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MULTILEVEL CALIBRATION STRATEGY FOR COMPLEX HYDROLOGIC SIMULATION MODELS

Silver Spring, Md.
February 1989.

U.S. DEPARTMENT OF COMMERCE
National Oceanic and Atmospheric Administration
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Robert A. Mosbacher, Sr.; Secretary

National Oceanic and Atmospheric Administration

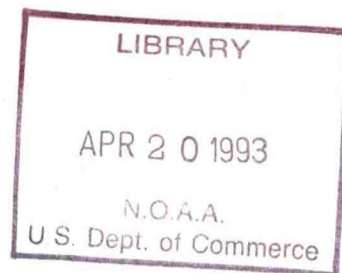
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PREFACE

This report is essentially a reproduction of the author's Ph. D. dissertation. The degree was obtained through the Department of Civil Engineering, Colorado State University, Fort Collins, Colorado, in May 1988.

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LIST OF SYMBOLS

<u>Symbol</u>	<u>Description</u>
d_u	Upper zone free water withdrawal rate
d_l'	Primary free water withdrawal rate
d_l''	Supplemental free water withdrawal rate
G	Input coefficient matrix
H	Measurement matrix
I	Identity matrix
K	Kalman gain matrix
m_1	Upper zone tension water reservoir exponent
m_2	Upper zone free water reservoir exponent
m_3	Lower zone tension water reservoir exponent
m_p	Mean of the precipitation time series
m_s	Mean of the streamflow time series
P	State estimate error covariance matrix
P_0	Initial state error covariance matrix
P_f	Decimal fraction of percolated water going directly to lower zone free water storage
P_x	Precipitation input for the time step
Q	System noise covariance matrix
R	Measurement noise covariance matrix
s_p	Standard deviation of the precipitation time series
s_s	Standard deviation of the streamflow time series

U	Input noise covariance matrix
u	Model input vector
u_e	Potential evapotranspiration demand
v	Measurement noise vector
v_r	Coefficient of variation of the precipitation time series
v_u	Coefficient of variation of the streamflow time series
w	System noise vector
x_l	Value of state at point of linearization
x_o	Observed state
x_p	Mean areal precipitation
x_u	Updated state
x_1	Upper zone tension water contents (mm)
x_2	Upper zone free water contents (mm)
x_3	Lower zone tension water contents (mm)
x_4	Lower zone free primary contents (mm)
x_5	Lower zone free supplemental contents (mm)
x_6	Tension water contents of the additional impervious area
x_1^0	Upper zone tension capacity (mm)
x_2^0	Upper zone free water capacity (mm)
x_3^0	Lower zone tension water capacity (mm)
x_4^0	Lower zone primary free water capacity (mm)
x_5^0	Lower zone free supplemental contents (mm)
Z	Measurement for updating
β_1	Additional impervious area (decimal fraction)
β_2	Minimum impervious area (decimal fraction)
δ	Kronecker delta function

Γ	System noise coefficient matrix
μ	Ratio of deep recharge to channel baseflow
Φ	State transition matrix
ε	Maximum percolation rate coefficient
θ	Percolation equation exponent

LIST OF ACRONYMS

<u>Acronym</u>	<u>Description</u>
ABSERR	Average absolute error between simulated and observed discharges
ABSMAX	Maximum deviation for the simulated period
ADIMC	Tension water contents of the additional impervious area
ADIMP	Additional impervious area (decimal fraction)
ARS	Adaptive Random Search
BASEFL	Base flow differences
BIAS	Summation of differences between simulated and observed discharges divided by observation
DINC	Time step length (day)
DT	User specified time step (day)
ESP	Extended Streamflow Prediction Program
INIT	Initial parameter estimation program
INSQPLOT	Operation to generate instantaneous discharge plot
LINDRV	Linear filter program
LZFPC	Lower zone free primary contents (mm)
LZFPM	Lower zone primary free water capacity (mm)
LZFSC	Lower zone free supplemental contents (mm)
LZFSM	Lower zone supplemental free water capacity (mm)
LZFW	Lower zone free water (mm)
LZPK	Fractional daily primary withdrawal rate
LZSK	Fractional daily supplemental withdrawal rate
LZTW	Lower zone tension water (mm)

LZTWC	Lower zone tension water contents (mm)
LZTWM	Lower zone tension water capacity (mm)
MAP	Maen Areal Precipitation
MAT	Mean Areal Temperature
MCP	Manual Calibration Program
MEAN-Q	Operation to compute of mean discharge from instantaneous discharges
MITLAND	MIT version of Sacramento soil moisture accounting model
NAS9000	National Advanced Systems Model 9000 computer
NCCF	National Weather Service Central Computer Facility
NINC	Number of computational intervals per user specified time step
NINF	Noninferior solution program
NWS	National Weather Service
NWSRFS	National Weather Service River Forecast System
OPT	Automatic Optimization Program
OSRCH	Random search optimization program
PCTIM	Minimum impervious area (decimal fraction)
PDIFF	Flood peak differences
PE	Potential Evapotranspiration
PEADJ	ET-demand adjustment factor
PFREE	Decimal fraction of percolated water going directly to lower zone free water storage
PXADJ	Precipitation adjustment factor
QIN	Instantaneous discharge
QME	Observed mean daily discharge
R'	Correlation coefficient
REDO-UHG	Reduced order unit hydrograph operation

REXP	Percolation equation exponent
RFC	River Forecast Center
RIVA	Riparian vegetation area (decimal fraction)
RMS	Root mean square error
RSERV	Decimal fraction of lower zone free water not transferrable to lower zone tension water
RVAR	Variance of residuals
SAC-SMA	Sacramento Soil Moisture Accounting Model
SIDE	Ratio of deep recharge to channel baseflow
STAT-QME	Operation to compute statistical summary for mean daily discharges
TASC	The Analytic Science Corporation
TCI	Total channel inflow
TMVOL	Total monthly volume
UGH	Unit hydrograph horizontal adjustment factor
UGV	Unit hydrograph vertical adjustment factor
UNIT-HG	Unit hydrograph operation
URS	Uniform Random Search
UZFW	Upper zone free water (mm)
UZFWC	Upper zone free water contents (mm)
UZFWM	Upper zone free water capacity (mm)
UZK	Fractional daily upper zone free water withdrawal rate
UZTW	Upper zone tension water (mm)
UZTWC	Upper zone tension water contents (mm)
UZTWM	Upper zone tension water capacity (mm)
WY-PLOT	Operation to compute water year flow plot
ZK	Daily recession coefficient
ZPERC	Maximum percolation rate coefficient

ABSTRACT

MULTILEVEL CALIBRATION STRATEGY FOR COMPLEX HYDROLOGIC SIMULATION MODELS

Larry E. Brazil

Office of Hydrology, National Weather Service, NOAA
Silver Spring, Md.

A systematic methodology was developed for calibrating conceptual hydrologic simulation models. A multilevel strategy which should be applicable to any complex simulation model was used to reduce the problem of model parameter estimation to a number of subproblems which could be solved using several different optimization techniques. The National Weather Service Sacramento Soil Moisture Accounting Model was chosen for implementation of the methodology. A state-space version of the model was formulated for use in some components of the study.

Three levels of optimization were used in the application of the strategy. Level I work consisted of the development of a guided interactive initial parameter estimator. The program uses computer generated graphics along with interactive input to lead an inexperienced user through some of the steps of initial data quality control and estimation of the model parameters. Two random search techniques were developed for use in the Level II analysis. The first procedure, a uniform random search technique, randomly selects parameter values and generates an output data set of various statistics which can be evaluated with a multi-objective post simulation analysis program. The second random search procedure converges as the simulation statistics improve. A recursive parameter estimation procedure was developed for Level III and tested against a direct search algorithm. The recursive technique uses the state-space model with a state augmentation form of the Kalman filter. The filter was tested for sensitivity to inputs. All of the procedures were tested and verified with synthetic data and a case study was performed for the Leaf River watershed near Collins, Mississippi. The study showed that the multilevel strategy provided a satisfactory calibration for the basin in far less time than using previous methods.

Chapter 1

INTRODUCTION

Calibration of computer simulation models is a topic of growing importance as sophisticated models continue to be developed to aid in the understanding and analysis of complex systems. Simulation models are used for a variety of purposes. Applications range from simulation of hydrologic systems to the prediction of earthquakes to preparation of financial forecasts. One item many of the models have in common is that they must be calibrated in some form in order to be effective. Calibration in this study refers to the selection of coefficients or parameters which minimize some measure of performance. The focus of this research is to develop and test a systematic approach to calibration of a conceptual hydrologic simulation model.

Hydrologic models, or more specifically, rainfall-runoff models, are widely used in engineering analyses and scientific studies. Hydrologic forecasting for the purpose of issuing flood forecasts and water management is one important use of the models. In addition, information obtained from forecast models is used as input to decisions concerning water supply, irrigation, power production, reservoir operation, recreation, and water quality.

Problem Definition

Hydrologic simulation models serve various purposes, such as estimation of runoff data, extension of runoff predictions to ungaged locations, simulation of extreme hydrologic phenomena and forecasting of future events. Models must be calibrated for the specific area for which they are to be used. Accuracy of a particular model usually is dependent on the accuracy of the calibration. Improvements in techniques which enhance users' abilities to calibrate hydrologic models will provide improved hydrologic simulation capabilities, potentially resulting in considerable savings in lives and reduction in property damage.

The calibration process generally consists of estimating the values for parameters which will minimize the differences between observed historical streamflows and streamflow values computed by the model. Parameters are the coefficients in model equations which allow the model to be adapted to long-term geographic or hydrologic conditions. Conceptual hydrologic simulation models have several parameters. The calibration problem is one of selecting the set of parameters from the many combinations which will produce the best simulation. A model with 12 parameters, for instance, each evaluated at only 10 values, would require 10^{12} iterations of the model. At one iteration per second, the time required to evaluate all the combinations would be approximately 32,000 years. Obviously, exhaustive enumeration is not feasible for most conceptual models. Although one combination of parameters may provide the best fit based on one or more statistics, most calibration problems have nonunique solutions. Several combinations of parameter values usually will provide acceptable

results. The real problem, then, is to find a suitable methodology for determining a set of parameters which produce a reasonable simulation.

The actual procedures used in calibrating conceptual rainfall-runoff models vary considerably, depending on the form of the model being calibrated. Most currently available calibration procedures are time-consuming and often result in suboptimal estimates of model parameters. In fact, the calibration process usually becomes a trade-off between time spent calibrating the model and model simulation accuracy. Calibration results are normally a function of the user's knowledge of the concepts in the model. Conceptual soil moisture models are usually quite complex and generally highly nonlinear, making it difficult to obtain a thorough understanding of the model.

Parameter estimation in hydrologic modeling is a topic which has been dealt with extensively in the literature; however, a considerable amount of research remains to be performed in this area. As of this time, no conceptual hydrologic forecast model has been shown to possess the characteristics necessary to provide accurate, continuous river forecasts and have the capability of being easily and accurately calibrated by a user not thoroughly familiar with the model components. Development of procedures which enable users of a proven forecast model to produce better or more efficient calibrations should be a valuable contribution to the hydrologic modeling field.

Study Objectives

The purpose of this research is to develop a methodology for systematically estimating the parameter values of a conceptual hydrologic forecast model and apply the methodology to an existing model. Specific objectives include:

1. Review current approaches to rainfall-runoff model calibration.
2. Analyze the structure of a conceptual hydrologic forecast model and decompose the model into components.
3. Develop a multilevel model calibration methodology which combines user experience, mathematical programming, and systematic search techniques based on stochastic estimation theory.
4. Demonstrate the use of the developed methodology on an actual watershed.

Thesis Organization

The thesis is divided into seven chapters. Chapter 2 presents a general description of calibration procedures and an outline of the proposed solution approach. A review of related research in rainfall-runoff modeling and optimization techniques is described in Chapter 3. Chapter 4 discusses the selection of the model for application of the methodology and presents the development of a state-space version of the model. Chapter 5 describes the development of the technical details of

the multilevel calibration system. The system consists of three levels of optimization: an initial parameter estimator, a random search procedure and a recursive estimation technique. The recursive technique is an application of the augmented Kalman filter to the state-space model developed in Chapter 4. A case study is presented in Chapter 6 to demonstrate the utility of the developed methodology for an actual watershed. Chapter 7 provides a summary of the work along with conclusions and recommendations for future research.

Chapter 2 CALIBRATION METHODOLOGY

Introduction

The purpose of this chapter is to present a methodology for systematic hydrologic model calibration. The approach was designed to combine the best aspects of existing optimization tools and newly developed techniques into a systematic procedure for estimating parameters. The approach incorporates the experience of hydrologists, mathematical programming, and systematic search techniques using optimal stochastic estimation theory concepts into a workable solution to many existing calibration problems.

The optimization techniques presented in this thesis represent a sample of tools which could be incorporated into an interactive calibration system. The methodology is the framework within which the tools are applied. The work presented in this study is part of a larger research project designed to develop an enhanced interactive modeling environment. Within the environment, a user will have the capability to perform interactive processing, analyze computer generated graphical displays with dynamic animation, converse with the system through interactive input devices, and submit background jobs to an efficient processor of mathematical instructions. Unlike many previous calibration research projects designed to develop enhanced fine-tuning techniques, the purpose of this study is to examine and improve the overall calibration process, beginning with initial parameter estimation.

The framework is patterned after procedures typically used by experienced hydrologists to perform model calibration. The overall goal of the process is to optimize the evaluation criteria, also called objective functions, which measure the difference between the observed and simulated flows. In most calibration studies, the most readily identifiable parameters are estimated first from soil or vegetation data or computed by analyzing hydrologic records. In many cases, specific parameters can be estimated by analyzing observed flows for isolated events where the parameters are known to have the greatest influence on simulated flows. When all parameters have been initially estimated or assigned nominal values, the user proceeds to make trial-and-error runs. Trial-and-error runs produce information concerning the sensitivity of output to changes in various parameters. The information is used to decide what adjustments should be made to parameters to begin to improve the model fit. Trial-and-error runs generally continue until the user has exhausted his patience or his ability to improve the simulation. Automatic calibration is used to further adjust parameter values according to programmed algorithms. Calibration typically ends with fine-tuning runs to try to eliminate any remaining biases. In addition, verification runs often are made for a period of data not in the original calibration analyses to check for biases in the simulation.

The underlying objective in current calibration procedures is to isolate and identify some of the components of the model in the initial

phase and then begin reducing the dimension of the calibration problem by systematically estimating the remaining parameters. The methodology presented in this thesis is designed to reduce the problem dimension in several levels as shown in Figure 2.1 and automate many of steps performed previously by hand. Projection is a concept which also can be incorporated into the multilevel strategy by iteratively fixing some parameters at specified levels and optimizing others. The following paragraphs describe the three levels of the strategy and the associated tools developed in this study. Guidance is given in later chapters concerning the appropriate parameters to be estimated in each level.

Multilevel Strategy

The first level of the calibration strategy was designed in an attempt to fix as many parameters as possible at reasonable values by performing computations similar to those currently used in manual calibration. The strategy is to decompose the specified model into some of its components so that some of the parameters can be estimated independently. An interactive program would provide the user with graphical displays that could be analyzed with the aid of computational algorithms. The program basically guides the user through initial parameter estimation.

The second level in the strategy is designed to be a global search procedure so that the full range of parameters not estimated in the Level I analysis can be examined. Since exhaustive enumeration is not possible; other techniques which analyze only portions of the response surface must be considered. A response surface is composed of the intersections of the various sets of parameter values and their corresponding evaluation criteria. A model with N parameters, for instance when evaluated with one objective function, will have a response surface of $N+1$ dimensions. Although they do not cover the entire response surface, random search procedures have been shown to be effective tools for optimizing response surfaces with several dimensions. The output from the Level II work should be a reasonable starting point for a fine-tuning analysis.

The objective of the third level is to perform a local search using a technique most applicable to the modeling situation. When the enhanced interactive environment is completed, several fine-tuning tools should be available. Some of the attractive candidates for a search of this type are existing gradient or hill-climbing procedures and recursive estimation techniques based on the concepts of linear and nonlinear filtering. Kalman filtering may be particularly suited for estimating some model parameters and provides an alternative to traditional response surface search procedures.

The final product from the multilevel research should be a workable procedure for systematically estimating the hydrologic model parameters without requiring a detailed knowledge of the models or years of calibration experience.

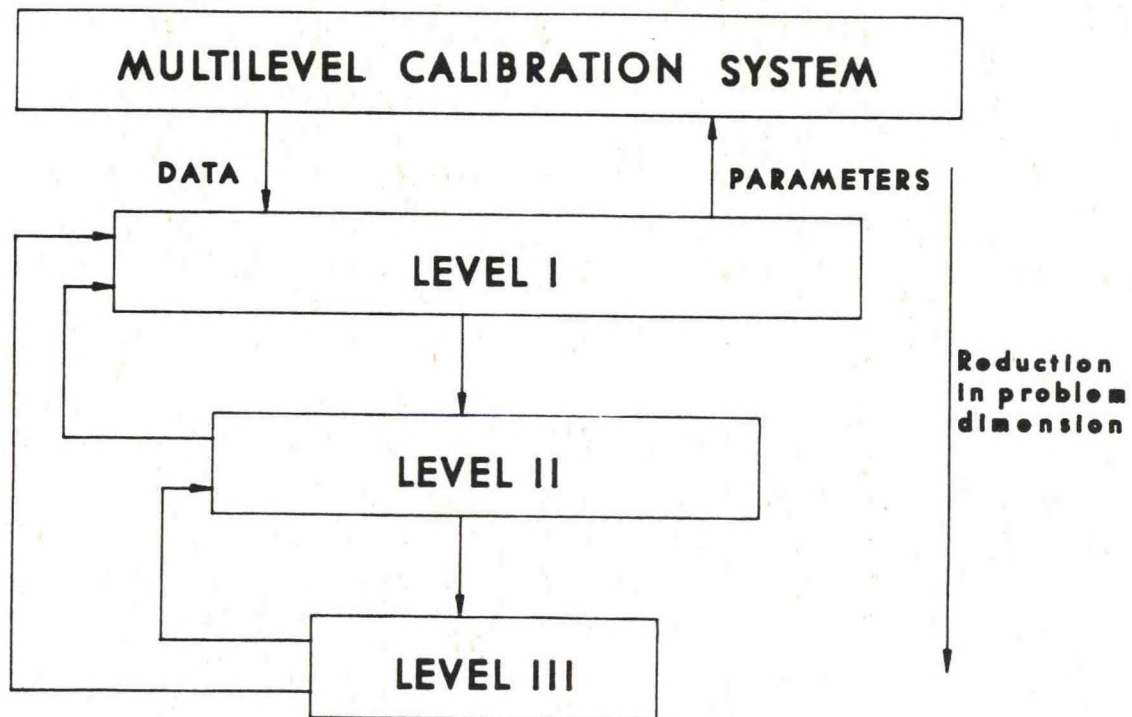


Figure 2.1. Multilevel Calibration Methodology

Chapter 3 RELATED RESEARCH

Introduction

The purpose of this research is to develop a generalized methodology for effectively estimating hydrologic simulation model parameters and demonstrate it using an existing conceptual rainfall-runoff model. The research work concerns several areas which have been dealt with extensively in published literature. The areas of rainfall-runoff modeling and model analysis have been the topic of numerous studies. Optimization, and more specifically, model calibration, is a subject of considerable interest in a wide range of scientific areas. As the review of literature will show, the field of hydrologic modeling has benefitted greatly from the application of results from several research disciplines.

This chapter provides an overview of numerous studies which are related to the research described in this thesis. Much of this work is built on the results of the previous projects. Applicable details of the most pertinent studies are given in appropriate sections throughout the thesis.

Rainfall-Runoff Modeling

Descriptions of conceptual rainfall-runoff models have been abundant in recent years in water resources publications. Many of the currently used models were developed in the 1960's and early 1970's as the use of computers for simulation modeling became common. One of the earliest and most widely publicized models was the Stanford Watershed Model (Crawford and Linsley, 1966). Other models include the Dawdy-O'Donnell model (Dawdy and O'Donnell, 1965), the Dawdy-Bergman U.S. Geological Survey Model (Dawdy, et al., 1972), the Haan model (Haan, 1972), and the Boughton model (Boughton, 1965). Burnash (1973) published a document describing the Sacramento soil moisture accounting model which is used by the National Weather Service (NWS) for hydrologic forecasting. Manley (1975) described a model which uses physically realistic parameters such as catchment shape and soil type in addition to hydrometeorological data. Many of the models are similar in that they conceptually represent the watershed as consisting of one or more soil moisture zones. Water generally is passed through the zones by means of infiltration and percolation algorithms. Soil moisture zones are depleted by evapotranspiration and lateral outflow which often is represented as outflow from a linear reservoir.

Several papers have been published reviewing various rainfall-runoff models. Clarke (1973) presented a thorough review of the use of mathematical models in hydrology and provided a classification system for the models. Probably the most thorough review of models was made by Fleming (1975). In this book, nineteen models are described in considerable detail. Weeks and Hebber (1980) published a comparison of five rainfall-runoff models, including the Boughton, Stanford and Sacramento models. The Sacramento model was selected as the

sophisticated conceptual model giving the best results, partly because of its "straightforward structure" (Weeks and Hebber, 1980, p. 23). The Boughton model was deemed inadequate.

Two more recent studies have investigated the components in the Sacramento model and the effect of model structure on parameter identifiability. Gupta and Sorooshian (1983) analyzed the percolation function in the model and demonstrated the difficulties in obtaining unique parameter values due to structural configuration. Sorooshian and Gupta (1985) later introduced an index for measuring parameter interaction and proposed procedures for reparameterizing model functions with identifiability problems.

In the 1970's researchers began to realize that developments in the field of control theory could provide hydrologic models with new capabilities. The use of mathematical filtering concepts became widespread. The Kalman filter was shown to be extremely useful in updating model state variables, separating model and measurement errors and estimating parameters in simplified models. The conference proceedings of Chiu (1978) and O'Connell (1977) give a thorough background on the use of the Kalman filter in parameter estimation. O'Connell and Clarke (1981) also have published a review of the use of filtering in adaptive hydrological forecasting. A more recent general description of the use of Kalman filtering in real-time forecasting is given by Wood and O'Connell (1985). Kitanidis and Bras (1980) reported on the development of the first state-space form of the Sacramento model. The model was coupled with the Kalman filter for automatic state updating. The Analytic Sciences Corporation (TASC, 1979 and TASC, 1980) also developed a state-space version of the model and routed the simulated flows using a state-space unit hydrograph model. Georgakakos (1986) coupled a state-space meteorological forecast model with a state-space version of the Sacramento model to form a stochastic hydrometeorological model for flood forecasting. Aboitiz (1986) used the Kalman filter with a daily water balance model to estimate and forecast soil water depletion and crop evaporation for irrigated fields. Investigation of the use of various forms of filtering in hydrologic forecasting was made by Puente and Bras (1987). Results showed that the extended Kalman filter was as effective as more complicated nonlinear filters.

Model Calibration

Most conceptual hydrologic forecast models are calibrated using a combination of trial-and-error and automatic parameter estimation procedures. Numerous studies have been performed to improve manual and automatic optimization techniques and determine better evaluation criteria. Some of the more recent projects have focused on applying research results from other fields to the parameter estimation problem. These include more extensive use of the Kalman filter and utilization of advances in computer science in the areas of hardware design and artificial intelligence.

Most of the recent papers have dealt with automatic fitting procedures, however, some authors have discussed first stage manual

calibration efforts. Manley (1978) described the three stages of the calibration procedure used on his own model (Manley, 1975). The first two stages consisted of manually assigning parameter values based on watershed characteristics and hydrograph analysis. Mein and Brown (1978) presented a parameter sensitivity analysis procedure based on the computation of the variance of each fitted parameter. Brazil and Hudlow (1980) described the trial-and-error calibration procedures used with the Sacramento model. Armstrong (1978) presented a method for deriving initial estimates of many of the Sacramento model parameters based on reported watershed soil properties. Abbi (1980) described his experience with trial-and-error calibration of the Sacramento model through a water balance study.

Automatic parameter estimation routines generally consist of gradient methods where first and second derivatives of the objective function are obtained or search methods where parameter changes are based on previous successful adjustments. Many of the basic optimization techniques currently in use today were developed in the 1960's. Examples include the methods presented by Hooke and Jeeves (1961), Rosenbrock (1960), Powell (1965), Fletcher and Powell (1963), Nelder and Mead (1965), Goldfeld, et al. (1966), and Beard (1967). One of the first comprehensive sources of FORTRAN optimization codes was the book by Kuester and Mize (1973) which includes coding for 26 optimization techniques. One of the most complete early reviews of automatic parameter estimation techniques in conceptual rainfall-runoff modeling was made by Ibbitt (1970), which considers a number of models and problems often encountered in model calibration. Ibbitt tested nine optimization techniques on the O'Donnell model (Dawdy and O'Donnell, 1965), including those by Beard (1967), Rosenbrock (1960), Powell (1964 and 1965), and Fletcher and Powell (1963). Four lesser known procedures also were used. Rosenbrock's hill climbing method was determined to be the most effective. Sorooshian (1980) made a comparison of Rosenbrock's search technique and Nelder and Mead's simplex algorithm concluding that each method showed different degrees of effectiveness depending on the objective function.

Numerous papers have been written on specific applications of automatic parameter optimization to hydrologic models. Only a representative sample will be described here. One of the first papers on this topic was written by Dawdy and O'Donnell (1965). They applied Rosenbrock's procedure to their model and showed favorable results. Liou (1970) reported on the application of automatic optimization techniques to the Stanford watershed model. James (1972) reported a favorable experience with Liou's program. He pointed out, however, that considerable research was still required in this area. Monroe (1971) applied Hooke and Jeeves' direct search method to the Stanford model with reasonable success. The same program also has been applied to the Sacramento model and unfortunately often tends to converge on local optima. The simplex method of Nelder and Mead was applied to the Boughton model by Johnston and Pilgrim (1976). They reported many of the same difficulties described by other researchers: interdependence among parameters, local optima, and indifference locations in the response surface. An attempt also was made to develop a form of the

Boughton model which could be optimized explicitly from the model equations; however, a complete set of algebraic solutions was never obtained.

Derivative based search procedures have never been popular for use with conceptual soil moisture accounting models because no effective technique was available for computing the derivatives other than numerical evaluation. Gupta and Sorooshian (1985) developed a procedure for calculating analytical derivatives of conceptual rainfall-runoff models with thresholds. The method is based on an analysis of the modality of behavior present in the model. Henderson (1987) applied the explicit derivative computation procedure with a gradient optimization algorithm to the Sacramento model. Problems were shown to exist in the technique due to discontinuities in the response surface. Another test of optimization algorithms was performed by Pickup (1977). He found that the techniques of Powell, Nelder and Mead, and Rosenbrock all performed reasonably well with the Boughton model. Pickup also concluded that the development of an optimization strategy which optimizes one select group of parameters at a time can improve the results.

Many of the studies of optimization techniques also have included analyses of objective functions and the effect of errors in the data. One of the most notable objective function investigations was made by Diskin and Simon (1977). They presented a procedure for selecting the appropriate objective function for a model. A study of general response surface analysis procedures was made by Sorooshian and Arfi (1982). The study provided two sensitivity measures, one for concentricity and one for interaction. Other studies by Sorooshian (Sorooshian, 1983 and Sorooshian, et al., 1983) have resulted in two objective functions: one which accounts for the presence of autocorrelated errors in streamflow and one which accounts for heteroscedastic streamflow errors. The objective functions have been shown to improve the reliability of models which simulate flows where the error conditions are known to exist. Other papers have since discussed the utility of the functions (Yeh, 1982 and Ibbitt and Hutchinson, 1984). Studies by Kuczera (1983) and Troutman (1985) have also addressed the importance of considering streamflow errors in estimating parameters. Troutman showed how bias in input error may contribute to bias in parameter estimation.

Numerous studies have shown the local convergence problems that exist with automatic search techniques (Brazil and Hudlow, 1980). A recent report by Croley and Hartman (1986) showed how the parameter set for the Large Basin Runoff Model converged to different optima based on the initial parameter values. Random search procedures tend to be independent of starting values, and can overcome many of the starting value problems associated with systematic searches. Advances in computer hardware capabilities have opened the door to the application of optimization procedures that are more computationally intensive. A project designed to produce a general purpose global optimizer resulted in the Adaptive Random Search (ARS) procedure (Pronzato, et al., 1984). Studies have shown that it can be an effective hydrologic model calibration tool (Brazil and Krajewski, 1987).

Use of the Kalman filter in parameter estimation has gained popularity in recent years. Groups from the Massachusetts Institute of Technology (MIT) (Restrepo-Posada, 1982) and the Analytic Sciences Corp. (TASC) (1981) performed studies incorporating a Kalman filter algorithm into a state-space version of the NWS model. The programs were designed to compute objective functions based on the residuals resulting from a run of the filtering form of the model through the data. The TASC and MIT programs optimized parameter values based on the Goldfeld, et al. (1966) and Fletcher-Powell (1963) procedures, respectively. In addition to state updating, filters have been used in some cases to estimate model parameters. Labadie, et al. (1980) used the Kalman filter in a state augmentation form to estimate transmissivities in a groundwater model. Bras and Restrepo-Posada (1980) used state augmentation and stochastic approximation to estimate three of the parameters of a simplified version of the Sacramento model. Georgakakos and Brazil (1987) reported on what appears to be the first application of state augmentation with the Kalman filter to a complex conceptual soil moisture accounting model, the Sacramento model. Since then, Rajaram and Georgakakos (1987) also have successfully presented a procedure for recursively estimating states and parameters for a conceptual watershed model, the Enhanced Trickle Down model.

In addition to the traditional parameter optimization procedures such as search algorithms and Kalman filter approaches, research in the field of water resources has produced a number of special application optimization techniques. The proposed research for this project includes an analysis of a technique called projection. Projection basically consists of holding certain complicating parameters constant while optimizing the remaining parameters, and then varying the complicating parameters to examine the resulting response surface. In other words, the simplifying parameters in the model are projected onto the complicating parameters. More details of the method are given by Geoffrion (1972). Labadie and Helweg (1975) reported success with projection in an application to the solution of a water well step-drawdown test equation. A highly nonconvex curve fitting problem with many nonunique local optima was transformed into a convex problem with a unique global optimum. An application of projection also was made to the estimation of parameters for a Muskingum river routing model (Gavilan and Houck, 1985).

Although most of the literature on model calibration has focused on the development of new optimization techniques, some studies have been made to address the issues of calibration strategy. Wildermuth and Yeh (1979), for instance, presented a "unified approach" to calibrating the Los Angeles County Flood Control District rainfall-runoff model. James and Burges (1982) described a systematic approach to model calibration and addressed the issues of handling data errors. Basically, they presented a methodology for performing stages of calibration designated as preliminary and refined. Willgoose (1987) performed a study in which a stochastic parameter estimation strategy was developed for the Sacramento model. He found that calibration of small groups of parameters overcame many problems associated with parameter

interaction. Carrera-Ramirez (1984) found while estimating parameters for a groundwater model that using a combination of search techniques can give good results. These strategies are consistent with the methodology presented in this thesis.

Recent advances in artificial intelligence, especially expert systems, are beginning to make their way into the field of hydrologic modeling. Expert systems are computer programs designed to perform computations or make decisions in a manner similar to an expert in the field. Studies were performed at the Stanford Research Institute to develop an expert system for estimating initial parameter values for the Stanford model (Reboh, et al., 1982). The values were computed based on a user's responses to questions concerning the watershed characteristics. Work also has been performed to develop an expert system for snowmelt modeling (Engman, et al., 1986). The system assists a user in preparing data, selecting parameters, and evaluating results.

Summary

This review of the literature covers only a small portion of the publications in this field. Obviously, a great deal of work has been performed in this area. The extensive interest of so many professionals in this field demonstrates the importance of improving the techniques used to calibrate hydrologic models.

Chapter 4

MODEL DEVELOPMENT

Introduction

The multilevel calibration scheme described in the previous chapters could be applied to a variety of hydrologic models. In fact, the methodology should be applicable to almost any type of simulation modeling system. Although model complexity is not a requirement for implementation of the strategy, users of a model which is characterized as being difficult to calibrate because of its large number of parameters and nonuniqueness of solution, stand to benefit most from the procedures. This chapter discusses the selection of the model for application of the methodology and describes development work performed to put the model into state-space form.

System Selection

Several existing models and modeling systems are potential candidates for application of the calibration methodology. Examples include any of the conceptual rainfall-runoff models discussed in Chapter 3 or systems of models such as SSARR (U.S. Army Engineer Division, 1975) or HSPF (Imhoff, 1981). For the reasons described below, a decision was made early in the research project to apply the methodology to the National Weather Service River Forecast System (NWSRFS) being implemented in various parts of the United States. The NWS is responsible for accurate and timely hydrologic forecasts for rivers and watersheds throughout the country. Most of the forecasting is performed with the aid of computer simulation models. One of the models used in NWSRFS is the Sacramento Soil Moisture Accounting (SAC-SMA) Model (Burnash, et al., 1973). As with any forecast system, forecast accuracy is significantly dependent on the accuracy of the calibration of the models. A major problem faced by the NWS is the large number of basins that need to be calibrated as new basins are added to the forecast network and others need to be recalibrated to reflect changing watershed conditions. Considerable effort will be put into calibrating NWS models within the next few years, making model calibration an area in which promising techniques will be given a high priority for testing and implementation. The potential payoff for improvements in this area in terms of saved lives and reduction in property damage is considerable. Various types of research work have been performed in recent years on the NWS calibration procedures which can be combined with new techniques to produce a systematic approach to NWS model calibration. These reasons combined with the fact that the conceptual rainfall-runoff model used by the NWS has been tested extensively and applied throughout the world make the NWSRFS an ideal system for testing a new calibration methodology.

NWSRFS

The NWSRFS is a set of interrelated computer programs developed to provide continuous hydrologic forecasting capabilities for NWS River Forecast Centers (RFC's). The system consists of an assortment of software components for hydrologic, hydraulic and data processing functions. A schematic diagram of the system is shown in Figure 4.1. The Operational Forecast System and the Extended Streamflow Prediction System have been described in various publications (Anderson, 1986; Brazil and Smith, 1981; and Day, 1985). The component of interest for this research is the Calibration System. The system is composed of the historical data access programs, the calibration data files, the data preprocessor and utility programs and the hydrologic simulation programs. The simulation programs currently consist of the Manual Calibration Program (MCP) and the Automatic Optimization Program (OPT). These programs will be discussed in more detail in Chapter 5.

The hydrologic simulation portion of the calibration system consists of three basic computational elements (Brazil and Hudlow, 1980): a snow accumulation and ablation model, a collection of rainfall-runoff models and a set of channel routing routines. Each model within the system is called an operation. An operation can be any computational algorithm which produces or modifies a time series of data or displays results. Appropriate operations are selected and sequenced into the proper computational order to simulate a watershed. A typical nonsnow headwater basin calibration setup is shown in Table 4.1. For this example, the watershed is modeled using the SAC-SMA operation to convert rainfall into runoff. The runoff is distributed in time using a unit hydrograph. Instantaneous discharges (QIN) are converted into mean daily flows using the MEAN-Q operation so that simulated flows can be compared statistically with the observed mean daily discharges (QME). Various routing models are available for routing the headwater flows to downstream points and combining local inflows. Input to the headwater models consists of mean areal precipitation (MAP) and estimates of potential evapotranspiration (PE) and, in the case of a snow basin, mean areal temperature (MAT). Programs are available within the calibration system to compute the mean areal estimates from the recorded point values.

Model Formulation

The work presented in this research deals primarily with application of the developed calibration methodology to the SAC-SMA and unit hydrograph models. For purposes of testing the methodology, several factors must be considered in selecting the form of the models to be used:

1. The purpose of the Level I work is to analyze the SAC-SMA model by components and estimate initial parameters based on the model decomposition. Any form of the model which facilitates analysis by components is desirable.

NATIONAL WEATHER SERVICE RIVER FORECAST SYSTEM

OPERATIONAL FORECAST SYSTEM

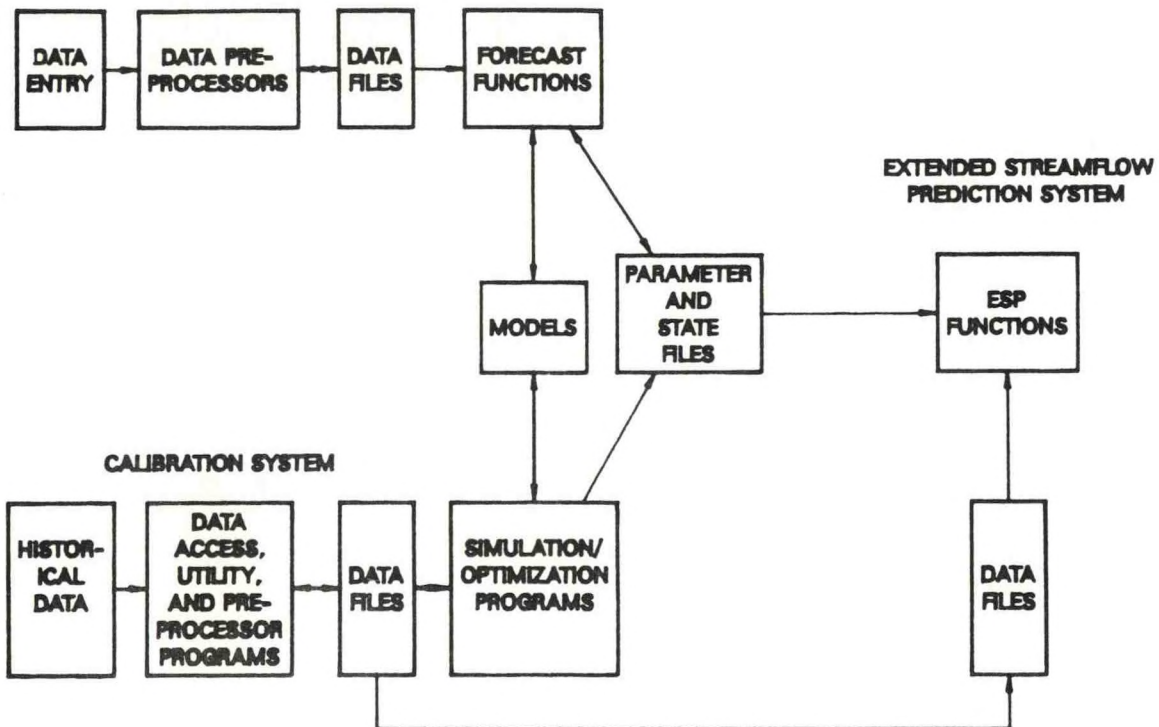


Figure 4.1. Schematic Overview of NWSRFS

Table 4.1

Sequence of Operations for Non-snow Headwater Basin

<u>Operation</u>	<u>Description</u>
1. SAC-SMA	Sacramento soil moisture accounting model
2. UNIT-HG	Unit hydrograph
3. MEAN-Q	Computation of mean discharge from instantaneous discharges
4. INSQPLOT	Instantaneous discharge plot (if observations are available)
5. WY-PLOT	Water year mean daily flow plot
6. STAT-QME	Statistical summary - mean daily discharge

2. The Level II analysis requires a form of the model which is efficient for use in a search program where many iterations of the model will be run.

3. The Level III design includes several types of fine-tuning tools. One of the techniques is recursive parameter estimation using the Kalman filter. Application of the filter requires a state-space form of the model so that function derivatives can be computed for each of the model states.

4. Any form of the model which deviates from the original model must have parameters and functional components which are consistent with the original model.

5. Implementation of a state-space SAC-SMA model in NWS programs will enhance the NWS capabilities to update hydrologic forecasts.

In light of these issues, a decision was made to develop and implement a state-space form of the SAC-SMA and unit hydrograph models by building on the work of other research projects. The state-space model should provide a suitable mechanism for testing some of the levels of the calibration strategy. The original model also can be used for some of the analysis. The following sections describe both the original and state-space SAC-SMA and unit hydrograph models.

Currently Used SAC-SMA and Unit Hydrograph

The SAC-SMA model is conceptual in design in that the authors have attempted to parameterize soil moisture characteristics. Numerous papers have been published about the model (Burnash, et al, 1973; Peck, 1976; Brazil and Hudlow, 1980), so only a brief description will be given here.

The SAC-SMA model is complex and has a number of nonlinear components. The model is deterministic and has lumped input and parameters within a soil moisture accounting area. A watershed may be subdivided into several soil moisture accounting areas to simulate a distributed system. The model was conceptualized as simulating a block of the soil mantle. Functions in the model account for the wetting and drying of the block of soil and the associated transfer of water from one layer to another within the soil. Drainage of water from the block also is simulated. The model vertically divides the soil into two main soil moisture zones. The upper zone represents interception and upper soil storage, while the lower zone represents most of the soil moisture and groundwater storage. Figure 4.2 (from Lawson and Shian, 1977) shows a schematic diagram of the model. A list of the parameters and state variables in the model is given in Table 4.2.

The upper and lower zones store both "tension" and "free" water. Tension water is assumed to be tightly bound to soil particles and can be moved only by evapotranspiration. Free water, however, can move both horizontally and vertically through the soil profile. The tension water requirements must be met in the upper zone before water can be

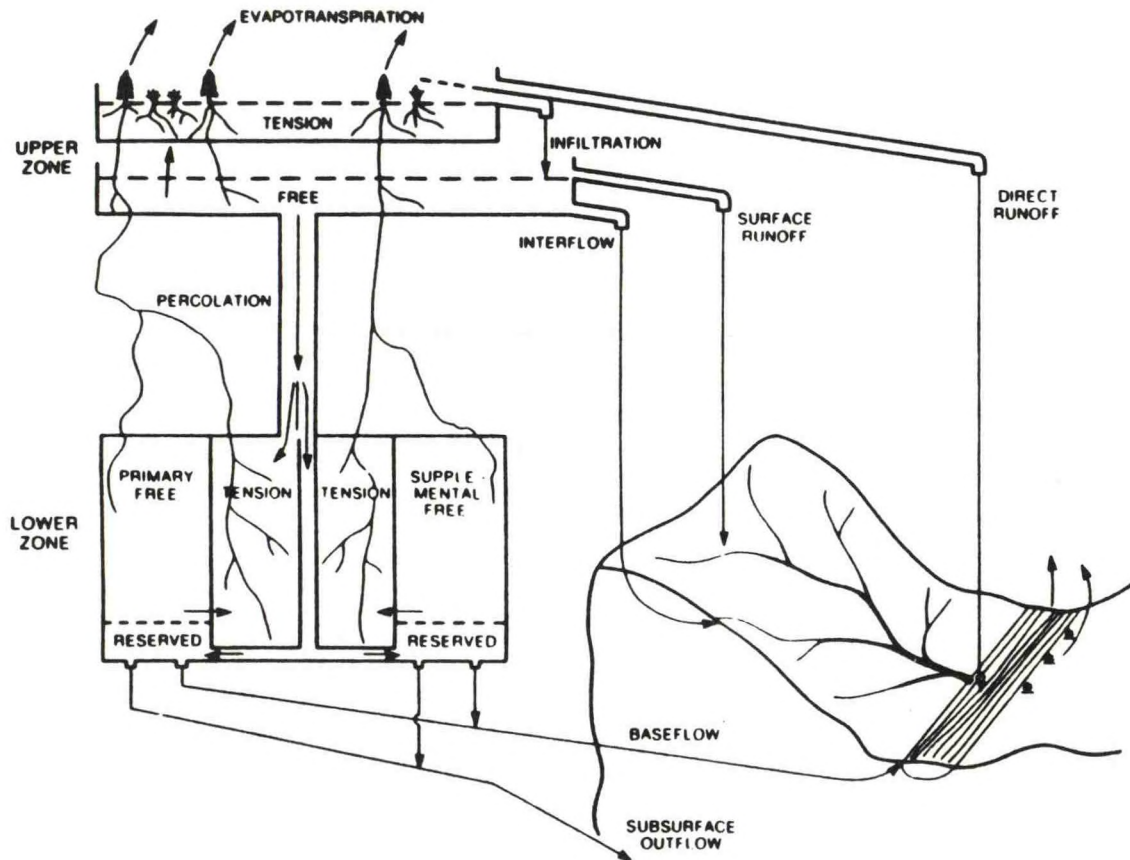


Figure 4.2. Schematic Representation of SAC-SMA Model
(from Lawson and Shiau, 1977)

Table 4.2

Parameters and State Variables Included in the
Soil Moisture Accounting Model

<u>Parameter</u>	<u>Description</u>
PXADJ	Precipitation adjustment factor
PEADJ	ET-demand adjustment factor
UZTWM	Upper zone tension water capacity (mm)
UZFWM	Upper zone free water capacity (mm)
UZK	Fractional daily upper zone free water withdrawal rate
PCTIM	Minimum impervious area (decimal fraction)
ADIMP	Additional impervious area (decimal fraction)
RIVA	Riparian vegetation area (decimal fraction)
ZPERC	Maximum percolation rate coefficient
REXP	Percolation equation exponent
LZTWM	Lower zone tension water capacity (mm)
LZFSP	Lower zone supplemental free water capacity (mm)
LZFPM	Lower zone primary free water capacity (mm)
LZSK	Fractional daily supplemental withdrawal rate
LZPK	Fractional daily primary withdrawal rate
PFREE	Decimal fraction of percolated water going directly to lower zone free water storage
RSERV	Decimal fraction of lower zone free water not transferrable to lower zone tension water
SIDE	Ratio of deep recharge to channel baseflow
<u>State Variables</u>	<u>Description</u>
UZTWC	Upper zone tension water contents (mm)
UZFWC	Upper zone free water contents (mm)
LZTWC	Lower zone tension water contents (mm)
LZFSC	Lower zone free supplemental contents (mm)
LZFPC	Lower zone free primary contents (mm)
ADIMC	Tension water contents of the ADIMP area (mm)

transferred to upper zone free water. The free water in the upper zone can be moved through percolation (to the lower zone), evapotranspiration, interflow, and tension water replacement.

During a time step (generally 6 hours), the model attempts to meet evapotranspiration demands before water is transferred by percolation or interflow. In the upper zone of the model, evapotranspiration occurs at the potential rate times the ratio of the contents of upper zone tension water (UZTW) to its maximum capacity. In the lower zone, the remaining evapotranspiration demand is attempted to be met by water from lower zone tension water (LZTW). If the demand exceeds the capacity of lower zone tension water to meet the demand, water from the lower zone free water storages is transferred to lower zone tension water.

Water moves from the upper zone to the lower zone by means of a percolation function. The function relates the capacities and contents of the upper and lower zones and is the key element in the transfer of water within the model. In general, water is transferred from upper zone free water (UZFW) to LZTW, however, the model has a feature which allows a fraction of the transferred water to be placed directly into the lower zone free water storage (LZFW) without fulfilling LZTW requirements. This allows a realistic simulation of basins where lower zone drainage is significant and total basin tension water requirements have not been met. Water also is transferred to LZFW by an overflow of LZTW.

The model has a feature which allows the impervious portion of the watershed to vary. This simulates basin response characteristics which are created by changes in the sizes of saturated areas along stream channels. The percentage of the area represented as being impervious is a function of the contents of the tension water zones.

The SAC-SMA model typically is used in conjunction with the unit hydrograph operation (UNIT-HG). UNIT-HG converts runoff generated from the SAC-SMA model into instantaneous discharges. The algorithm within the operation is based on the concepts presented by Linsley, Kohler, and Paulhus (1975). It is a simple, yet effective mechanism for temporally distributing simulated runoff (OH, 1987). Being a linear and time invariant system, it is particularly adaptable to updating techniques which are based on assumptions of linearity.

State-Space Model Development

Considerable resources have been expended in recent years to develop state-space forms of the SAC-SMA model (Kitanidis and Bras, 1980; TASC, 1980; and Georgakakos, 1986). In this form the states are expressed through individual equations as functions of the model parameters, inputs and other states. The formulation facilitates the transformation of the model into a structure which easily can be coupled with a linear filter for updating. Similar modifications have been made to the UNIT-HG operation in order to produce a reduced order state-space unit hydrograph algorithm (TASC, 1980).

