.06	-.05	.92	.46	-.01	-.03	-.01	.21	.98	1.00				
PCTIM	-.37	.13	.24	.09	-.33	-.88	-.22	.27	-.16	.06	.02	1.00			
RIVA	-.27	.06	.09	.25	-.33	-.26	-.48	.15	.21	.18	.12	.37	1.00		
PFREE	.84	-.86	-.97	.11	.79	.17	.81	-.98	.79	-.12	.00	-.32	-.18	1.00	
SIDE	-.21	.68	.65	-.44	-.25	.06	-.26	.57	-.62	-.17	-.17	.09	-.58	-.52	1.00

Table 8.3. Parameter elongation matrix for synthetic data at true parameter set

	UZTWM	UZFWM	LZTWM	LZFPM	LZFSM	ADIMP	UZK	LZPK	LZSK	ZPERC	REXP	PCTIM	RIVA	PFREE	SIDE
UZTWM	.00														
UZFWM	.45	.00													
LZTWM	.14	.12	.00												
LZFPM	.20	.15	.15	.00											
LZFSM	.44	.36	.11	.04	.00										
ADIMP	.01	.01	.00	.00	.00	.00									
UZK	.03	.05	.01	.01	.02	.29	.00								
LZPK	.00	.00	.00	.00	.00	.05	.04	.00							
LZSK	.01	.02	.00	.00	.00	.12	.39	.02	.00						
ZPERC	.08	.06	.17	.05	.01	.00	.00	.00	.00	.00					
REXP	.07	.13	.01	.00	.00	.03	.26	.00	.02	.00	.00				
PCTIM	.01	.01	.00	.00	.00	.08	.25	.07	.13	.00	.03	.00			
RIVA	.33	.20	.56	.66	.43	.00	.01	.00	.00	.31	.03	.00	.00		
PFREE	.28	.18	.37	.47	.31	.00	.01	.00	.00	.28	.02	.00	.82	.00	
SIDE	.69	.70	.13	.16	.37	.01	.00	.00	.01	.07	.08	.01	.16	.25	.00

Table 8.4. Parameter interaction matrix for synthetic data at true parameter set in degrees from the parameter axis

	UZTWM	UZFWM	LZTWM	LZFPM	LZFSM	ADIMP	UZK	LZPK	LZSK	ZPERC	REXP	PCTIM	RIVA	PFREE	SIDE
UZTWM	0														
UZFWM	-23														
LZTWM	-80	-87	0												
LZFPM	-79	-85	-38	0											
LZFSM	-58	-75	-16	-20	0										
ADIMP	0	1	0	0	0	0									
UZK	0	-1	0	0	1	-82	0								
LZPK	0	0	0	0	0	7	1	0							
LZSK	-1	-1	0	0	-1	57	17	-85	0						
ZPERC	-86	-88	-64	-68	-81	90	90	-90	-90	0					
REXP	4	5	1	2	4	-84	-79	89	81	1	0				
PCTIM	0	1	0	0	0	-40	-6	82	28	0	-5	0			
RIVA	-86	89	-19	-29	-80	90	90	-90	-90	-6	89	90	0		
PFREE	-83	-89	-33	-40	-75	90	90	-90	-90	-13	89	61	61	0	
SIDE	-32	88	-8	-10	-28	90	89	-90	-89	-4	86	-14	-14	-4	0

Table 8.5. First derivatives of SLS estimation criterion for synthetic calibration data near true parameter values

Parameter	First partial derivative of SLS estimation with respect to parameter
UZTWM	-33.0
UZFWM	-58.0
LZTWM	-7.0
LZFPM	-9.5
LZFSM	-28.0
ADIMP	4211.0
UZK	94.0
LZPK	-28000.0
LZSK	-2495.0
ZPERC	-3.4
REXP	338.0
PCTIM	4974.0
RIVA	-2.6
PFREE	-3.4
SIDE	-23.0

CHAPTER 9

CONCLUSIONS

In the past, derivative-based optimization algorithms have not frequently been used to calibrate conceptual rainfall-runoff (CRR) models, partly due to difficulties associated with obtaining the required derivatives. Since the estimation criterion is not available in closed form, it was thought that analytical derivatives could not be obtained, or were too difficult to obtain. Finite difference derivatives could be calculated but were of unknown numerical accuracy and were computationally expensive. With the introduction by Gupta and Sorooshian (1985) of a new method to compute analytic derivatives, new explorations of gradient methods became possible. One of the primary contributions of this thesis is to demonstrate the feasibility of computing analytic derivatives of a complex CRR model, and to perform gradient-type calibration and derivative-based sensitivity and identifiability analyses for that model. The model used was the Soil Moisture Accounting model of the U.S. National Weather Service.

One of the interesting results of this investigation concerns a comparison between analytic and finite difference derivatives of the Soil Moisture Accounting model. Analytic and numeric derivatives of model output with respect to parameters were found to be identical to at least the sixth decimal place. It appears that finite difference derivatives are sufficiently accurate for many applications, providing that an appropriate step size and large computer word size are used. Numerical derivatives have the advantage of being easier to program. Comparison of computational effort would depend of details of the implementataion.