Kitanidis was first to develop the state-space equations for the SAC-SMA model (Kitanidis and Bras, 1978). The purpose of the research

was to reformulate the SAC-SMA model into a framework amenable to linear estimation theory, so that the Kalman filter could be used to update the states of the system. The work involved development of procedures to account for the nonlinear properties in the model. In the original model the conceptual reservoirs behave as discontinuous functions. Tension water reservoirs, for example, produce no outflow until the contents exceed capacity. When this occurs outflow is equal to inflow. This nonlinear behavior is inconsistent with basic assumptions in the estimation theory concepts. Kitanidis' approach was to use the "describing function technique" discussed by Gelb (1974) for the most strongly nonlinear responses and Taylor expansion for the rest. Two states were added to the original model to account for linear channel routing. The research produced a discrete state-space version of SAC-SMA and demonstrated how the states of the model could be updated automatically using observations of instantaneous discharges and an extended Kalman filter.

The Analytic Sciences Corporation (TASC) developed a set of state equations to produce a continuous version of the SAC-SMA model at approximately the same time as Kitanidis (TASC, 1981). Although minor differences existed between the two models, mostly due to differences between discrete and continuous formulations, both models seemed to represent the primary simulation capabilities of the original Sacramento model. In addition to the SAC-SMA state equations, TASC developed a state-space model to approximate the impulse response of a unit hydrograph. Details of the unit hydrograph model formulation are given later in this section.

Georgakakos developed a real-time hydrometeorological forecast model by coupling the Kitanidis formulation of SAC-SMA with a meteorological model (Georgakakos, 1986). Runoff was distributed in time using a nonlinear channel routing model developed previously by Georgakakos and Bras (1980) and automatic state updating was performed through the use of the extended Kalman filter. Several modifications were made to the original Kitanidis state equations as a result of further model testing. In order to simplify the computations, Georgakakos replaced Kitanidis' describing function techniques with a nonlinear reservoir response. The procedure allows reservoirs to produce outflow as a function of saturation and prior to reaching capacity. Because of the spatially lumped nature of the model, this form probably is more consistent with soil inhomogeneity found in natural watersheds than the original model. Modifications also were made to the Kitanidis formulation to improve the allocation of percolating water between the lower zone free water reservoirs and to include surface runoff from the additional impervious area (Georgakakos, 1986).

Considerable progress has been made toward the development of a state-space Sacramento model for use with NWSRFS. Any of the described forms of the model could be formulated into an operation. It should be kept in mind that the purpose of the development of each of the previous state-space formulations was to facilitate updating. The purpose of selecting a model formulation for this research is to enhance calibration through updating techniques and other procedures.

Therefore, it is important to select a form of the model which accurately mimics the original SAC-SMA model in both update and non-update modes.

The Kalman filter algorithm consists of a forecast step and an update step. In the Kitanidis formulation, the forecast step used an enhanced version of the SAC-SMA model code which accounted for the modified thresholds. The Georgakakos formulation used the state equations with a variable time step integration scheme to produce forecasts. When rigid integration tolerances are imposed, this implementation essentially becomes a continuous model. Several test runs were made to compare the Kitanidis and Georgakakos models in a non-update mode. Only slight differences were found to exist between the channel inflows generated by the two models. Because of the enhancements the Georgakakos model offered over the Kitanidis model and the more simplified approach to threshold linearization, a decision was made to use the Georgakakos equations for the simulation step for this research.

Model Equations

The model equation symbols are described in Table 4.3. Most of the symbols were introduced by TASC (1981). Also, to simplify notation the following expressions are used:

$$c_1 = d'_\ell x_4^0 + d''_\ell x_5^0 \quad (4.1)$$

$$c_2 = \frac{d'_\ell x_4^0}{d'_\ell x_4^0 + d''_\ell x_5^0} \quad (4.2)$$

$$y = 1 - \frac{x_3 + x_4 + x_5}{x_3^0 + x_4^0 + x_5^0} \quad (4.3)$$

The model equations are:

Upper zone tension water(f_1) --

$$\frac{dx_1}{dt} = \left[1 - \left(\frac{x_1}{x_1^0} \right)^{m_1} \right] \phi x_p - u_e \frac{x_1}{x_1^0} \quad (4.4)$$

Upper zone free water(f_2) --

$$\frac{dx_2}{dt} = \left(\frac{x_1}{x_1^0}\right)^{m_1} \phi x_p \left[1 - \left(\frac{x_2}{x_2^0}\right)^{m_2}\right] - d_u x_2 - C_1(1 + \epsilon y^\theta) \frac{x_2}{x_2^0} \quad (4.5)$$

Lower zone tension water(f_3) --

$$\begin{aligned} \frac{dx_3}{dt} = & C_1(1 + \epsilon y^\theta) \frac{x_2}{x_2^0} (1 - P_f) \left[1 - \left(\frac{x_3}{x_3^0}\right)^{m_3}\right] \\ & - u_e \left(1 - \frac{x_1}{x_1^0}\right) \frac{x_3}{x_1^0 + x_3^0} \end{aligned} \quad (4.6)$$

Lower zone primary free water(f_4) --

$$\begin{aligned} \frac{dx_4}{dt} = & -d'_l x_4 + c_1(1 + \epsilon y^\theta) \frac{x_2}{x_2^0} \left[1 - (1 - P_f) \left[1 - \left(\frac{x_3}{x_3^0}\right)^{m_3}\right]\right] \\ & \left[\left(c_2 \frac{x_5}{x_5^0} - 1\right) \frac{x_4}{x_4^0} + 1\right] \end{aligned} \quad (4.7)$$

Lower zone secondary free water(f_5) --

$$\begin{aligned} \frac{dx_5}{dt} = & -d''_l x_5 + c_1(1 + \epsilon y^\theta) \frac{x_2}{x_2^0} \left[1 - (1 - P_f) \left[1 - \left(\frac{x_3}{x_3^0}\right)^{m_3}\right]\right] \\ & \left(1 - c_2 \frac{x_5}{x_5^0}\right) \frac{x_4}{x_4^0} \end{aligned} \quad (4.8)$$

Additional impervious area water(f_6) --

$$\begin{aligned} \frac{dx_6}{dt} = & \left[1 - \left(\frac{x_6 - x_1}{x_3^0} \right)^2 \left(\frac{x_1}{x_1^0} \right)^{m_1} \right] \Phi x_p - u_e \left(1 - \frac{x_1}{x_1^0} \right) \left(1 - \frac{x_6 - x_1}{x_3^0 + x_1^0} \right) \\ & - u_e \frac{x_1}{x_1^0} - \left[1 - \left(\frac{x_6 - x_1}{x_3^0} \right)^2 \right] \left(\frac{x_2}{x_2^0} \right)^{m_2} \left(\frac{x_1}{x_1^0} \right)^{m_1} \Phi x_p \end{aligned} \quad (4.9)$$

The output TCI from the soil moisture accounting model, referred to as total channel inflow per unit time is given by --

$$\begin{aligned} \text{TCI} = & (d_u x_2 + \frac{d'_l x_4 + d''_l x_5}{1 + \mu}) (1 - \beta_1 - \beta_2) \\ & + \Phi x_p \beta_2 = \left(\frac{x_6 - x_1}{x_3^0} \right)^2 \Phi x_p \left(\frac{x_1}{x_1^0} \right)^{m_1} \beta_1 \\ & + \Phi x_p \left(\frac{x_1}{x_1^0} \right)^{m_1} \left(\frac{x_2}{x_2^0} \right)^{m_2} (1 - \beta_1 - \beta_2) \\ & + \left[1 - \left(\frac{x_6 - x_1}{x_3^0} \right)^2 \right] \left(\frac{x_2}{x_2^0} \right)^{m_2} \left(\frac{x_1}{x_1^0} \right)^{m_1} \Phi x_p \beta_1 \end{aligned} \quad (4.10)$$

The state variables are constrained by:

$$0 \leq x_i \leq x_i^0 \quad i = 1, 2, \dots, 5$$

Computational Algorithm

Implementation of the state equations in a forecast mode can be done in several different ways. As mentioned previously, Georgakakos used an integration scheme which resulted in very small time steps. The issue is to determine a suitable implementation algorithm for solving the differential equations which will adequately emulate the original Sacramento model and will be an appropriate forecast step for propagating the system states in an updating scheme.

The left side of Figure 4.3 shows the various levels of complexity that can be used to calculate the forecast step. The original SAC-SMA model computes the new states for each time step by executing the

Table 4.3

State-space Model Equation Variables

State-space Notation

Original SAC-SMA

States:

x_1
 x_2
 x_3
 x_4
 x_5
 x_6

UZTWC (mm)
 UZFWC (mm)
 LZTWC (mm)
 LZFPC (mm)
 LZFSC (mm)
 ADIMC (mm)

Inputs:

x_p
 u_e

Mean areal precipitation (mm/ Δt)
 Potential evapotranspiration demand (mm/ Δt)

Parameters:

x_1^0

UZTWM (mm)

x_2^0

UZFWM (mm)

x_3^0

LZTWM (mm)

x_4^0

LZFPM (mm)

x_5^0

LZFSM (mm)

d_u

$1. - (1. - UZK)^{\Delta t}$

d_l

$1. - (1. - LZPK)^{\Delta t}$

d_l

$1. - (1. - LZSK)^{\Delta t}$

d_l

ϵ

ZPERC

θ

REXP

p_f

PFREE

μ

SIDE

β_1

ADIMP

β_2

PCTIM

m_1

UZTW nonlinear reservoir exponent

m_2

UZFW nonlinear reservoir exponent

m_3

LZTW nonlinear reservoir exponent

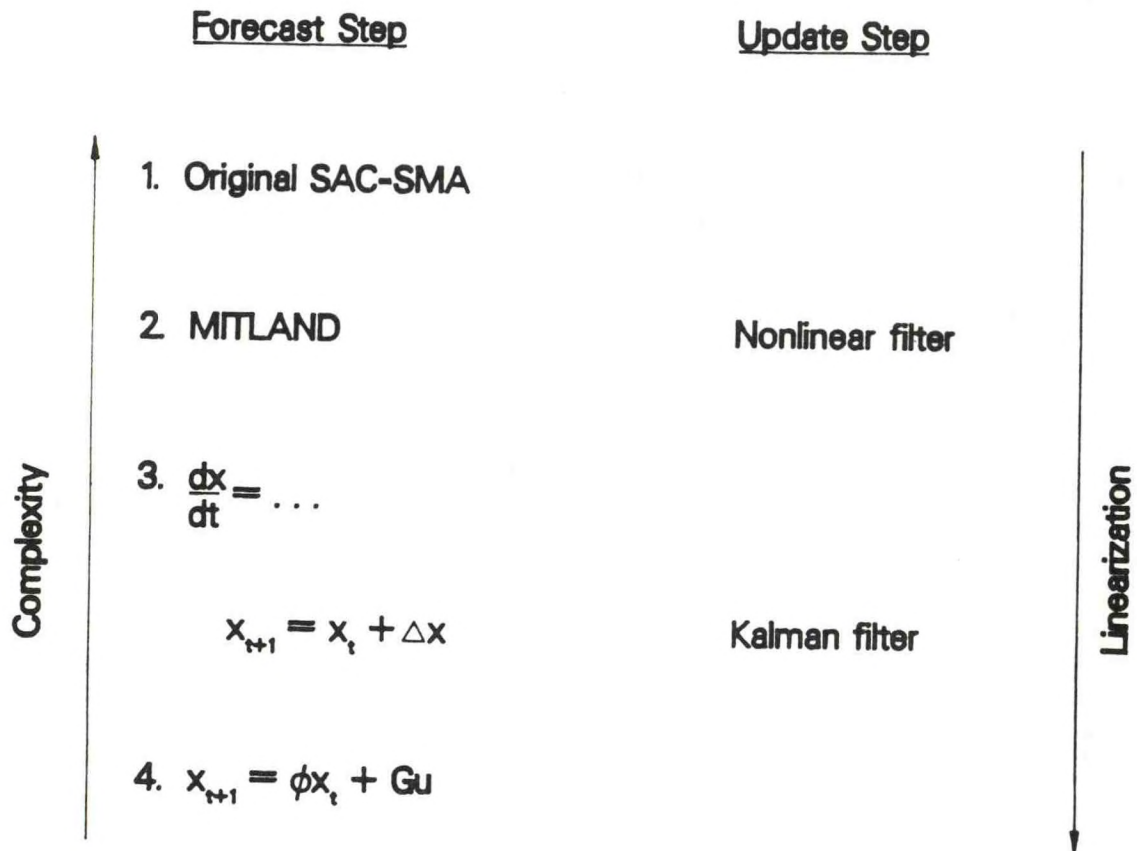


Figure 4.3. Complexity Levels of Forecast and Update Steps

nonlinear FORTRAN algorithms. As shown in Figure 4.3, this solution is the most complex and nonlinear of the possible forecast steps. The Kitanidis version of the model with its threshold approximations was called MITLAND. The simulation step in the Kalman filter algorithm is a linear translation and is shown as Step No. 4 in Figure 4.3. Details of the filter equations are presented in Chapter 5. The linear translation forecast model does not preserve the nonlinear features of the original model. Simulation runs were made with each form of the forecast step. Results showed that the models lost some capability to reproduce the original SAC-SMA results with each step towards the filter state equation form. In general, the models tend to overrespond to precipitation because of the nonlinear reservoirs.

The right side of Figure 4.3 represents the spectrum of updating procedures. They range from the purely linear form of the Kalman filter to complex nonlinear filtering, such as iterated or second-order filters. In this application, complex nonlinear filtering probably is not warranted because of the large number of assumptions in the model and the many errors in the areally averaged inputs. The conclusions are that the choice of updating for this application should be the extended Kalman filter (the Kalman filter extended to a linear approximation of a nonlinear problem). Forecast Step No. 3 is the chosen form for the forecast step. This form of the model serves as a compromise, as it preserves some of the nonlinear features of the original model, yet computes the states from the same equations used in the updating step.

A new procedure was developed for solving the differential equations. Instead of the 6-hour integration scheme, an algorithm which more closely resembles the discretization interval within the original SAC-SMA model was used. The original SAC-SMA model has a provision which limits the amount of water to be processed at any one time step to 5 mm. This allows the algorithms in the model to function in a more continuous mode which is closer to natural conditions. When large amounts of precipitation are input, the model can operate at extremely small time steps and when little or no precipitation is experienced, the model can resume computations at the original time interval.

This variable time step algorithm was included in the newly formulated model. Three elements in the model are functions of time. These are the three recession coefficients: UZK, LZSK, and LZPK. The functional relationship between the daily recession coefficients and the incremental time step coefficients is:

$$d = 1.0 - (1.0 - ZK)^{DINC} \quad (4.11)$$

where d=Recession coefficient for the specified time step;
 ZK=Daily recession coefficient;
 DINC=Time step length (day)

DINC is computed as:

$$DINC = (1./NINC) \cdot DT \quad (4.12)$$

where $NINC = 1. + .2 \cdot (UZFWC + Px)$;
 DT = user specified time step (day);
 Px = precipitation input for the time step.

This variable time step solution of the model differential equations more closely approximates the computations of the original Sacramento model than some of the earlier state-space models.

The differential state equations are of the form:

$$\frac{dx}{dt} = f(x, p, u) \quad (4.13)$$

where x = states,
 p = parameters,
 u = inputs,
 t = time step.

In each computational loop of length DINC, the incremental state changes are computed and accumulated:

$$dx_{t+1} = f(x_t, p, u) \cdot dt \quad (4.14)$$

$$x_{t+1} = dx_{t+1} + x_t \quad (4.15)$$

The state-space SAC-SMA was coupled with the unit hydrograph and tested for several years of data. The state-space simulation seems to approximate the original SAC-SMA output under a variety of conditions. Verification results are discussed following the description of the state-space unit hydrograph.

Unit Hydrograph

Output from the state-space soil moisture model is in the form of total channel inflow (TCI). TCI typically is distributed in time using the UNIT-HG operation. TASC developed the reduced order unit hydrograph (REDO-UHG) operation so that the time distribution algorithm would be consistent with the state-space SAC-SMA model. The formulation of REDO-UHG was based on the concept of canonical variate decomposition (TASC, 1981). A relationship between a past (input) and future (output) vector of random variables is modeled by a Markov process of a specified order of states (k). This leads to a model which can predict the best statistical estimate of the output from k linear combinations of the input. The REDO-UHG operation produces a measurement matrix based on the input unit hydrograph ordinates which can be multiplied by TCI to produce simulated instantaneous discharges. Details of the computations are described in Chapter 5 in relation to the use of the models with the Kalman filter.

Although the focus of the application of this research is on estimation of parameters for the SAC-SMA model, determination of the

proper unit hydrograph ordinates for a basin is a major part of the overall calibration process. Part of this research project was devoted to the development of an efficient mechanism for parameterizing unit hydrographs. The concept originally was proposed (Sittner and Krouse, 1979) as a means of updating a simulated hydrograph to more closely match discharge observations. The algorithms developed in this study provide a way to adjust unit hydrograph ordinates vertically and horizontally using two adjustment factors UGV and UGH, respectively. Vertical adjustment is performed by computing a discharge, above which ordinates are adjusted proportional to the ratio of UGV to 1.0 and below which they are moved in inverse proportion, all while maintaining the original hydrograph volume. Horizontal adjustment is made by moving the unit hydrograph curve in direct proportion to the ratio of UGH to 1.0 and inversely proportional to the distance from the time of peak. Thus, points close to the peak move farther, so that the shape is actually distorted rather than the base shifted. The advantage of this parameterization is that the shape of the unit hydrograph can be optimized by adjusting only 2 parameters in an optimization algorithm. Although the algorithms were tested and verified, the studies performed for the purpose of this thesis assumed the unit hydrograph ordinates had been previously optimized and were not included in the analysis. The algorithms have already become a part of NWS calibration procedures.

Model Verification

The new state-space SAC-SMA was coupled with the REDO-UHG measurement matrix to form a state-space watershed model which uses estimates of precipitation and potential evapotranspiration to generate instantaneous discharges. Test runs were made to compare the output of the new model with results from the original SAC-SMA and UNIT-HG operations. Both systems were used to generate instantaneous discharges for the Bird Creek watershed in Oklahoma. The watershed is primarily semi-arid grassland with some forested areas. The drainage area is approximately 2340 square kilometers. The parameter values and unit hydrograph ordinates used in the models were those determined by manual and automatic calibrations of the basin in previous studies. The discharges were routed to a gaging point using the same lag and K channel routing procedure. The resulting mean daily simulated discharges for both systems were compared with observed records. Statistical results are shown in Table 4.4. The statistics are similar for the two models, with the state-space model actually statistically outperforming the original model in some areas. An examination of plots of the three time series (2 simulated and 1 observed) showed that the two models have similar simulations for most events. The correlation coefficient relating the two time series of simulated discharges was 0.9972.

Summary

NWSRFS was selected as the system to be used for implementation of the calibration methodology. The SAC-SMA and unit hydrograph models are used to simulate and forecast hydrologic conditions. Issues were discussed concerning the appropriate forms of the models to be used in the research project. The current SAC-SMA model was described and details were given on the development of the state-space version of the model.

Table 4.4

Statistical Comparison of State-space and Original Sacramento Models
versus Bird Creek Mean Daily Flow Observations

Period of Record: Water years 1956 - 1962

Observed monthly mean (CMSD) : 16.32

<u>Statistic</u>	<u>Original Model</u>	<u>State-space Model</u>
Monthly mean (CMSD)	15.32	16.019
Percent bias	-6.12	-1.84
Daily RMS error (CMSD)	18.61	18.82
Daily average absolute error (CMSD)	5.99	6.37
Average absolute monthly volume error (mm)	2.98	3.41
Monthly volume RMS error (mm)	5.36	5.85
Correlation Coefficient	.9659	.9662

Chapter 5

TECHNICAL DEVELOPMENT OF METHODOLOGY COMPONENTS

Introduction

This chapter describes the current SAC-SMA model calibration procedures and the development of the technical details related to the implementation of the calibration methodology. The purpose of the multilevel approach is to reduce the parameter estimation problem into several subproblems which can be dealt with individually. The procedures described in this chapter are the tools which seem appropriate for solving each of the subproblems.

Current SAC-SMA Calibration Procedures

Techniques currently used for calibrating a typical headwater basin with the NWSRFS conceptual model (SAC-SMA Model and corresponding unit hydrograph operation) are time consuming and often result in sub-optimal estimates of model parameters. Calibration results are normally a function of the user's knowledge of the concepts in the model. A typical calibration for a watershed consists of three stages. In the first stage, initial parameter values are estimated from nearby basins or manually derived through an analysis of the hydrograph and other available information. In the second stage trial and error simulation runs are made using MCP so that the parameters can be adjusted manually. MCP allows a user to perform one simulation run with the model and print the observed and simulated hydrographs plus a variety of statistics describing the model fit. The third stage consists of a series of automatic optimization runs using OPT where the parameters are varied by a nonlinear search scheme. In the current version of OPT, the optimization algorithm is the direct search routine of Hooke and Jeeves (1961). Daily root mean square error is the most commonly used objective function. More details of OPT are provided later in this chapter.

Because the soil moisture model is complex, few users have a thorough understanding of all the model components. In many cases, this results in trial and error runs which give unreasonable parameter values. Poor second stage results also can affect the results of the third stage. Numerous problems have been encountered with the automatic optimization procedures converging to unrealistic parameter values when inconsistent initial parameter values were specified. The final result can be a poorly calibrated model. Details of the currently available calibration procedures are provided in several publications (Peck, 1976; Armstrong, 1978; Brazil and Hudlow, 1980).

Level I Development

Although years of developmental effort have been spent by numerous contractors in improving and automating calibration procedures, the most effective calibration technique for the NWS hydrologic models has always been the manual procedure performed by an experienced hydrologist. In fact, some experienced hydrologists believe that this may always be the

way to obtain the best calibrations. This theory is evidenced somewhat in this field and others by the amount of effort being put into the development of expert systems which attempt to mimic the decision process of experts (Reboh, et al., 1982, and Engman, et al., 1986). The Level I phase of this research is a first attempt at automating some of the procedures used by NWS experts to estimate initial parameter values for the SAC-SMA model. By estimating those parameters which are readily identifiable from the hydrometeorological data, the calibration problem dimension is reduced to a level that may be solvable using mathematical optimization tools.

The purpose of the Level I strategy is to provide an interactive environment for the calibrator to analyze the available data such as mean areal precipitation (MAP), mean areal temperature (MAT), instantaneous discharges (QIN), and mean daily discharges (QME) and make intelligent decisions concerning the quality of the data and what information can be learned from the data for the purpose of selecting initial parameter values. As a first step towards producing this interactive software, a program (INIT) was developed to guide a user through an analysis of the quality of data and the initial phases of SAC-SMA model parameter estimation. As more effort is put into this project, the software will be expanded to include other data analysis tools. INIT eventually will expand into an interactive session where a user can perform trial-and-error analyses as well as initial parameter estimation.

INIT Program

Program INIT was developed as a result of analyzing the SAC-SMA model, holding discussions with experts and referring to previous work by others (Peck, 1976, and Restrepo-Posada, 1982). Experience with the model has shown that reasonable values can be obtained for a number of the parameters by analyzing portions of the hydrologic record where parameters are known to have the most influence on the simulated flows. For instance, the baseflow component of the SAC-SMA model is the component most easily identifiable from analysis of streamflow records. During periods of baseflow, only the lower zone free water elements are contributing to TCI. This allows the model to be decoupled so that the lower zone components can be analyzed independently. The impervious portion of the watershed also is represented by a parameter which often can be estimated from the hydrometeorological record.

At the beginning of a session in INIT, a user specifies the file names for the watershed to be analyzed, period of record to be examined, and tolerance for the model fit. The program begins with quality control of the data. Although this currently is limited to a comparison of the sums of MAP, PE, and QME, the values provide the user with enough information to know that the input data appear to be reasonable. Ongoing research will provide other quality control measures, such as outlier detection, which will be incorporated into INIT.

Program INIT next begins analyses of the lower zone drainage coefficients. Lower zone free water within the SAC-SMA model is made up of two components, primary and supplemental. Four parameters, LZPK, LZSK, LZFPM, and LZFSM, control the amount of runoff which occurs during baseflow periods. LZPK and LZSK are the recession coefficients for the primary and supplemental reservoirs, respectively. LZFPM and LZFSM are the reservoir capacities. The recession rates are exponential. The rates can be computed from the following relationships:

$$LZPK = 1.0 - \left(\frac{Q_2}{Q_1} \right)^{1/t_1} \quad (5.1)$$

$$LZSK = 1.0 - \left(\frac{Q_4}{Q_3} \right)^{1/t_2} \quad (5.2)$$

Where Q_1 , Q_2 , Q_3 , Q_4 , t_1 and t_2 are defined as shown in Figure 5.1.

Although the equations for computing the coefficients are straightforward, actual estimation of the parameters for real data can be a difficult and time consuming task. Various procedures have been attempted for computing the parameters. Restrepo-Posada (1982) developed an automated technique for estimating baseflow parameters by looking for the minimum flow during a year and trying to fit a model of baseflow to the period preceeding it. The procedure was never implemented due to various problems. The current research has produced a procedure for guiding the user through a manual identification process. It was decided that the user probably would benefit from a program which could aid the user in understanding the workings of the model.

Program INIT is an interactive program with graphical displays similar to Figure 5.2. The user selects a period of data to be displayed and then looks for a period of baseflow within the displayed hydrograph. Baseflow is typically a long recession with little or no precipitation. The user is prompted for beginning and ending dates of primary baseflow. Response is given by moving the terminal cursor to the appropriate location and entering a character from the keyboard. The program computes the corresponding value of LZPK and then simulates the selected baseflow period to see if the model is an accurate representation. Accuracy is determined by the tolerance the user specified at the beginning of the program. If the percent deviation between simulated and observed flows exceeds the tolerance, the date and simulated flow are displayed. The user is given a chance to drop the period from the analysis if the simulation fails to give good results. INIT continues prompting the user until the entire period of record has been examined. Finally, the list of LZPK estimates is printed and the user is given a final chance to discard outliers. The mean and standard deviation for LZPK are computed from the remaining values.

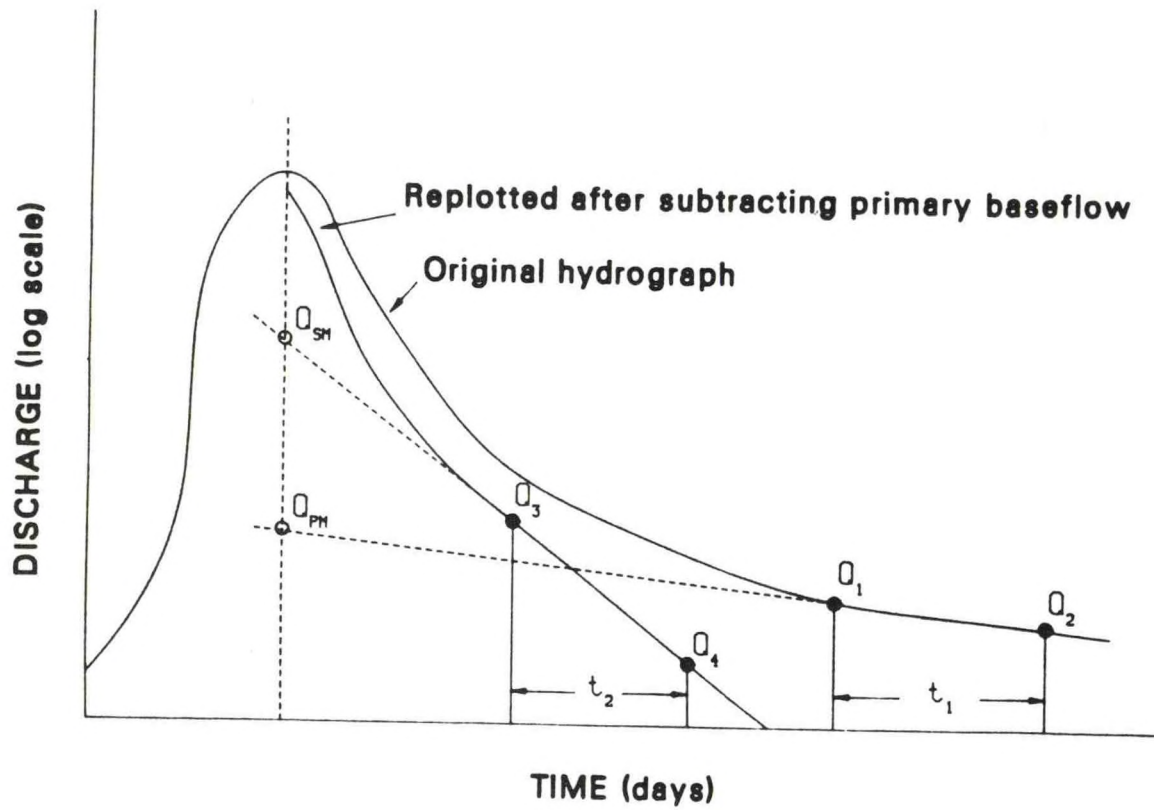
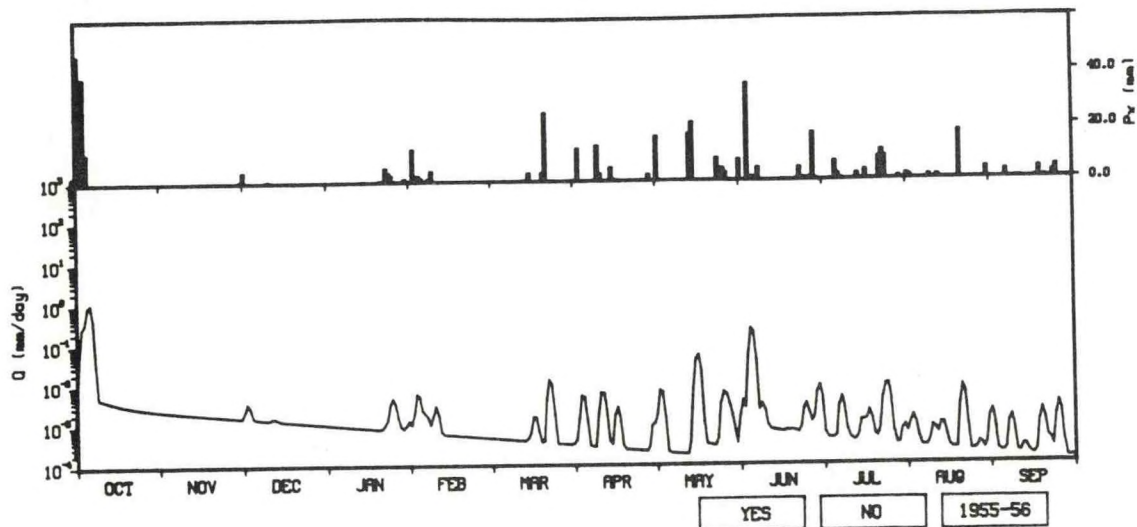


Figure 5.1. Hydrograph Decomposition with Program INIT
(Initial Parameter Estimation Program).



ENTER BEGINNING & ENDING PRIMARY BASEFLOW DATES
 DATES SELECTED ARE: 11 18 1955 11 24 1955
 LZPK- .013 ACCEPTABLE?
 OTHER LZPK EVENTS?
 IS THE EVENT IN THE DISPLAYED YEAR?
 ENTER BEGINNING & ENDING PRIMARY BASEFLOW DATES
 DATES SELECTED ARE: 12 13 1955 1 17 1956
 LZPK- .014 ACCEPTABLE?
 OTHER LZPK EVENTS?
 IS THE EVENT IN THE DISPLAYED YEAR?
 ENTER BEGINNING & ENDING PRIMARY BASEFLOW DATES
 DATES SELECTED ARE: 3 25 1956 3 30 1956
 LZPK- .014 ACCEPTABLE?
 OTHER LZPK EVENTS?
 IS THE EVENT IN THE DISPLAYED YEAR?
 OTHER LZPK EVENTS?
 LZPK ESTIMATES:
 1 0.013
 2 0.014
 3 0.014

DELETE ANY LZPK ESTIMATES?
 MEAN- 0.014 ST. DEV.- 0.00055
 WHEN READY TO CONTINUE PRESS RETURN

Figure 5.2. Interactive Display from Program INIT
 (Initial Parameter Estimation Program).

Similar calculations are performed for LZSK and the user is prompted for the corresponding inputs. In the case of LZSK, the mean LZPK value is used to subtract primary baseflow from the total discharge so that the remaining flow can be modeled with the supplemental component. Checks similar to those for LZPK are made to verify that the supplemental baseflow model represents the data.

In addition to LZPK and LZSK, program INIT guides users through the estimation of LZFPM and LZFSM. The parameters are traditionally estimated by selecting large events, extending baseflow back to the peak of the hydrograph and estimating the content of moisture in the lower zones. The technique is shown graphically in Figure 5.1. The program allows users to specify periods of data for estimating the values. The reservoir capacities are estimated from a combination of the previously computed LZPK and LZSK values and the observed hydrograph peak. The equations are:

$$\text{LZFPM} = Q_{PM} / \text{LZPK} \quad (5.3)$$

$$\text{LZFSM} = Q_{SM} / \text{LZSK} \quad (5.4)$$

where Q_{PM} , Q_{SM} are defined as shown in Figure 5.1. The values actually used for the capacities are typically greater than the largest of the estimates since these baseflow reservoirs rarely fill completely.

Checks are made to see that the backwards extended baseflow recessions do not violate the assumptions in the algorithms (i.e. extended simulated baseflows exceeding observed discharges). Figure 5.1 shows an example of the extension technique.

The fifth parameter estimated with INIT is PCTIM, the percentage of the basin considered impervious and connected to the stream. The user is asked to select beginning and ending dates for a period during which streamflow occurs in excess of baseflow and appears to have been generated only by runoff from impervious areas. This typically would be a small event during the summer which follows several days with little or no precipitation. The algorithm in INIT uses the discharge on the beginning and ending dates as baseflow and computes the amount of impervious runoff as that streamflow which exceeds the baseflow. PCTIM is the result of dividing the impervious runoff by the observed precipitation over N days.

$$\text{PCTIM} = \frac{\sum_{t=1}^N \text{Runoff}}{\sum_{t=1}^N \text{Precipitation}} \quad (5.5)$$

The user is encouraged to select a number of these events and take the average of the computed values.

INIT Verification

Each component in the multilevel methodology was tested as it was developed using synthetic data. Seven years of six-hourly streamflow were generated with the state-space SAC-SMA model using seven years of

actual precipitation from the Bird Creek watershed near Sperry, Oklahoma (water years 1956-1962). No errors were introduced into the synthetic flows, except in cases specifically described, so the only differences between simulated and observed flows were due to parameter differences.

Test runs were made for INIT using the Bird Creek synthetic data. Results are shown in Table 5.1. The Level I work is a first step towards the development of a workable interactive calibration system. If used properly, the system should provide a reduction in the dimension of the calibration problem. The rules which are incorporated into the algorithm for checking the assumptions in the estimation procedures should aid the user in learning how to better select appropriate periods for calculating the various parameter values. The Level I system also provides a structure for adding algorithms and quality control features to the overall process. As new features are added, more information can be generated which will be useful as the input to the Level II programs.

Level II Development

The purpose of the Level II strategy is to further reduce the dimensionality of the calibration problem through use of an effective parameter space search procedure. As described in Chapter 3, numerous research projects have been aimed at developing efficient and robust search algorithms for estimating parameters of rainfall-runoff models. Many of the projects have adapted search tools from other scientific fields. Most of the approaches have a major point in common: they generally are hill climbing procedures which give results that are strongly influenced by parameter starting values. If the initial values are inaccurate, the procedures often can converge to unrealistic optima (Brazil and Krajewski, 1987). Studies (Gupta and Sorooshian, 1983 and Hendrickson, 1987) have shown that the surface may be highly irregular, making a climb to the true optimum a difficult task. Also, search techniques typically are driven by one objective function which may or may not be the best criterion for the model or application.

The focus of the current work is to develop an effective search algorithm which is not dependent on accurate starting values, although can make use of reasonable estimates, and is not adversely affected by severe parameter interaction. Several candidate search procedures were considered. Random search techniques offer a means for overcoming many of the disadvantages of hill climbing procedures. The random procedures search within an area rather than along a line determined from a starting point, and therefore, tend to be less prone to converge at a local optimum. Random procedures do not have to be driven by a single evaluation criterion. Although they typically are more computationally expensive than hill climbing searches, random search techniques are becoming more attractive as computer hardware prices decrease and processing time becomes more readily available (Brazil and Krajewski, 1987).

This project produced two search procedures for the Level II strategy. Both techniques are based on random search algorithms. The first procedure is Uniform Random Search (URS). As the name indicates,

Table 5.1

Summary of INIT Analysis for Bird Creek Synthetic Data

LZPK = .013 (True value = .013)

Event beginning date	Event ending date	Estimated parameter value
* 11/18/55	11/24/55	.013
* 12/13/55	1/17/56	.014
* 3/25/56	3/30/56	.014
10/01/56	10/10/56	.013
11/03/58	11/10/58	.013
9/29/60	10/10/60	.013
.....		

LZSK = .125 (True value = .126)

Event beginning date	Event ending date	Primary flow date	Est. parameter value
10/11/55	11/06/55	11/18/55	.135
7/08/57	8/05/57	8/06/57	.130
6/16/60	7/11/60	7/16/60	.109
.....			

LZFPM = 160. (True value = 140.)

Event beginning date	Event ending date	Est. contents
5/26/57	8/07/57	103
6/13/57	7/16/57	89
3/30/58	5/01/58	78

therefore, $LZFPM = 103. / (50\% \text{ to } 90\%) = 114. - 206.$

.....

LZFSM = 20. (True value = 14)

Event beginning date	Event ending date	Primary flow date	Est contents
10/03/59	11/28/59	10/20/59	13

therefore, $LZFSM = 13. / (50\% \text{ to } 90\%) = 14. - 26.$

Table 5.1 (Continued)

PCTIM = .001 (True value = .001)

Event beginning date	Event ending date	Estimated parameter value
1/18/56	2/09/56	.001
3/12/56	3/23/56	.001
4/25/56	5/05/56	.001
9/15/56	9/26/56	.001
10/11/56	10/18/56	.001
10/20/57	10/25/57	.001

* Shown in figure 5.2

the technique is based on an algorithm which selects parameter values randomly between bounds using a uniform distribution. The second procedure is based on an Adaptive Random Search (ARS) (Pronzato, 1984). Instead of uniformly searching the entire feasible parameter space, ARS concentrates on areas which show greater potential for containing the global optimum (Brazil and Krajewski, 1987).

Program OSRCH was developed to test and implement the two random search procedures with the SAC-SMA model. The user input consists of optional starting parameter values, parameter bounds, stopping criteria, and a random number seed. If the user does not specify initial parameter values, ARS uses the parameter range midpoints. URS does not use starting values. The program performs simulations by running the original SAC-SMA model or the state-space SAC-SMA model and corresponding reduced-order unit hydrograph for the specified period. Each pass through the data is a trial. Statistics are computed for each trial to determine how well the simulated discharges for a particular parameter set match the observed flows. The statistics can be computed for instantaneous or mean daily discharges depending on the time interval of the observations. Several types of statistics are computed for each trial. Table 5.2 shows the equations used to compute the statistics in OSRCH.

The statistics represent a variety of evaluation criteria. They include bias (BIAS), maximum deviation for the simulation period (ABSMAX), root mean square error (RMS), average absolute error (ABSERR), the variance of the residuals (RVAR) and correlation coefficient (R'). PDIFF and BASEFL are computed for user specified events. They represent the difference in the magnitudes of the simulated and observed peak flows and the sum of the differences of flows during a baseflow period, respectively. TMVOL is a measure of the monthly volume differences and would be useful in a situation where the model is being used to forecast volumes rather than peak discharges. NSC is computed by summing the number of times the sign of the residual changes from one time period to the next. Venot (1986) showed this to be a robust identification measure. Each of the evaluation criteria is computed every time OSRCH performs an iteration of the model.

A user typically would run OSRCH after having run INIT to determine initial values for several of the parameters. Using the current version of INIT, the user should have accurate estimates for five parameters and some information about their variability. The variability information is useful in determining the bounds for the random search. Future versions of INIT will have the capability to aid the user in estimating most of the model parameters and determining their variability through sensitivity analyses and interactive trial and error simulations. OSRCH is run to examine the parameter space within the bounds set by the user. This step in the calibration process further refines the feasible region of the problem solution and hopefully provides a good point for performing Level III fine tuning analyses or returning to Level I for more manual adjustments.

A synthetic data experiment was conducted to test the OSRCH program. Results from the experimental runs are described later in this section after each of the algorithms in the program has been discussed.

Table 5.2
Statistics Computed for Each OSRCH Trial

$$\text{BIAS} = \frac{\sum_{t=1}^N (s_t - o_t)}{\sum_{t=1}^N o_t}$$

$$\text{ABSMAX} = \max_{t=1, \dots, N} |s_t - o_t|$$

$$\text{RMS} = \left(\frac{\sum_{t=1}^N (s_t - o_t)^2}{N} \right)^{.5}$$

$$\text{ABSERR} = \left(\frac{\sum_{t=1}^N |s_t - o_t|}{N} \right)$$

$$\text{RVAR} = \left(\frac{\sum_{t=1}^N (s_t - o_t)^2 - \left(\sum_{t=1}^N (s_t - o_t) \right)^2 / N}{N-1} \right)$$

$$\text{PDIFF} = |s_{pk} - o_{pk}|$$

$$\text{BASEFL} = \sum_{t=1}^{NB} |s_t - o_t|$$

$$\text{TMVOL} = \frac{\sum_{t=1}^{NM} \left(\sum_{t=1}^{NP} s_t - \sum_{t=1}^{NP} o_t \right)^2}{NP}$$

$$R' = \frac{N \cdot \sum_{t=1}^N (s_t \cdot o_t) - \sum_{t=1}^N s_t \cdot \sum_{t=1}^N o_t}{\left(\left(N \cdot \sum_{t=1}^N s_t^2 - \sum_{t=1}^N s_t \cdot \sum_{t=1}^N s_t \right) \left(N \cdot \sum_{t=1}^N o_t^2 - \sum_{t=1}^N o_t \cdot \sum_{t=1}^N o_t \right) \right)^{.5}}$$

$$\text{NSC} = \sum_{t=1}^N (IS)$$

Where
 s_t = Simulated discharge @ time t (Volume/time step)
 o_t = Observed discharge @ time t (Volume/time step)

[continued on following page]

Table 5.2 (Continued)

s_{pk}	=	Simulated peak discharge for the specified peak period (Volume/time step)
o_{pk}	=	Observed peak discharge for the specified peak period (Volume/time step)
N	=	Number of time steps
NB	=	Number of time steps in the specified baseflow period
NM	=	Number of months
NP	=	Number of time steps per month
IS	=	Residual sign change from one time step to the next

Sensitivity Analyses

An option within OSRCH allows a user to perform sensitivity analyses. The user specifies a set of parameters to be used as the base and a corresponding range for each parameter. One hundred trials are run as each parameter is incremented through its range, all other parameters remaining fixed. Both synthetic and real streamflow observations were used for Bird Creek to demonstrate the sensitivity analysis capabilities. The objective functions were normalized so that comparisons could be made without concern about units. Conclusions can be drawn about the sensitivity of the various evaluation criteria to changes in each parameter and also about the relative sensitivity of the different parameters. Synthetic and real results for representative parameters are shown in Figures 5.3 a, b, and c and in Figures 5.4 a, b, and c, respectively. As expected, the plots show that LZPK is far more sensitive than LZTWM, one reason for identifying LZPK in the Level I analysis. Because it is a sensitive parameter and interacts with several other parameters, identification of LZPK in Level I reduces the problem dimension significantly. Figures 5.4 a, b and c emphasize the fact that the problem is multi-objective. An analysis of the plots could yield far different parameter values depending upon which objective function is used.

Uniform Random Search

The user must specify the number of trials to be run when using the URS option, since URS does not converge. In test cases run during the development of the program for the seven years of synthetic data, 10,000 trials typically were specified. This number seemed to give reasonable results without overburdening the computer. Runs were made during the night on the NWS Central Computer Facility (NCCF) NAS9000 system and typically took approximately four hours of CPU time. Results from the runs are shown and discussed later in this chapter.

One of the main advantages of URS is the fact that it is not driven by an objective function. Instead it runs multiple trials through the data, computing and recording various statistics, using an assortment of parameter combinations. This type of run allows a user to perform a postsimulation multi-objective analysis of the results. All of the objective functions are normalized so that trade-offs can be made among the values.

Program NINF was developed to aid a user in analyzing the results of a URS run. In order to further reduce the problem dimension, the program determines the set of noninferior points in the true multi-objective sense. Cohen (1978, p.70) defines a feasible solution as being noninferior "if there exists no other feasible solution that will yield an improvement in one objective without causing a degradation in at least one other objective." Figure 5.5 shows the concept of noninferiority. NINF examines the statistics from each trial against previous trials and keeps track of the noninferior points. For the test runs made during the development of the program, the noninferiority analysis reduced the number of possible solutions to about 3 percent of the original sample. This reduction in points is critical because in

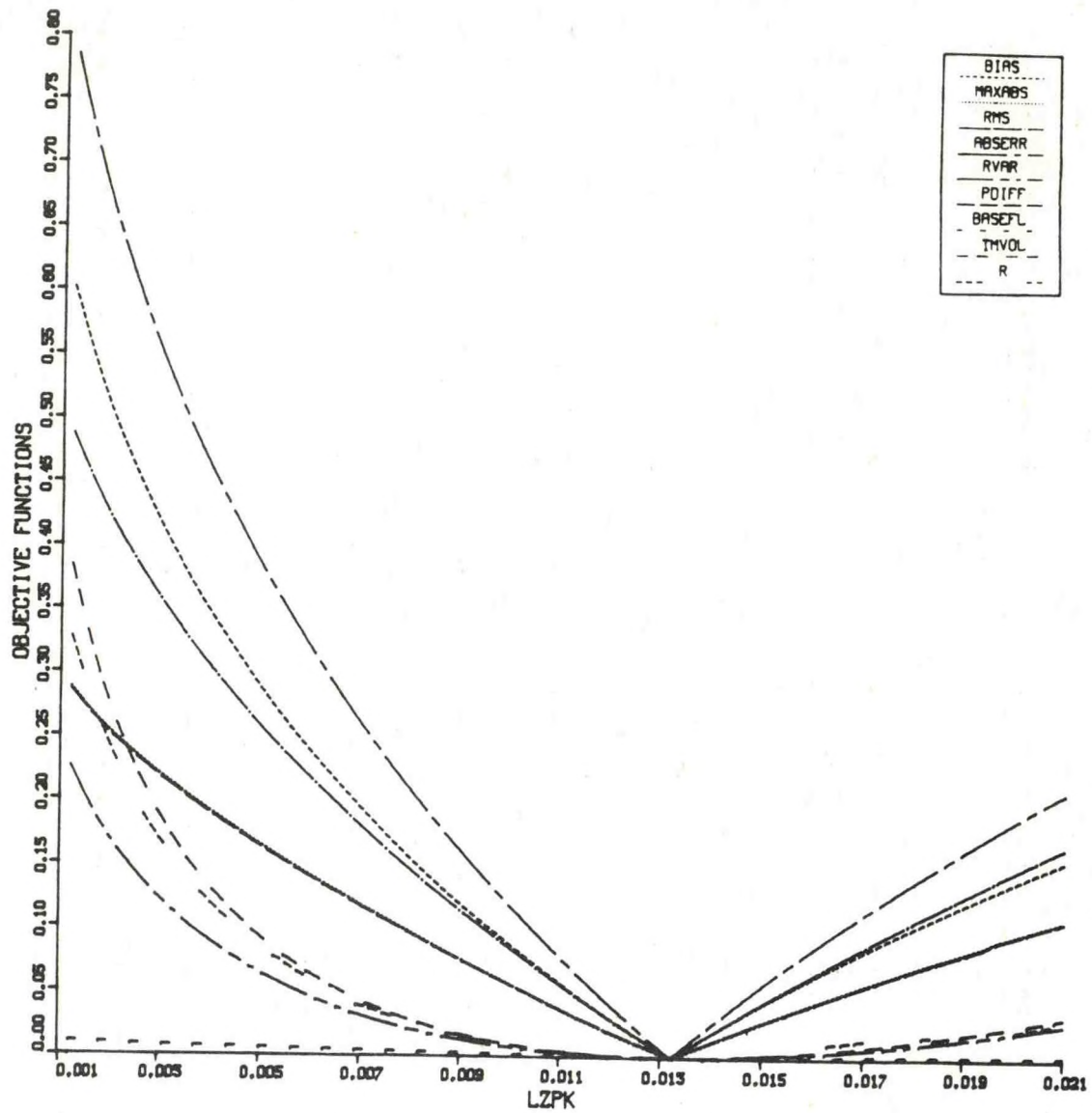


Figure 5.3a. Synthetic Data Sensitivity Analysis Results for LZPK (Fractional daily primary withdrawal rate). (Objective function definitions shown in Table 5.2).

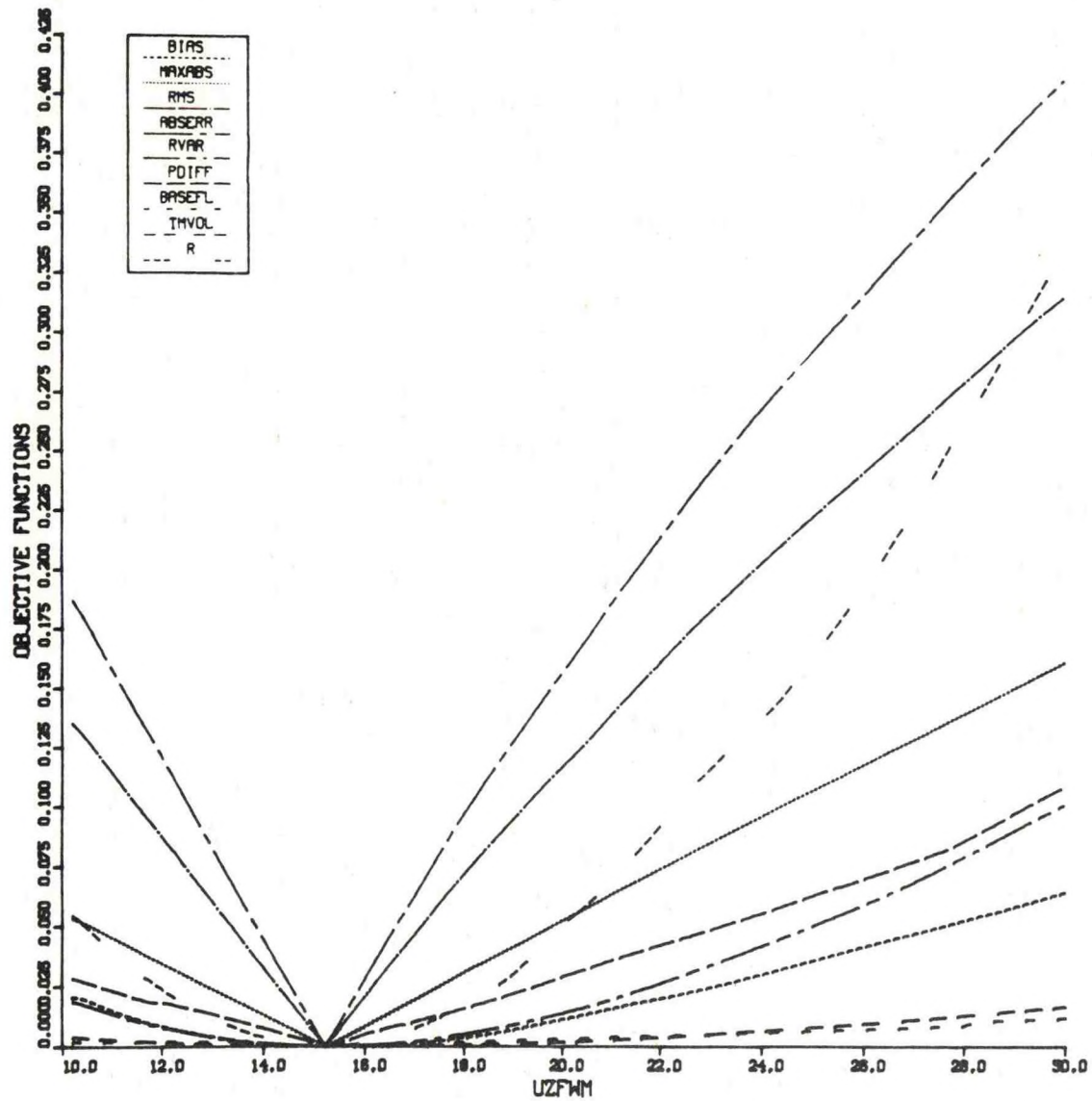


Figure 5.3b. Synthetic Data Sensitivity Analysis Results for UZFWM (Upper zone free water capacity). (Objective function definitions shown in Table 5.2).

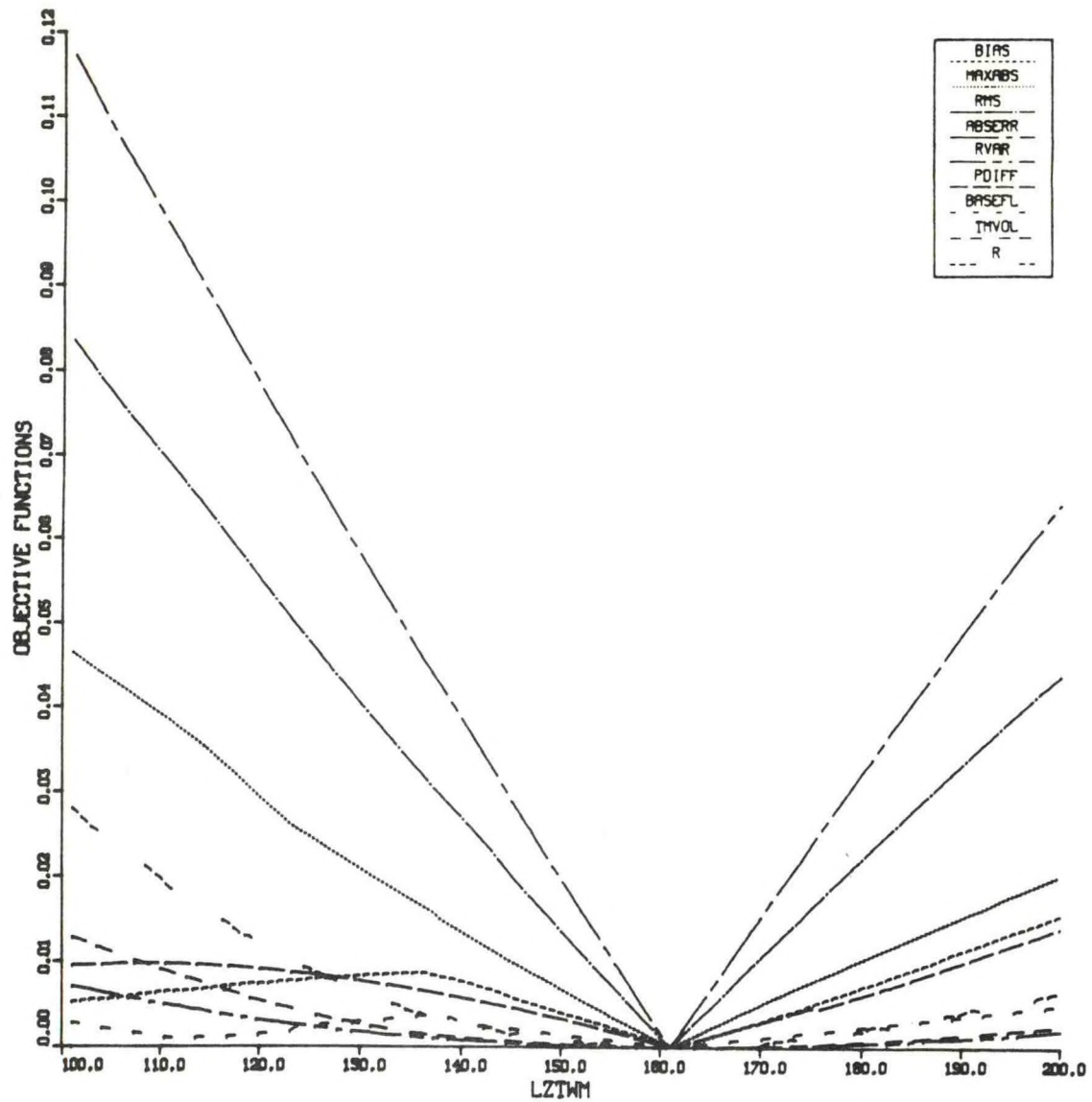


Figure 5.3c. Synthetic Data Sensitivity Analysis Results for LZTWM (Lower zone tension water capacity). (Objective function definitions shown in Table 5.2).

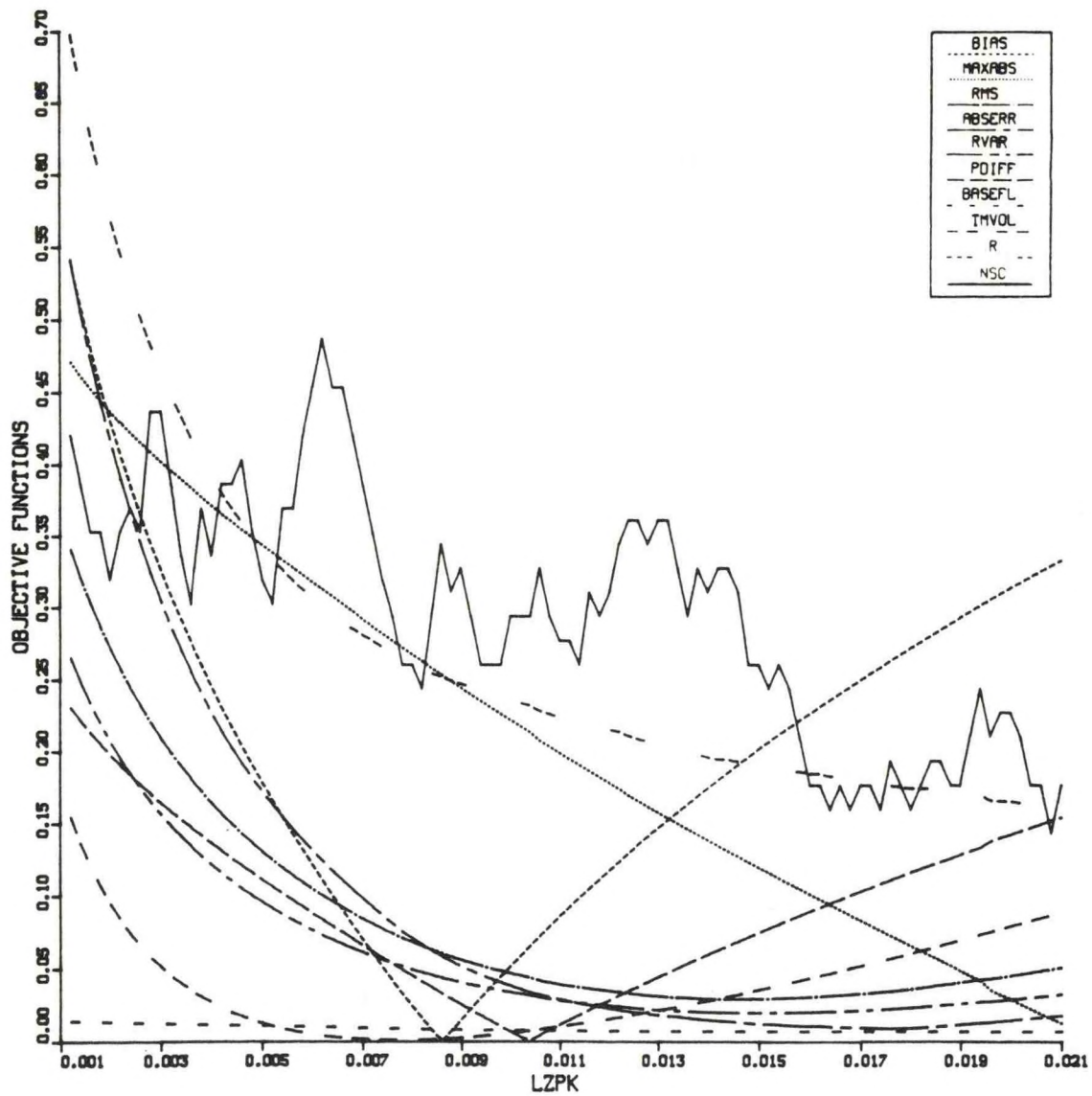


Figure 5.4a. Bird Creek Sensitivity Analysis Results for LZPK
 (Fractional daily primary withdrawal rate).
 (Objective function definitions shown in Table 5.2).

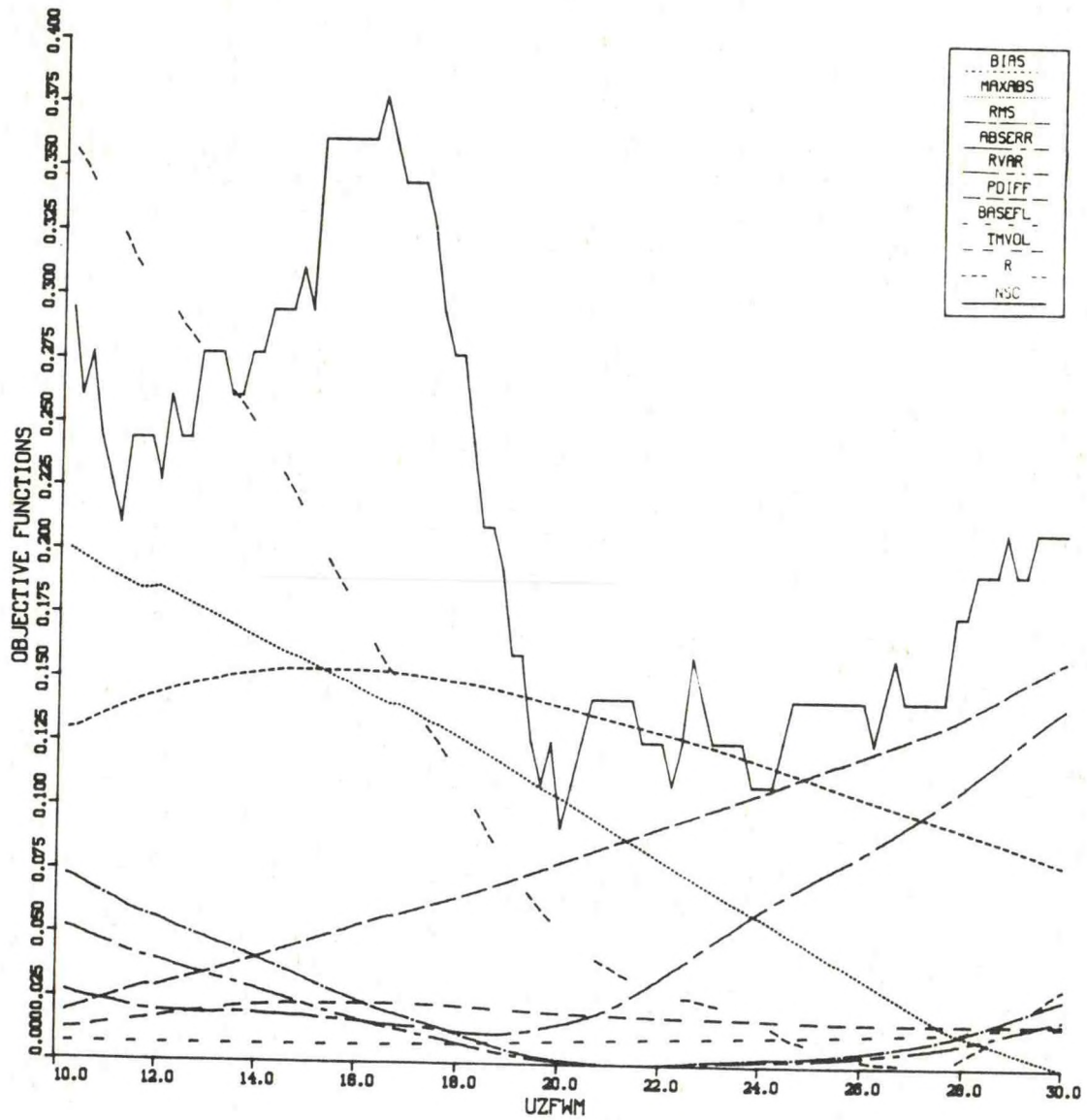


Figure 5.4b. Bird Creek Sensitivity Analysis Results for UZFWM (Upper zone free water capacity). (Objective function definitions shown in Table 5.2).

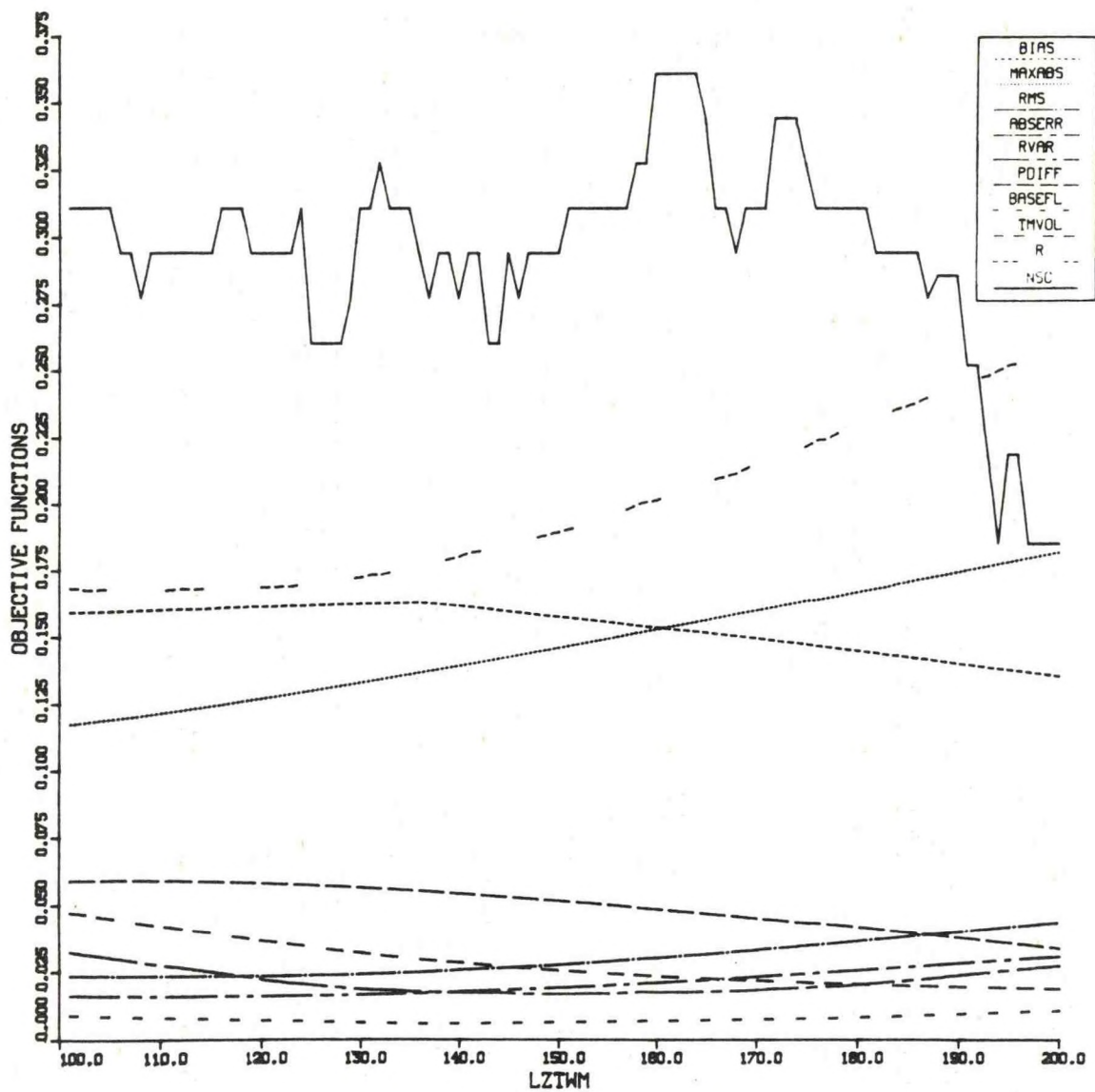


Figure 5.4c. Bird Creek Sensitivity Analysis Results for LZTWM (Lower zone tension water capacity). (Objective function definitions shown in Table 5.2).

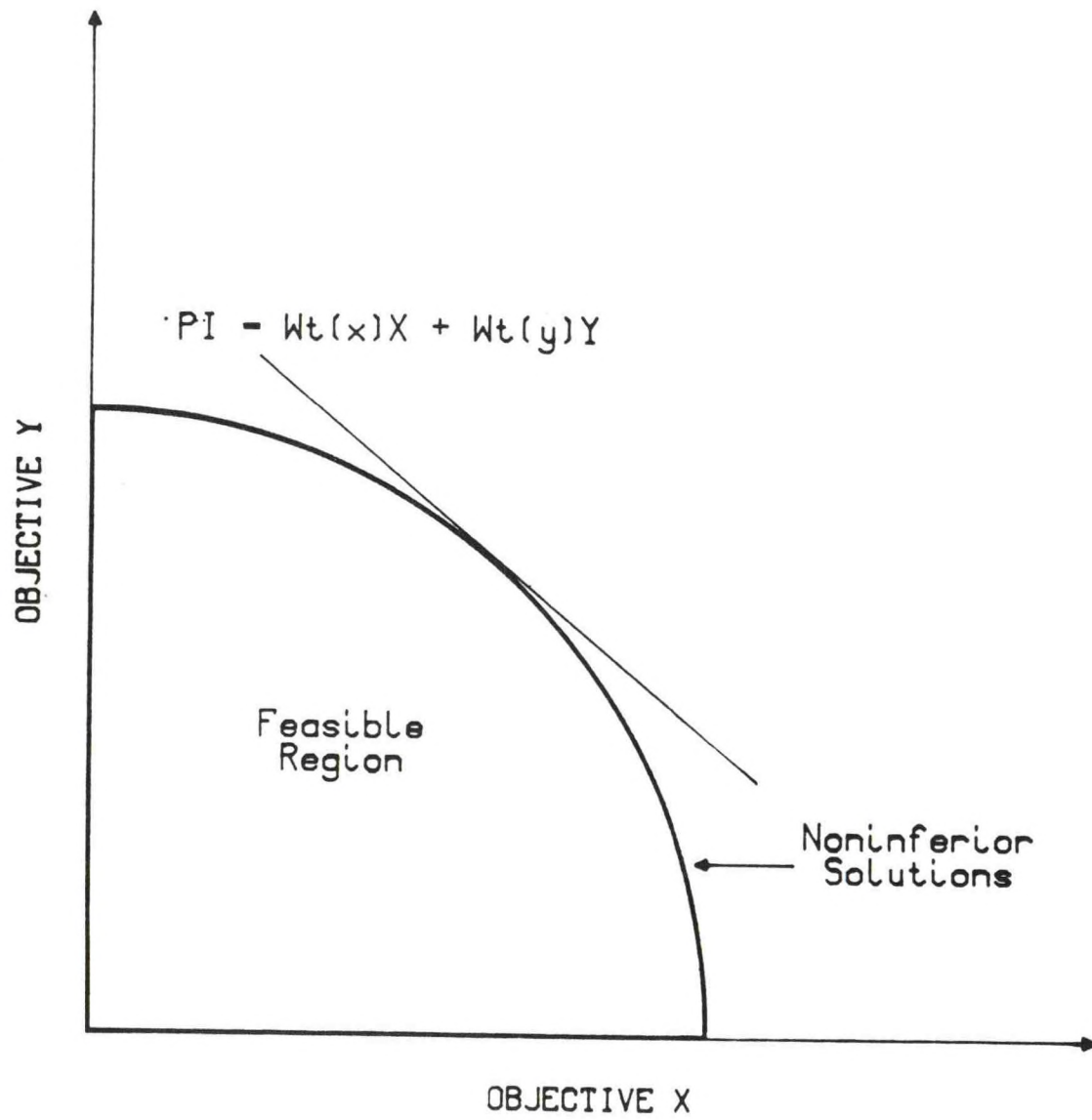


Figure 5.5. Multi-objective Analysis Solutions.

the case of a 10,000 iteration run, it transforms the multi-objective analysis from a batch job to an interactive program. Program CMPTPI was developed to assist a user in performing a multi-objective analysis of the noninferior points. A user specifies weights to be assigned to each objective function and the program selects the trial with the best set of weighted objective functions. A synthetic data experiment was conducted to test the program. Results are provided later in this chapter. The computations within CMPTPI for a typical 10,000 trial OSRCH run take only a few seconds, enabling a user to try various combinations of weights within one interactive session.

Experience with the model has shown that relationships sometimes exist between some of the parameters in the SAC-SMA model. Identification of parametric relationships can help to restrict the search space if some of the parameters can be shown to be dependent on the values of other parameters. An experiment was conducted to determine what relationships might exist among parameters. Parameter values were analyzed for 28 basins selected from various parts of the U.S. and other countries. The basins were calibrated by experienced hydrologists and were considered to have good simulations. Plots were made for every parameter against every other parameter to see if any obvious relationships could be determined. Little or no correlation was detected for most parameters. This is a sign that the model is not over parameterized--no parameter can be expressed as a combination of other parameters. However, this does not help the effort to restrict the search space. Experience with the model and discussions with experts indicated that three pairs of parameters should be examined more closely: REXP vs. ZPERC, UZK vs. LZSK, and UZFWM vs. PBASE. PBASE is an intermediate variable in the SAC-SMA model which is a function of four parameters:

$$\text{PBASE} = \text{LZFPM} * \text{LZPK} + \text{LZFSM} * \text{LZSK} \quad (5.6)$$

Experience in calibration has shown that the strongest correlation probably exists between REXP and ZPERC. Research by Gupta and Sorooshian (1983) verified that interaction is strong between these two parameters. Hydrologists generally adjust the two parameters simultaneously when calibrating. NWS experience with the SAC-SMA model has shown that the parameters probably are related in a quadratic manner. A relationship similar to the curve in Figure 5.6 was used in the current study.

The relationships for UZK vs. LZSK and UZFWM vs. PBASE are less known. It can be argued that some positive correlation exists between UZK and LZSK. As the interflow rate increases, the supplemental baseflow rate probably will increase proportionately. A ratio of UZK to LZSK of 2.5 was assumed for the experiment with bounds of 0.2 and 0.5 for UZK. In general, lower zone permeability is positively correlated with upper zone permeability. A linear relationship was assumed between UZFWM and PBASE. The experiment and its results are explained later in this chapter after the development of all the components of the experiment have been described.

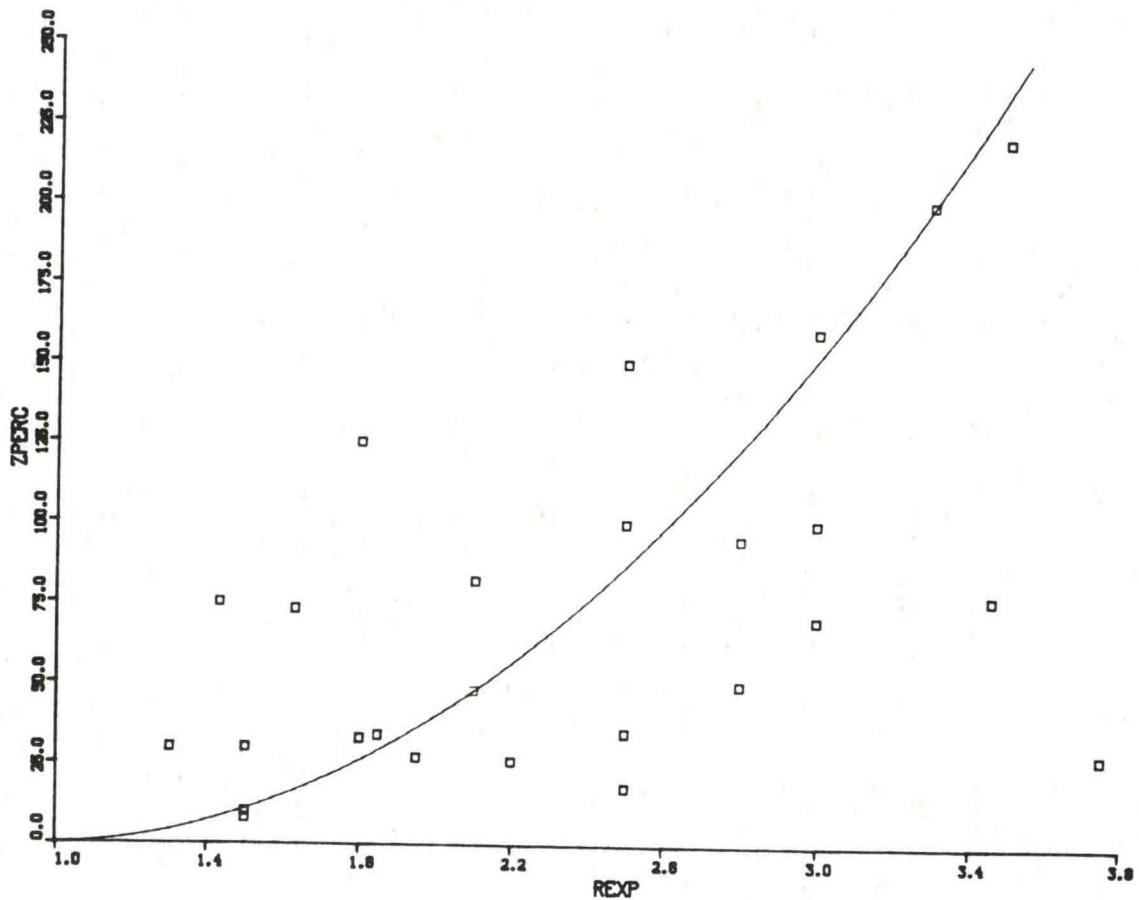


Figure 5.6. Results from Multi-basin Parameter Analysis. Combinations of REXP (Percolation equation exponent) and ZPERC (Maximum percolation rate coefficient) with assumed relationship shown as solid curve.

Adaptive Random Search

The ARS procedure was included in OSRCH to provide the user with a converging random search. Previous studies have shown ARS to be a particularly effective technique for optimizing multidimensional problems (Pronzato, 1984). Although the procedure uses a single objective function to drive the convergence, the technique can be extremely useful when the proper statistic or combination of statistics is selected. Details of the algorithm are given by Pronzato (1984). Basically, the procedure consists of uniform random searches over various defined search spaces. The initial search is over the entire feasible region. The best point found is assumed to be near the optimum and a new uniform random search is made near its vicinity. This cycle of restricting the space and resuming the search is continued for a user specified number of times. When the smallest search space has been examined, the program begins the cycle again with the largest area. This enables the procedure to escape from local optima. When the search returns to the same vicinity a predetermined number of times, the best point in the vicinity is assumed to be the best point within the search space.

The algorithm was summarized by Brazil and Krajewski (1987):

1. Select the criterion to be minimized $f(\underline{\alpha})$ and the admissible range of the parameters

$$\alpha_i^L \leq \alpha_i \leq \alpha_i^U \quad \text{for } i = 1, \dots, N$$

$$R_i = \alpha_i^U - \alpha_i^L$$

2. Select the starting point as

$$\alpha_i^0 = \frac{1}{2} (\alpha_i^L + \alpha_i^U) \quad \text{for } i = 1, \dots, N$$

3. Set MAX, LOC, K, L_{stop} , and $K = 1$, $L_{\text{opt}} = 0$

4. Compute $R_i^{(k)} = 10^{1-k} R_i$ for $i = 1, \dots, N$

5. Perform MAX iterations of uniform random search so that

$$\alpha_i^{j+1} = \alpha_i^j + U(\beta_i^L, \beta_i^U) \quad \text{for } i = 1, \dots, N$$

where

$$\beta_i^L = \max \left\{ \alpha_i^L, \alpha_i^j - \frac{1}{2} R_i^{(k)} \right\}$$

$$\beta_i^U = \min \left\{ \alpha_i^U, \alpha_i^j + \frac{1}{2} R_i^{(k)} \right\}$$

Store the best found point and the corresponding k as $\underline{\alpha}^*(k)$

6. Set $k = k + 1$.
If $k > K$, go to 7, otherwise $MAX = MAX/k$, go to 4.
7. Select $\min\{\alpha^*(k): k = 1, \dots, K\}$. Record the best k as k^* .
If $k^* = K$, the $L_{opt} = L_{opt} + 1$. If $L_{opt} = L_{stop}$, go to 10.
If $k^* \neq K$, set $L_{opt} = 0$.
8. Perform LOC iterations of uniform random search around $\underline{\alpha}^*(k)$ within the neighborhood $\underline{R}^{(k^*)}$ corresponding to the best k^* .
9. Reset the parameters MAX and $k = 1$. Go to 4.
10. Stop. The best point is $\underline{\alpha}_{OPT} = \underline{\alpha}^*(k)$.

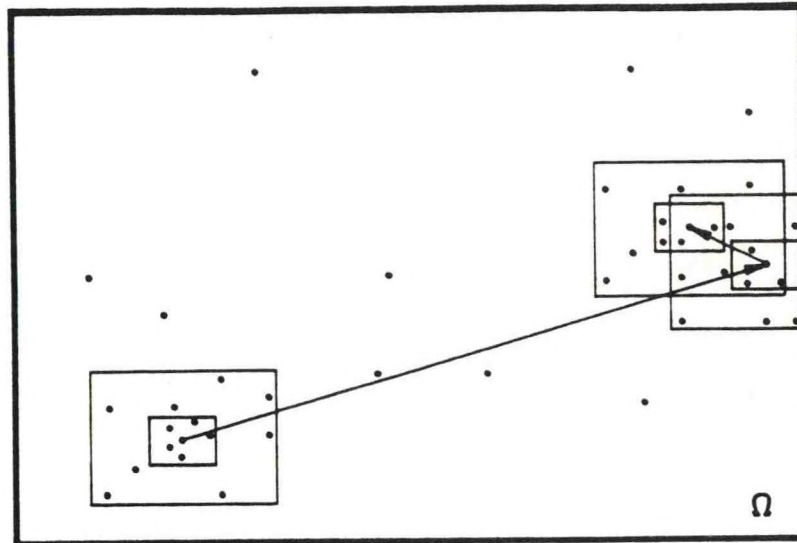
The ARS algorithm also was coupled with the parametric relationship algorithm to restrict the search space. Figure 5.7 shows the concept representation of ARS with and without the restricted space.

Synthetic Data Experiment

A synthetic data experiment was designed and conducted to evaluate the performance of the OSRCH algorithms. The seven years of Bird Creek synthetic data were used for all the runs. Four algorithms were used to estimate parameters: URS (1), ARS (2), and URS and ARS with restricted search spaces, (3) and (4), respectively. Five runs were made for each algorithm, each with a different random number seed. Root mean square error (RMS) was used as the objective function for all runs. The results from the experiment are shown in Table 5.3. The columns show the parameter values for the best run for each algorithm. The unmodified ARS algorithm gave the run with the lowest objective function value. On the average, ARS with the modified search space provided slightly better results. The small difference between the algorithms with and without parametric relationships might be explained by the fact that the search spaces were only slightly modified and the fact that only five realizations were made for each algorithm. Because the trials are generated randomly, one would expect more runs to produce a larger average difference. Identifiable parameters have more of a tendency to converge to the same value in each run. It is obvious from the results that some parameters are more identifiable than others.

The programs developed for the Level II system provide an effective mechanism for selecting values for any or all of the model parameters. When used in conjunction with Levels I and III, the Level II objectives

(a)



(b)

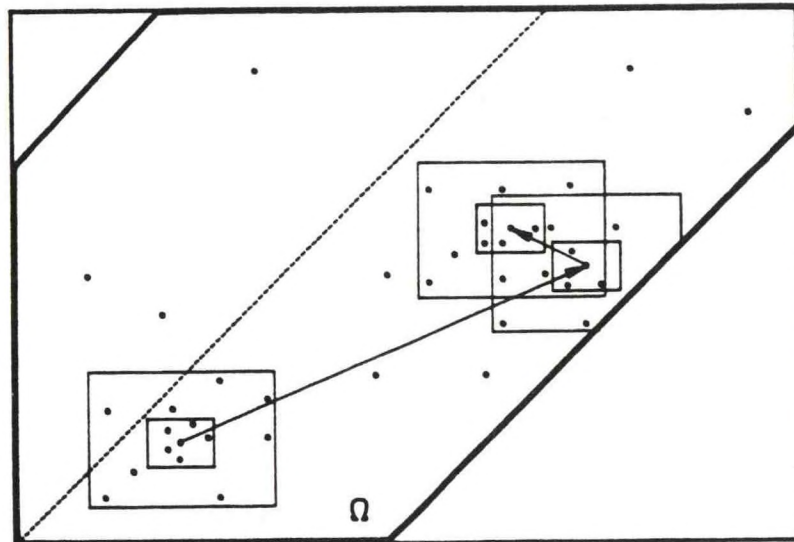


Figure 5.7. ARS Concept Representation

- a. Search of two-parameter space with upper and lower bounds.
- b. Search restricted by parametric relationship.

Table 5.3

Results from Random Search Synthetic Data Experiment -
Best Run for each Optimization Algorithm

Parameter	Algorithm*				True Value	Lower Bound	Upper Bound
	1	2	3	4			
UZTWM	131.	121.	111.	117.	120.	100.	150.
UZFWM	15.1	15.1	14.8	15.6	15.0	10.	30.
LZTWM	200.	165.	193.	159.	160.	100.	200.
LZFPM	167.	168.	158.	150.	140.	100.	200.
LZFSM	14.	14.	15.	12.	14.	10.	60.
UZK	.280	.303	.382	.276	.300	.2	.4
LZPK	.0144	.0150	.0098	.0140	.0130	.001	.02
LZSK	.138	.102	.167	.130	.126	.02	.2
ZPERC	62.	53.	81.	49.	48.	10.	100.
REXP	2.90	2.70	2.57	2.29	2.10	1.5	4.
PFREE	.017	.053	.073	.037	.020	0.	.1
ADIMP	.135	.171	.175	.188	.170	.1	.2
PCTIM	.015	.000	.000	.000	.001	0.	.05
RMS (mm)	.0141	.0026	.0148	.0031			
Average RMS (mm)	.0158	.0060	.0166	.0058			

- *1 URS
2 ARS
3 Restricted URS
4 Restricted ARS

should give users a way of optimally selecting parameter values which could not be identified with Level I procedures. The results from Level II should give users the information necessary to perform additional Level I computations or proceed to Level III to adjust parameters using a filtering approach.

Level III Development

The purpose of the Level III strategy is to perform a search of the response surface in the immediate vicinity of the location determined to be optimal by the Level I and II analyses. The objective of the search is to find the local optimum and determine if the point provides a satisfactory set of parameters for the simulation model or if additional Level I or II analyses are required. This process is commonly called fine-tuning.

Numerous fine-tuning tools have been used in previous hydrologic studies. Several of these were discussed in Chapter 3. Most of the procedures are gradient based or hill-climbing techniques with stringent convergence criteria. Probably the most frequently used fine-tuning tool is trial-and-error analyses, commonly called manual calibration. The work presented in this study assumes that manual calibration will always be available for use and probably should normally be the final fine-tuning step in any calibration.

Two very different types of fine-tuning procedures were included for testing and evaluation in this study. The first tool is the current version of the NWS OPT program (OH, 1987). The program uses the Pattern Search (Hooke and Jeeves, 1961) algorithm and has been shown to be an efficient local search procedure (Hendrickson, 1987) when started at reasonable and consistent parameter values. The program uses the deterministic version of the SAC-SMA model and is run with batch processing. This means that all data are processed in a single trial before a parameter is adjusted. In contrast to this is the program LINDRV. LINDRV is a recursive stochastic parameter estimator which was developed for this study and uses the extended Kalman filter to adjust model states and parameters at every observation. The LINDRV work is believed to be the first application of Kalman filtering to simultaneous state and parameter estimation of a complex soil moisture accounting model (Georgakakos & Brazil, 1987).

OPT

The OPT program is a general optimization program which was designed to be used to select parameters for the models within NWSRFS. The program adjusts model parameter values automatically based on a statistical comparison of simulated and observed data. The only optimization routine currently available is Pattern Search. The ARS algorithm described in Level II currently is being added to the OPT code. Five objective functions are available in the program: three are based on differences between simulated and observed mean daily

discharges, one is based on monthly volumes, and one is a modified form of the correlation coefficient. Daily RMS error is the most commonly used objective function:

$$\text{Index} = \left(\frac{\sum (Q_{\text{SIM}} - Q_{\text{OBS}})^2}{\text{No. Days}} \right)^{.5} \quad (5.7)$$

Although this objective function tends to be influenced more by large errors, typically from high flows, experience has shown that this function normally results in parameters which allow the model to simulate flows adequately in most situations (Brazil and Hudlow, 1980).

User input to OPT consists of initial parameter values, parameter adjustment increments, upper and lower parameter bounds, and convergence criteria. The Pattern Search algorithm establishes a pattern of adjustments based on the success of parameter moves using the specified increments. Studies have shown, however, that the algorithm can have difficulties when irregular response surfaces are encountered (Brazil & Hudlow, 1980). The irregularities typically are caused by interactions among parameters. Gupta and Sorooshian (1983) investigated and reported on some of these interactions. The irregular response surface often causes the Pattern Search algorithm to converge at a local suboptimal point. Although the random search algorithms described as part of the Level II work do not have an effect on the shape of the response surface, they are not directly driven by its slopes and appear to produce a point on the surface which is a suitable position for beginning a local search. The Pattern Search algorithm shows promise of being an effective tool when applied in such a situation.

Previous studies have confirmed the utility of the OPT program, so no developmental results are given here (Brazil & Hudlow, 1980 and Sorooshian and Hendrickson, 1987). Results from OPT runs are presented as a part of the case study described in Chapter 6.

LINDRV

The LINDRV program was developed to provide users with a fine-tuning parameter adjustment tool that could be used to recursively estimate model states and parameters and give information concerning the statistical properties of the data and uncertainties associated with the estimates. The estimation algorithm is based on the extended Kalman filter. The program allows users to run the state-space version of the SAC-SMA and reduced order unit hydrograph models for any length of record and observe the filter as it updates model states and parameters at each time step. The user can specify how many and which parameters are to be estimated for any given run. Estimates of the variance of the input errors (U), system errors (Q), and measurement errors (R) can be specified by the user. Observation data can consist of instantaneous or mean daily discharges. The following sections describe the Kalman filter algorithm steps, the application of the filter to the hydrologic model, the computational steps in adaptive filtering, and computer runs that were made to test the program.

The Kalman filter provides a linear unbiased minimum variance estimate of a model state (Gelb, 1974). Details of the development of the filter were described by Kalman (1960) and Kalman and Bucy (1961). Numerous sources are available which describe the derivation of the filter equation (Gelb, 1974, and Jazwinski, 1970). A schematic diagram of the filtering process is shown in Figure 5.8. The first step in applying the filter is to express the system and measurement equations as linear functions of the model states. The discrete form of these equations expresses the state vector at time, $t + 1$, as a function of the state vector at time, t , external inputs and system noise. The measurement equation shows the relationship between the observations and the system states. The system and measurement equations are:

$$x_{t+1} = \Phi_t x_t + G_t u_t + \Gamma_t w_t \quad (5.8)$$

$$z_t = H_t x_t + v_t \quad (5.9)$$

with

$$E(w_t) = 0, E(w_t w_s^T) = Q \delta_{ts},$$

$$E(v_t) = 0, E(v_t v_s^T) = R \delta_{ts},$$

$$E(w_t v_s^T) = 0 \text{ for all } t, s;$$

where

x_t = state vector estimate at time t , $(n \times 1)$

Φ_t = state transition matrix at time t , $(n \times n)$

G_t = input coefficient matrix at time t , $(n \times j)$

u_t = input vector at time t , $(j \times 1)$

Γ_t = system noise coefficient matrix at time t , $(n \times k)$

w_t = system noise vector at time t , $(k \times 1)$

v_t = measurement noise vector at time t , $(m \times 1)$

H_t = measurement matrix at time t , $(m \times n)$

z_t = measurement at time t , $(m \times 1)$

Q = system noise covariance matrix, $(n \times n)$

R = measurement noise covariance matrix, $(m \times 1)$

δ_{ts} = Kronecker delta function $\delta_{ts} = 1, t = s,$
 $\delta_{ts} = 0, t \neq s.$

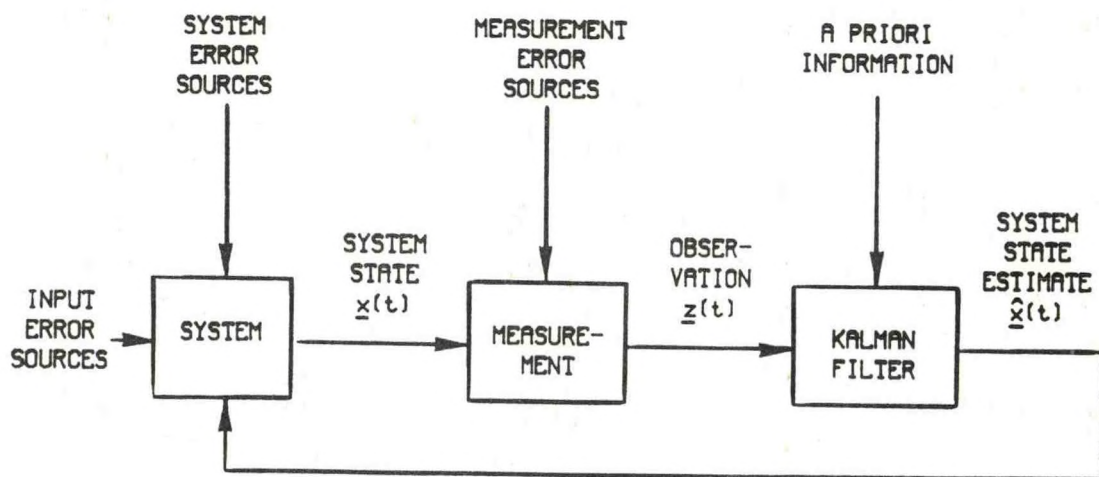


Figure 5.8. Concept of Forecasting and Updating (after Gelb, 1974).

The Kalman filter is used to estimate the optimal state as a linear function of the observation and the state estimate prior to the observation. The system equation is used to forecast the state. The computational steps in updating the state are:

- (a) Predict the error covariance, $P_{t+1|t}$

$$P_{t+1|t} = \Phi_t P_{t|t} \Phi_t^T + G_t U_t G_t^T + \Gamma_t Q \Gamma_t^T \quad (5.10)$$

- (b) Compute the Kalman gain, K

$$K_{t+1} = P_{t+1|t} H_{t+1}^T (H_{t+1} P_{t+1|t} H_{t+1}^T + R_{t+1})^{-1} \quad (5.11)$$

- (c) Process the observations

$$\hat{x}_{t+1|t+1} = \hat{x}_{t+1|t} + K_{t+1} (z_{t+1} - H_{t+1} \hat{x}_{t+1|t}) \quad (5.12)$$

- (d) Update the error covariance, $P_{t+1|t+1}$

$$P_{t+1|t+1} = [I - K_{t+1} H_{t+1}] P_{t+1|t} [I - K_{t+1} H_{t+1}]^T + K_{t+1} R_{t+1} K_{t+1}^T \quad (5.13)$$

where

$$\begin{aligned} \hat{x}_{t|s} &= \text{state vector estimate at time } t, \\ &\quad \text{given observation at time } s, \quad (n \times 1) \\ P_{t|s} &= \text{state estimate error covariance matrix at time } t, \\ &\quad \text{given observation at time } s, \quad (n \times n) \\ U_t &= \text{input noise covariance matrix, } (j \times 1) \\ K_t &= \text{Kalman gain matrix at time } t, \quad (n \times m) \\ I &= \text{identity matrix, } (n \times n). \end{aligned}$$

The result is a linear unbiased minimum variance estimate of the state and the associated state error covariance.