Studies of a least squares response surface created by the Soil Moisture Accounting model using error-free synthetic data indicate that the surface is convex and approximately quadratic in the region of the optimal parameters. This is a desirable property from the point of view of convergence of calibration algorithms. Using the synthetic data, the model was found to be completely insensitive to the parameter SAVED, leading to the recommendation that parameter SAVED not be optimized.

Close inspection of the response surface generated by synthetic data confirmed the existence of discontinuities in the surface itself and in its first and second derivatives. An investigation revealed that the cause of these discontinuities is the existence of threshold behavior, which is described by threshold parameters such as maximum moisture storage, in conjunction with a discrete time step. Discontinuities are very undesirable features which adversely affect the calibration process, especially when using gradient-type algorithms. Since threshold parameters and discrete time steps are fundamental properties of watershed models, and natural watersheds do indeed exhibit threshold behavior, the suggestion of eliminating the thresholds seems neither fruitful nor practical.

One of the questions explored in this thesis involves the choice of the most appropriate optimization algorithm for automatic calibration of the Soil Moisture Accounting model. Of course, the choice of the "most appropriate" algorithm hinges on the relative emphasis placed on robustness, efficiency of computer time, and other factors. The results of the Chapter 7 calibration studies indicate that for the Soil Moisture Accounting model, the pattern search (direct) algorithm is more robust than the Newton-Raphson (gradient) algorithm. However, the Newton-Raphson algorithm used substantially less computer time than the pattern search algorithm when using analytic derivatives.

If the response surface was smooth, continuous, and quadratic, there is little question that least squares gradient methods such as Newton-Rapahson would be more robust than direct-search methods. However, it appears that poor conditioning of the Soil Moisture Accounting model response surface is responsible for the poor performance of the Newton-Raphson algorithm. It is expected that the result would be similar for any CRR model. Aspects of poor conditioning include discontinuities and surface "roughness", and "potholes".

If a gradient algorithm sampled the estimation criterion at a discontinuity at which the derivatives blow up, the algorithm would also blow up. However, extensive sampling of the Soil Moisture Accounting model's estimation criterion has always yielded finite values of derivatives. Therefore, it appears that both the criterion and its first and second derivatives are piecewise continuous, and everywhere finite. It is to be expected that these discontinuities will adversely affect a gradient algorithm. They do not, however, prevent its use.

The robustness of gradient algorithms would be enhanced by any technique which would result in better conditioning of the response surface, such as the use of maximum likelihood estimators. Since the study presented here used error-free synthetic data, however, use of a maximum likelihood estimator would not have affected results.

It appears that for the Soil Moisture Accounting model, the SLS estimator is approximately quadratic, while the DRMS estimator is not. Since the Newton-Raphson and other gradient algorithms assume that the response surface is quadratic, SLS or other least squares estimators should be the choice for gradient calibration, and possibly direct search calibration as well. If desired, the DRMS value, which has a physically-intuitive meaning, can be evaluated at the final parameter values of a calibration run.

In general, due to poor robustness, the author would not recommend the exclusive use of gradient algorithms for the calibration of CRR models. However, since it appears that the use of several algorithms is better than one, researchers may wish to consider the use of a gradient algorithm to supplement use of a direct-search algorithm.

Situations in which a gradient algorithm may be useful include:

(1) Assisting in finding new search directions when a direct-search algorithm is stuck in an apparent minimum; and

(2) Providing derivatives which can be useful for sensitivity and identifiability analysis, both during and after calibration.

The results of the response surface studies and calibration studies highlighted the considerable influence of poor response surface conditioning and parameter interaction on the calibration process for CRR models. It appears that these are serious problems which adversely affect the ability to obtain optimal and unique parameter estimates which are necessary for the best utilization of these models. Although there is certainly progress which can be made to alleviate the problems of response surface condition and a parameter interaction, for the most part, they seem to be problems inherent to CRR models.

APPENDIX A

SAMPLE PROGRAM ILLUSTRATING ANALYTIC COMPUTATION OF DERIVATIVES

This appendix gives an example of the computation of analytical derivatives of a CRR model using the techniques presented in Chapter 5. To illustrate the practical application of these techniques, a short FORTRAN program is given below in which the derivatives of a simple CRR model and its estimation criterion are computed. For clarity, variables which represent derivatives have been shown using mathematical notation, instead of a correct FORTRAN name.