In this study the Kalman filter is applied to a nonlinear model and therefore referred to as the extended Kalman filter. The extended filter was first applied to the SAC-SMA model by Kitanidis and Bras (1980a). The filter was used to demonstrate how streamflow observations can be used to update states and improve hydrologic forecasts. Kitanidis and Bras (1978) and others (Bras and Rodriguez-Iturbe, 1985) have shown how the nonlinear models can be linearized using a technique such as Taylor series expansion.

Linearization for this study was done using the procedures outlined by Kitanidis and Bras (1980a). The highly nonlinear SAC-SMA model described earlier in this chapter can be expressed in general form as:

$$\dot{x} = f(x, u) \quad (5.14)$$

Linearization results in a system equation:

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}_t + \mathbf{B}\mathbf{u}_t + \mathbf{f}_0. \quad (5.15)$$

The system of equations which comprise the state-space model (equations 4.1 through 4.10) can be linearized into the form of equation (5.15). The elements of A and B are:

$$A_{ij} = \delta f_i(x,u)/\delta x_j; \quad (5.16)$$

$$B_{ij} = \delta f_i(x,u)/\delta u_j. \quad (5.17)$$

The last step in implementing the filter is the integration of equation (5.15) into the form of equation (5.8). Kitanidis and Bras (1978a) developed an accurate integration scheme which produces a solution for Φ and G in equation (5.8). The matrices are:

$$\Phi = \left(\mathbf{I} - \mathbf{A} \frac{\Delta t}{2} + \mathbf{A}^2 \frac{\Delta t^2}{12} \right)^{-1} \left(\mathbf{I} + \mathbf{A} \frac{\Delta t}{2} + \mathbf{A}^2 \frac{\Delta t^2}{12} \right) \quad (5.18)$$

$$= \left(\mathbf{I} - \mathbf{A} \frac{\Delta t}{2} + \mathbf{A}^2 \frac{\Delta t^2}{12} \right) \mathbf{B} \Delta t. \quad (5.19)$$

The state-space SAC-SMA and reduced order unit hydrograph (REDO-UHG) models were coupled for the purposes of this study into one set of system and measurement equations. The output from the original SAC-SMA model and input to the unit hydrograph operation, is total channel inflow (TCI). TCI, therefore, is the link between the state-space SAC-SMA and REDO-UHG matrix elements. The state vector consists of the six soil moisture states, TCI, and the REDO-UHG states. Elements in the SAC-SMA portion of Φ and G come from equations (5.18) and (5.19). The elements in the REDO-UHG component of Φ , G and H are produced by the REDO-UHG operation from the original unit hydrograph ordinates.

The purpose of the Kalman filter development work is to produce a parameter estimation procedure which has the same properties as the state estimator. Parameter estimation is accomplished by augmenting the state vector with parameters, thus producing parameters which are updated in the same way as model states. The parameters have essentially become model states for the purpose of filtering. The objective function in OPT typically is based on a least squares statistic for the observed and simulated discharges. In the Kalman filter, optimization of parameters is performed by updating the parameters according to the Kalman gain which minimizes the weighted sum of the diagonal elements of the error covariance matrix. Although optimality cannot be guaranteed with the extended and augmented filter, the variance of the error of the state and parameter estimates is reduced by adjusting both states and parameters. Parameters converge because the elements in the covariance matrix are reduced as more information is processed.

The matrices in the program are quite complex and vary considerably depending on how many parameters are being estimated and how many states are being used to describe the unit hydrograph. Subroutines in LINDRV build the matrices according to the user specified inputs. The states representing parameters are inserted in the matrices in the rows and

columns following the actual model states. The general forms of the filter matrices are shown below. There are n parameters and m unit hydrograph states.

State vector, x :

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ \cdot \\ x_6 \\ \alpha_1 \\ \alpha_2 \\ \cdot \\ \cdot \\ \cdot \\ \alpha_n \\ f_7 \\ UG_1 \\ UG_2 \\ \cdot \\ \cdot \\ \cdot \\ UG_m \end{bmatrix} \quad (5.20)$$

where X = actual model states
 α = parameter states
 f_7 = TCI
 UG = Unit hydrograph states.

A matrix, for equation (5.16):

$$A = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_6} & \frac{\partial f_1}{\partial \alpha_1} & \cdots & \frac{\partial f_1}{\partial \alpha_n} \\ \vdots & & \vdots & \vdots & & \vdots \\ \frac{\partial f_6}{\partial x_1} & \cdots & \frac{\partial f_6}{\partial x_6} & \frac{\partial f_6}{\partial \alpha_1} & \cdots & \frac{\partial f_6}{\partial \alpha_n} \\ 0 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & & \vdots & \vdots & & \vdots \\ \vdots & & \vdots & \vdots & & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & 0 \end{bmatrix} \quad (5.21)$$

B matrix, for equation (5.17):

$$B = \begin{bmatrix} \frac{\partial f_1}{\partial u} \\ \vdots \\ \frac{\partial f_6}{\partial u} \\ 0 \\ \vdots \\ 0_n \\ \frac{\partial f_7}{\partial u} \end{bmatrix} \quad (5.22)$$

Φ matrix:

$$\Phi = \left[\begin{array}{cccccc} (I - A \frac{\Delta t}{2} + A^2 \frac{\Delta t^2}{12})^{-1} * & 0 & 0 & \dots & 0 \\ (I + A \frac{\Delta t}{2} + A^2 \frac{\Delta t^2}{12}) & \cdot & \cdot & & \cdot \\ \text{for } n+6 \text{ by } n+6 \text{ elements} & \cdot & \cdot & & \cdot \\ \frac{\partial f_7}{\partial x_1} \dots \frac{\partial f_7}{\partial x_6} \frac{\partial f_7}{\partial \alpha_1} \dots \frac{\partial f_7}{\partial \alpha_n} & 0 & 0 & \dots & 0 \\ 0 & \dots & 0 & G_{UG_1} & \Phi_{UG_1,1} \dots \Phi_{UG_1,m} \\ \cdot & & \cdot & \cdot & \cdot \\ \cdot & & \cdot & \cdot & \cdot \\ 0 & \dots & 0 & G_{UG_m} & \Phi_{UG_m,1} \dots \Phi_{UG_m,m} \end{array} \right] \quad (5.23)$$

G matrix:

$$G = \left[\begin{array}{c} n+6 \text{ elements from} \\ (I - A \frac{\Delta t}{2} + A^2 \frac{\Delta t^2}{12})^{-1} * B \Delta t \\ B (n+7) * \Delta t \\ 0 \\ \cdot \\ \cdot \\ 0_m \end{array} \right] \quad (5.24)$$

H matrix:

$$H = \begin{bmatrix} 0 \\ \vdots \\ 0_{n+7} \\ H_{UG_1} \\ \vdots \\ H_{UG_m} \end{bmatrix} \quad (5.25)$$

The 147 derivative equations (derivatives of 7 functions with respect to 6 states, 14 parameters, and 1 input) calculated to determine the elements in the A and B matrices are given in Appendix A.

The computational steps in LINDRV closely follow the steps outlined in equations (5.10) through (5.13). Input data consist of estimates of mean areal precipitation and potential evaporation. The computational time interval of the forecast model is variable and can be set to agree with the interval of the precipitation data. The only current restriction is that the time interval of the REDO-UHG model must match the time step of the SAC-SMA, and only multiples of hour time steps which are evenly divided into 24 hours currently are allowed in REDO-UHG. Six hour precipitation observations typically are used with the model and potential evaporation usually is expressed as total for a day.

Inputs to LINDRV also consist of the initial state error covariance matrix (P_0), the system noise covariance matrix (Q), the input noise covariance matrix (U), and the measurement noise covariance matrix (R). The P_0 diagonal elements must be specified by the user. Off diagonal elements are set to 0.0. If the filter is stable, the choice of P_0 should not be crucial to its performance (Georgakakos, 1980). It may, however, affect the results and should be tested with various values to assess its impact. The case study in Chapter 6 addresses the P_0 sensitivity. The Q matrix diagonal elements represent the variance of the errors in the system model. These values are estimated for the model states and typically are set to zero for the parameters. The parameter estimation procedure is based on the assumption that no system error exists for the parameter states. Bowles and Grenney (1978) and Rajaram and Georgakakos (1987) have described some of the problems associated with estimating values for Q. The covariance characteristics

also can be included in the parameter space and recursively estimated. Information concerning the choice of Q for this research is given in Chapter 6.

Only one input (precipitation) is treated as a driving variable in LINDRV and only one measurement (streamflow) value is observed, making U and R scalars rather than matrices. The values of U and R are both functions of time and vary with the magnitude of the estimate with which they are associated.

U is expressed as a function of the precipitation value and the coefficient of variation of the precipitation time series (v_u).

$$U = (v_u \cdot \text{precipitation value})^2 \quad (5.26)$$

where

$$\begin{aligned} v_u &= s_p / m_p \\ s_p &= \text{standard deviation of the precipitation time series} \\ m_p &= \text{mean of the precipitation time series} \end{aligned}$$

R is a function of the streamflow measurement and the coefficient of variation of the streamflow time series (v_r).

$$R = (v_r \cdot \text{streamflow value})^2 \quad (5.27)$$

where

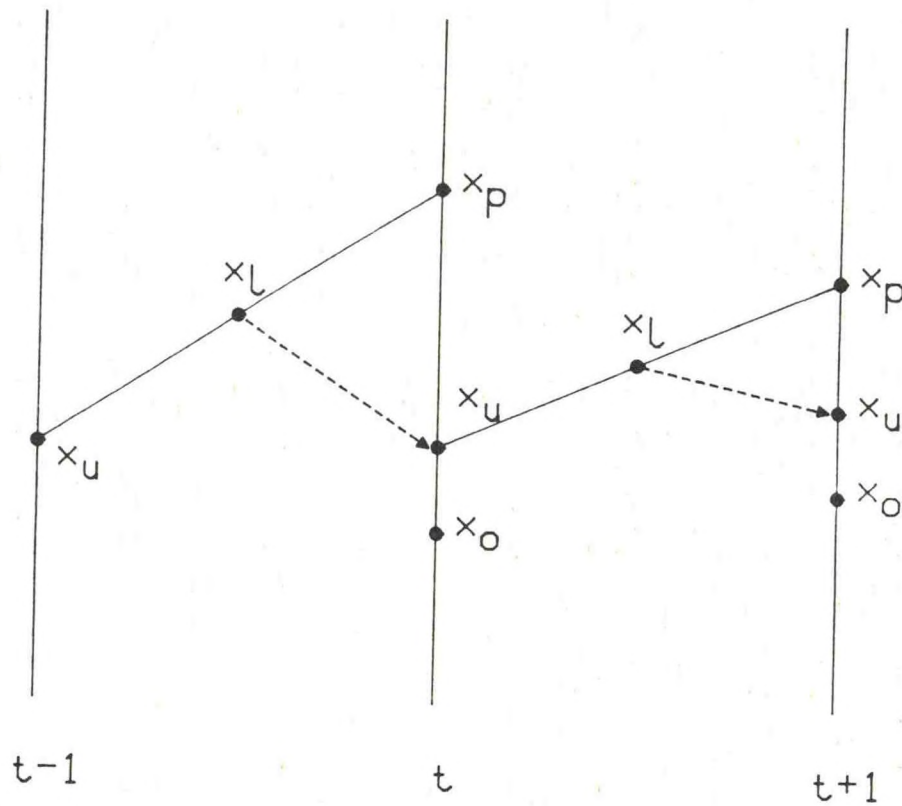
$$\begin{aligned} v_r &= s_s / m_s \\ s_s &= \text{standard deviation of the streamflow time series} \\ m_s &= \text{mean of the streamflow time series} \end{aligned}$$

A discussion of how the values for v_u and v_r should be estimated is included in the case study description in Chapter 6.

The forecast step in LINDRV is performed by running the deterministic state-space SAC-SMA and REDO-UHG models for one time step. As discussed in Chapter 4, the nonlinear state-space model appears to be a reasonable compromise which produces output statistically close to the original SAC-SMA model and gives results which are superior to the linear expression in equation (5.8). The forecast step results in predicted estimates of the model system states.

The updating step requires evaluation of the A and B and resulting Φ and G matrices. The point at which matrices A and B are evaluated becomes the point about which linearization takes place. Several LINDRV runs were made to try to determine the best point of linearization. The points evaluated included the points at both the beginning and end of time steps and the point represented by the mean of the beginning and ending state values. Kitanidis (1978) used the mean point and the results from the runs for this study showed no reason to differ. The mean point was used for linearization as shown in figure 5.9.

The only other source of information needed to process the observation and update the states is the observation itself. Equation



x_p = predicted state

x_l = value of state at
point of linearization

x_o = observed state

x_u = updated state

Figure 5.9. Point of Linearization for Computation of State Transition Matrix.

(5.12) shows the computation for the update step. Observations can consist of instantaneous or mean daily streamflow values. The most straightforward procedure for updating is to have a measurement observation at the same time interval as the model time step. Unfortunately, for most watersheds, streamflow observations at less than daily time intervals are available only for isolated periods. Typically, streamflow records for extended periods consist of mean daily flows. LINDRV was developed such that the streamflow observation can be an instantaneous or mean daily value. This is done by choosing the point of linearization as the midpoint of the time interval of the observation. Instantaneous output from the model is averaged to compute a mean daily simulated flow which can be compared to the observed mean daily flow for the purpose of processing the observation. The result is a filter which has the forecast step driven by the time interval of the input and the update step driven by the time interval of the observation.

Synthetic Data Development Runs

Numerous computer runs were made to test the features of LINDRV. Because the experiment involved tests of the first implementation of adaptive filtering to such a complex hydrologic model, the developmental runs were for synthetic data. Synthetic discharges were generated using actual 6-hour mean areal precipitation values and daily potential evaporation estimates for the Bird Creek watershed near Sperry, Oklahoma for water years 1956-62.

The first set of LINDRV runs were made to determine if perturbed parameter values could converge to their true values. Runs were made for every parameter in the SAC-SMA model. A representative sample of run results are shown in figure 5.10 a-f. The discharge observations were instantaneous 6-hour values and contained no errors. The initial error covariances for the parameters were set at 10 percent of the parameter values. The results show that the parameters tend to converge from both high and low initial values. Some of the parameters converge faster than others. Parameter adjustments generally occur in steps and correspond to events where the parameters tend to have the most effect on the simulation. For instance ADIMP is corrected abruptly during the first event where significant direct runoff occurs since ADIMP affects direct runoff most. In fact, the first occurrence of simulated direct runoff was on February 9. Direct runoff accounted for 80 percent of the total flow on February 9 and 10, the dates of change in ADIMP. SIDE which is controlled more by overall volume tends to move more slowly throughout the period.

The same runs were made over again for all parameters with observations of mean daily discharge. Results are shown in figure 5.11 a-f. The plots are similar to the results shown in figure 5.10, except a certain amount of overcorrection can be seen to occur as a result of the averaging effect of the discharges. Because updating occurs only after every four steps of forecasting, flows are allowed to deviate more from their optimal estimates before they are corrected. The result is

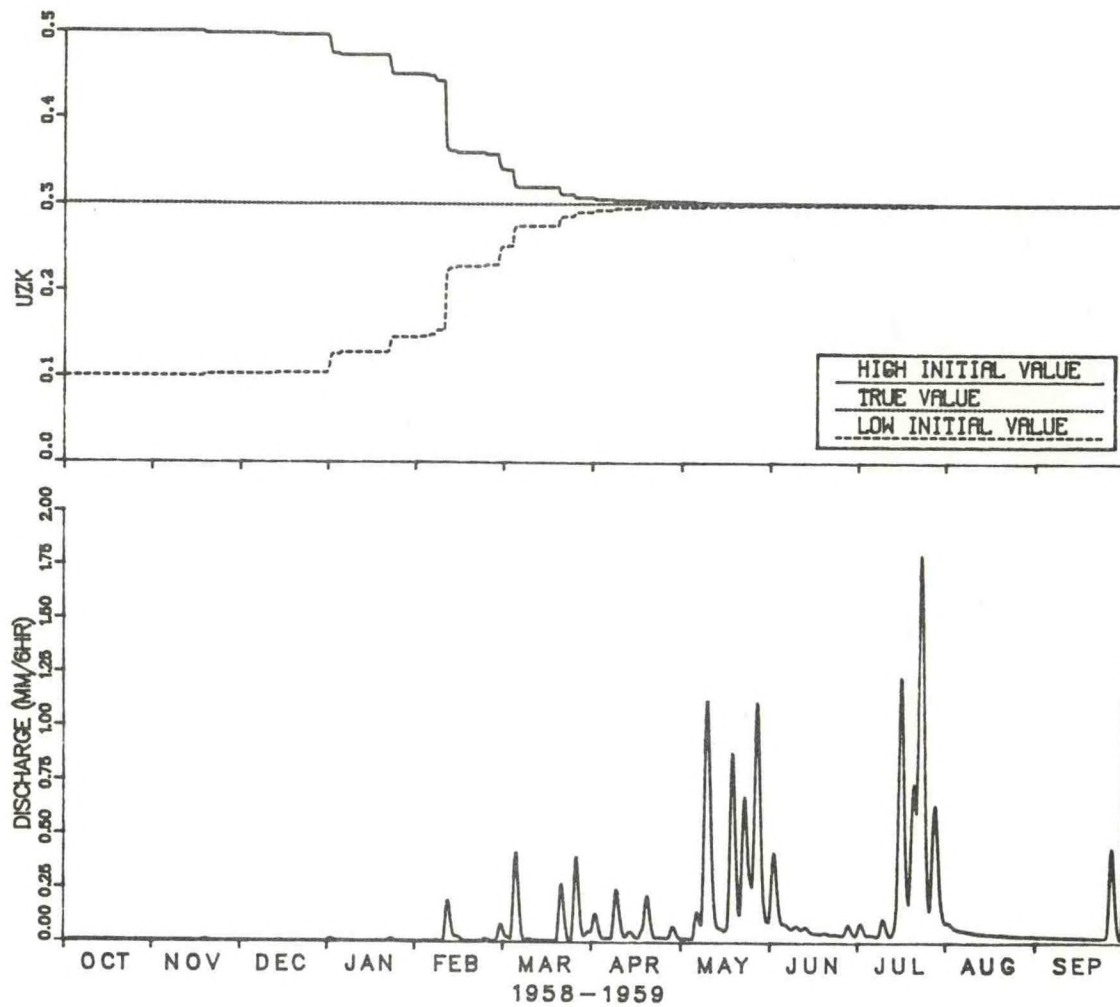


Figure 5.10a. LINDRV Results for UZK (Fractional daily upper zone free water withdrawal rate) using 6-hour Synthetic Streamflows.

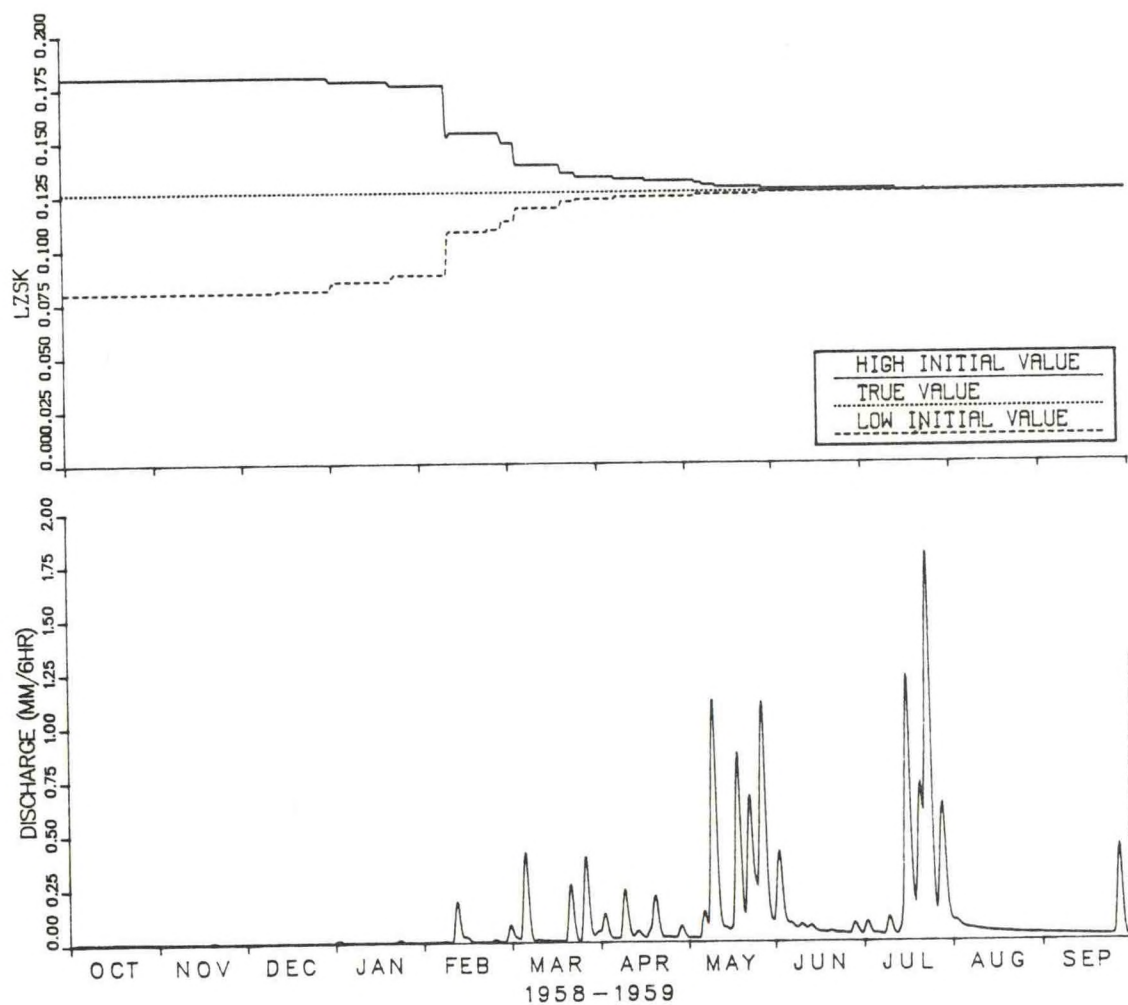


Figure 5.10b. LINDRV Results for LZSK (Fractional daily supplemental withdrawal rate) using 6-hour Synthetic Streamflows.

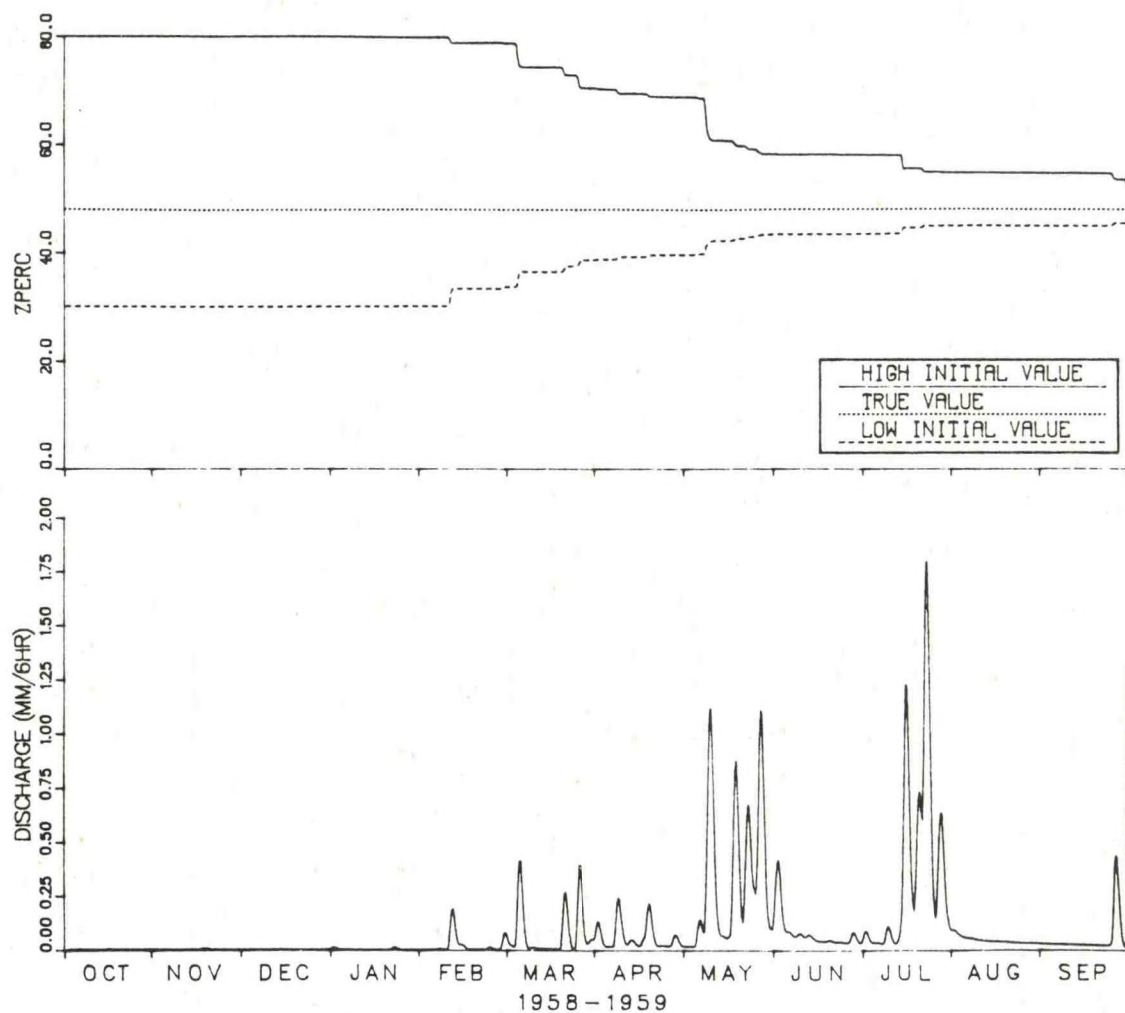


Figure 5.10c. LINDRV results for ZPERC (Maximum percolation rate coefficient) using 6-hour Synthetic Streamflows.

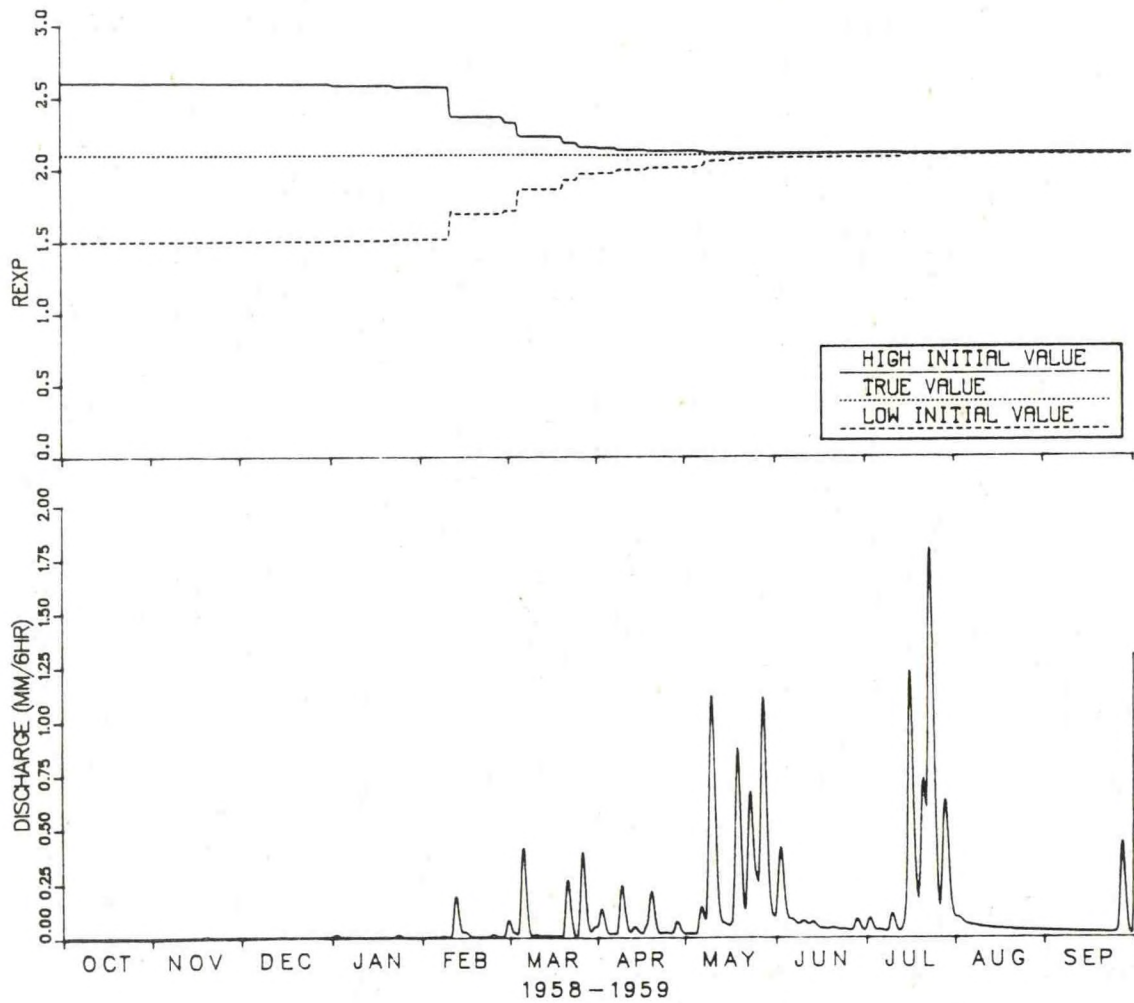


Figure 5.10d. LINDRV Results for REXP (Percolation equation exponent) using 6-hour Synthetic Streamflows.

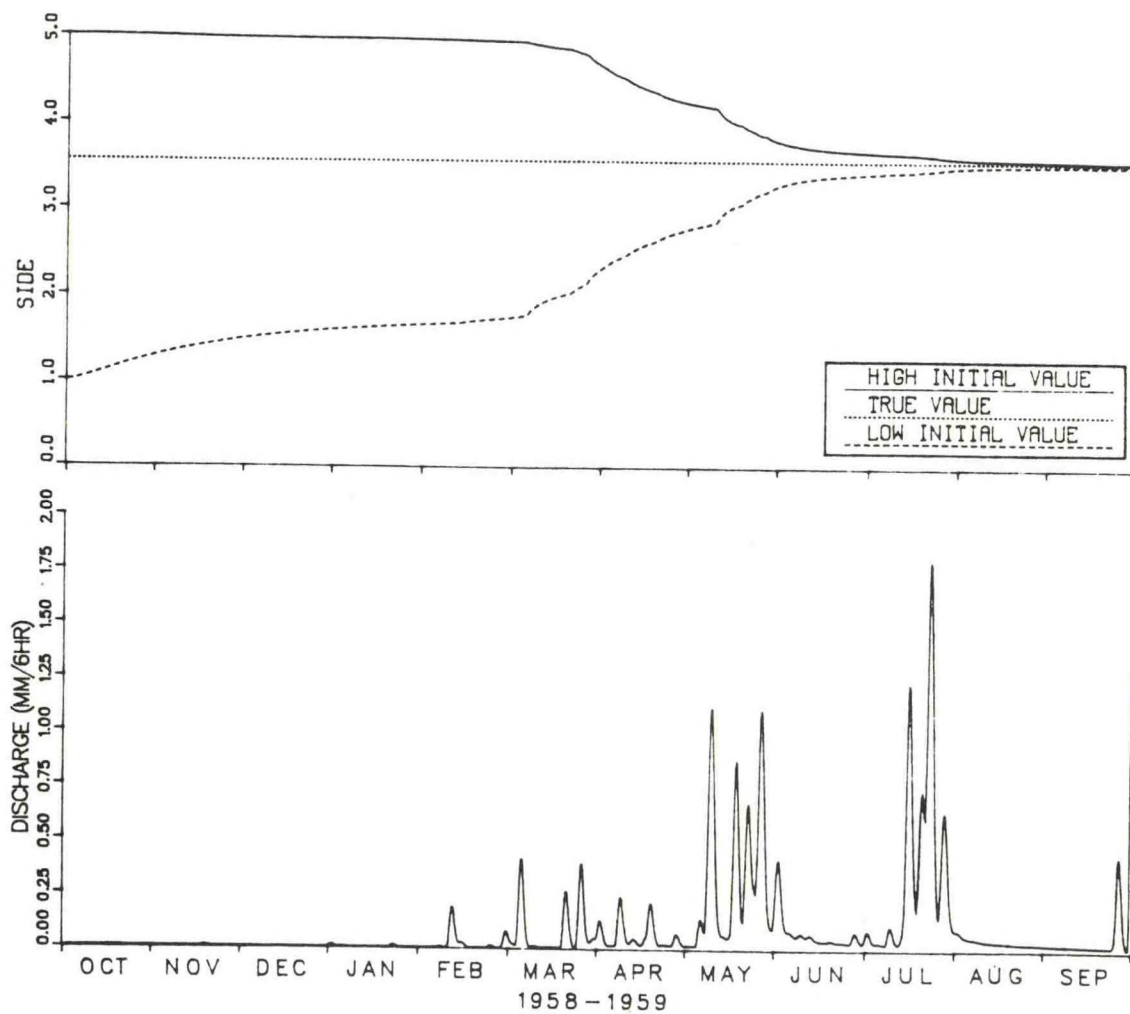


Figure 5.10e. LINDRV Results for SIDE (Ratio of deep recharge to channel baseflow) using 6-hour Synthetic Streamflows.

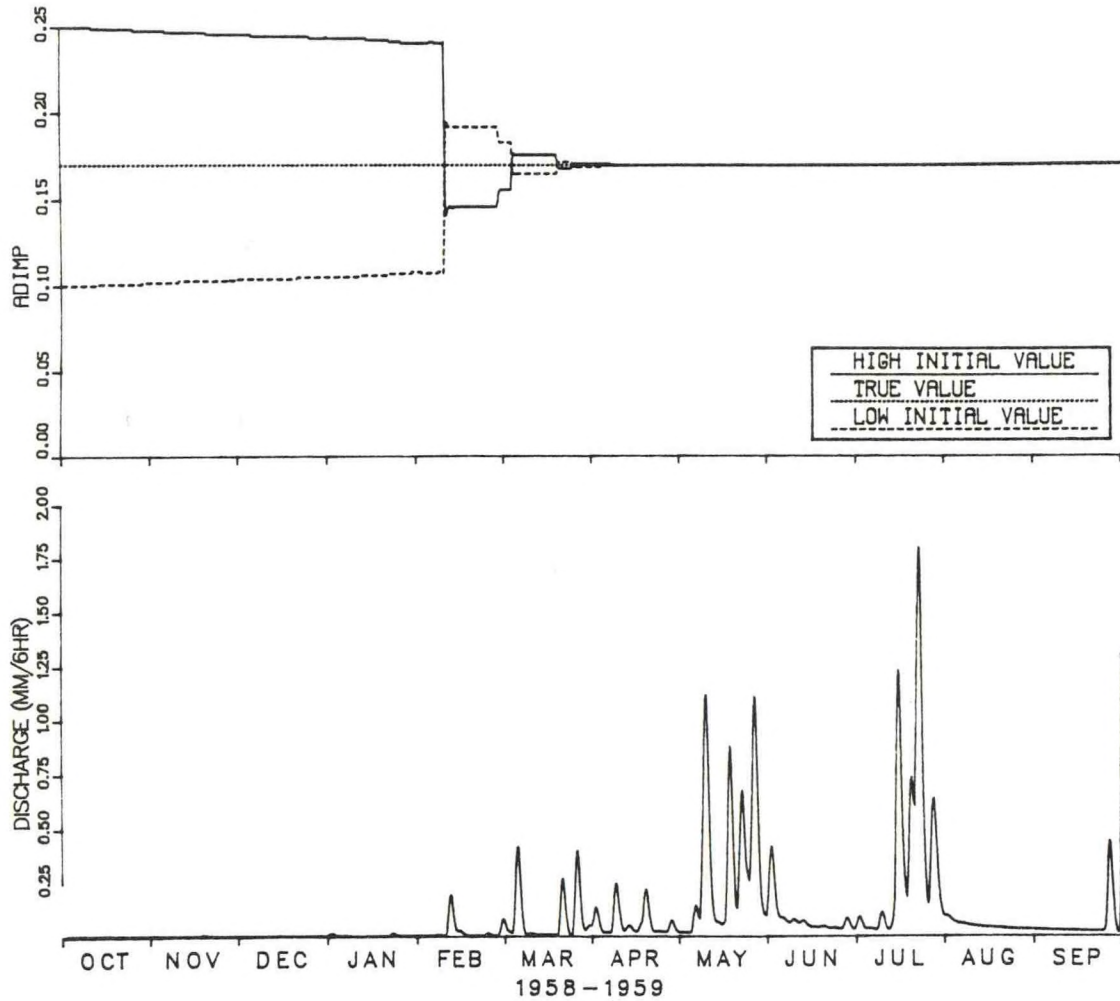


Figure 5.10f. LINDRV Results for ADIMP
(Additional impervious area) using 6-hour
Synthetic Streamflows.

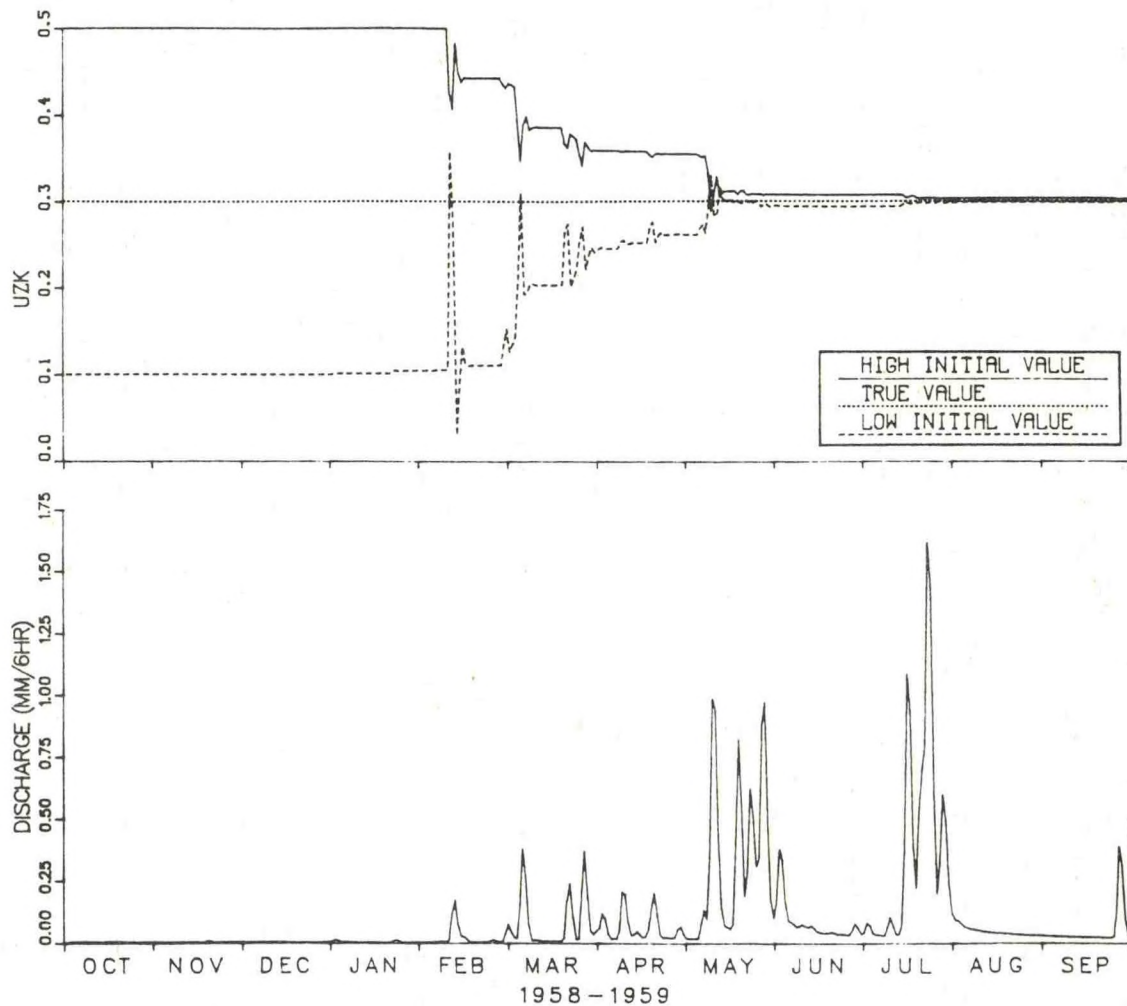


Figure 5.11a. LINDRV Results for UZK (Fractional daily upper zone free water withdrawal rate) using Mean Daily Synthetic Streamflows.

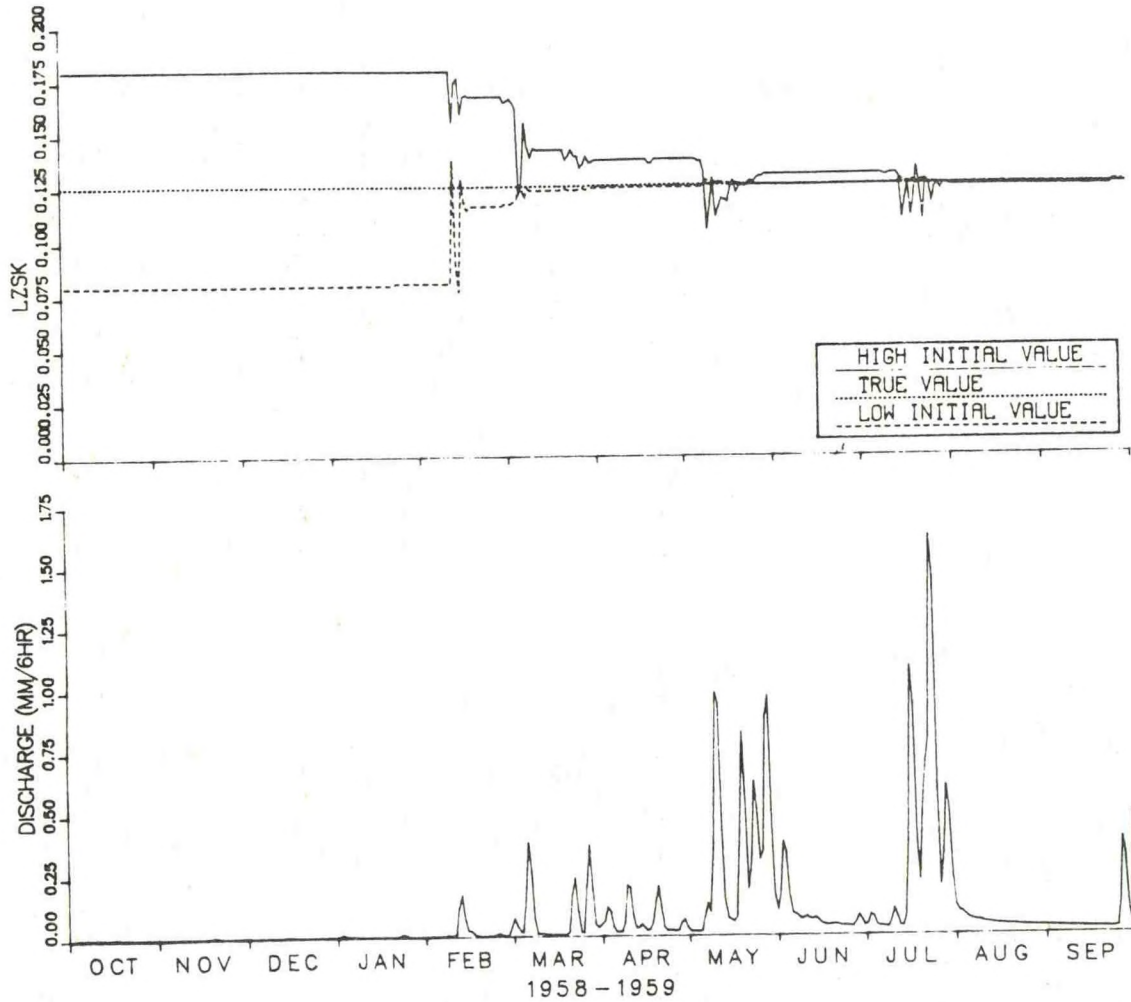


Figure 5.11b. LINDRV Results for LZSK (Fractional daily supplemental withdrawal rate) using Mean Daily Synthetic Streamflows.

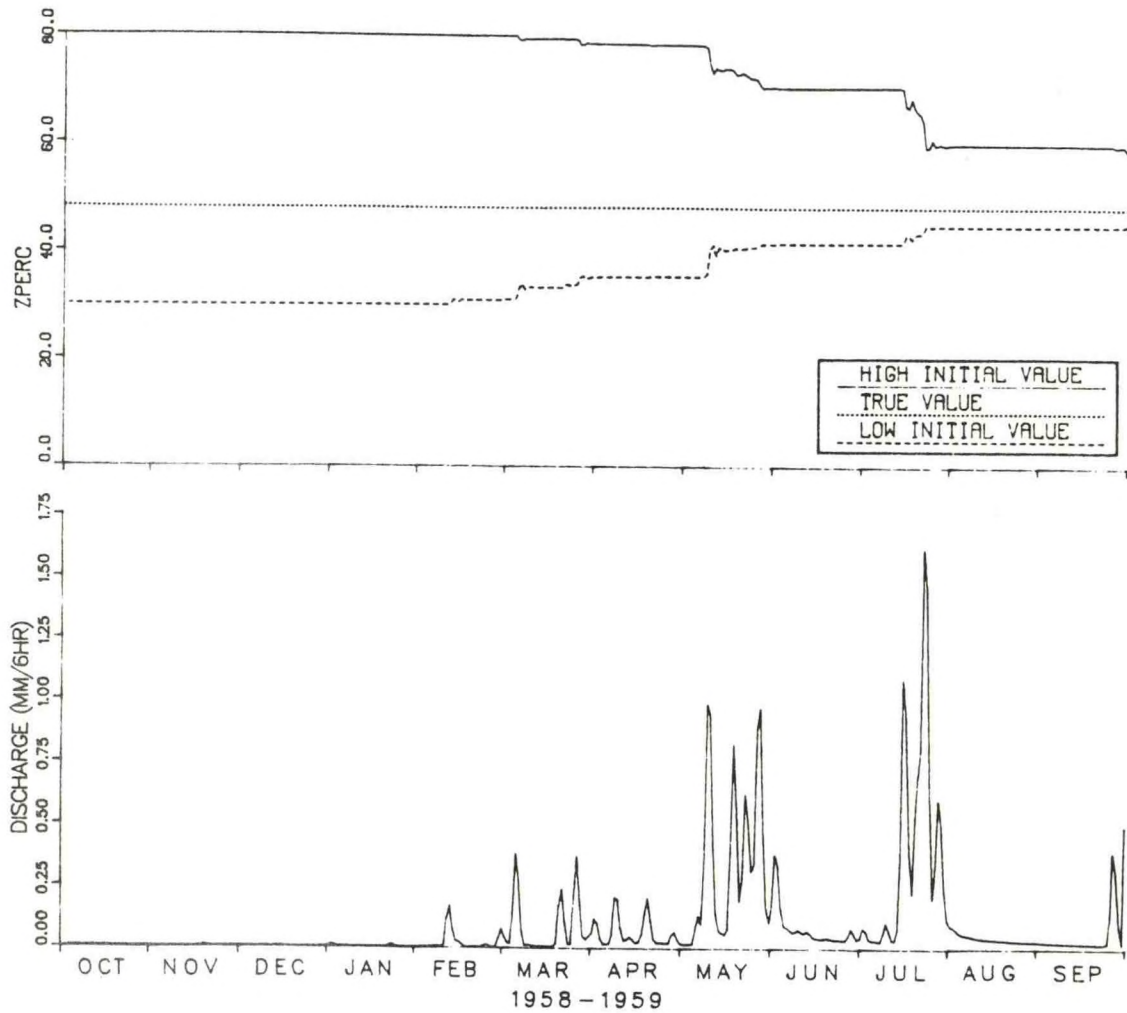


Figure 5.11c. LINDRV Results for ZPERC (Maximum percolation rate coefficient) using Mean Daily Synthetic Streamflows.

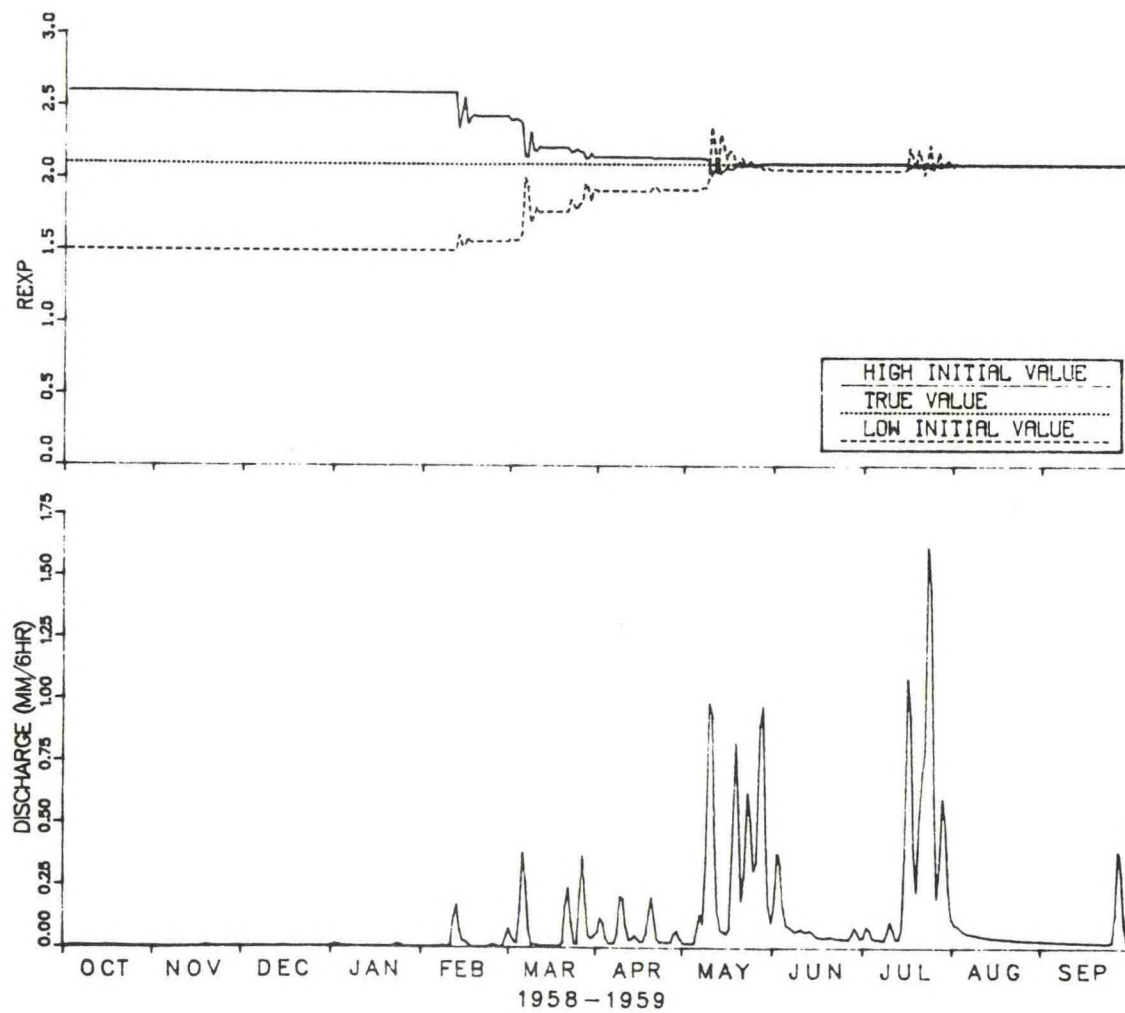


Figure 5.11d. LINDRV Results for REXP
(Percolation equation exponent) using
Mean Daily Synthetic Streamflows.

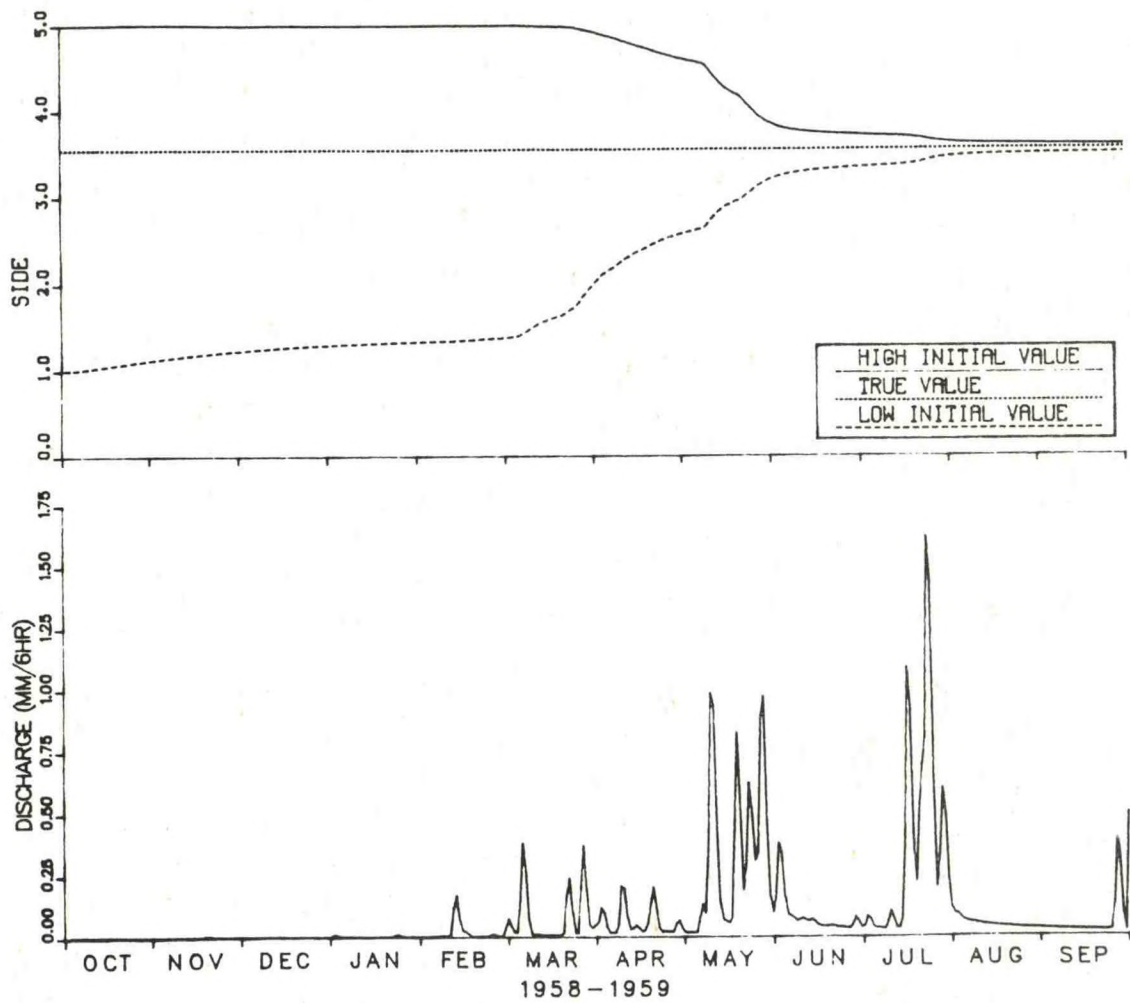


Figure 5.11e. LINDRV Results for SIDE (Ratio of deep recharge to channel baseflow) using Mean Daily Synthetic Streamflows.

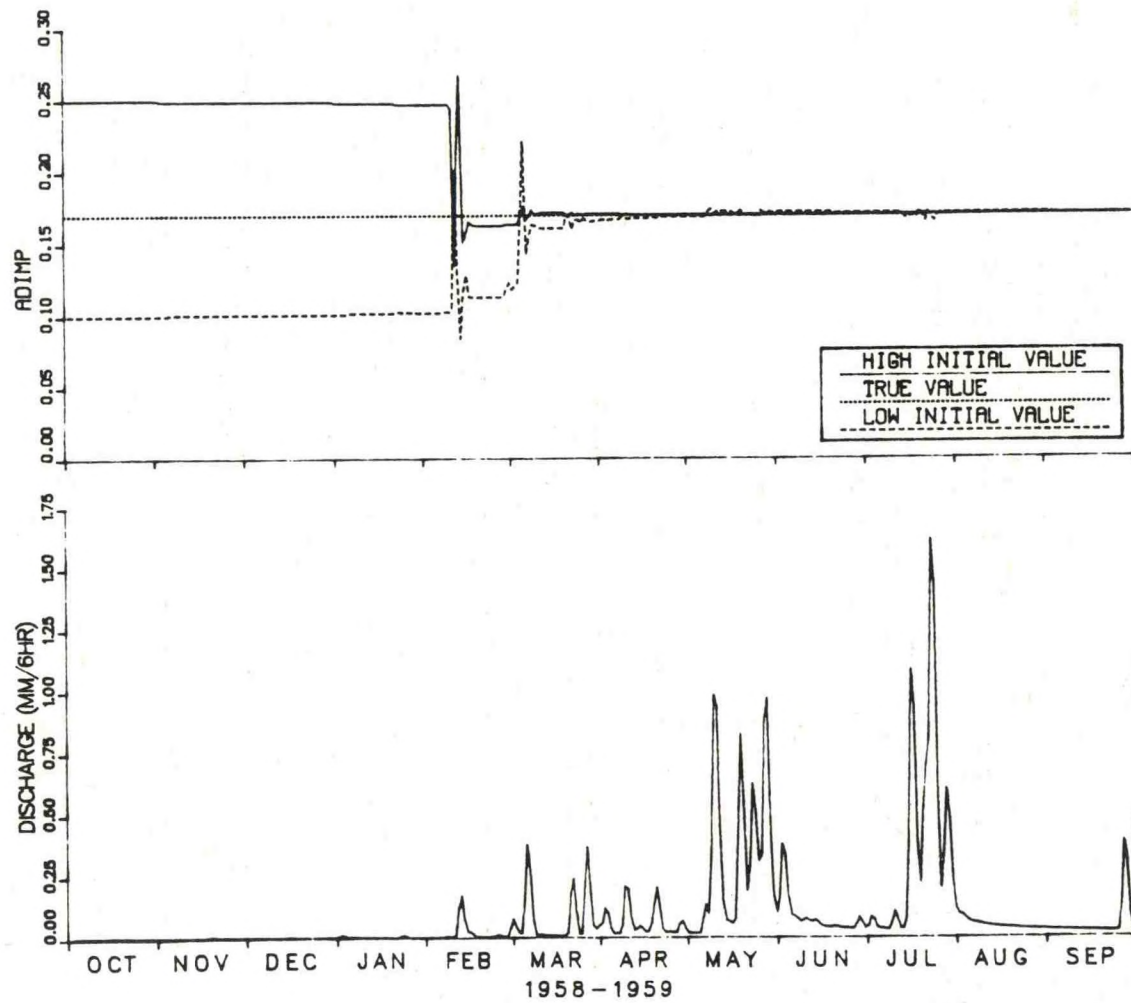


Figure 5.11f. LINDRV Results for ADIMP (Additional impervious area) using Mean Daily Synthetic Streamflows.

an overcompensation in many of the time steps. Convergence is still evident in the runs, though. SIDE exhibits a slowly converging trend, even for mean daily flows.

One criticism of previous studies of Kalman filtering in hydrologic forecasting has been the limited amount of data used in the analysis. Studies have tended to focus on only one year of data. For this reason, LINDRV was run to estimate UZK from instantaneous discharge for each of the seven water years in the synthetic period of record. Results are shown in Figure 5.12 a-f. Results for water year 1959 were given in Figure 5.10a. The figures show how the filter adjusts a parameter at different rates depending on the type of streamflow activity within the simulation period.

One problem commonly associated with model calibration is the simultaneous estimation of several parameters. Numerous runs were made with various combinations of parameters. In general the parameters moved toward their true values, however, the adjustments were sensitive to changes in elements in P_0 and Q . Figure 5.13 shows results from a run where UZK and LZSK were estimated simultaneously. The two parameters were assigned each others true value as their starting value and converged to their correct values.

The parameter UZK became the focus of most of the remaining developmental runs because it showed relatively predictable sensitivity to changes in inputs. A number of runs were made to examine the behavior of the algorithms using data with a known error structure. Figure 5.14 shows results from a run where the instantaneous streamflow observations included a measurement error corresponding to a coefficient of variation of 10 percent. Results were similar to previous runs, however, convergence occurs before the parameter reaches its true value. Figure 5.15 shows results from a run where error also was introduced into the precipitation. The precipitation error coefficient of variation also was 10 percent.

Two final runs show the effect of not using a Q matrix diagonal element of zero for parameter values. Figures 5.16 and 5.17 show results from runs analogous to Figures 5.14 and 5.15 except for parameter Q values equal to 1 percent of their values. Although the parameters still exhibit convergence, the nonzero Q values introduce an unnecessary element of uncertainty in the parameter estimation procedure.

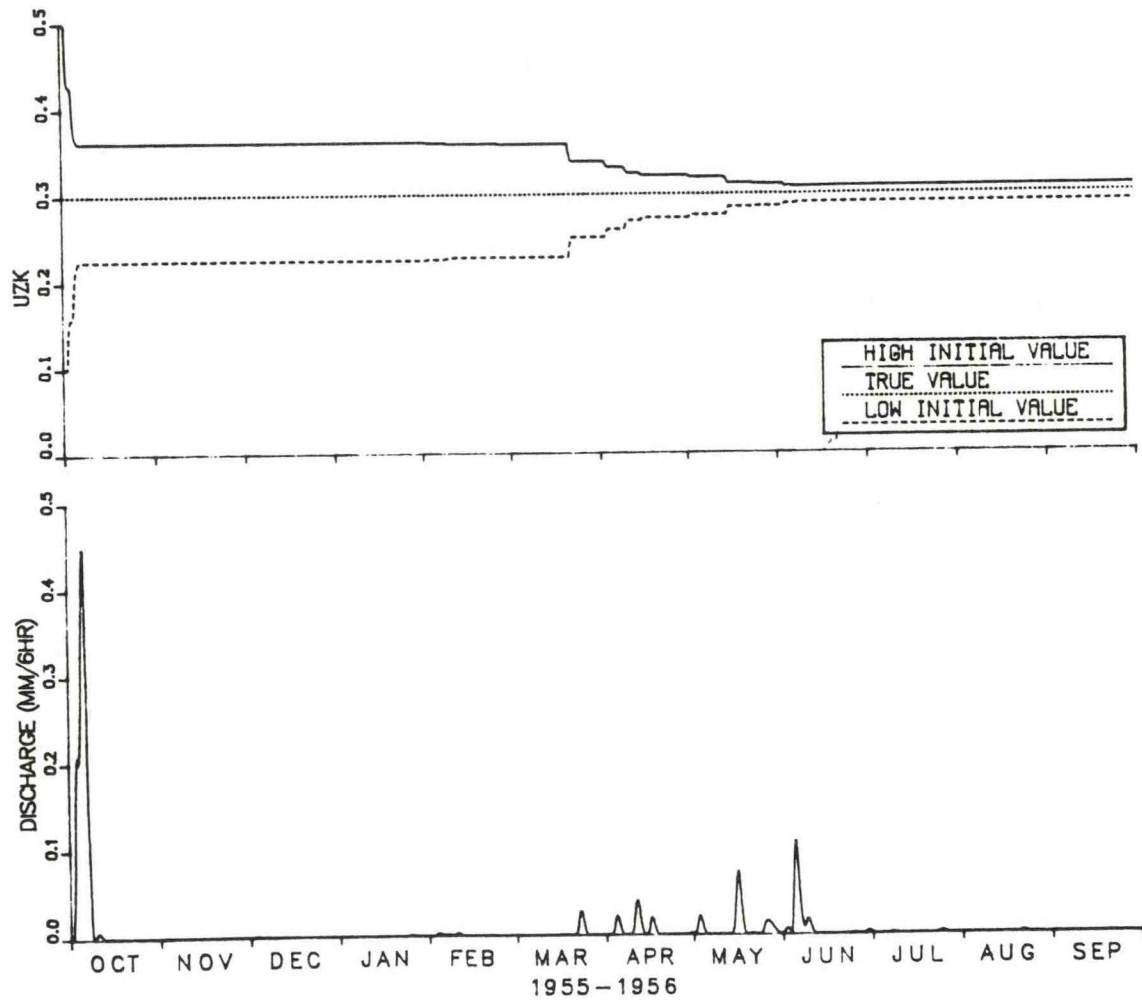


Figure 5.12a. LINDRV Results for UZK (Fractional daily upper zone free water withdrawal rate) using 6-hour Synthetic Streamflows (WY1956).

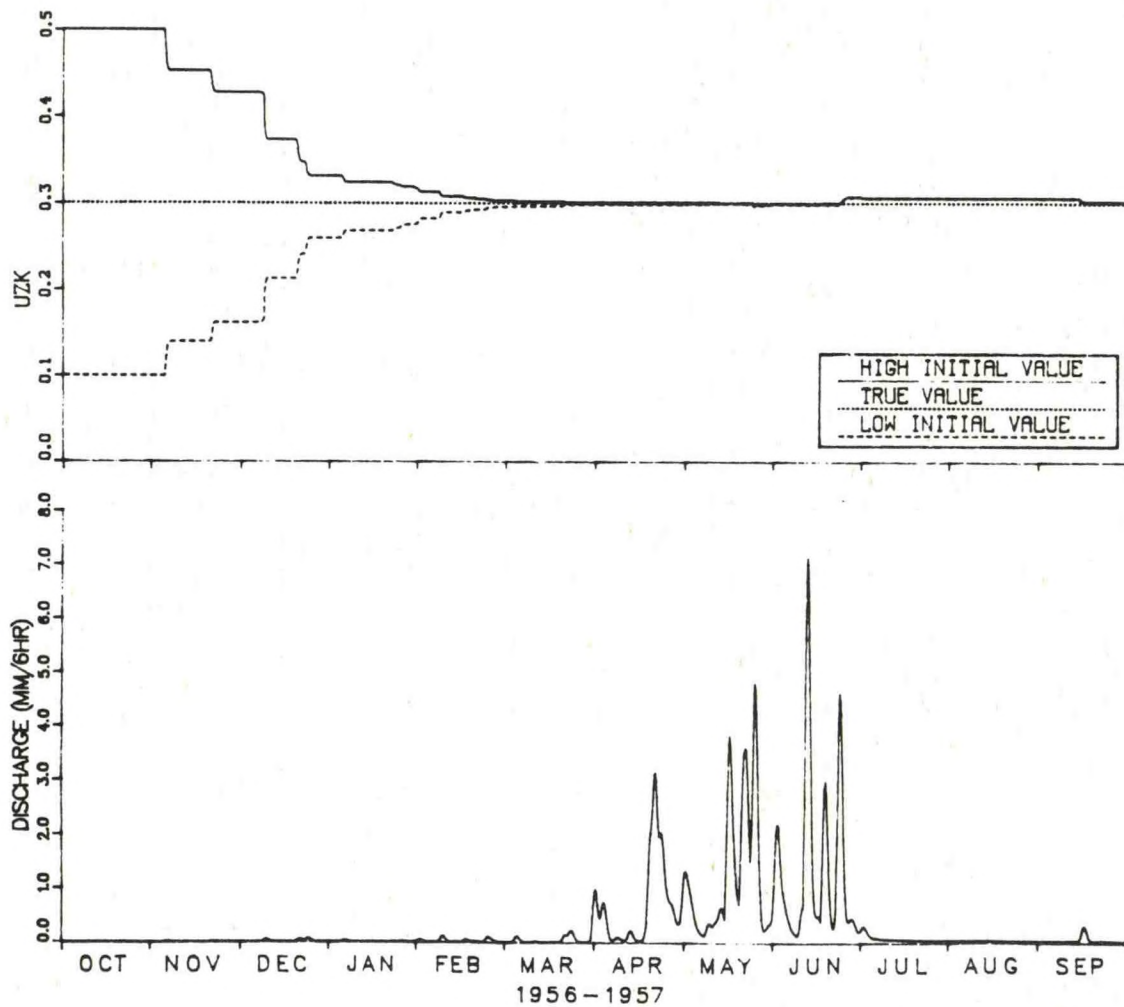


Figure 5.12b. LINDRV Results for UZK (Fractional daily upper zone free water withdrawal rate) using 6-hour Synthetic Streamflows (WY1957).

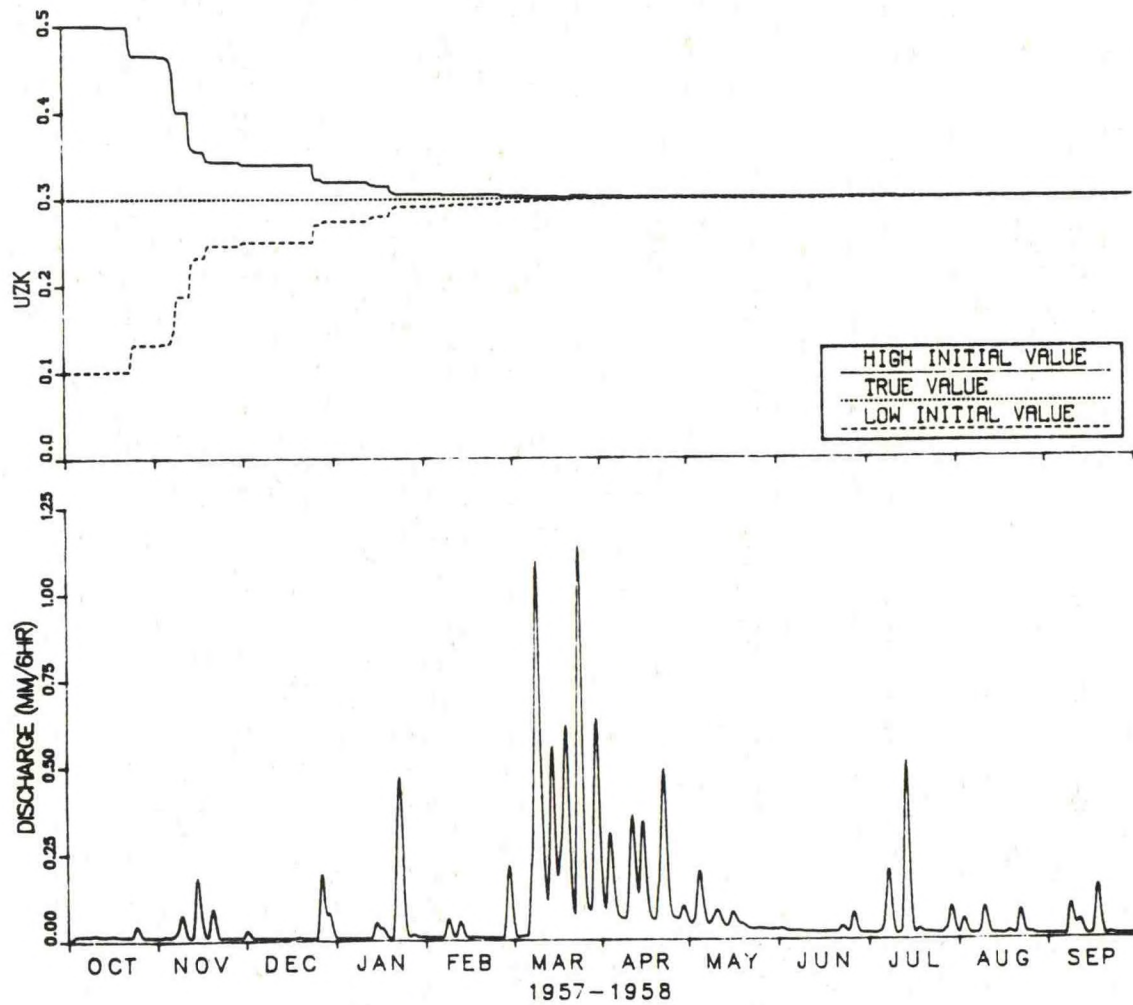


Figure 5.12c. LINDRV Results for UZK (Fractional daily upper zone free water withdrawal rate) using 6-hour Synthetic Streamflows (WY1958).

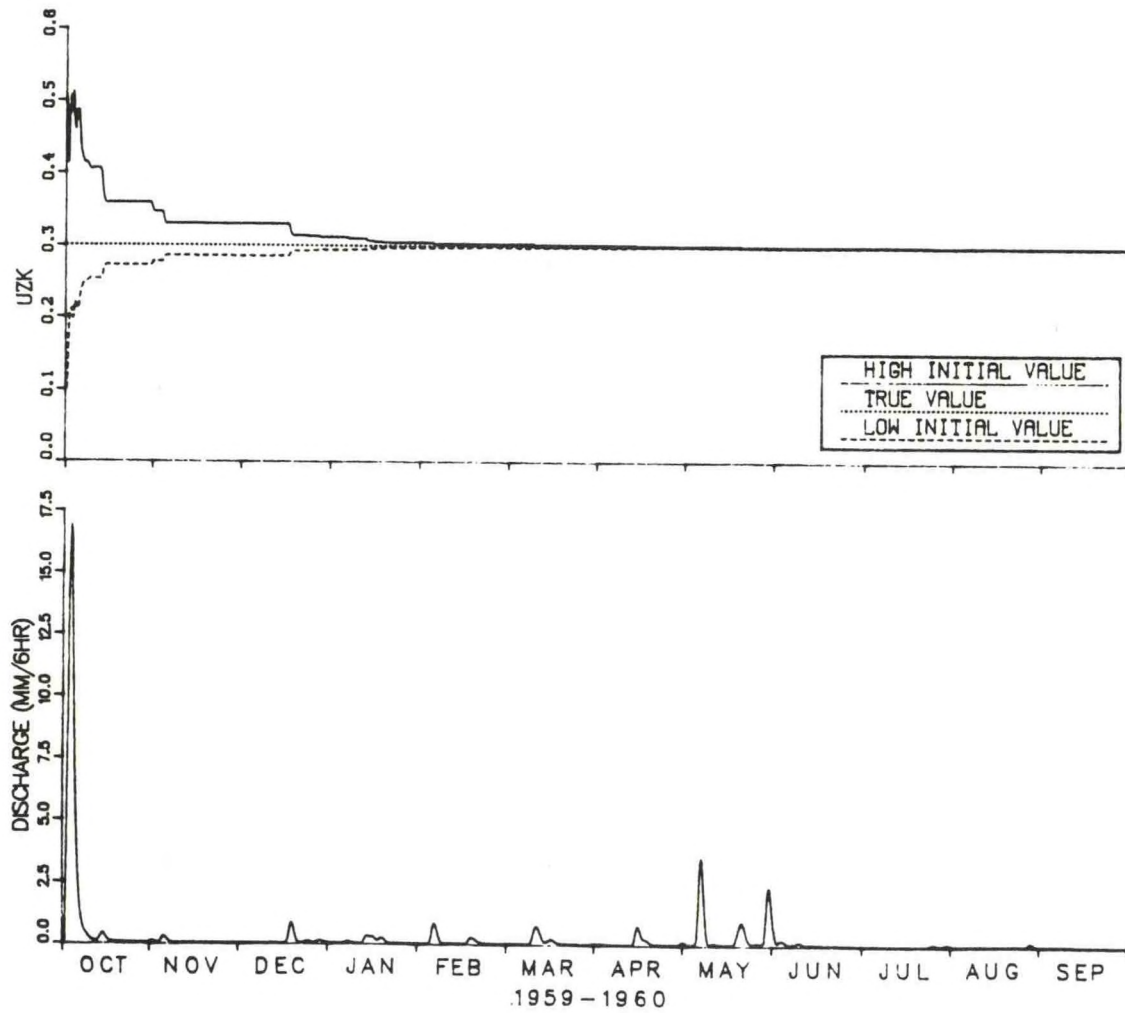


Figure 5.12d. LINDRV Results for UZK (Fractional daily upper zone free water withdrawal rate) using 6-hour Synthetic Streamflows (WY1960).

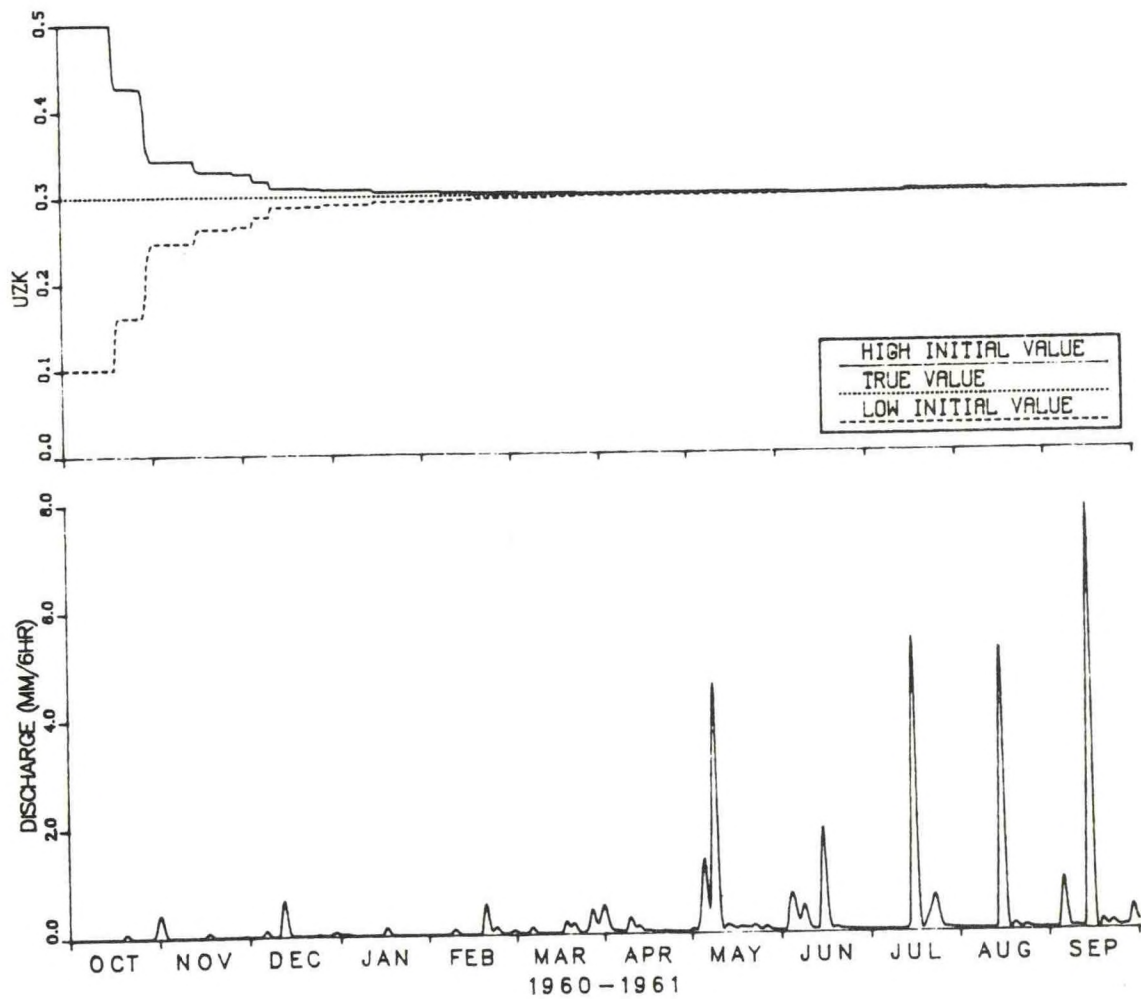


Figure 5.12e. LINDRV Results for UZK (Fractional daily upper zone free water withdrawal rate) using 6-hour Synthetic Streamflows (WY1961).

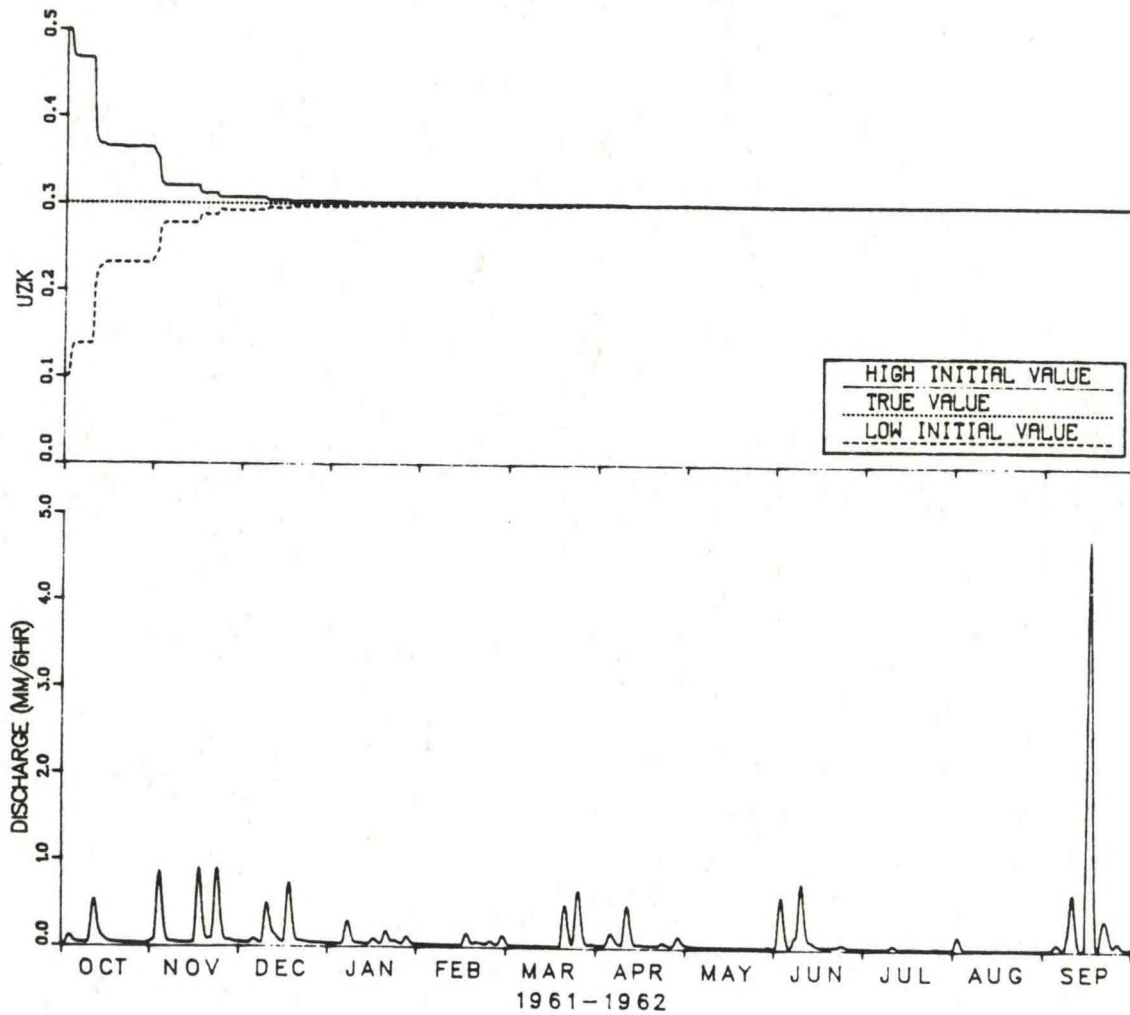


Figure 5.12f. LINDRV Results for UZK (Fractional daily upper zone free water withdrawal rate) using 6-hour Synthetic Streamflows (WY1962).

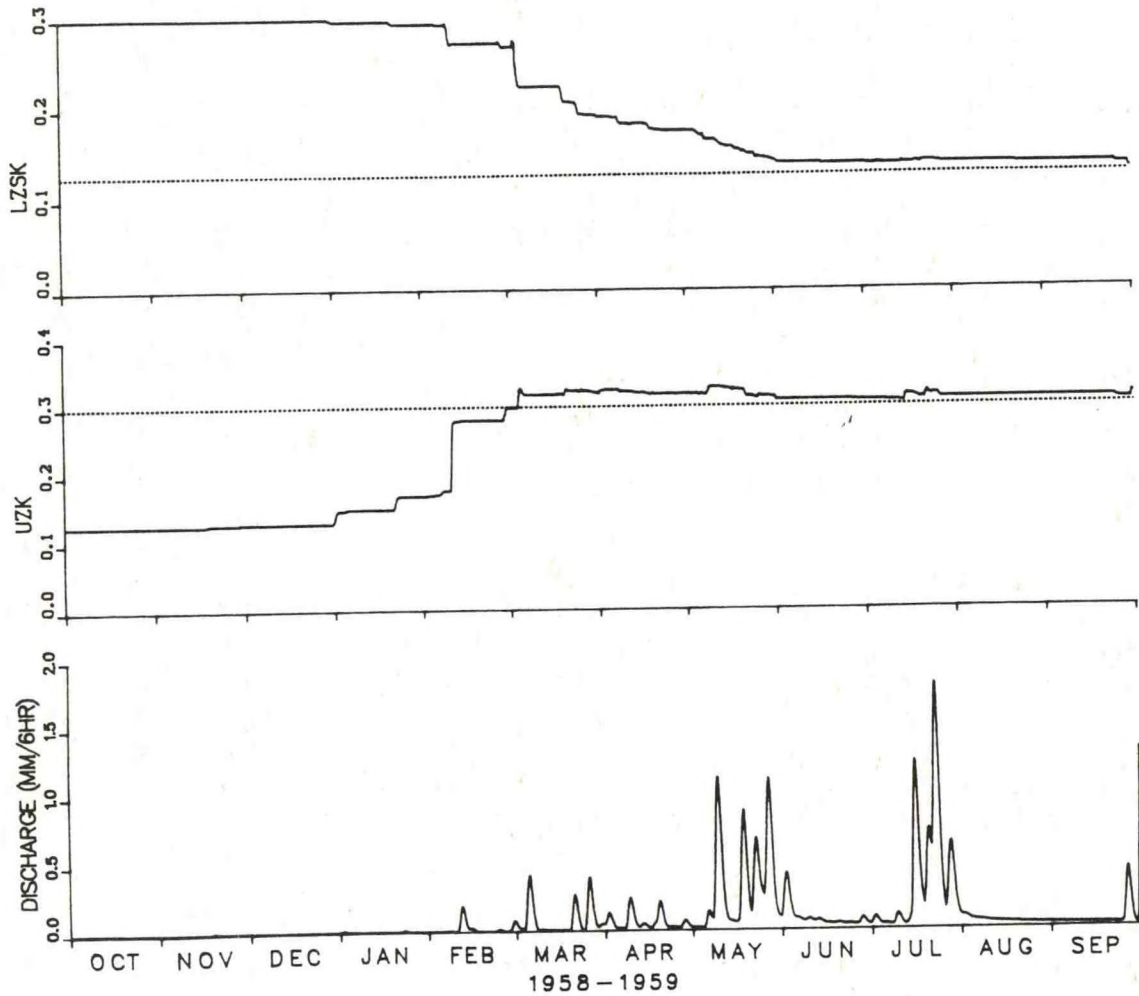


Figure 5.13. LINDRV Results for UZK (Fractional daily upper zone free water withdrawal rate) and LZSK (Fractional daily supplemental withdrawal rate) using 6-hour Synthetic Streamflows.

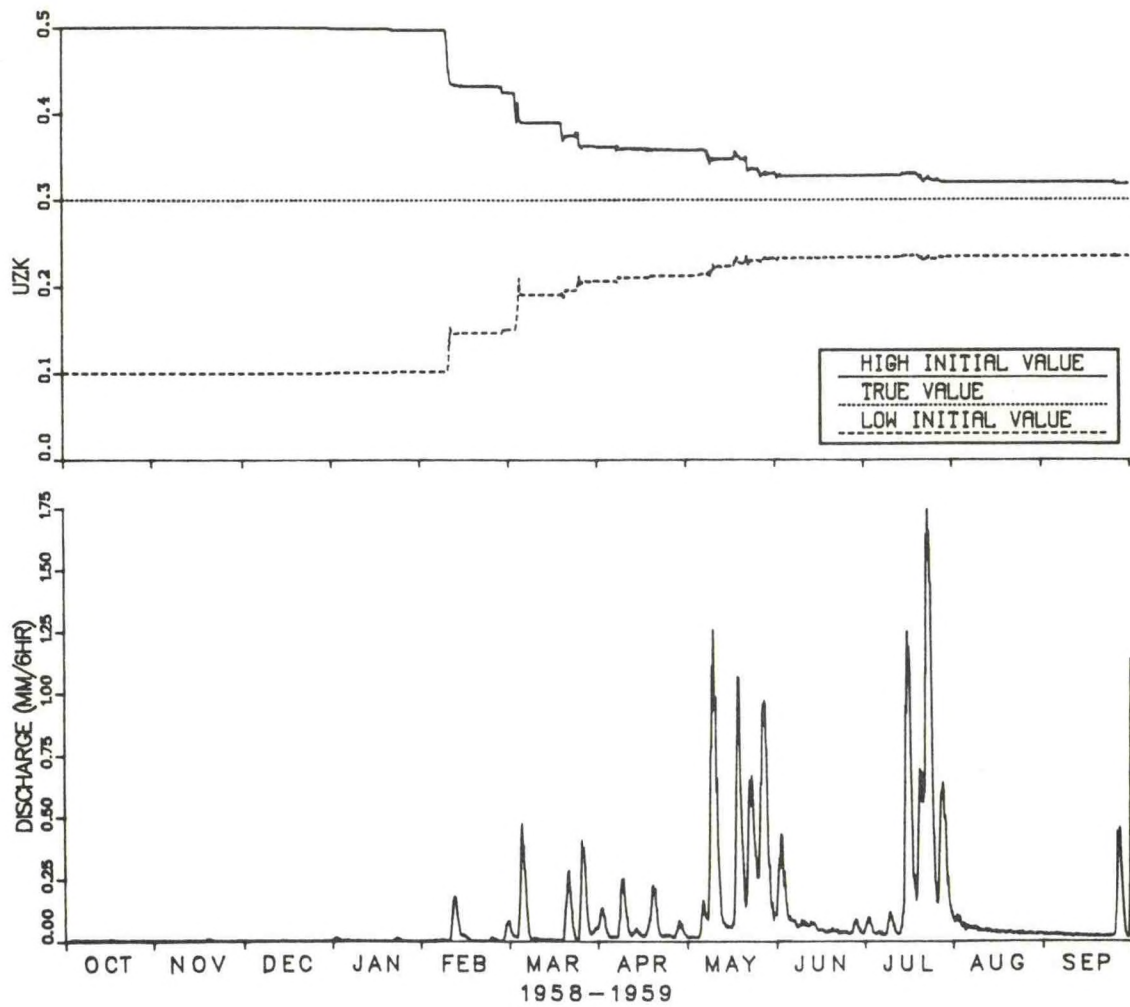


Figure 5.14. LINDRV Results for UZK (Fractional daily upper zone free water withdrawal rate) using 6-hour Synthetic Streamflows ($v_r=0.1$).

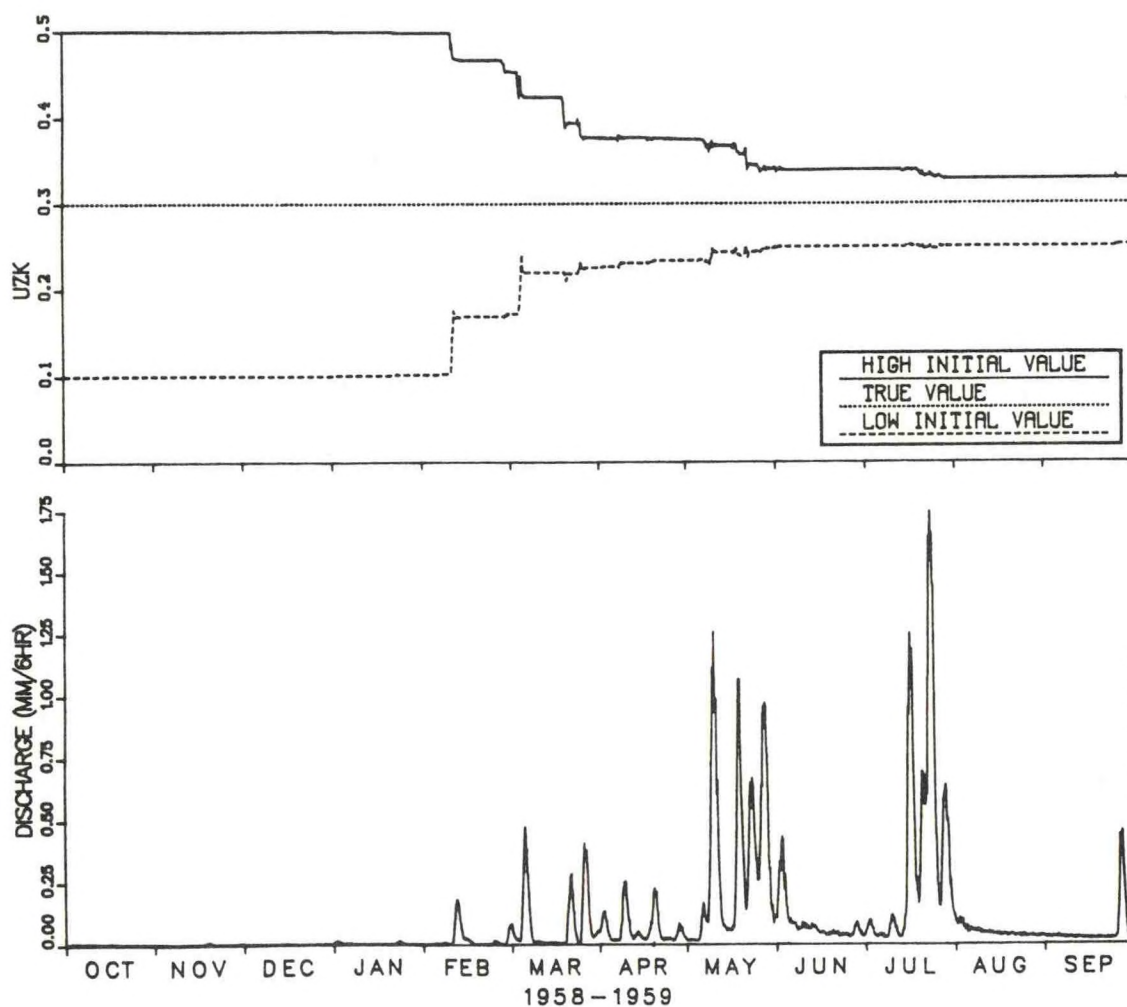


Figure 5.15. LINDRV Results for UZK (Fractional daily upper zone free water withdrawal rate) using 6-hour Synthetic Streamflows ($v_r=0.1, v_u=0.1$).