The first derivatives of the estimation criterion with respect to parameters are exact; the second derivatives are approximations to the exact analytical derivatives in which higher order terms were omitted.

```
      PROGRAM DERIVATIVE
      REAL MAX
      DIMENSION PRECIP(100), TOTALQ(100),QOBS(100)
C EXPLANATION OF VARIABLES
C PARAMETERS:
C            MAX = MAXIMUM LEVEL IN RESERVOIR
C              K = RECESSION COEFFICIENT OF RESERVOIR
C              F = ESTIMATION CRITERION
```

```
C STATE VARIABLE:

                X = LEVEL OF RESERVOIR

C OTHER VARIABLES:

C            QWKQ = SPILL OVER TOP OF RESERVOIR (STORM RUNOFF)

C           BASEQ = OUTFLOW OF RESERVOIR (BASEFLOW)

C          TOTALQ = TOTAL STREAMFLOW

C                 = QWKQ + BASEQ

C            QOBS = OBSERVED FLOWS

CXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX

C     INITIALIZE DERIVATIVES
```

$$\frac{\partial X}{\partial K} = 0$$

$$\frac{\partial X}{\partial MAX} = 0$$

```
CCCCC   READ IN DATA CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

      READ(5,*)K,MAX,X,NDATA

      READ(5,*)(PRECIP(I),I=1,NDATA),(QOBS(I),I=1,NDATA)

CCCCC   BEGIN TIME LOOP     CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

      DO 100 ITIME = 1,NDATA

          X = X + PRECIP(ITIME)
```

$$\frac{\partial X}{\partial K} = \frac{\partial X}{\partial K}$$

$$\frac{\partial X}{\partial MAX} = \frac{\partial X}{\partial MAX}$$

C CALCULATE BASEFLOW IF THERE IS NO SPILL

IF(X.LE.MAX) THEN

BASEQ = X * K

$$\frac{\partial BASEQ}{\partial K} = K * \frac{\partial X}{\partial K} + X$$

$$\frac{\partial BASEQ}{\partial MAX} = K * \frac{\partial X}{\partial MAX}$$

X = X*(1-K)

$$\frac{\partial X}{\partial K} = (1-K) * \frac{\partial X}{\partial K} - X$$

$$\frac{\partial X}{\partial MAX} = (1-K) * \frac{\partial X}{\partial MAX}$$

END IF

C IF SPILL OCCURS, CALCULATE BASEFLOW AND STORM RUNOFF

IF (X.GT.MAX) THEN

QWKQ = X - MAX

$$\frac{\partial QWKQ}{\partial K} = \frac{\partial X}{\partial K}$$

$$\frac{\partial QWKQ}{\partial MAX} = \frac{\partial X}{\partial MAX} - 1$$

BASEQ = MAX * K

$$\frac{\partial BASEQ}{\partial K} = MAX$$

$$\frac{\partial BASEQ}{\partial MAX} = K$$

X = MAX * (1-K)

$$\frac{\partial X}{\partial K} = -MAX$$

$$\frac{\partial X}{\partial MAX} = (1-K)$$

END IF

C CALCULATE TOTAL STREAMFLOW

TOTALQ(ITIME) = QWKQ + BASEQ

$$\frac{\partial TOTALQ(ITIME)}{\partial K} = \frac{\partial QWKQ}{\partial K} + \frac{\partial BASEQ}{\partial K}$$

$$\frac{\partial TOTALQ(ITIME)}{\partial MAX} = \frac{\partial QWKQ}{\partial MAX} + \frac{\partial BASEQ}{\partial MAX}$$

100 CONTINUE

C CALCULATE ESTIMATION CRITERION

F = 0.0

$$\frac{\partial F}{\partial K} = 0.0$$

$$\frac{\partial F}{\partial MAX} = 0.0$$

$$\frac{\partial^2 F}{\partial K^2} = 0.0$$

$$\frac{\partial^2 F}{\partial MAX^2} = 0.0$$

$$\frac{\partial^2 F}{\partial K \partial MAX} = 0.0$$

DO 200 ITIME = I, NDATA

RESIDUAL = TOTALQ(ITIME) - QOBS(ITIME)

F = F + RESIDUAL**2

$$\frac{\partial F}{\partial K} = \frac{\partial F}{\partial K} + 2 * RESIDUAL * \frac{\partial TOTALQ(ITIME)}{\partial K}$$

$$\frac{\partial F}{\partial MAX} = \frac{\partial F}{\partial MAX} + 2 * RESIDUAL * \frac{\partial TOTALQ(ITIME)}{\partial MAX}$$

$$\frac{\partial^2 F}{\partial K^2} = \frac{\partial^2 F}{\partial K^2} + 2 * \frac{\partial TOTALQ(ITIME)}{\partial K} * \frac{\partial TOTALQ(ITIME)}{\partial K}$$

$$\frac{\partial^2 F}{\partial MAX^2} = \frac{\partial^2 F}{\partial MAX^2} + 2 * \frac{\partial TOTALQ(ITIME)}{\partial MAX} * \frac{\partial TOTALQ(ITIME)}{\partial MAX}$$

$$\frac{\partial^2 F}{\partial K \partial MAX} = \frac{\partial^2 F}{\partial K \partial MAX} + 2 * \frac{\partial TOTALQ(ITIME)}{\partial K} * \frac{\partial TOTALQ(ITIME)}{\partial MAX}$$

```
200 CONTINUE
STOP
END
```

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