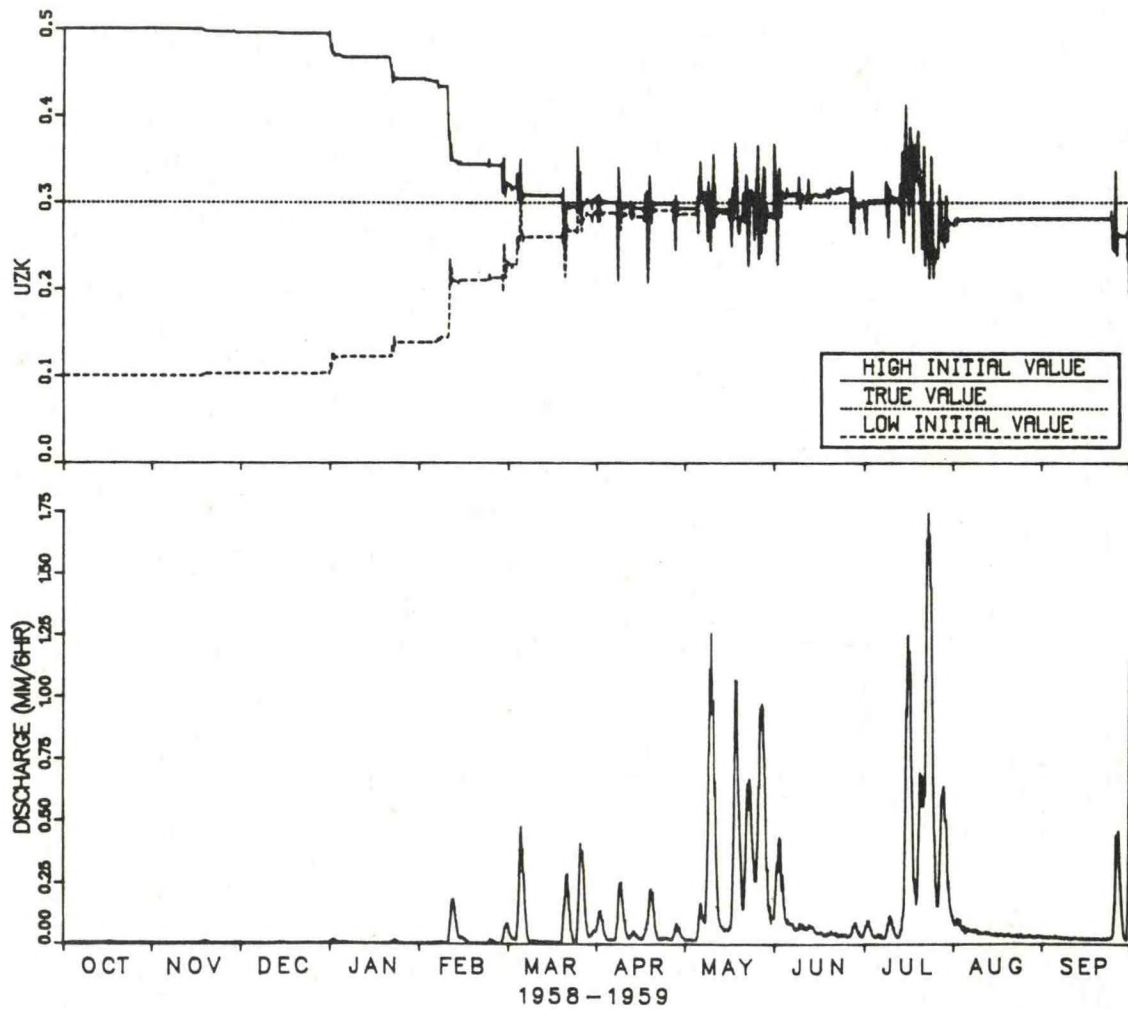


Figure 5.16. LINDRV Results for UZK (Fractional daily upper zone free water withdrawal rate) using 6-hour Synthetic Streamflows ($v_r=0.1$; $Q=0.1$ times initial parameter value).

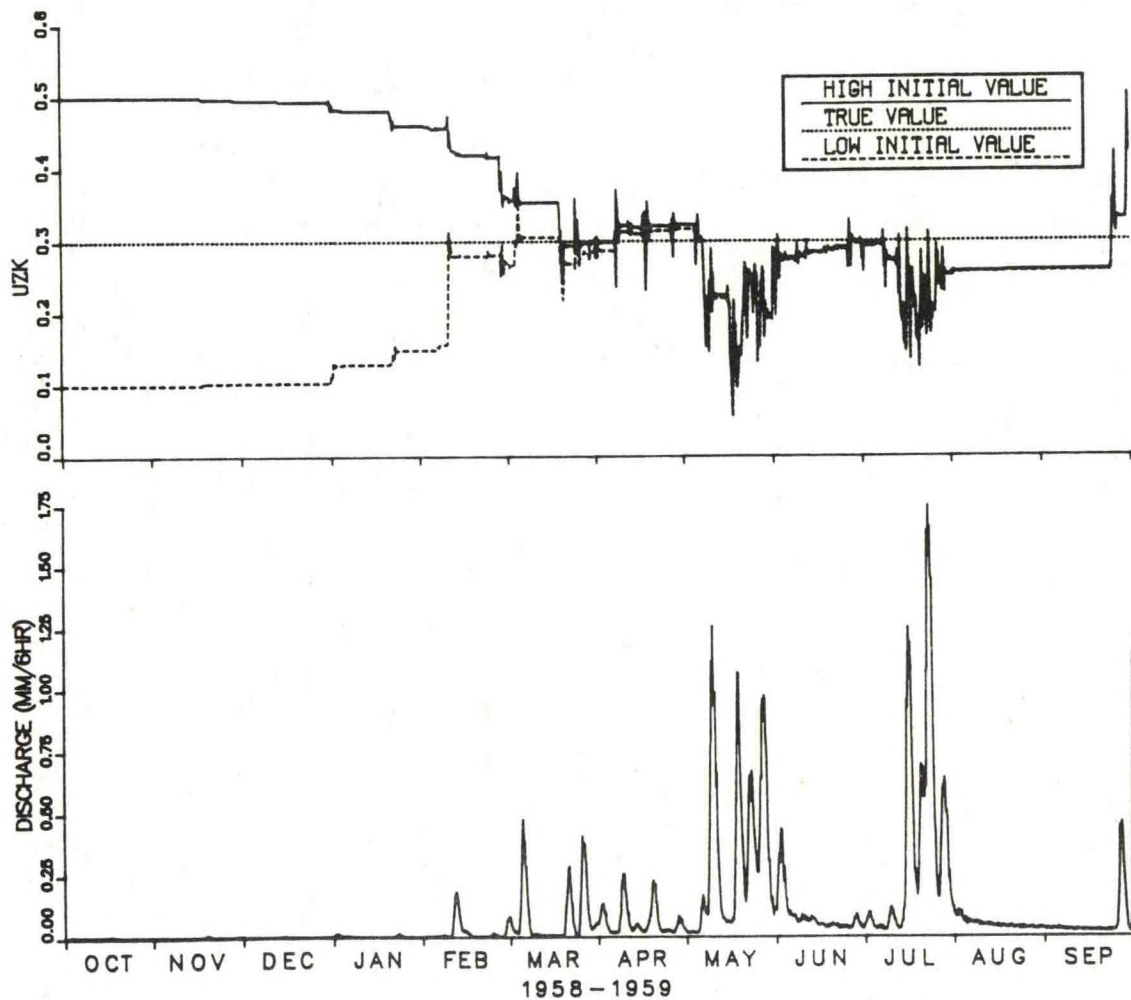


Figure 5.17. LINDRV Results for UZK (Fractional daily upper zone free water withdrawal rate) using 6-hour Synthetic Streamflows ($v_r=0.1, v_u=0.1; Q=0.1$ times initial parameter value).

Summary

Chapter 5 provided the technical details of the development of the various levels in the calibration strategy. The first level consists of an interactive program which uses computer generated graphical displays to guide a user through the process of estimating initial values for some of the model parameters. The Level II work was aimed at developing an effective random search procedure which would overcome many of the problems associated with hill-climbing techniques that are dependent on consistent parameter starting values. Two random search techniques were developed. The first procedure, a uniform random search technique, randomly selects parameter values and generates an output data set of various statistics which can be evaluated with a multi-objective post simulation analysis program. The second random search procedure converges as the simulation statistics improve. Level III work resulted in the development of a recursive parameter estimation procedure using the extended Kalman filter. Each of the calibration tools was tested using synthetic data for a seven year period.

Chapter 6

CASE STUDY

Introduction

A case study was conducted to demonstrate and evaluate the calibration strategy developed in the previous chapter for an actual watershed. The case study provided a mechanism for testing the various parameter estimation tools on real data and fine tuning the details of the strategies and procedures. The study also gave information relating to the sensitivity of the results to alternative ways of applying some of the optimization algorithms.

Selection of a suitable test basin can be key to the success of a case study. In order to adequately evaluate the calibration strategy for the complete set of model parameters, the watershed should produce a variety of flows: floods, periods of baseflow, and occasional small events dominated by impervious or direct runoff. The data for the basin must be reliable and cover a period long enough to represent a heterogeneous mixture of climatic and hydrologic conditions.

Case Study Design

Test Watershed

The Leaf River above Collins, Mississippi was chosen to be the case study watershed. The basin exhibits the characteristics described above and has been used in a variety of previous studies (Brazil and Hudlow, 1981; Sorooshian and Gupta, 1983; and Sorooshian et al., 1983). The watershed is primarily forested and has a drainage area of approximately 1948 square kilometers. The location is shown in Figure 6.1. Average annual runoff is 450 millimeters. Data are readily available for water years 1952-1969 and consist of mean daily discharges, daily potential evaporation estimates, and 6-hour mean areal precipitation totals. The mean areal values were computed in previous studies.

Strategy

The purpose of the case study was to calibrate the SAC-SMA model for the Leaf River using the newly developed procedures and compare the results to a calibration performed previously for the basin. The calibration was performed by an experienced hydrologist using manual and automatic procedures. Although it was not necessarily the best possible calibration, it was considered adequate for conducting tests on the watershed for this and other studies. Data are available for 18 years of record. A five to ten year period generally is considered adequate for calibration. For this study calibration was performed on the first eleven years of data (water years 1952-1962). Several assumptions were made so that the calibration could focus only on the SAC-SMA model. The evapotranspiration adjustment curve was assumed to have been previously optimized, although this typically is estimated in conjunction with the other model parameters. The ordinates for the unit hydrograph also were



Figure 6.1. Leaf River Watershed Location.

assumed to be known prior to the case study. Ongoing work in this research area will provide a mechanism for simultaneously estimating these model inputs along with the SAC-SMA parameters.

The case study was designed to demonstrate the steps a model user would perform to utilize the parameter estimation procedures outlined previously as Levels I, II, and III. Level I constitutes running the INIT program on an interactive computer using a terminal with dynamic graphics capabilities. The results were interpreted and used as input to Level II. The Level II work consists of running the OSRCH program with various options to perform either uniform or adaptive random searches and sensitivity analyses. The results from Level II dictate if additional Level I work is required, more Level II runs should be made or Level III work should be started. Level III consists of fine tuning some parameters by further adjustment or checking for applicability of Kalman filter estimation techniques.

Case Study Results

Level I

The purpose of the Level I work is to identify some of the model parameters and their ranges by analyzing the hydrometeorological record using interactive computer generated graphics. Program INIT, which contains algorithms for estimating some of the parameters normally identified by hand calculations, was developed to guide the user through this process. The program uses interactive graphical displays to allow a user to scan through a hydrometeorological record to identify periods where the effects of individual model components can be isolated. Peck (1976) presented procedures for estimating several of the SAC-SMA parameters using similar hand calculation techniques.

For this case study 24-hour time series were developed for precipitation and discharge. Precipitation values were computed by summing 6-hour observations. The program begins with a comparison of total precipitation, potential evaporation and runoff for the period of interest. Although only a crude first attempt at establishing data quality control, this simple test verifies that the data being used in the analysis have been read correctly by the program. For the Leaf River for the period October 1951 to September 1962, the ratio of precipitation to runoff was 3.0 (14,636 mm vs. 4875 mm). The total potential evaporation was approximately 90 percent of the total precipitation. The precipitation/runoff ratio seems reasonable for the area. The potential evaporation/precipitation value is high, but it is within the acceptable range.

The period of record was scanned for each of the five parameters: LZPK, LZSK, LZFPM, LZFSM and PCTIM. Displays similar to Figure 5.2 were analyzed and events of interest were identified. Table 6.1 shows the events and the corresponding estimates of the parameters. Based on the analysis of the data, it was assumed that the lower zone primary and supplemental components had filled to one-half and two-thirds of their capacity, respectively, during the peaks examined. The table shows that the estimates were reasonably consistent for LZPK, LZSK and PCTIM, with

Table 6.1

Summary of Initial Parameter Estimation Analysis for Leaf River

LZPK = .008

Event beginning date	Event ending date	Estimated parameter value
10/08/51	10/20/51	.006
01/13/52	01/20/52	.012
09/22/53	10/25/53	.006
08/18/54	09/06/54	.008

LZSK = .195

Event beginning date	Event ending date	Primary flow date	Est parameter value
04/18/52	04/22/52	05/17/52	.223
06/04/52	06/14/52	06/22/52	.182
05/24/53	06/06/53	07/07/53	.184
09/06/53	09/11/53	09/23/53	.195
03/03/55	03/15/55	03/18/55	.203
04/23/55	05/03/55	05/19/55	.182
12/26/55	01/01/56	01/13/56	.231
04/19/56	04/30/56	05/12/56	.131
10/08/58	10/22/58	10/29/58	.184
04/11/60	04/25/60	04/26/60	.231

LZFPM = 128.

Event beginning date	Event ending date	Est. contents
05/02/58	06/01/58	47.
02/23/61	06/03/61	64.

LZFPM = $64./5 = 128.$

LZFSM = 52.

Event beginning date	Event ending date	Primary flow date	Est Contents
02/23/61	03/16/61	03/06/61	33.
04/01/61	04/08/61	04/07/61	35.

LZFSM = $35./67 = 52.$

Table 6.1 (Continued)

PCTIM = .006

Event beginning date	Event ending date	Est. parameter
08/31/52	09/04/52	.003
09/10/52	09/25/52	.008
08/18/54	08/26/54	.000
09/14/54	09/24/54	.007
11/03/54	11/09/54	.006
09/21/55	09/26/55	.005
10/22/55	11/01/55	.002
10/25/56	10/30/56	.005
11/06/56	11/13/56	.008
10/01/61	10/06/61	.012

the maximum scatter occurring for PCTIM. This was interpreted as a sign that considerable confidence could be placed in the three parameters, and that they could be assigned fairly tight ranges in the Level II analyses. Estimates for LZFP and LZFSM were based on fewer events, but appear to be reasonable values. Examination of the data and computation of the parameters took approximately one hour using program INIT. The primary advantage of the program is the capability it gives the user to rapidly estimate parameters for numerous events and decide whether or not to include them in the final analyses.

Level II

The Level II analysis was performed by running the random search procedures outlined in Chapter 5 for the Leaf River. Input to the program consisted of the ranges for the parameters being optimized, program options, and observed data. The input data were 6-hour mean areal estimates of precipitation computed from point observations and 24-hour estimates of potential evaporation. Streamflows consisted of observed mean daily discharges. As in the Level I analyses, the unit hydrograph ordinates and potential evaporation demand curve were assumed to have been optimized previously.

Program OSRCH can simulate discharges with either the original SAC-SMA model and traditional unit hydrograph operation or the state-space soil moisture accounting and unit hydrograph models. Because previous calibrations had been made with the original model and comparisons would be easier, and because no current version of the state-space models are available for use in forecasting, the original model was used for this analysis. A few runs actually were made with both models to be sure there were no major differences. The only notable difference is that the original model uses approximately 35 percent less CPU time. This can be a considerable advantage in long random search runs.

Program OSRCH can be used to run either the ARS or URS algorithms. Runs with both options were made for this case study. Two runs were made using the ARS algorithm. Different random number seeds were used to minimize bias due to the choice of seed. Daily RMS error was used as the objective function. The period run was water years 1956 to 1962. The inputs and results are shown in Table 6.2. Also shown in the table are statistical results from the calibration done for previous studies. The values in Table 6.2 represent the results from implementation of the Level I and II strategies. The statistical output indicate that Runs #1 and #2 gave slightly better results than the previous calibration studies for the Leaf basin. In general, the runs produced reasonable parameters with statistics comparable to those produced after numerous trial-and-error runs.

One run also was made to show the advantage of having the Level I analysis as input to the OSRCH runs. Results are given in Table 6.3. The only difference in the inputs between Runs #1 - #2 and Run #3 are the initial values and ranges used for the five parameters estimated in using INIT. The initial values for the five INIT parameters were the midpoints of their ranges. The results show that the run without the INIT input converged at an inferior point on the response surface.

Table 6.2

Results from ARS Case Study Runs #1 and #2

Parameter	Base Run	ARS Run #1	ARS Run #2	ARS Starting Value	Lower Bound	Upper Bound
UZWIM	20.	10.	10.	25.	10.	150.
UZFWM	25.	36.9	37.9	30.	10.	75.
LZWIM	200.	222.	231.	175.	75.	400.
LZFPM	140.	129.	131.	128.	120.	140.
LZFSM	45.	51.	44.	52.	40.	60.
UZK	.35	.329	.307	.3	.2	.4
LZPK	.004	.0068	.0082	.008	.006	.01
LZSK	.15	.171	.193	.195	.15	.20
ZPERC	200.	141.	135.	175.	5.	250.
REXP	3.3	3.99	3.93	3.	1.1	4.
PFREE	.10	.055	.029	.1	0.	.6
SIDE	0.	0.	0.	0.	0.	0.
ADIMP	.15	.20	.20	.1	0.	.2
PCTIM	.025	.003	.016	.006	0.	.02

Obj. Function (Computed from mean daily flows in mm.)

RMS	.8539	.7922	.7927
BIAS	.0123	-.0019	.0063
ABSMAX	11.8264	10.8484	10.8373
ABSERR	.3710	.3492	.3571
RVAR	.7292	.6278	.6285
PDIFF	8.5182	10.8484	10.8373
BASEFL	2.5632	.7056	1.0347
TMVOL	213.7851	164.9763	165.8239
R'	.9633	.9692	.9632
NSC	298	336	341

Table 6.3

Results from ARS Case Study Run #3

<u>Parameter</u>	<u>ARS Run #3</u>	<u>Starting Value</u>	<u>Lower Bound</u>	<u>Upper Bound</u>
UZW	56.	25.	10.	150.
UZF	46.	30.	10.	75.
LZW	131.	175.	75.	400.
LZFP	162.	525.	50.	1000.
LZFS	23.	155.	10.	300.
UZK	.245	.3	.2	.4
LZPK	.0086	.011	.001	.02
LZSK	.0429	.135	.02	.25
ZPERC	226.	175.	5.	250.
REXP	3.65	3.	1.1	4.
PFREE	.063	.1	0.	.6
SIDE	0.	0.	0.	0.
ADIMP	.173	.1	0.	.2
PCTIM	.043	.05	0.	.1

Obj. Function (Computed from mean daily flows in mm.)

RMS	.8393
BIAS	.0658
ABSMAX	10.5917
ABSERR	.4016
PVAR	.6961
PDIFF	9.1315
BASEFL	4.7085
TMVOL	242.8958
R'	.9654
NSC	298

One run was made using the URS algorithm. Ten thousand iterations were run, each with the original SAC-SMA and unit hydrograph models. The ten objective functions discussed in Chapter 5 were computed at each iteration. The period of record was the same seven years as that used for the ARS runs. Parameter ranges also were the same as in ARS Runs #1 and #2. Program OSRCH generated an output file consisting of 10,000 parameter combinations and their associated evaluation criteria. The data set was analyzed using program NINF to determine the noninferior set of objective functions. Output from NINF consisted of 192 parameter combinations/evaluation criteria. The number of noninferior points is consistent with the 2-3 percent range of noninferior points found during the development of the programs using synthetic data. Program CMPTPI was run interactively to analyze the noninferior points and select the optimum parameter set. Twelve different weighting combinations were used. The combinations included one analysis where each objective function was given a weight of 0.1, ten analyses where each objective function in turn was given a weight of 1., and one analysis where RMS error and correlation coefficient were each given weights of 0.5. The results are shown in Table 6.4. The clear winner from the analysis is iteration number 7853. Six of the twelve weighting schemes selected number 7853 as the optimum. Because the problem truly is multi-objective, though, six other iterations also were selected as optimal for six of the weighting schemes.

A comparison between Tables 6.2 and 6.4 show that considering the ranges of possible values for the parameters, the parameter sets representing Run #1 in Table 6.2 and Trial #7853 are quite similar. A number of observations can be made about Table 6.4. For instance, the trial selected as producing the best simulation for the designated baseflow period (#3955) had the UZTWM which deviated most from the ARS results. UZTWM typically has an insignificant effect on baseflow. Trial #7457 was considered optimal using PDIFF as the objective function. ZPERC has little effect on the simulated peak flow, and therefore has a value for the #7457 parameter set which differs most from the other ZPERC values. In other words, ZPERC probably was not identifiable using PDIFF. It is interesting to note that the parameter set which produced the best peak event scored the worst on six of the other nine evaluation criteria.

Sensitivity Runs - Program OSRCH also was used to make three sets of sensitivity runs for the Leaf River. The runs were designed to show the effect that each level of the calibration procedure had on the smoothing of the response surface. Figures 6.2a, b and c represent the objective functions over the full range of parameter values where all other parameters were given the values of the midpoints of their full range of values. In this case, the parameter bounds were the same as those shown in Table 6.3. Figures 6.3a, b and c show the same objective functions, however, the five parameters analyzed using INIT were assigned their estimated values rather than their range midpoints. Figures 6.4a, b and c represent the surface about the parameters when assigned the values resulting from the best ARS run (Run #1 in Table 6.2). The figures show that the response surface becomes better defined

Table 6.4

Results from URS Case Study Runs

Parameter	Trials							Lower Bound	Upper Bound
	7853	1165	2944	3955	7457	6076	1761		
UZWMM	15.	110.	47.	141.	14.	15.	57.	10.	150.
UZFWM	30.	16.	16.	55.	26.	41.	12.	10.	75.
LZTWM	245.	110.	121.	310.	152.	243.	133.	75.	400.
LZFPM	128.	137.	121.	122.	125.	136.	136.	120.	140.
LZFSM	53.	60.	41.	41.	45.	44.	42.	40.	60.
UZK	.278	.301	.373	.274	.275	.376	.318	.2	.4
LZPK	.0077	.0065	.0085	.0098	.0064	.0081	.0082	.006	.01
LZSK	.154	.162	.199	.166	.157	.162	.151	.15	.20
ZPERC	154.	62.	69.	118	12.	175.	37.	5.	250.
REXP	3.77	1.95	3.27	3.70	3.81	3.87	2.82	1.1	4.
PFREE	.035	.396	.078	.138	.207	.296	.241	0.	.6
SIDE	0	0	0	0	0	0	0	0	0
ADIMP	.188	.185	.036	.140	.172	.152	.154	0	.2
PCTIM	.019	.015	.011	.011	.004	.005	.001	0	.02

Obj. Functions (Computed from mean daily flows in mm)

Parameter	7853	1165	2944	3955	7457	6076	1761
RMS	.8247*	1.0441	.9230	1.1217	1.3646	.8631	1.0156
BIAS	-.0243	.0000*	.0366	-.1887	.1466	.0163	.0042
ABSMAX	11.3275	15.0874	8.5171*	18.1547	18.8882	14.4096	9.6173
ABSERR	.3605*	.4653	.4389	.4683	.5240	.3928	.4327
RVAR	.6792*	1.0906	.8496	1.1877	1.8199	.7448	1.0319
PDIFF	10.0706	15.0874	8.5171	18.1547	7.066*	14.4096	8.7679
BASEFL	.6160	8.3515	5.8250	.2420*	2.3439	7.6490	4.0890
TMVOL	191.21*	303.58	275.22	623.71	831.01	271.93	302.65
R'	.9670	.9508	.9571	.9494	.9191	.9671*	.9483
NSC	329	302	286	229	266	276	342*

.1 EACH *

.5 RMS, .5 R' *

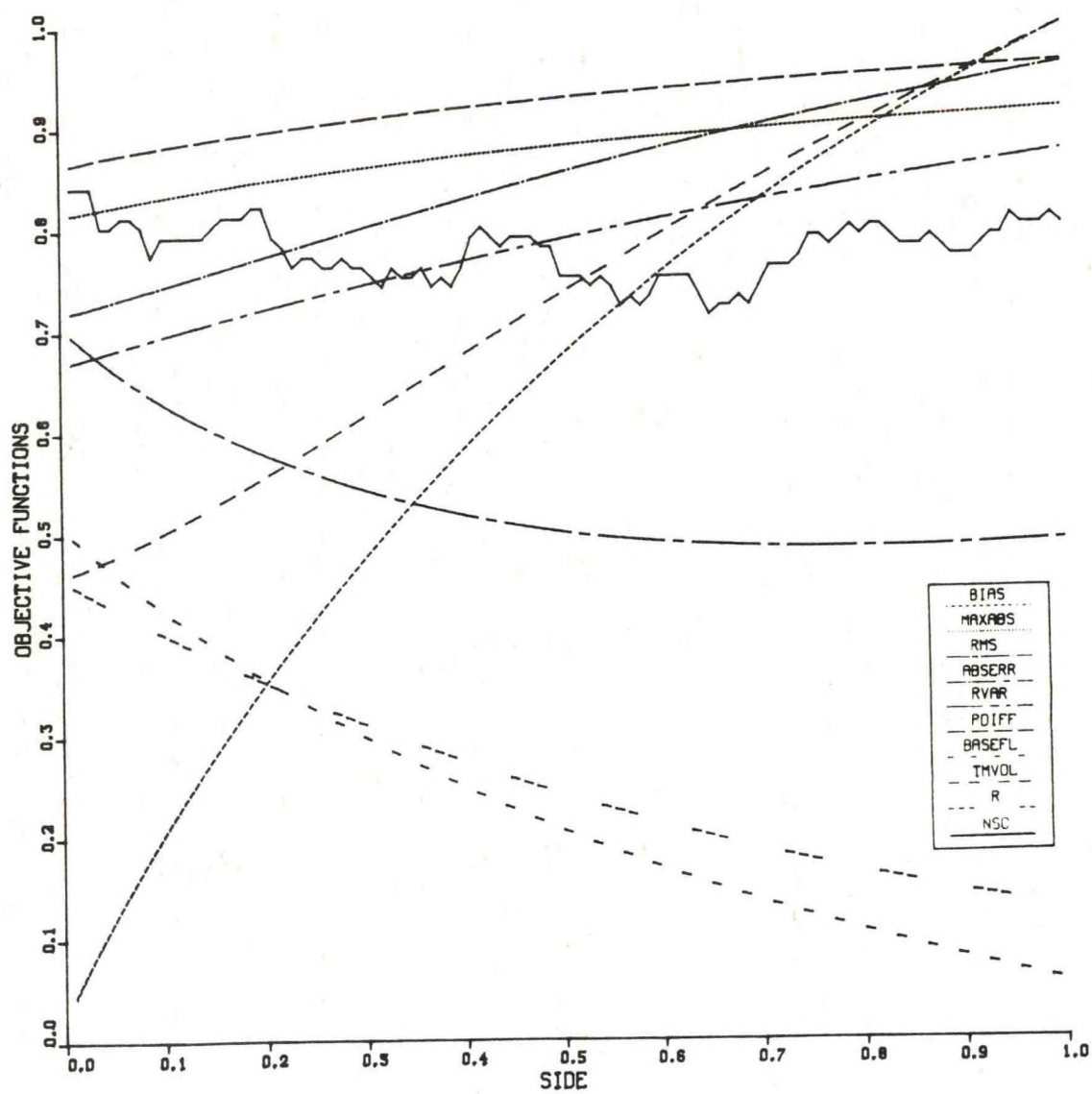


Figure 6.2a. Leaf River Sensitivity Analysis Results for SIDE (Ratio of deep recharge to channel baseflow) prior to Level I analyses. (Objective function definitions shown in Table 5.2.)

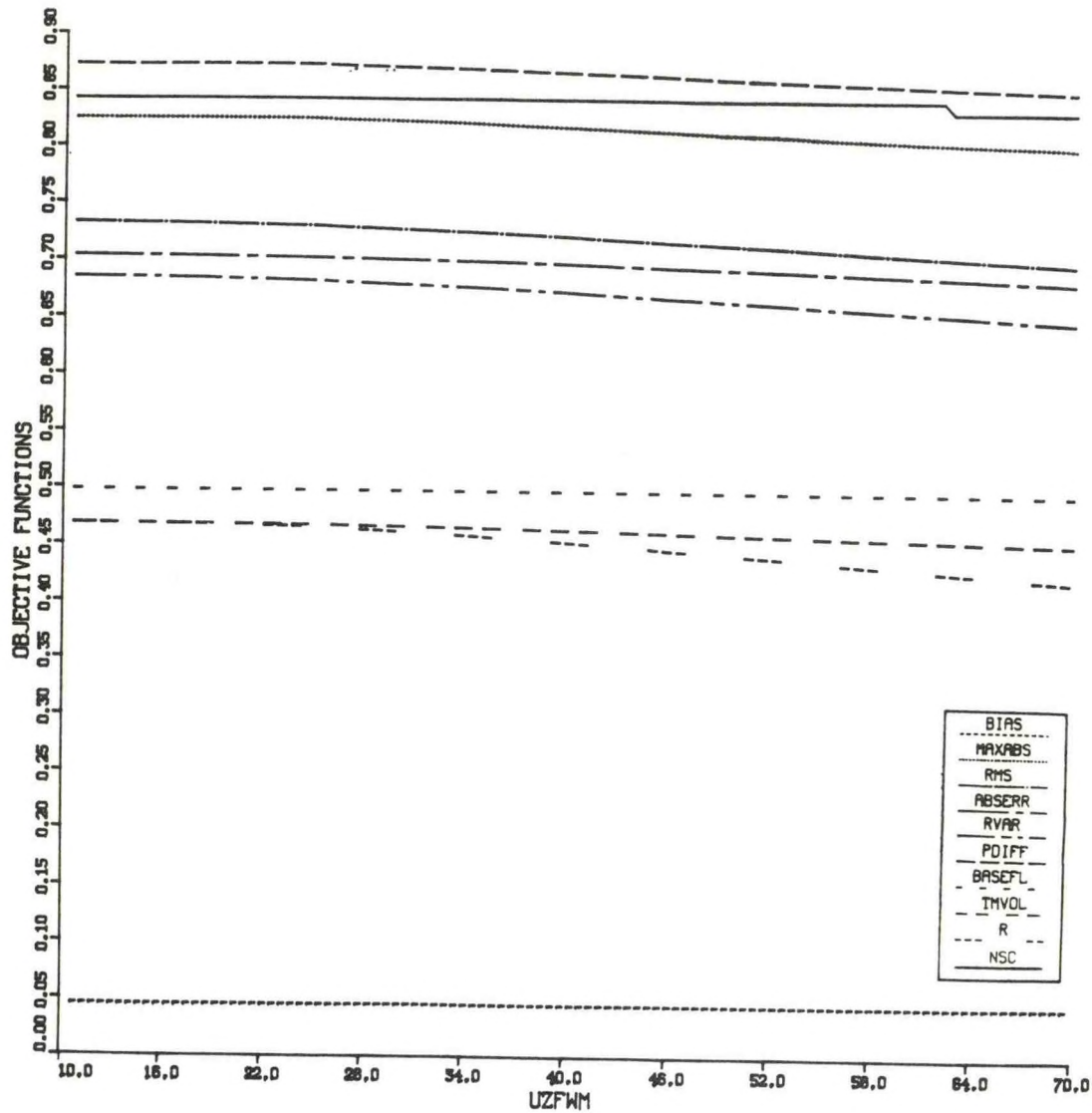


Figure 6.2b. Leaf River Sensitivity Analysis Results for UZFWM (Upper zone free water capacity) prior to Level I analyses. (Objective function definitions shown in Table 5.2).

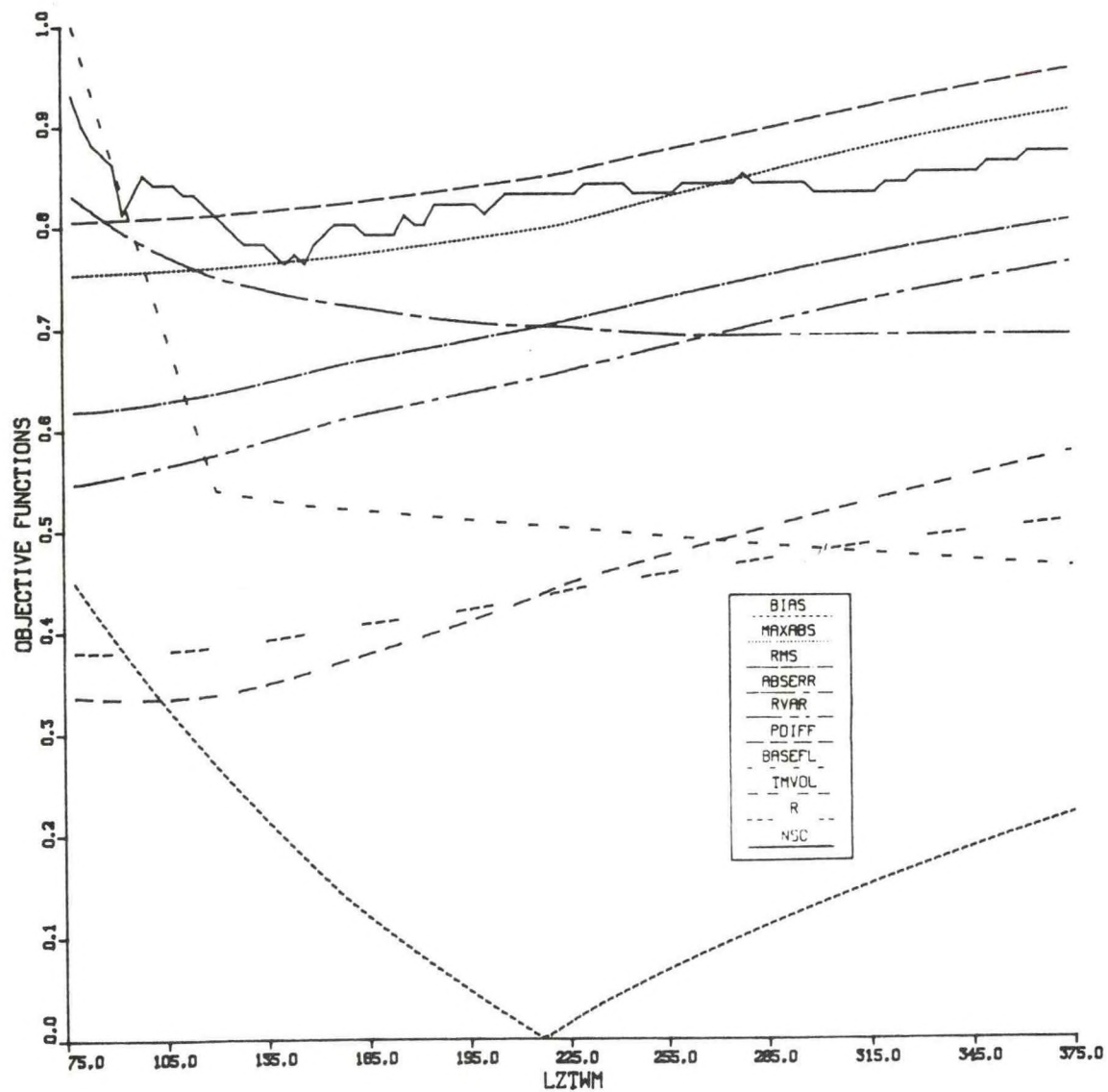


Figure 6.2c. Leaf River Sensitivity Analysis Results for LZTWM (Lower zone tension water capacity) prior to Level I analyses. (Objective function definitions shown in Table 5.2).

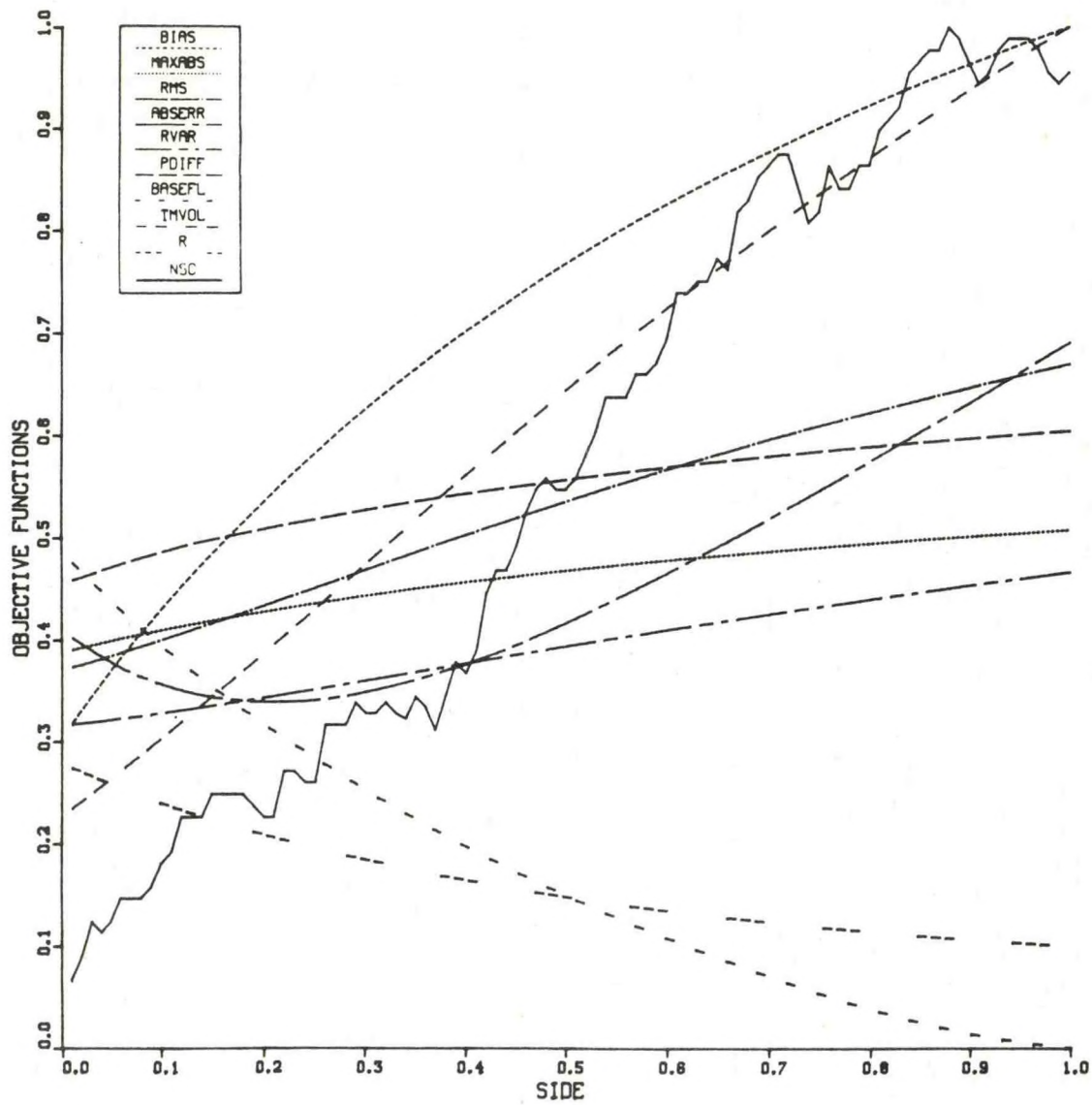


Figure 6.3a. Leaf River Sensitivity Analysis Results for SIDE (Ratio of deep recharge to channel baseflow) following Level I analyses. (Objective function definitions shown in Table 5.2.)

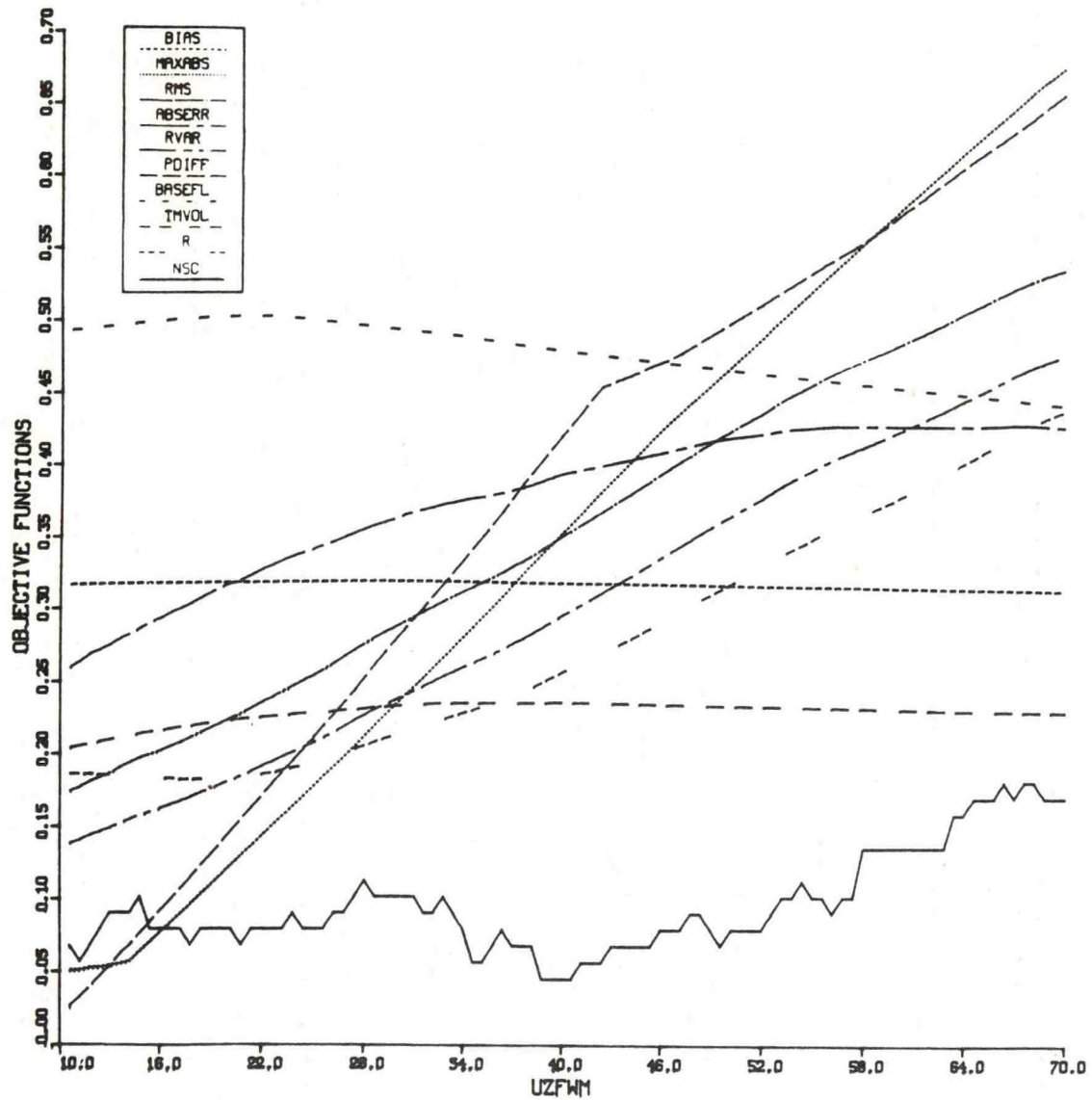


Figure 6.3b. Leaf River Sensitivity Analysis Results for UZFWM (Upper zone free water capacity) following Level I analyses. (Objective function definitions shown in Table 5.2.)

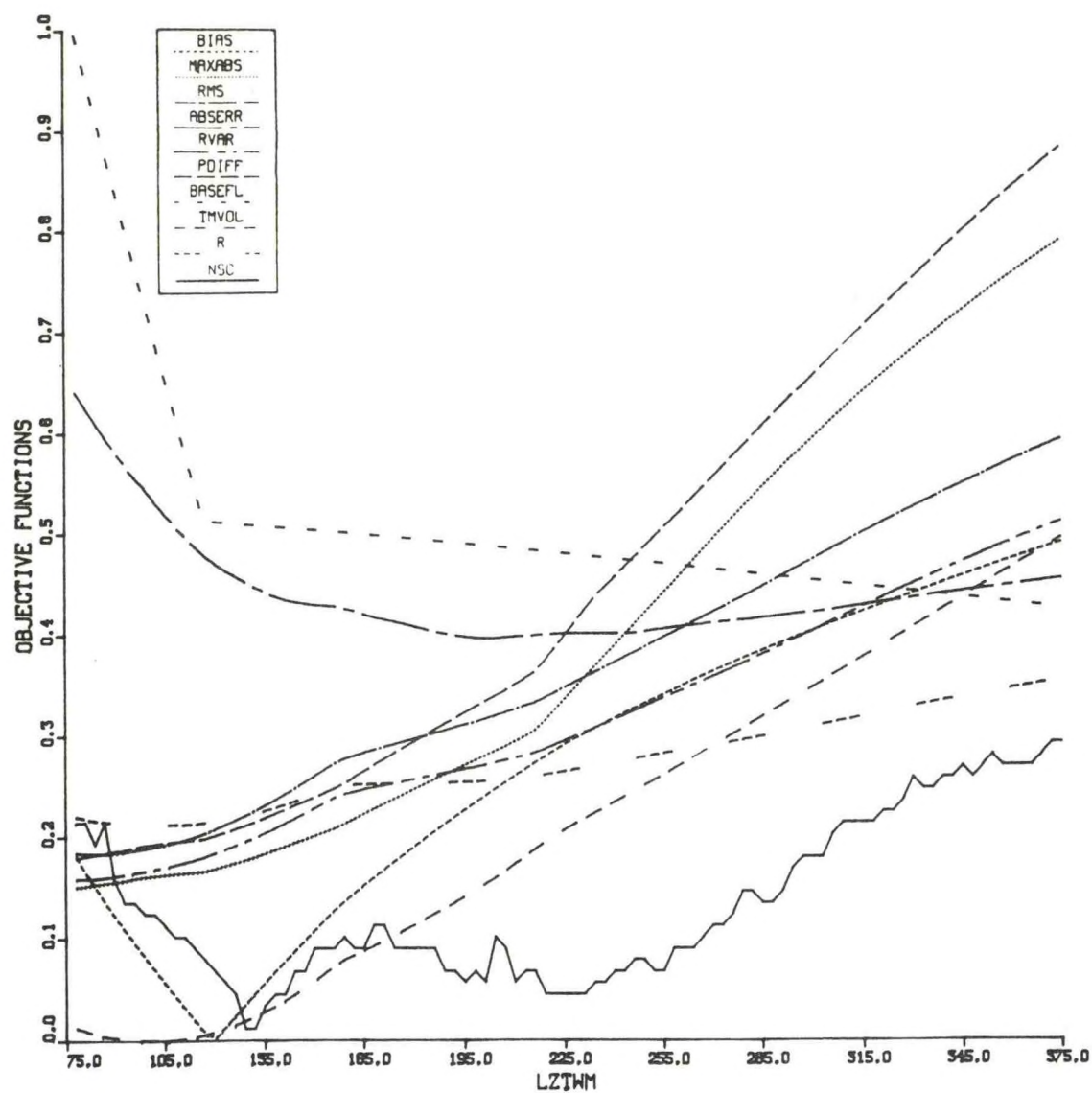


Figure 6.3c. Leaf River Sensitivity Analysis Results for LZTWM (Lower zone tension water capacity) following Level I analyses. (Objective function definitions shown in Table 5.2.)

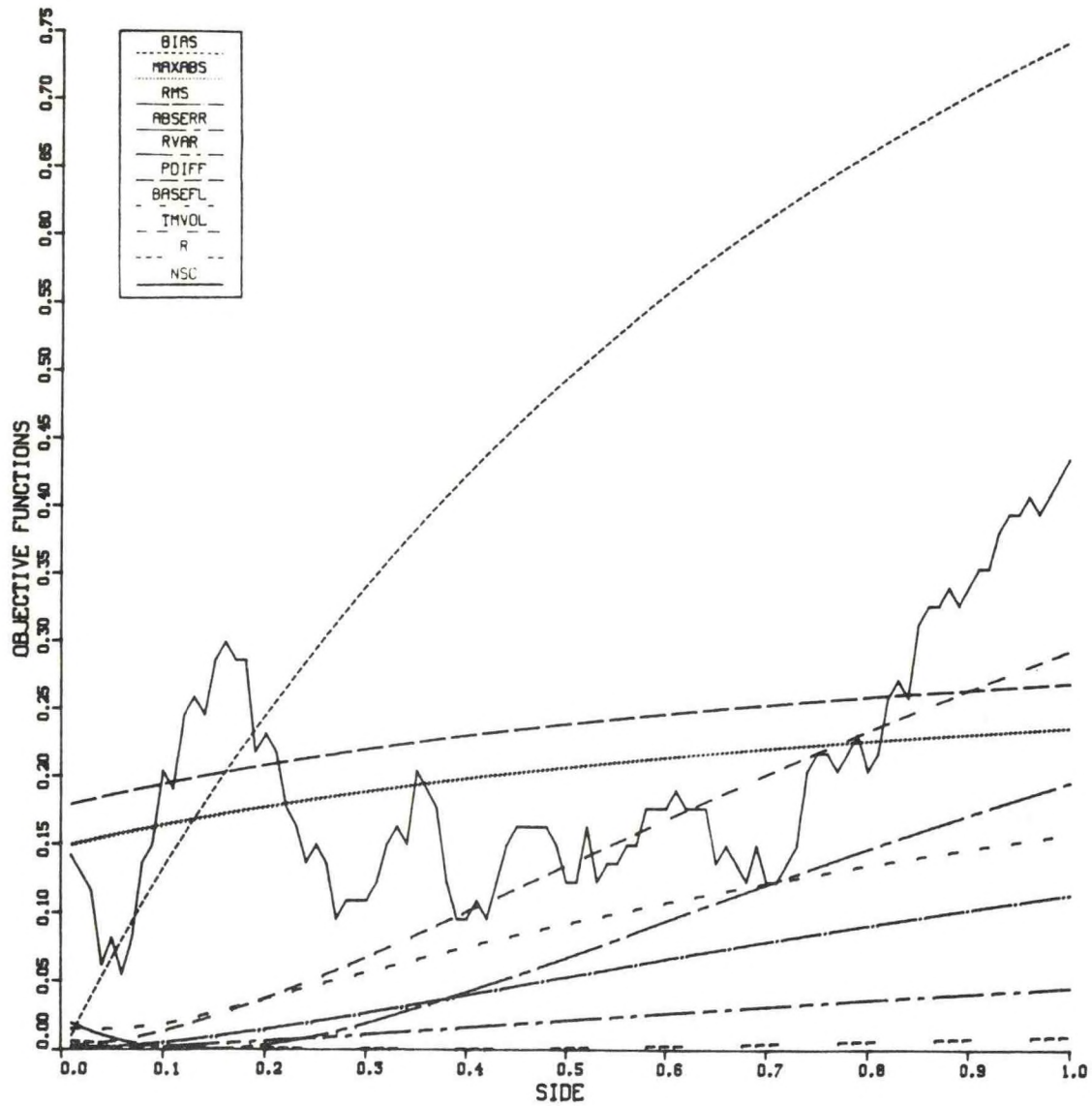


Figure 6.4a. Leaf River Sensitivity Analysis Results for SIDE (Ratio of deep recharge to channel baseflow) following Level II analyses. (Objective function definitions shown in Table 5.2.)

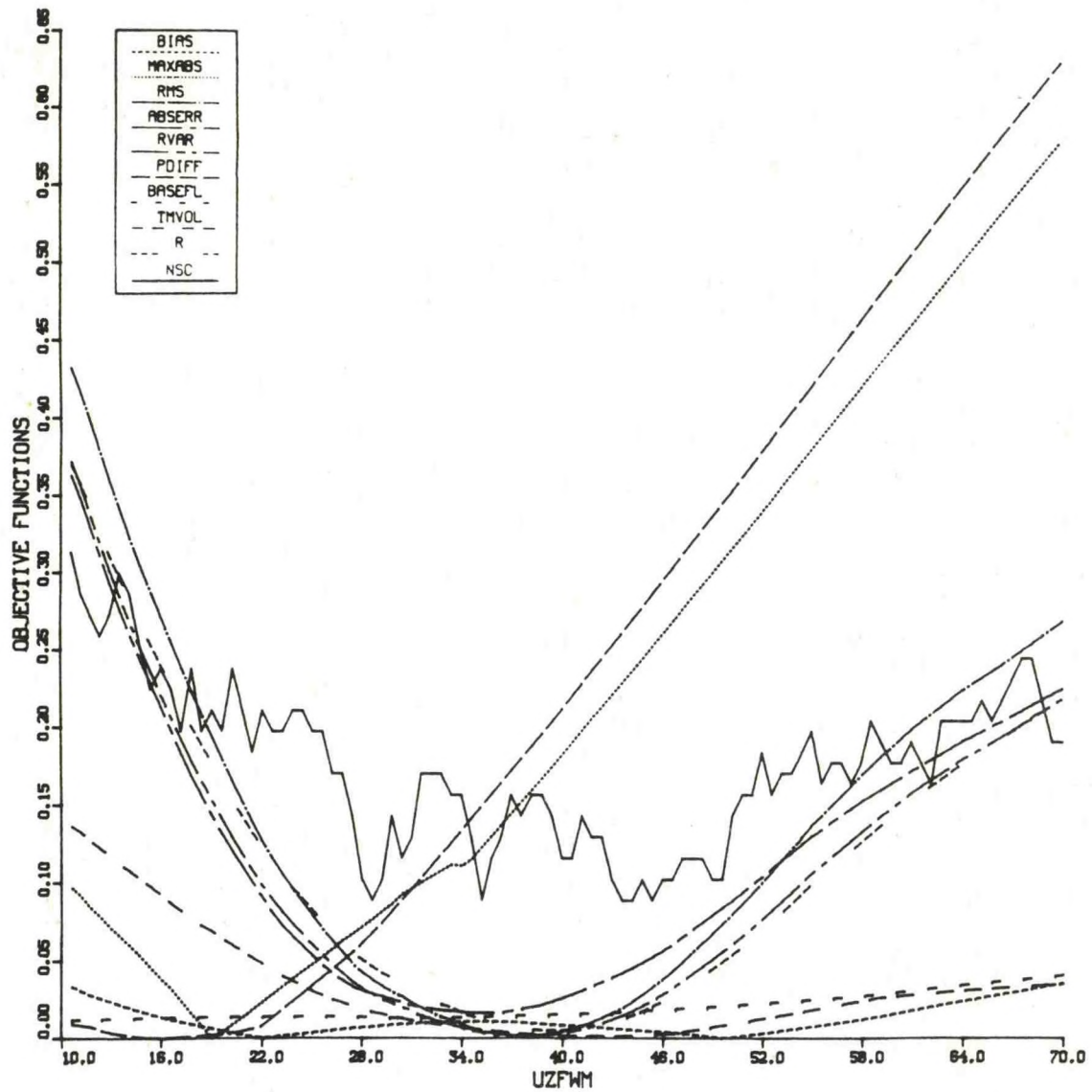


Figure 6.4b. Leaf River Sensitivity Analysis Results for UZFWM (Upper zone free water capacity) following Level II analyses. (Objective function definitions shown in Table 5.2.)

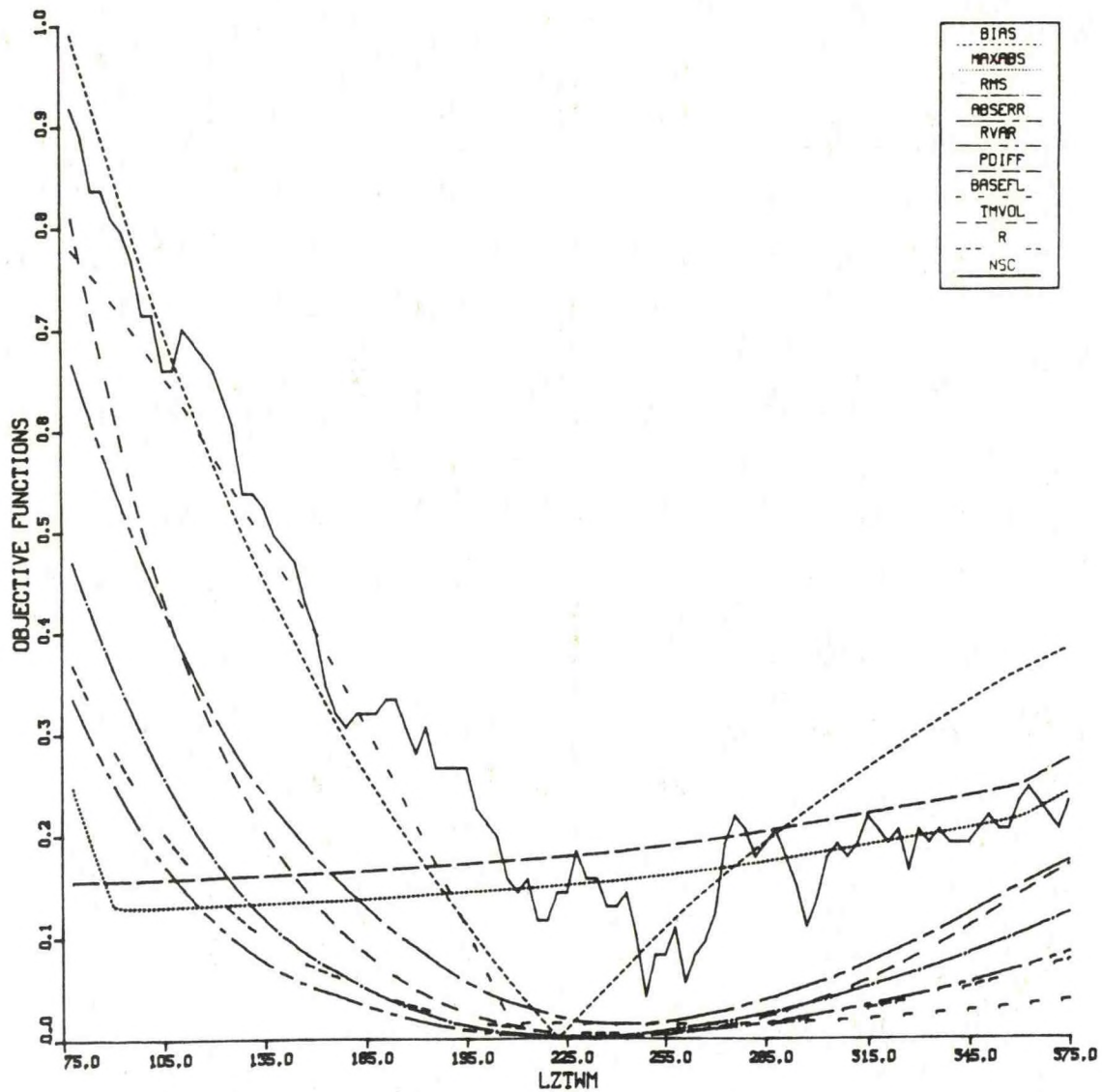


Figure 6.4c. Leaf River Sensitivity Analysis Results for LZTWM (Lower zone tension water capacity) following Level II analyses. (Objective function definitions shown in Table 5.2.)

at each level. That is, the individual parameters become more identifiable from the objective function curves as the entire parameter set moves closer to the optimum.

Level III

The purpose of the Level III analyses is to fine tune the parameters resulting from the Level II work. This is done by examining the response surface of the objective functions in the immediate vicinity of the parameter values. The Level II results provide information concerning sensitivity analyses which can be helpful. Two programs were described in Chapter 5 which can be used for fine tuning: OPT3 and LINDRV. Each program has advantages and disadvantages. OPT3 uses the Pattern Search procedure which has been shown to be an efficient optimization algorithm when the starting parameter values are close to the true optimum. LINDRV is a new procedure developed for this study which uses the Kalman filter for recursive parameter estimation and therefore can account for errors in the inputs or streamflow observations. The filter also can provide information regarding the confidence in states and parameters. Several runs were made using both programs for this case study.

A number of OPT3 runs were made in an attempt to improve upon the results from the Level II analyses. Table 6.5 shows results from the run where all thirteen parameters were optimized. The run was for the same seven years as the Level II runs, water years 1956 - 1962, and used the results from the best ARS run as its starting point. The range of acceptable values as well as the starting and ending parameter values are shown in the table. The statistics for RMS error and R' show that the fit was improved slightly. One run also was made where all parameters were optimized for only water year 1956 so that comparisons could be made with the LINDRV results.

An analysis of the results in Table 6.4 show that most of the significant parameters were adjusted very little. In some cases compensating adjustments were made. For instance, consider the percolation function. Most of the parameters which determine percolation (LZPK, LZSK, LZFP, LZFSM, ZPERC and REXP) were adjusted, some significantly from the base parameters. Considering the range of feasible values the percolation curve can assume, the net effect on the percolation curve was insignificant. Figure 6.5 shows the percolation curves for the base, ARS, and ARS+OPT parameter sets.

As the statistics indicate (Tables 6.2 and 6.4) the simulations for the base, ARS, and ARS+OPT runs were quite similar for the calibration period. Verification runs were made for two periods. One period consisted of the calibration period (water years 1956-1962) plus water years 1963-1969. The other period consisted of only the extension (water years 1963-1969). Results are shown in Table 6.6. Once again, the statistics were very close for all three runs. Plots of the three simulation time series coincide for most events. Figures 6.6a and b show a baseflow period where the different streamflows could be differentiated. Figures 6.7a and b show the same period where flow differences are exaggerated because of the logarithmic discharge

Table 6.5

Results from Level III Opt Case Study Runs

<u>Parameter</u>	<u>Starting Value (ARS Run #1)</u>	<u>7Yr OPT Run</u>	<u>1Yr OPT Run</u>	<u>Lower Bound</u>	<u>Upper Bound</u>
UZTWM	10.	9.	10.	9.	150.
UZFWM	36.9	39.8	23.	10.	75.
LZTWM	222.	240.	140.	75.	400.
LZFPM	129.	120.	120.	120.	140.
LZFMS	51.	40.	40.	40.	60.
UZK	.329	.200	.253	.2	.4
LZPK	.0068	.006	.006	.006	.01
LZSK	.171	.15	.15	.15	.20
ZPERC	141.	250.	105.	5.	250.
REXP	3.99	4.27	4.5	1.1	4.5
PFREE	.055	.027	.012	0.	.6
SIDE	0.	0.	0.	0.	0.
ADIMP	.20	.25	.081	0.	.25
PCTIM	.003	.003	.001	0.	.02

Obj. Functions

RMS (CMSD)	18.04	17.26	10.42
R'	.9686	.9708	.9887

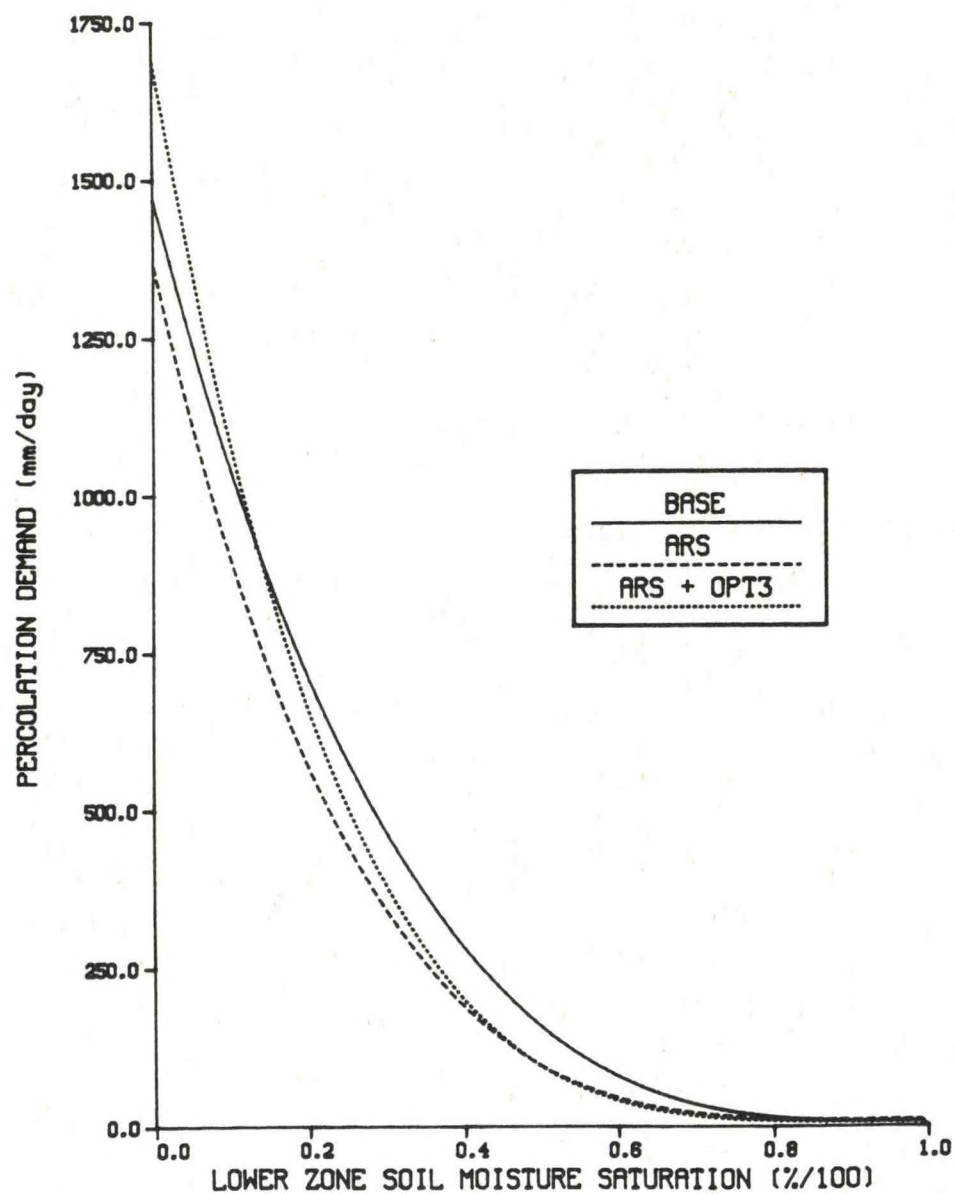


Figure 6.5. Percolation Functions for 3 Sets of Parameter Values.

Table 6.6

Verification Runs Using BASE, ARS, and ARS + OPT Parameters

<u>Obj. Function</u>	<u>Period of Record</u>	<u>BASE Parameters</u>	<u>ARS Parameters</u>	<u>ARS & OPT Parameters</u>
RMS (CMSD)	10/1955 -	16.687	16.274	15.762
R'	9/1969	.9626	.9640	.9664
RMS (CMSD)	10/1962	14.063	14.300	14.100
R'	9/1969	.9615	.9585	.9611

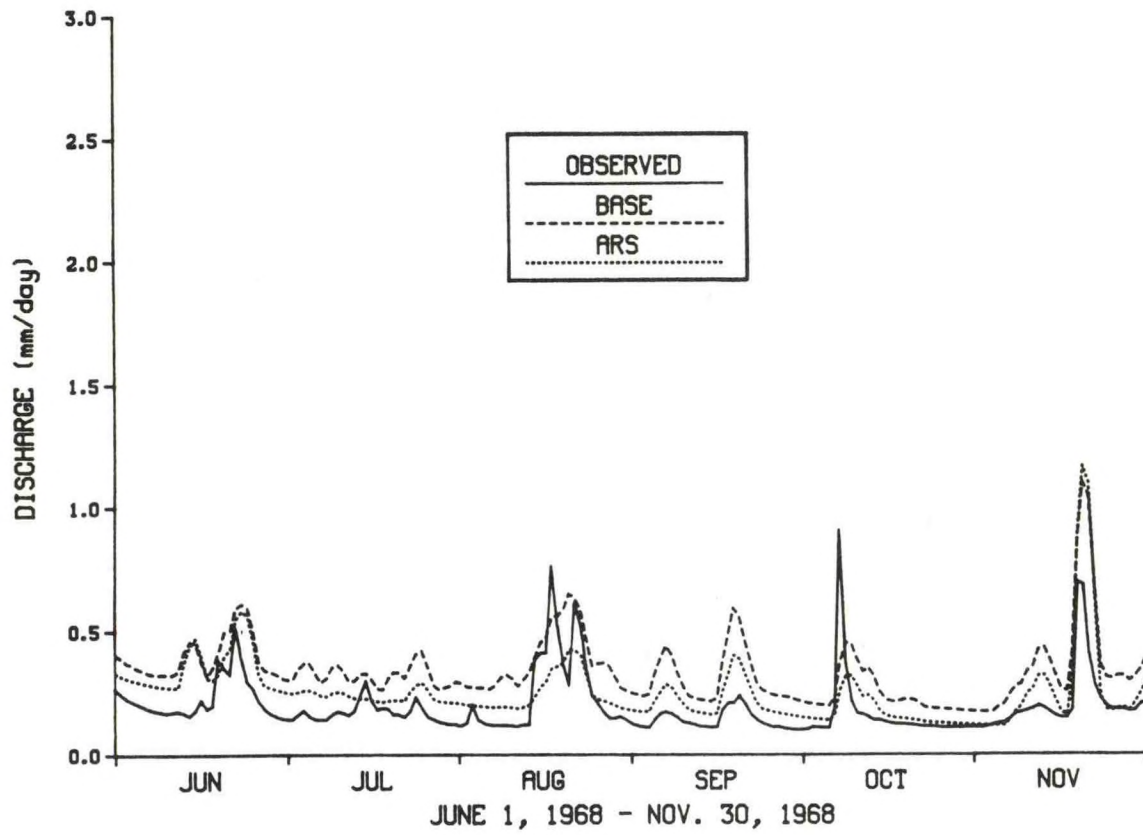


Figure 6.6a. Baseflow Hydrograph for Comparison of Base and ARS Parameter Sets.

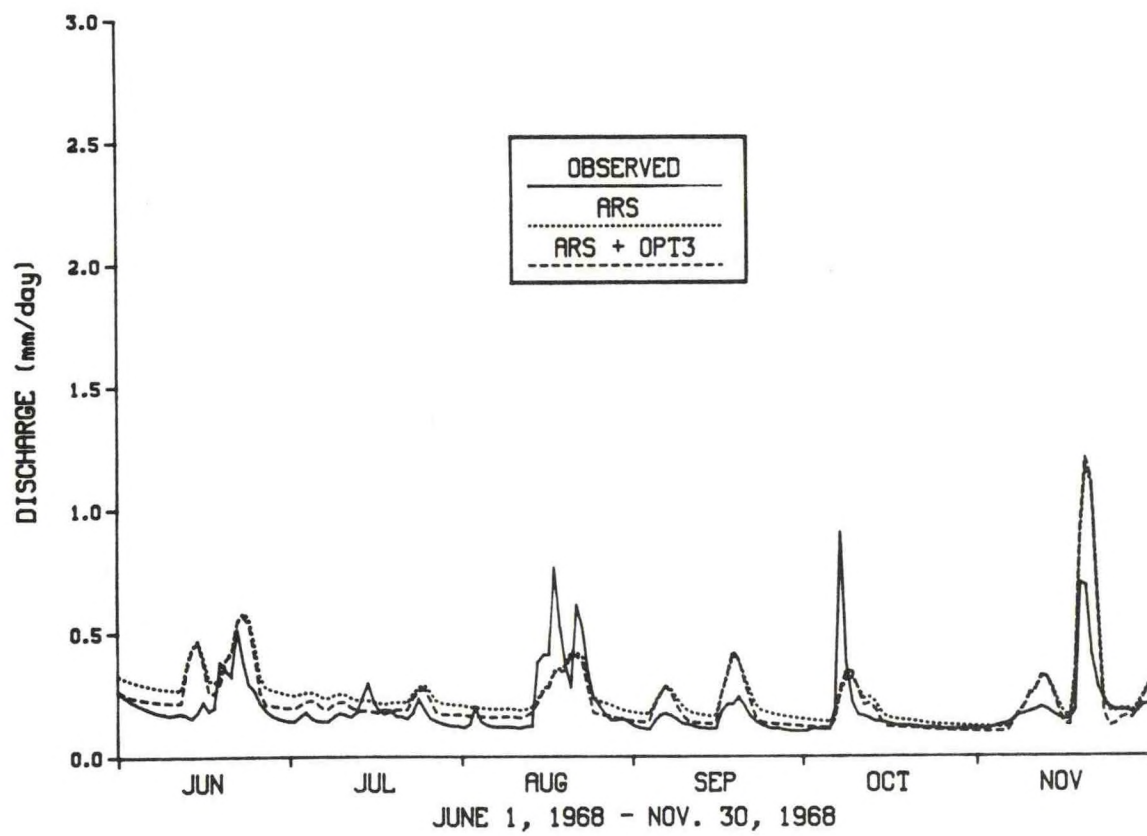


Figure 6.6b. Baseflow Hydrograph for Comparison of ARS and ARS +OPT Parameter Sets.

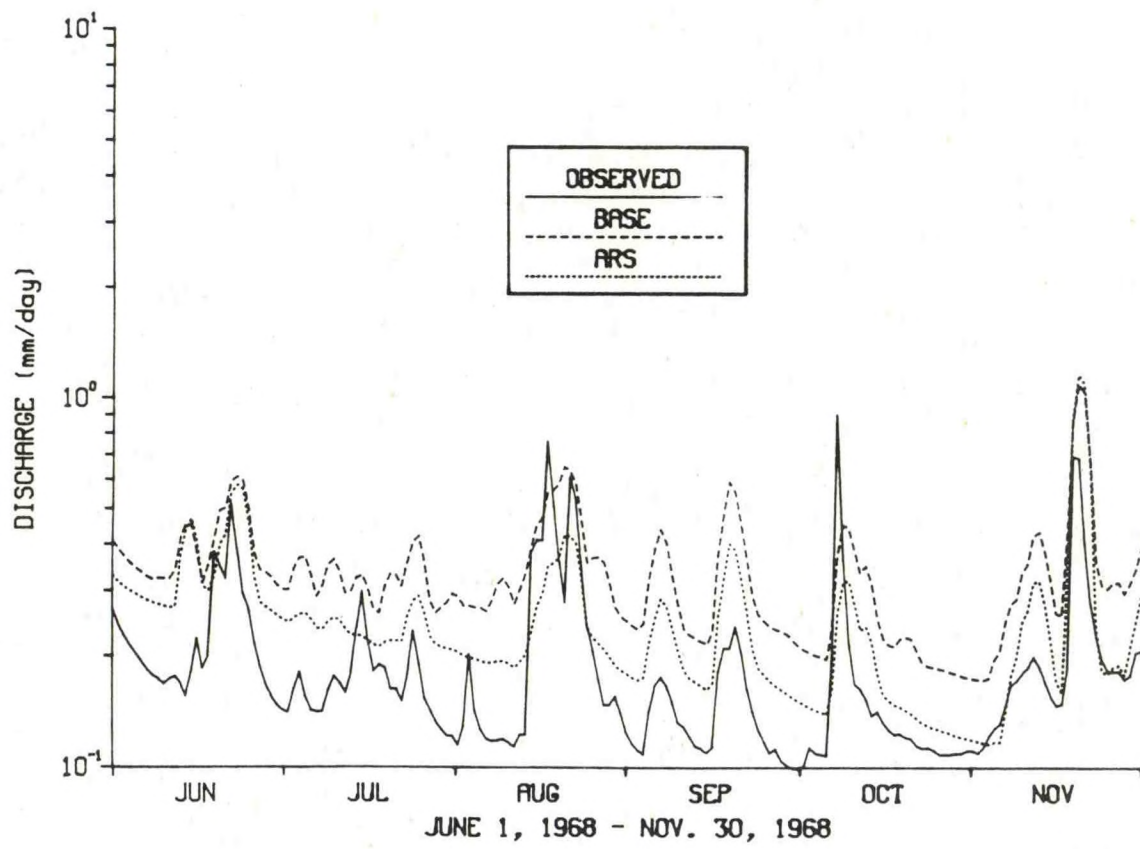


Figure 6.7a. Logarithmic Baseflow Hydrograph for Comparison of Base and ARS Parameter Sets.

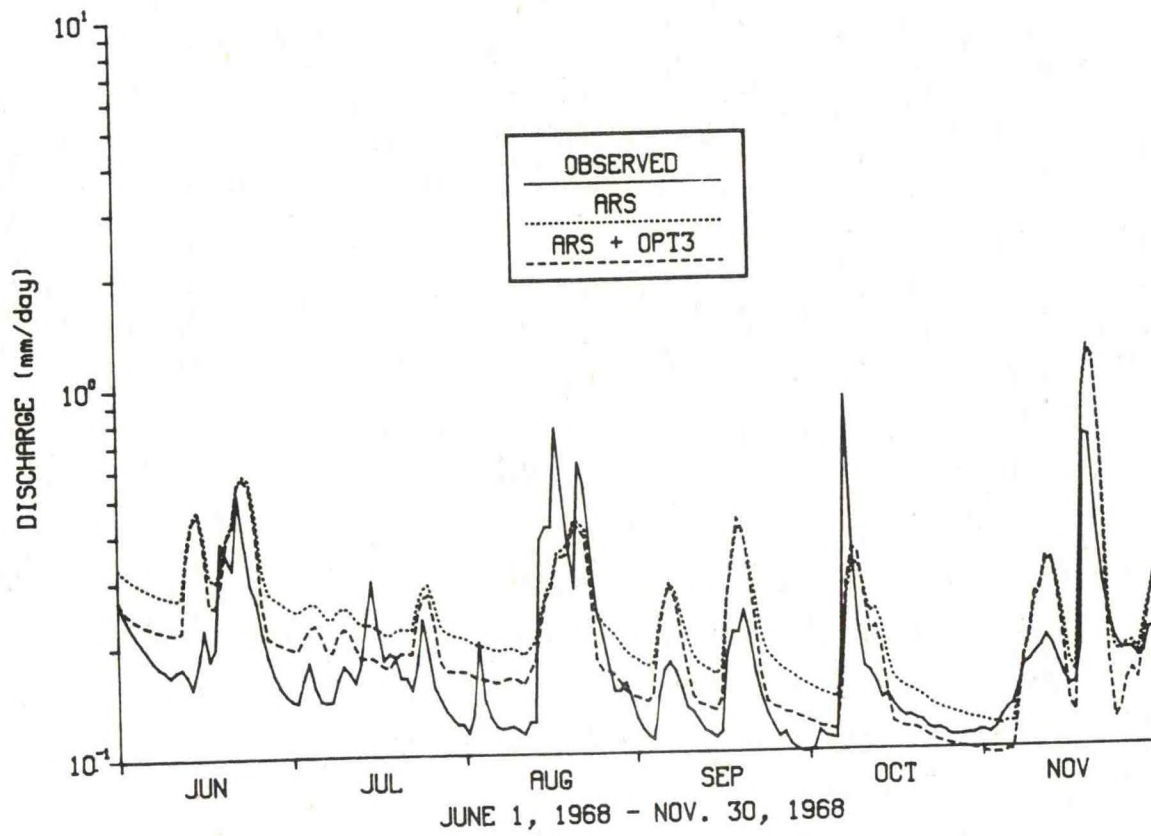


Figure 6.7b. Logarithmic Baseflow Hydrograph for Comparison of ARS and ARS + OPT Parameter Sets.

scales. The main difference between the base run and the ARS run is attributable to the fact that the ARS run has a slightly faster baseflow recession. The ARS+OPT run has longer periods of interflow and more direct runoff.

Considerable testing was made with the parameter UZK during the development of the Level III procedures. Several runs were made using OPT3 to optimize UZK so that results could be compared to LINDRV optimization runs. The runs optimized UZK while all other parameters were held at their ARS optimal values. The first run used data for the entire seven year period. Although found to be one of the most sensitive parameters in these studies, the OPT3 search produced a converged UZK value of 0.333. This was within one percent of the starting value. The results are an indication that the parameter values obtained by the Level II analysis (ARS algorithm) probably are reliable consistent values. Other runs for UZK, using variations in input, gave similar results. One run was made using only the first year of data (water year 1956). Results were quite different. With all other parameters fixed, UZK converged at a value of 0.6. Apparently, events during water year 1956 (or possibly data errors) are not adequately modeled by the ARS parameter set and cause the optimization algorithm to drastically change the UZK parameter. This also is evident in the LINDRV runs.

Numerous runs were made with LINDRV for comparison with OPT3 and to test its capabilities as a fine tuning tool and to assess the sensitivity of the filter to variations in the initial covariance of the state error (P), the variance of the measurement noise (R), and the variance of the error in the precipitation input (U). The initial LINDRV runs continued with the estimation of UZK, since it had been analyzed most in the previous runs. Later runs included other parameters in an attempt to begin to develop a strategic selection of parameters to be examined in fine tuning. Unlike a search procedure where the period of record to be analyzed is determined prior to a run, the filter estimation algorithm estimates the parameters as each data point is processed. This means that parameter values can be assessed for any length of record, beginning with the first day, by running the filter for the entire period of record. This information can be useful in determining how rapidly a parameter tends to converge. It also can be used to indicate seasonal variations in parameters.

The first few case study runs with LINDRV were made to determine the sensitivity of the results to the initial P matrix. All elements other than those on the diagonal were set to zero. The nonparameter elements of P and Q were set to nominal values of 0.1. In the first two runs R and U were computed according to the equations in Chapter 5 from coefficients of variation of 0.2 and 0.1, respectively. In other words, the standard deviation of the error in the streamflow observation was assumed to be twice that for the precipitation input. Element P was set to be 0.1 percent of the parameter value, an initial value assumed to be severely constraining. The full seven years of data (water years 1956-1962) were processed with the filter with little change being observed in the UZK parameter. At the end of one year the parameter had moved from its starting value of 0.329 to 0.322. By the end of year seven the

value had converged to 0.295, and because of contraction of the P matrix, was no longer changing. Another run was made with initial P set to one percent of UZK. The initial P restricted movement of the parameter, however, the final value of convergence was 0.253. Results are shown in Figures 6.8 and 6.9. The filter has a tendency to slightly reduce UZK, whereas, the OPT3 pattern search algorithm with the RMS objection function left UZK essentially unchanged when the other parameters were fixed.

Several runs were made to determine the sensitivity of the filter to changes in R and U. R represents an estimate of the variance of the error in the streamflow. The observation can contain errors from several sources: the rating curve, bed scour or deposition, backwater effects or faulty recording equipment. R is computed from the coefficient of variation (v_r) and is a function of the streamflow observation. A v_r value of 0.2 means that the true streamflow associated with a measurement of 100 cms has a 0.67 probability of being between 80 and 120 cms. For this case study, a value of v_r between 0.1 and 0.3 seems reasonable. Ongoing research is being conducted to assess the effect of using a time varying coefficient of variation so that R can be adjusted to reflect seasonal as well as streamflow magnitude differences.

Errors in precipitation also can be accounted for in the filter. The errors generally are attributable to problems with the precipitation gages or in the procedure for estimating mean areal values from the point observations. The latter error can be significant when dealing with areas where flooding is caused by localized events. The coefficient of variation for the precipitation (v_u) was assumed to range from 0.1 to 0.3 also. Seasonal adjustments may be appropriate for computing v_u and will be considered in ongoing research.

Figure 6.10 shows the results from a run where UZK was estimated when both the observed streamflow and precipitation were assumed to contain no errors (v_r and $v_u = 0$). Similarly to the OPT3 results for water year 1956, the filter attempts to adjust UZK upward to a value much greater than its starting point. Although subject to further correction during the following years, the parameter never converges to a more realistic value. Figure 6.11 shows the results from a run with the same input as Figure 6.10 except for v_r being assigned a value of 0.2. In this case the filter adjusted the parameter for the events of water year 1956, but managed to correct to reasonable values and finally converge to an acceptable level. One other case was run where v_r and v_u were both set to 0.2. Slight changes were made in the output values, however, no significant differences could be seen in the plot. The results indicate that the parameter estimation algorithm is quite sensitive to changes in v_r and, as expected, produces reasonable results only when allowed to filter the data with an assumed error structure.

One of the development runs described in Chapter 5 was used to estimate both UZK and LZSK. In that case the starting values were switched with each others true value. One run was made with LINDRV to estimate UZK and LZSK for the Leaf River. All other parameters were held at their best ARS values. Both v_r and v_u were set to 0.2. The

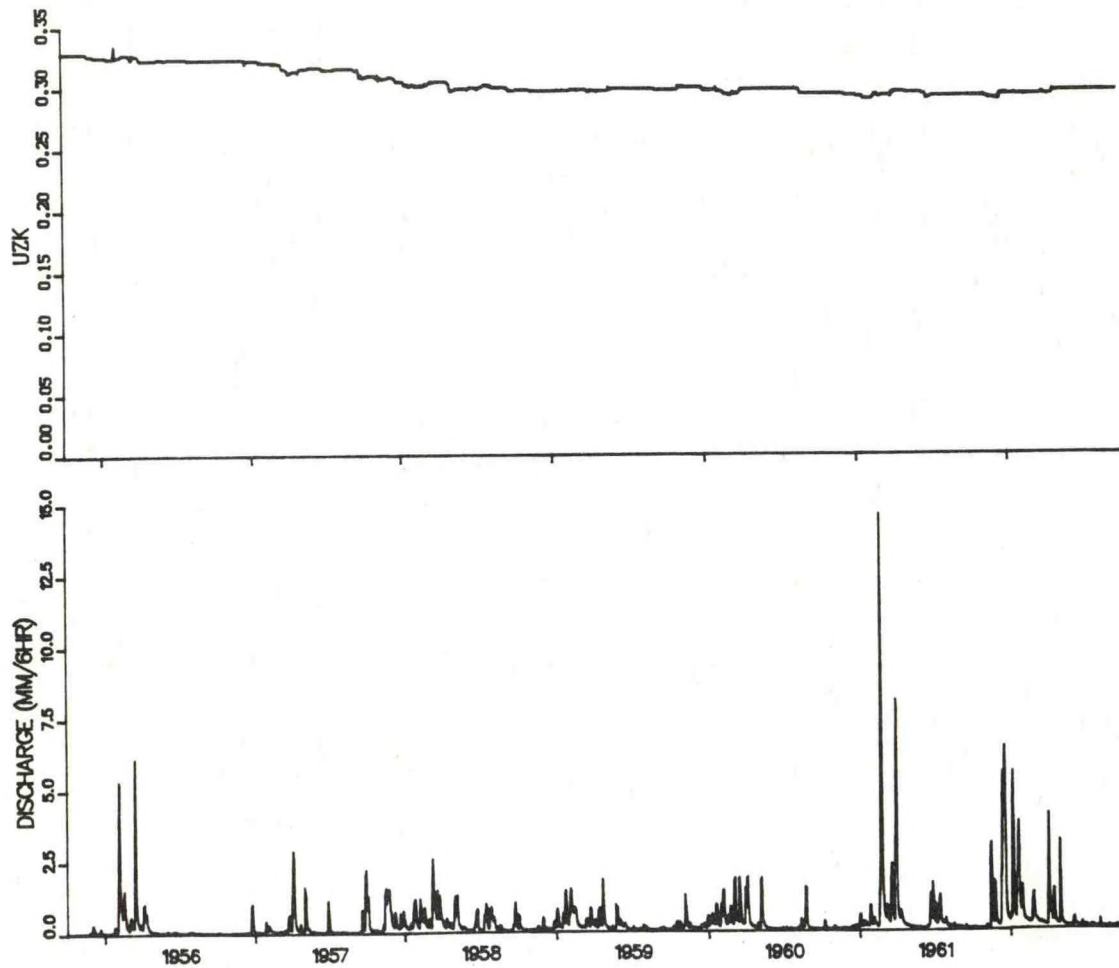


Figure 6.8. LINDRV Results for UZK (Fractional daily upper zone free water withdrawal rate) for Leaf River Data ($P_0=0.1\%$ initial parameter value, $v_r=0.2$, $v_u=0.1$).

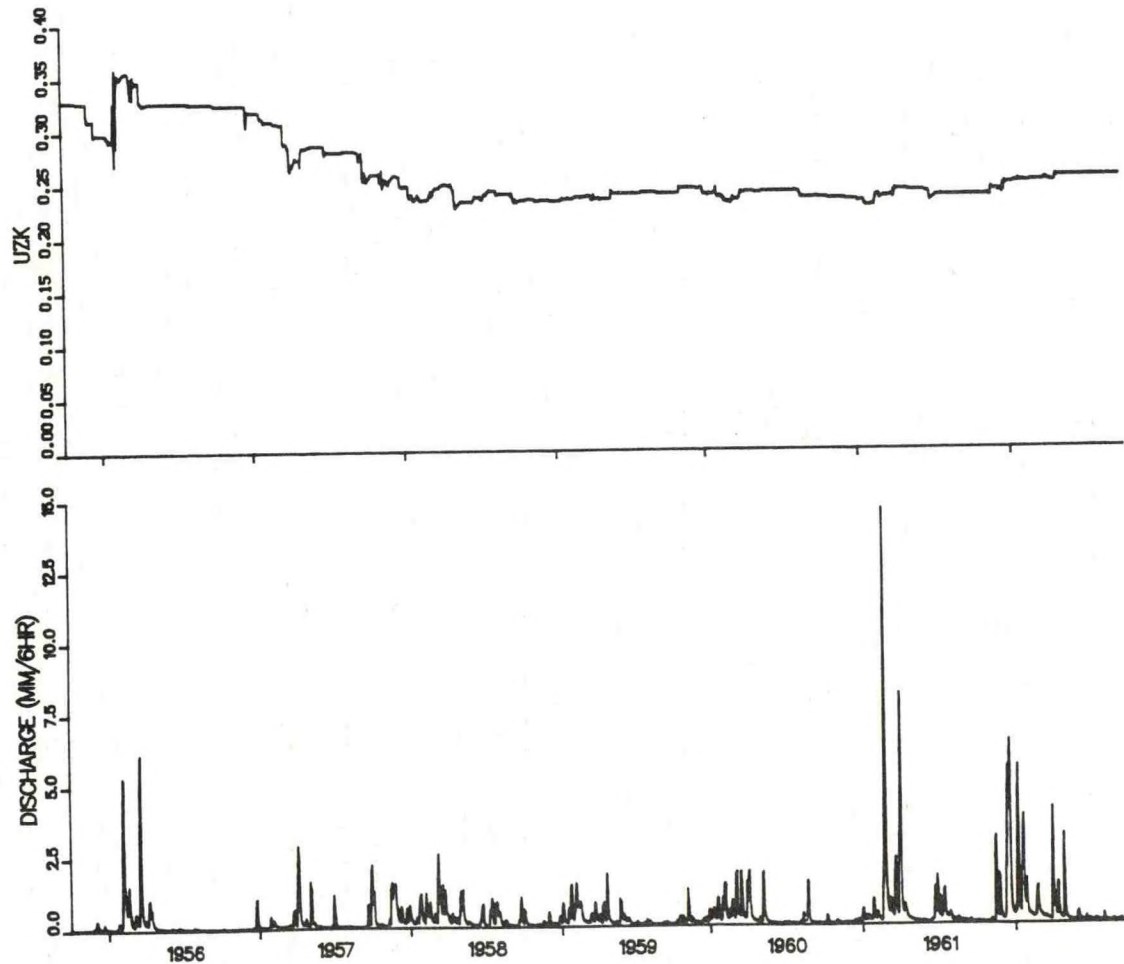


Figure 6.9. LINDRV Results for UZK (Fractional daily upper zone free water withdrawal rate) for Leaf River Data ($P_0=1\%$ initial parameter value, $v_r=0.2$, $v_u=0.1$).

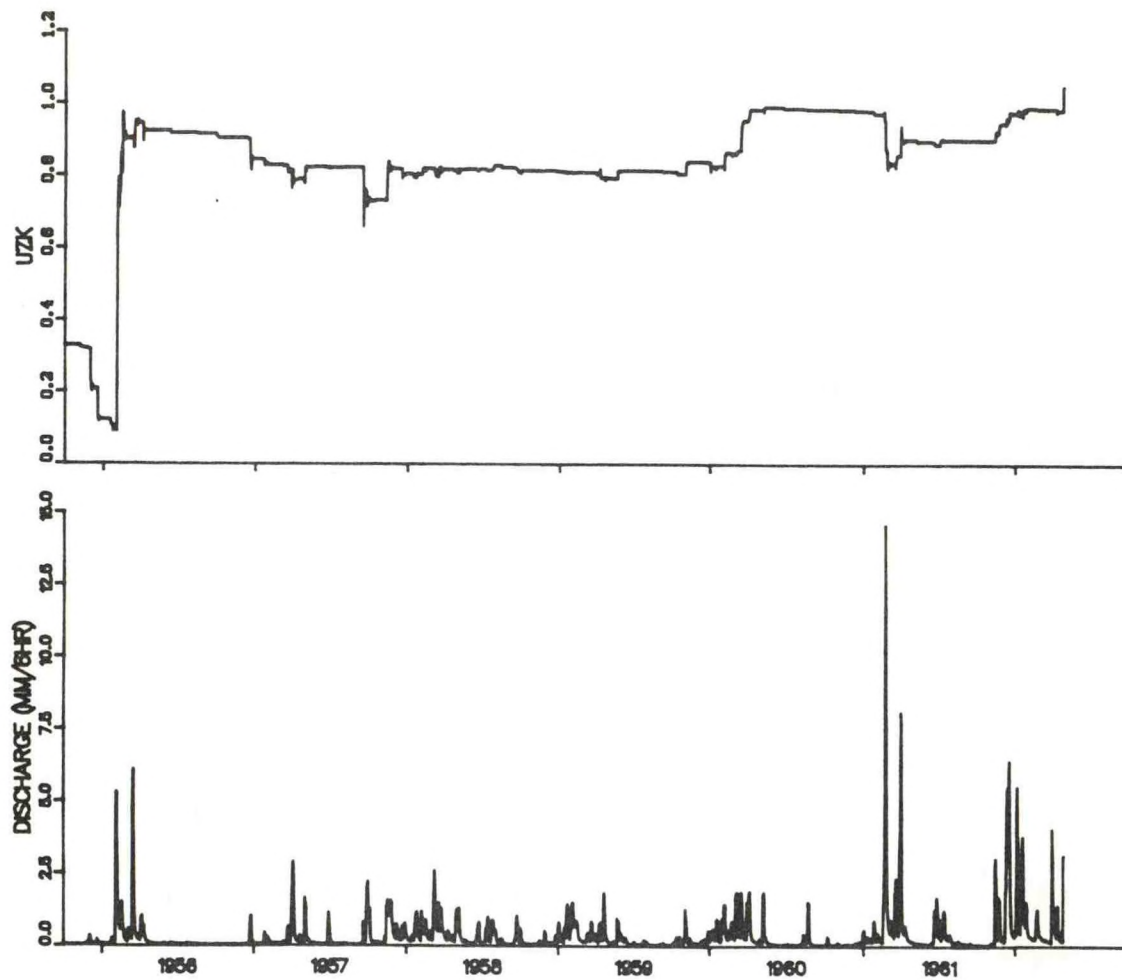


Figure 6.10. LINDRV Results for UZK (Fractional daily upper zone free water withdrawal rate) for Leaf River Data ($P_0=1\%$ initial parameter value, $v_r = v_u = 0$).

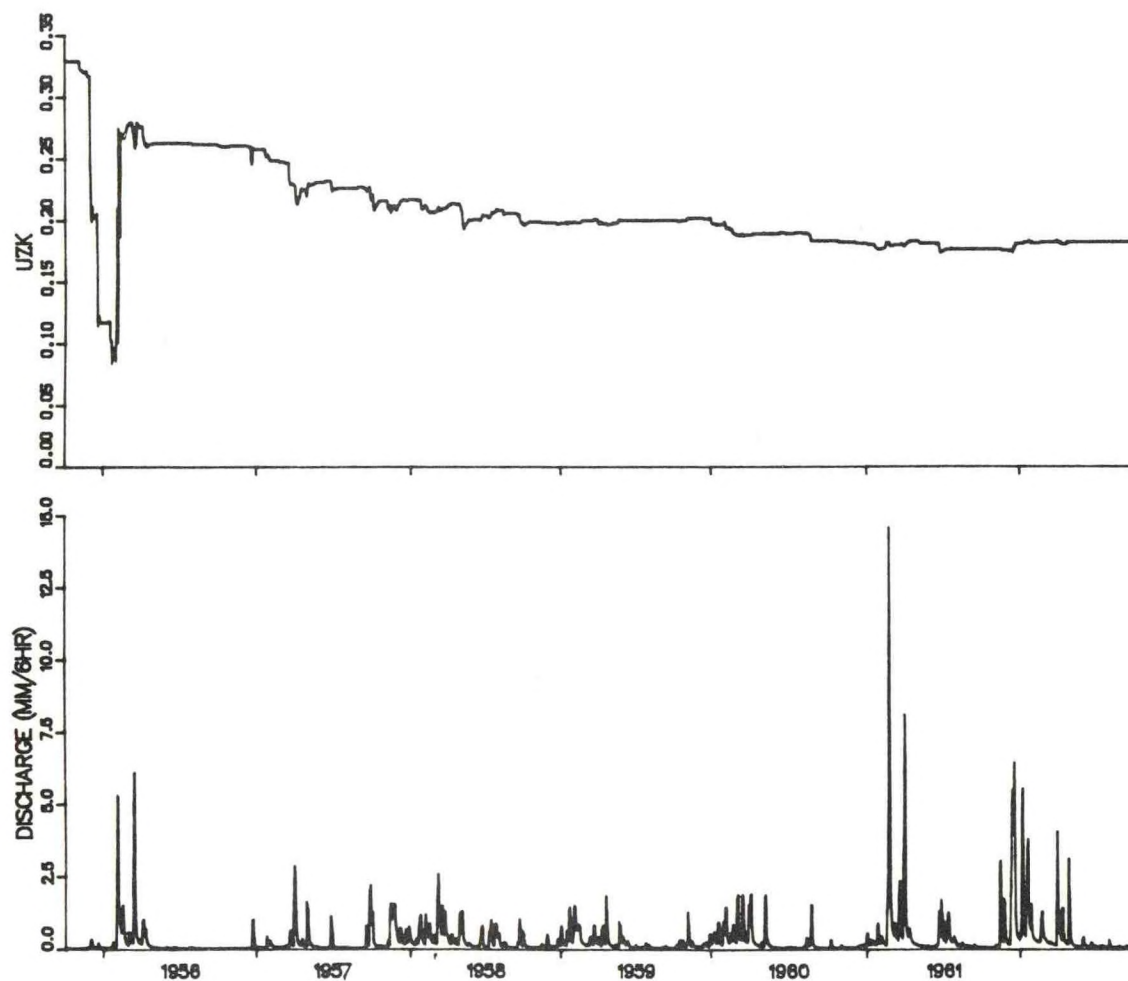


Figure 6.11. LINDRV Results for UZK (Fractional daily upper zone free water withdrawal rate) for Leaf River Data ($P_0=1\%$ initial parameter value, $v_r=0.2$, $v_u=0$).

results are shown in Figure 6.12. After both downward and upward corrections, both parameter values converged to lower values. This result is consistent with the OPT3 run shown in Table 6.5 where both parameters were decreased to their lower bounds.

Several runs were made with an estimation of all parameters to further test the effects of the initial P matrix. Table 6.7 shows the results for initial P diagonal elements equal to 1 percent and 10 percent of the parameter values. As shown in the table, the increase in P gives the filter more freedom to adjust the parameter values. The indication is that the inclusion of all parameters in the filter gives the algorithm too many degrees of freedom. Some parameter adjustments tend to dominate others and result in parameter values which may be outside the range considered to be acceptable. This may be an indication of model structural errors. Although model parameter compensation may be controlled somewhat by arbitrarily adjusting the filter parameters, a more structured approach which limits the number of parameters estimated at any one time seems more reasonable.

The results from these runs provided valuable information to be used in development of a strategy for using the filter in a parameter estimation mode. Selection of initial P values and estimates for v_r and v_u can be critical to the estimation process. Initial P elements must be large enough to give the filter freedom to move parameters but may need to be adjusted so that not all the correction between observed and simulated streamflow is accounted for in one parameter. Also, reasonable estimates of R and U are necessary. With these thoughts in mind, several more runs were made to estimate various combinations of parameters.

Results from previous runs showed that some of the parameters were better candidates for recursive parameter estimation than others. This conclusion is consistent with the objectives of the study: estimation of the parameters through projection and reduction in problem dimension. Although optimized in some of the previous LINDRV runs, the five parameters estimated with INIT were assumed to be fixed at their best ARS values. Two levels of calibration analysis were devoted to their estimation, thus, they are assumed to be at their optimum. Because of the nonlinearities associated with threshold elements (UZTWM, UZFWM, LZTWM) they were considered to be undesirable candidates for recursive filter estimation. The same argument can be made against ADIMP, however, it was included in some of the runs. The remaining five parameters also were the parameters showing the most adjustment during the OPT3 runs.

The results from three of the final LINDRV runs are presented in the following paragraphs. Five parameters were estimated in the first run: UZK, ZPERC, REXP, PFREE, and ADIMP. ADIMP was eliminated from the final two runs. All other parameters were held at their best ARS values. Results from the first run are shown in Figures 6.13a, b and c. Initial values of P were set at 10 percent of the initial parameter value with the exception of UZK. Prior runs showed that UZK was too sensitive when P was initiated at 10 percent; therefore its value was set at one percent instead. Parameters ZPERC, REXP, UZK, and ADIMP all

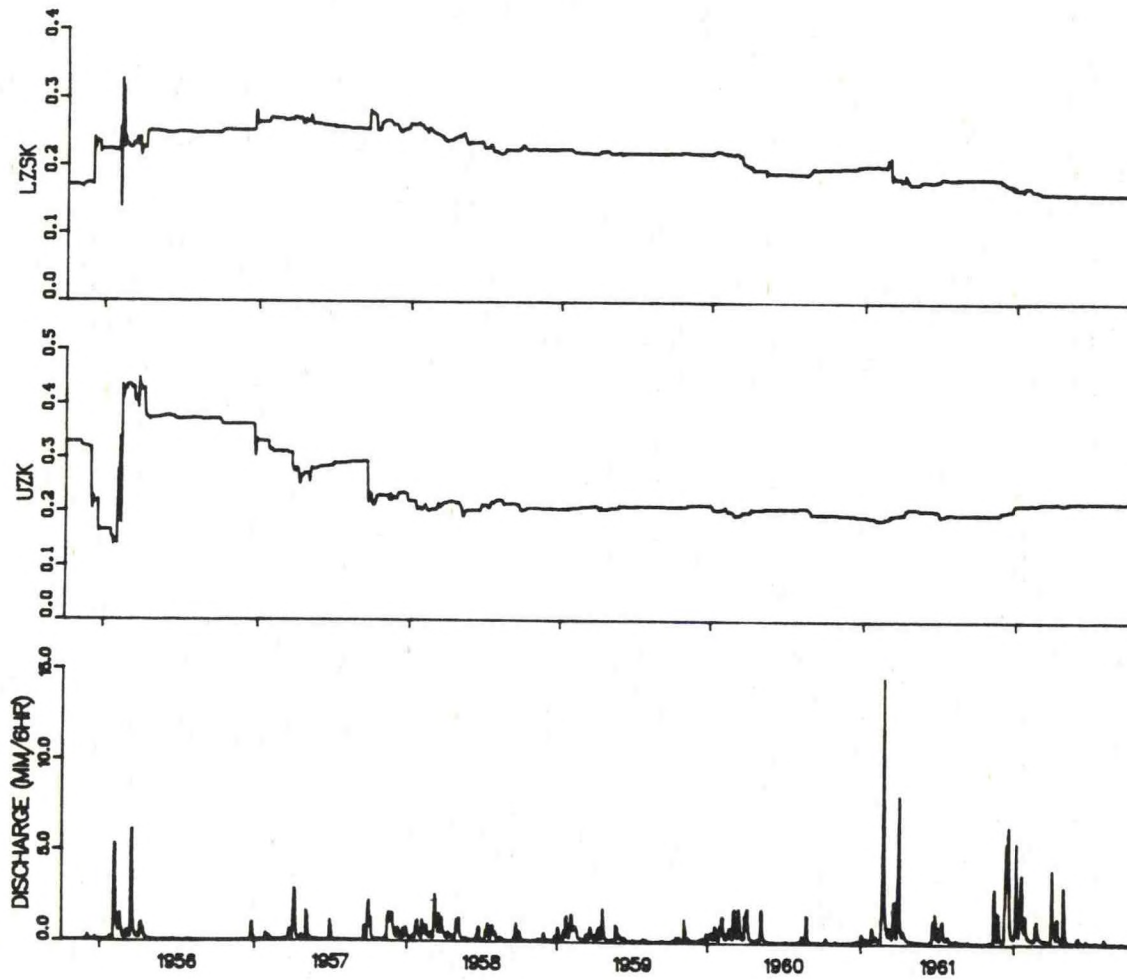


Figure 6.12. LINDRV Results for UZK (Fractional daily upper zone free water withdrawal rate) and LZSK (Fractional daily supplemental withdrawal rate) for Leaf River Data ($P_0=1\%$ initial parameter value, $v_r = v_u=0.2$).

Table 6.7

Results from LINDRV Runs with Varying P_{INIT}

<u>Parameter</u>	<u>Starting Value</u>	<u>Results with $P_{INIT} = 1\%$</u>	<u>Results with $P_{INIT} = 10\%$</u>
UZTWM	10.	10.02	12.27
UZFWM	36.9	36.89	39.40
LZTWM	222	222.04	221.9
LZFPM	129.	128.97	129.0
LZFSM	51.	50.99	51.3
UZK	.329	.274	.036
LZPK	.0068	.006	.006
LZSK	.171	.169	.335
ZPERC	141.	140.97	140.4
REXP	3.99	3.985	5.098
PFREE	.055	.052	.195
ADIMP	.20	.277	.608
PCTIM	.003	.000	.002

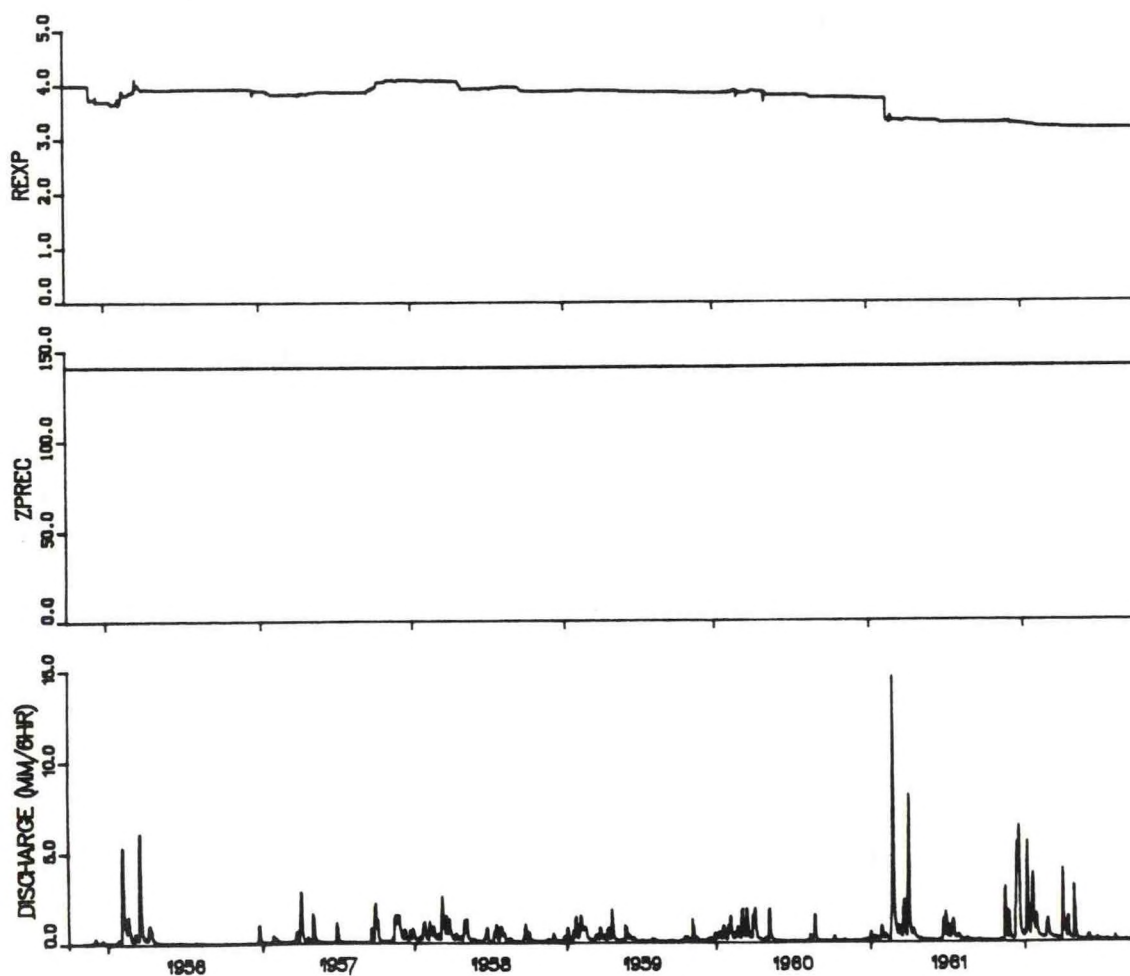


Figure 6.13a. LINDRV Results for 5-parameter Run for Leaf River Data.
REXP (Percolation equation exponent)
ZPERC (Maximum percolation rate coefficient)

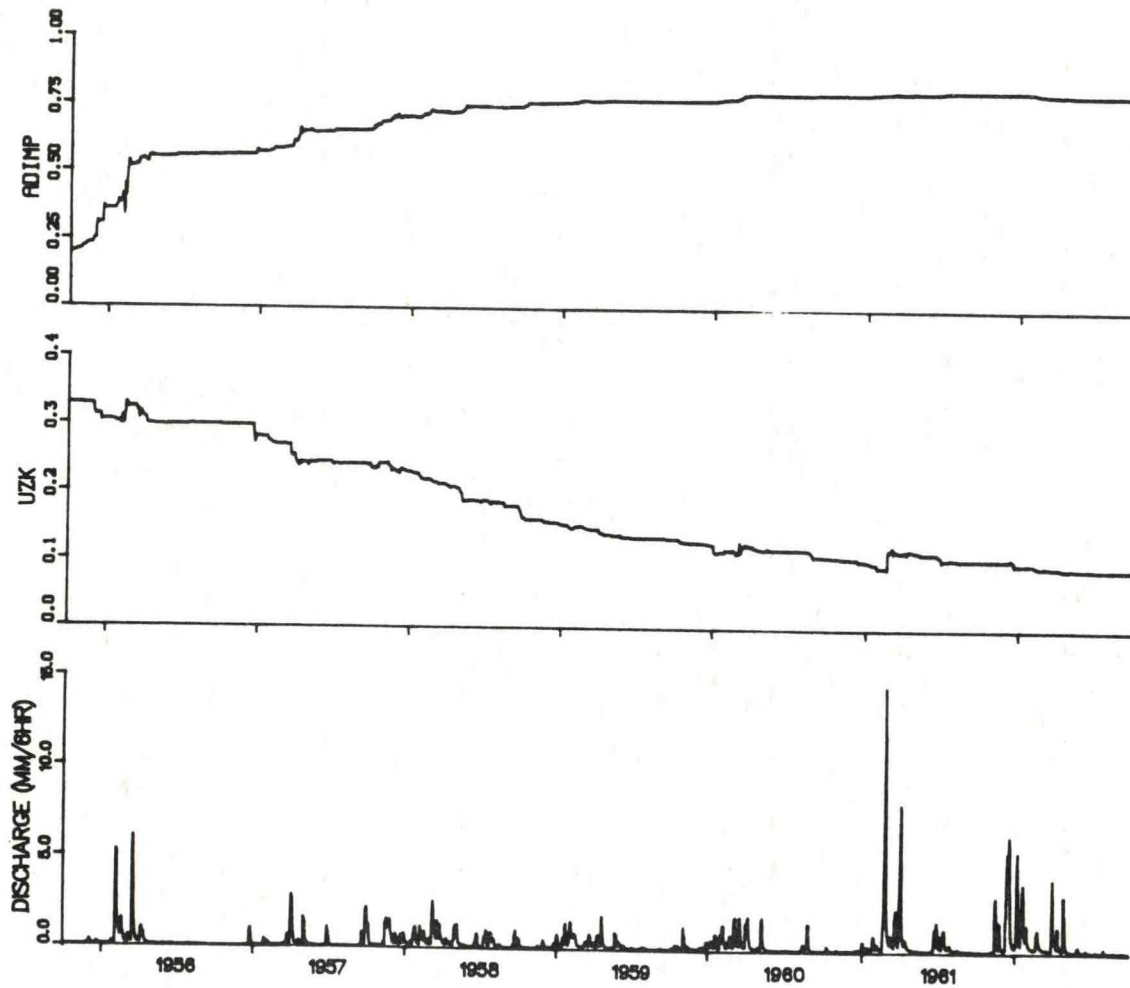


Figure 6.13b. LINDRV Results for 5-parameter Run for Leaf River Data.
ADIMP (Additional impervious area)
UZK (Fractional daily upper zone free water withdrawal rate)

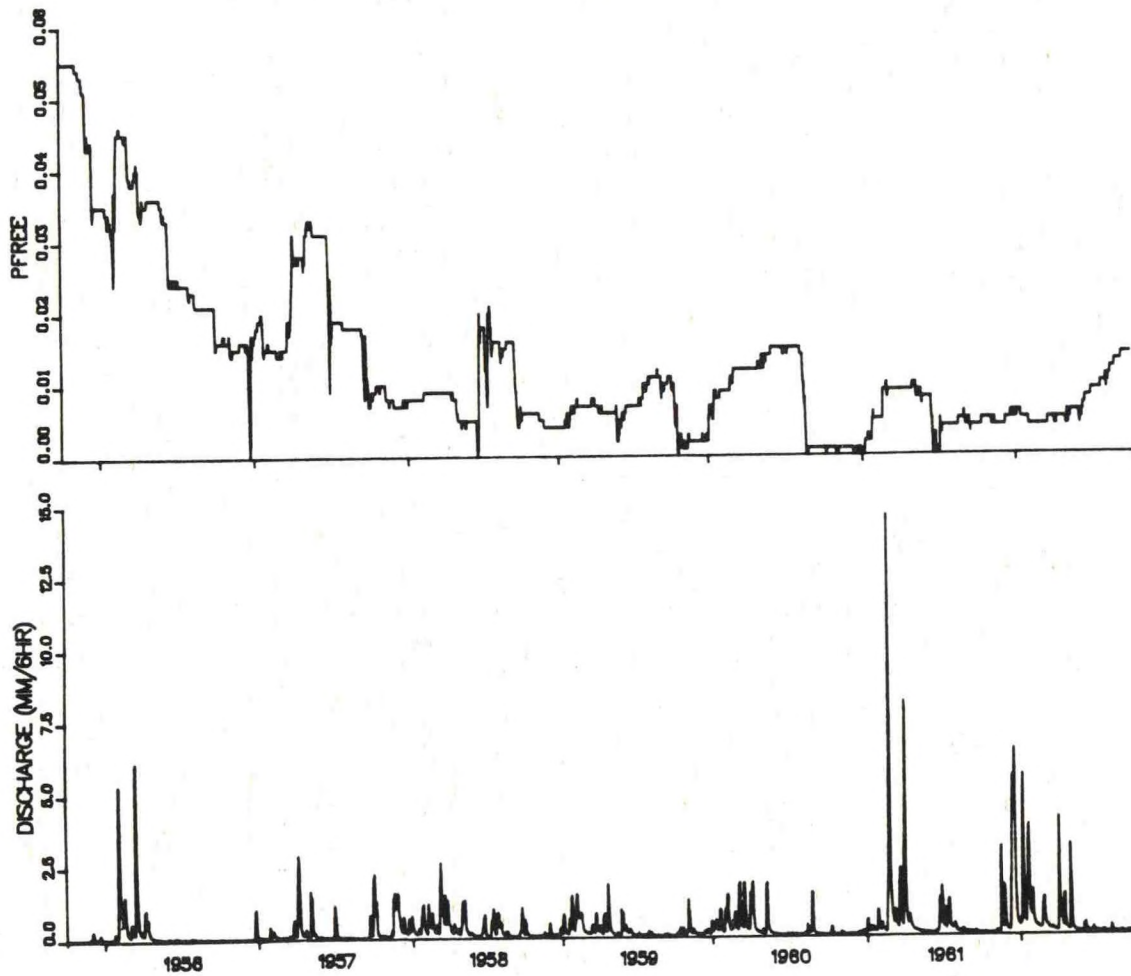


Figure 6.13c. LINDRV Results for 5-parameter Run for Leaf River Data.
PFREE (Decimal fraction of percolated water going
directly to lower zone free water storage)

appear to converge by the end of the seventh year. ADIMP moves to a value considered larger than the normal range and UZK is adjusted below what is generally considered acceptable. The UZK move is consistent with the seven year OPT3 run shown in Table 6.5, where UZK was adjusted to its lower limit. It appears that the increase in ADIMP has resulted in a change in the components which sum to generate the peaks and has essentially eliminated the need for interflow controlled by UZK. PFREE continues to be corrected throughout the period. The scale of the plot makes the parameter appear to be less stable than it actually is. The movement of PFREE to a lower value also was consistent with the OPT3 run.

A second run was made with ADIMP fixed at its ARS value. The results are shown in Figures 6.14a, b and c. UZK again moved to a lower value, but not as small as in Figure 6.13b. REXP did not decrease as it did in Figure 6.13a. The differences between the two runs are indicative of the complex interrelationships that exist among the parameters in the model. A third run was made with doubled initial P values. Results were basically the same, indicating that the initial P value in the second run probably was adequate for the estimation procedure.

As an independent check on the validity of the LINDRV runs, two runs were made with MCP to compute the statistics for a simulation produced by the parameters resulting from the final two LINDRV runs. The results from the runs plus the statistics from the best ARS run are shown in Table 6.8. The statistics show that the LINDRV program produced parameters which slightly degraded the model fit according to the OPT3 evaluation criteria, however, the results are all within a highly acceptable range. This probably is due to the fact that the recursive estimation procedure uses an objective function different from OPT3. One run also was made with OPT3 to optimize the same four parameters that were adjusted in LINDRV. Parameter corrections were insignificant, with three of the four parameters moving in the same direction as the Figure 6.14 run. The conclusion that can be drawn from these final runs is that the parameters must be close to their optimum, at least for this vicinity of the response surface, and any further adjustments will consist of insignificant trade-offs among parameter values. Some of the runs showed that the adjustment of parameters can be sensitive to initial values of the P matrix elements. In some cases, such as UZK, the parameters are just more sensitive than others, and this can be controlled somewhat by adjustments to the initial value of P. Further studies will be made in the future to test filter sensitivity to P, R, and U.

Several conclusions can be drawn from the analysis of the LINDRV runs. The filter algorithm provides the user with a tool for assessing and accounting for errors in the inputs and in the streamflow observations. The results from the water year 1956 data show how valuable this capability can be, particularly if short data periods are being used or the data are known to contain errors.

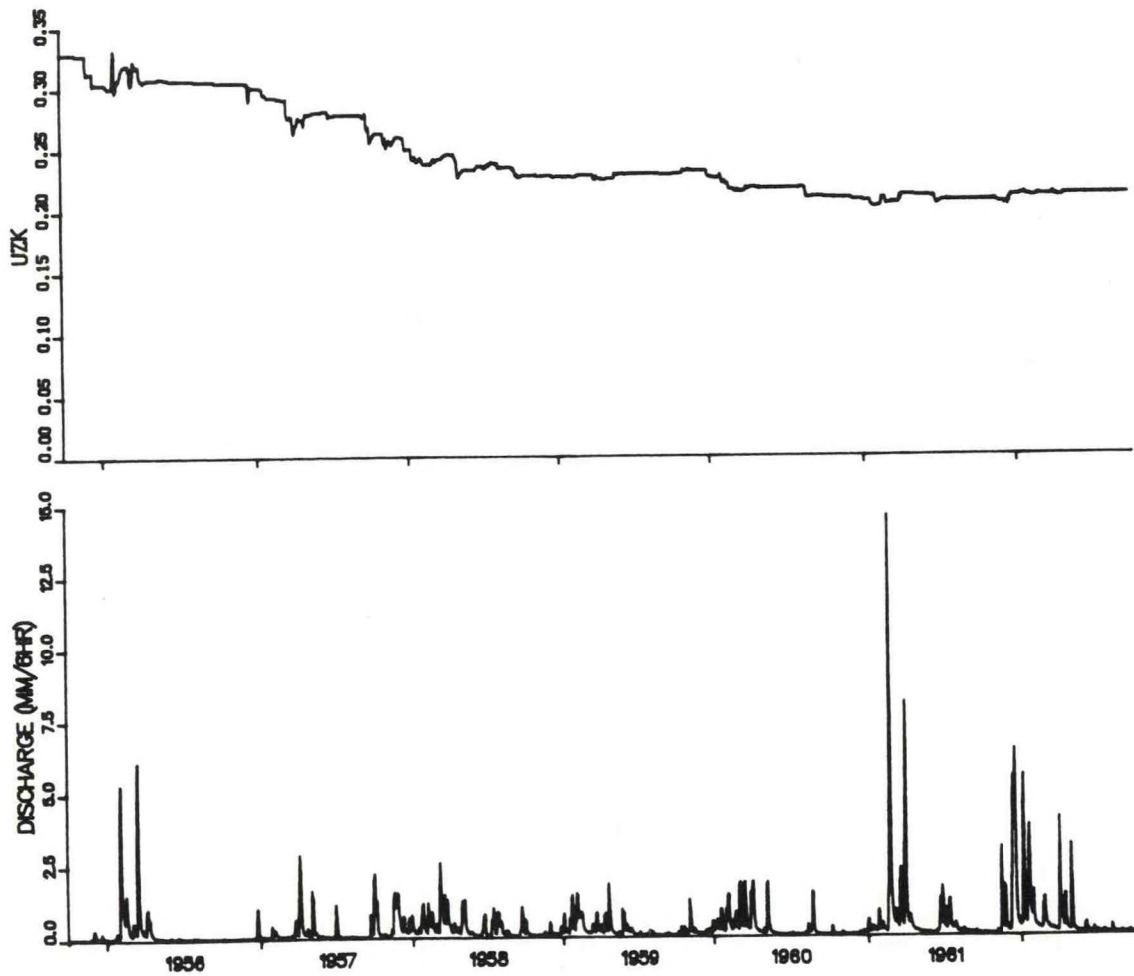


Figure 6.14a. LINDRV Results for 4-parameter Run for Leaf River Data.
UZK (Fractional daily upper zone free water withdrawal
rate)

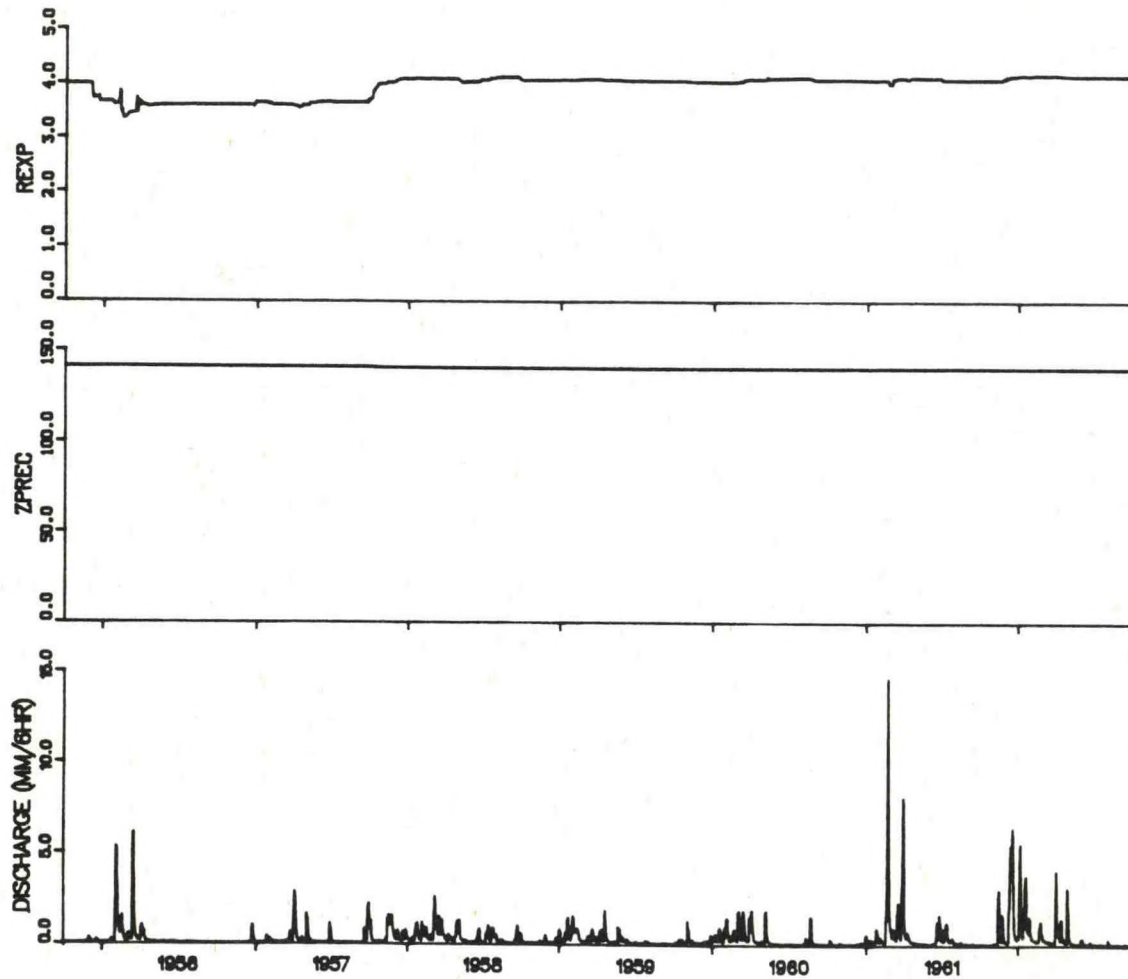


Figure 6.14b. LINDRV Results for 4-parameter Run for Leaf River Data.
REXP (Percolation equation exponent)
ZPERC (Maximum percolation rate coefficient)

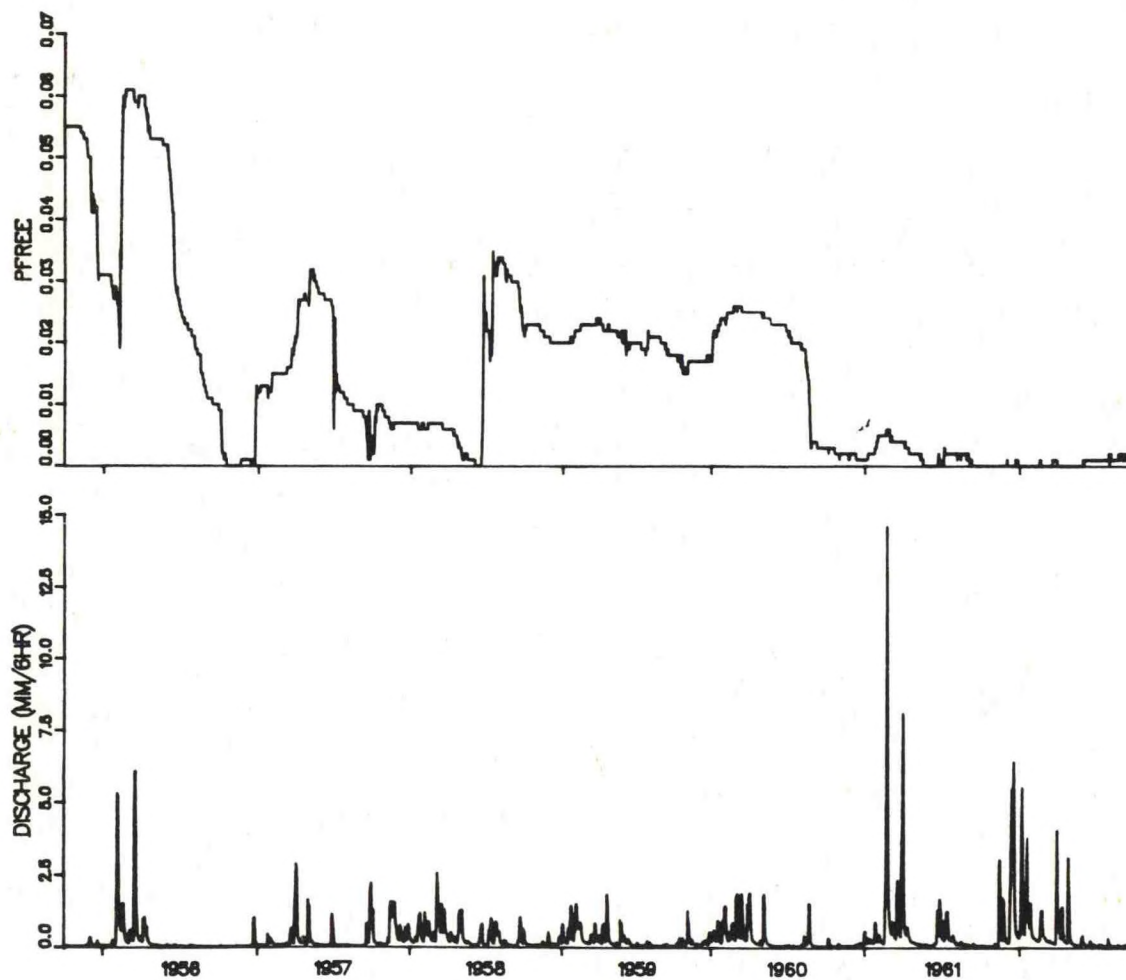


Figure 6.14c. LINDRV Results for 4-parameter Run for Leaf River Data.
PFREE (Decimal fraction of percolated water going
directly to lower zone free water storage)

Table 6.8

Results from MCP Runs with LINDRV Parameters and OPT Run

<u>Parameters</u>	<u>ARS Run #1 Values</u>	<u>Fig. 6.13 Values</u>	<u>Fig. 6.14 Values</u>	<u>OPT^{1/} Values</u>
UZW	10.	Same	Same	Same
UZF	37.	"	"	"
LZW	222.	"	"	"
LZFP	129.	"	"	"
LZFS	51.	"	"	"
UZK	.329	.090	.212	.312
LZPK	.0068	Same	Same	Same
LZSK	.171	"	"	"
ZPERC	141.	141.2	140.	150.
REXP	3.99	3.177	4.126	4.233
PFREE	.055	.014	.001	.050
SIDE	0.	Same	Same	Same
ADIMP	.20	.795	"	"
PCTIM	.003	Same	"	"

Obj. Functions

RMS (CMSD)	18.04	26.117	18.257	17.99
R'	.9686	.9459	.9605	.9686

^{1/} No parameters were constrained by bounds.

The Level III analysis showed that both the OPT3 Pattern Search algorithm and the LINDRV filter are capable of providing useful information about the local response surface. In this particular case study, the Level III work probably was insignificant due to the success of the calibration results from Levels I and II. This may be different for other watersheds. The choice of which fine tuning tool is appropriate will be dependent on the application of the results. State-space modeling and automatic updating soon will become part of the standard tools available for operational forecasting. As this occurs recursive parameter estimation which is consistent with the forecast system will begin to play a larger role in model calibration.

Case Study Conclusions

The multilevel calibration strategy developed in previous chapters was applied to the Leaf River watershed near Collins, Mississippi. Program INIT was used to estimate five of the SAC-SMA model parameters. The five parameters along with ranges for the remaining parameters were used as input to program OSRCH. Both the ARS and URS procedures were used to estimate the remaining parameters. Results were similar for both types of runs and comparable in fit to simulations after several hours worth of hand calculations and trial-and-error runs. Fine tuning was performed using both deterministic and stochastic techniques. Results from the Level III work showed that only small improvements could be seen in the fit of the model beyond the Level II analysis. There were no indications that further runs were necessary. The case study reveals that the multilevel approach provided satisfactory results for this basin in far less time than using previous methods.

Chapter 7

SUMMARY, CONCLUSIONS AND RECOMMENDATIONS

Summary

The purpose of this research was to develop and test a systematic methodology for calibrating conceptual hydrologic simulation models. A multilevel approach was proposed to reduce the problem to a number of subproblems which could be solved using several different optimization techniques. The NWS SAC-SMA model was chosen for implementation of the methodology. A state-space version of the model was formulated for use in some components of the study.

Three levels of optimization were proposed for the model. Level I consisted of the development of a guided interactive initial parameter estimator. The program uses computer generated graphics along with interactive input to lead an inexperienced user through some of the steps of initial data quality control and estimation of the model parameters. The Level II work was designed to overcome some of the convergence problems commonly associated with direct search procedures. Two random search techniques were developed for use with the SAC-SMA model. URS performs a random search by randomly selecting parameter values and creating an output data set of various statistics for each iteration. Programs NINF and CMPTPI were created to allow a user to perform a multi-objective post simulation analysis of the results. ARS is a converging random search procedure that was shown to produce effective results. A program for generating sensitivity analysis plots for various objective functions also was presented. Level III was designed to be a fine-tuning analysis. A recursive parameter estimation procedure was developed and tested against a direct search algorithm. The recursive technique uses the state-space version of the SAC-SMA model with a state augmentation form of the Kalman filter. The filter was tested for sensitivity to inputs. All of the procedures were tested and verified with synthetic data. A case study was presented where the multilevel strategy was applied to the Leaf River.

Conclusions and Recommendations

The general strategy of dimension reduction and projection should be applicable to almost any type of complex simulation model. The multilevel methodology was shown in this case to be a valid approach to the problem of hydrologic model calibration. The procedures produced results in a case study which were comparable to those obtained using traditional manual techniques, but in considerably less time. The results from this research will serve as a framework for building a hierarchical structure of procedures for analyzing the components of a conceptual hydrologic model.

The resulting strategy consists of the identification of different parameters in each level of optimization. The choice of which parameters to include in the various levels obviously is up to the modeler, however, several conclusions can be drawn from this research.

The dimension of the calibration problem can be tremendously reduced when certain components in the model can be isolated and the corresponding parameters identified. In the case of the SAC-SMA model, the baseflow parameters were readily identifiable and were shown to be some of the most sensitive. The net effect of computing and fixing their values, as shown in the case study, was to restrict the remaining search to a more quadratic region on the response surface. Any other available tools, such as trial-and-error calibration runs, also should be used to gain information and establish bounds prior to running the large scale search techniques. The random search procedures can be run for all parameters, however, the number of trials required to obtain convergence in the ARS case will be correlated with the number of parameters. In this application of the methodology, all parameters were estimated with ARS, but the Level I parameters were given tight constraints. The parameters included in Level III should be those which still show considerable uncertainty after Level II. In the initial applications of the projection technique, the parameters causing the least complications were included in the inner problem. This philosophy was used in the Leaf River case study, where the inner problem (Level III) was restricted to those parameters least associated with the model nonlinearities. In this case, the inner problem delineation works well because the Kalman filter algorithm is based on assumptions of linearity. In general, the selection of parameters for each level should be based on identifiability, sensitivity, complication factors and the assumptions corresponding to the optimization tools.

Tools were developed for use in each level of the strategy. The procedures serve as initial steps towards the development of an enhanced interactive modeling system for hydrologic simulation and forecasting. The INIT program was shown to be a useful calibration tool and will be expanded in the future to include other parameters. The area of initial parameter estimation seems particularly suitable for application of expert system technology. Both of the random search procedures offer users several advantages over direct or gradient search techniques. The multi-objective aspects of URS allow users to emphasize the importance of various evaluation criteria, much as experts typically do in manual calibration. The URS and ARS procedures should be tested further and compared for results. URS offers a user more flexibility, but costs considerably more to run. The ARS procedure should be analyzed carefully to be sure that convergence is taking place most efficiently. This is an area with large potential benefits because of the vast amounts of computer time being used by the program. As processing time becomes more available, random search techniques will become more significant in optimization problems.

If the initial parameter estimation procedure and random search programs typically produce results similar to the Leaf River case study, the choice of a local search procedure may not matter. In this study, neither Pattern Search nor the Kalman filter parameter estimation algorithm significantly improved the model performance, because the Level II results produced a simulation considered to be a final calibration for most purposes. Research will continue, however, in the development of the LINDRV program. The primary advantage of the Kalman filter in this application appears to be the generation of error

covariance information which can be used to assess the reliability of parameters in calibration and states in forecasting. In fact, the form of the model used in LINDRV could be used in a forecast mode where the parameters could be updated as well as states, and the covariance information could be used to determine confidence in both parameters and states. Filter inputs, such as the Q and R matrix elements, could be adjusted to reflect relative user confidence in the states and parameters.

Several areas have been considered for enhancing the Kalman filtering work. Selection of error covariances is always a concern when using the filter. Techniques for estimating the values, such as adaptive filtering, will be examined. Also, additional information concerning the active components and parameters in the model is available from the function derivatives, the filter gain vector and the computed error covariances and should be incorporated into the parameter estimation procedure. Future research plans in this area should consider exploring items such as selective filtering, where some parameters are updated only during periods when they are active, and techniques for artificially propagating error covariances for periods not updated. The results from this research represent another step towards the development of a system of state-space models. Current research in state-space snow modeling and previous work in state-space routing modeling (Smith, 1983) eventually will be coupled with the work in this thesis to produce an operational hydrologic forecast system with automatic updating. When this occurs, recursive parameter estimation which is consistent with the forecast system will play a more significant role in model calibration.

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Appendix

STATE TRANSITION AND INPUT COEFFICIENT MATRIX DERIVATIVE COMPUTATIONS

This appendix contains the derivatives of the functions in equations 4.4 to 4.10. The derivatives represent the elements in the A and B matrices in Chapter 5. A and B are used to compute ϕ and G as shown in equations 5.18 and 5.19.

The symbols defined in Table 4.3 are used in the equations. Additional symbols are defined below to simplify notation in the derivatives.

$$r_1 = \frac{x_1}{x_1^0} \quad (\text{A.1})$$

$$r_2 = \frac{x_2}{x_2^0} \quad (\text{A.2})$$

$$\begin{array}{c} \cdot \\ \cdot \\ \cdot \\ r_5 = \frac{x_5}{x_5^0} \end{array} \quad (\text{A.3})$$

$$mr_1 = \frac{m_1 \cdot x_1^{m_1-1}}{x_1^0 m_1} \quad (\text{A.4})$$

$$mr_2 = \frac{m_2 \cdot x_2^{m_2-1}}{x_2^0 m_2} \quad (\text{A.5})$$

$$mr_3 = \frac{m_3 \cdot x_3^{m_3-1}}{x_3^0 m_3} \quad (\text{A.6})$$

$$dxr_1 = \frac{m_1 \cdot x_1^{m_1}}{x_1^0 m_1 + 1} \quad (\text{A.7})$$

$$dxr_2 = \frac{m_2 \cdot x_2^{m_2}}{x_2^0 m_2 + 1} \quad (\text{A.8})$$

$$dxr_3 = \frac{m_3 \cdot x_3^{m_3}}{x_3^0 m_3 + 1} \quad (A.9)$$

$$y = 1. - \left(\frac{x_3 + x_4 + x_5}{x_3^0 + x_4^0 + x_5^0} \right) \quad (A.10)$$

$$z = 1. + \varepsilon \cdot y^\theta \quad (A.11)$$

$$dy = \frac{x_3 + x_4 + x_5}{(x_3^0 + x_4^0 + x_5^0)^2} \quad (A.12)$$

$$\theta r = (\theta \cdot y)^{\theta-1} \cdot dy \quad (A.13)$$

$$d\theta y = \frac{\varepsilon \cdot \theta \cdot y^{\theta-1}}{x_3^0 + x_4^0 + x_5^0} \quad (A.14)$$

$$P_{f3} = (1. - P_f) \cdot (1. - r_3^{m_3}) \quad (A.15)$$

$$c_1 = d'_\ell \cdot x_4^0 + d''_\ell \cdot x_5^0 \quad (A.16)$$

$$c_2 = \frac{d'_\ell \cdot x_4^0}{c_1} \quad (A.17)$$

$$c_2 f_4 = (c_2 \cdot r_5 - 1.) \cdot r_4 + 1. \quad (A.18)$$

$$c_2 f_5 = (1. - c_2 \cdot r_5) \cdot r_4 \quad (A.19)$$

Derivatives for UZTWM (x_1^0):

$$\frac{\partial f_1}{\partial x_1^0} = (dxr_1 \cdot Px) + (u_e \cdot \frac{r_1}{x_1^0}) \quad (A.20)$$

$$\frac{\partial f_2}{\partial x_1^0} = -dxr_1 \cdot Px \cdot (1. - r_2^{m_2}) \quad (A.21)$$

$$\begin{aligned} \frac{\partial f_3}{\partial x_1^0} = & -u_e \cdot ((1. - r_1) \cdot (\frac{-x_3}{(x_1^0 + x_3^0)^2}) + \\ & (\frac{x_3}{x_1^0 + x_3^0}) \cdot (\frac{r_1}{x_1^0})) \end{aligned} \quad (A.22)$$

$$\frac{\partial f_4}{\partial x_1^0} = 0. \quad (A.23)$$

$$\frac{\partial f_5}{\partial x_1^0} = 0. \quad (A.24)$$

$$\begin{aligned} \frac{\partial f_6}{\partial x_1^0} = & (\frac{x_6 - x_1}{x_3^0})^2 \cdot dxr_1 \cdot Px + u_e \cdot (1. - r_1) \cdot (\frac{x_6 - x_1}{(x_1^0 + x_3^0)^2}) - \\ & u_e \cdot (\frac{x_6 - x_1}{x_1^0 + x_3^0}) \cdot \frac{r_1}{x_1^0} + u_e \cdot \frac{r_1}{x_1^0} + \\ & (1. - (\frac{x_6 - x_1}{x_3^0})^2) \cdot r_2^{m_2} \cdot dxr_1 \cdot Px \end{aligned} \quad (A.25)$$

$$\begin{aligned} \frac{\partial f_7}{\partial x_1^0} = & (\frac{x_6 - x_1}{x_3^0})^2 \cdot Px \cdot (-dxr_1) \cdot \beta_1 + Px \cdot (-dxr_1) \cdot r_2^{m_2} \cdot \\ & (1. - \beta_1 - \beta_2) + (1. - (\frac{x_6 - x_1}{x_3^0})^2) \cdot r_2^{m_2} \cdot \\ & (-dxr_1) \cdot Px \cdot \beta_1 \end{aligned} \quad (A.26)$$

Derivatives for UZFWM (x_2^0):

$$\frac{\partial f_1}{\partial x_2^0} = 0 \quad (\text{A.27})$$

$$\frac{\partial f_2}{\partial x_2^0} = r_1^{m_1} \cdot P_x \cdot dxr_2 + c_1 \cdot z \cdot \frac{r_2}{x_2^0} \quad (\text{A.28})$$

$$\frac{\partial f_3}{\partial x_2^0} = -\frac{r_2}{x_2^0} \cdot c_1 \cdot z \cdot P_{f_3} \quad (\text{A.29})$$

$$\frac{\partial f_4}{\partial x_2^0} = c_1 \cdot z \cdot \left(\frac{-r_2}{x_2^0}\right) \cdot (1. - P_{f_3}) \cdot c_2 f_4 \quad (\text{A.30})$$

$$\frac{\partial f_5}{\partial x_2^0} = c_1 \cdot z \cdot \left(\frac{-r_2}{x_2^0}\right) \cdot (1. - P_{f_3}) \cdot c_2 f_5 \quad (\text{A.31})$$

$$\frac{\partial f_6}{\partial x_2^0} = \left(1. - \left(\frac{x_6 - x_1}{x_3^0}\right)^2\right) \cdot dxr_2 \cdot r_1^{m_1} \cdot P_x \quad (\text{A.32})$$

$$\frac{\partial f_7}{\partial x_2^0} = P_x \cdot r_1^{m_1} (-dxd_2) \cdot (1. - \beta_1 - \beta_2) +$$

$$\left(1. - \left(\frac{x_6 - x_1}{x_3^0}\right)^2\right) \cdot (-dxd_2) \cdot$$

$$r_1^{m_1} \cdot P_x \cdot \beta_1 \quad (\text{A.33})$$

Derivatives for LZTWM (x_3^0):

$$\frac{\partial f_1}{\partial x_3^0} = 0 \quad (\text{A.34})$$

$$\frac{\partial f_2}{\partial x_3^0} = -c_1 \cdot \varepsilon \cdot \Theta r \cdot r_2 \quad (\text{A.35})$$

$$\frac{\partial f_3}{\partial x_3^0} = c_1 \cdot z \cdot r_2 \cdot (1. - P_f) \cdot dxr_3 +$$

$$P_{f3} \cdot c_1 \cdot \varepsilon \cdot \Theta r \cdot r_2 +$$

$$u_e \cdot (1. - r_1) \cdot \left(\frac{x_3}{(x_1^0 + x_3^0)^2} \right) \quad (\text{A.36})$$

$$\frac{\partial f_4}{\partial x_3^0} = c_1 \cdot z \cdot r_2 \cdot -((1. - P_f) \cdot dxr_3) \cdot$$

$$c_2 f_4 + (1. - P_{f3}) \cdot$$

$$c_2 f_4 \cdot c_1 \cdot \varepsilon \cdot \Theta r \cdot r_2 \quad (\text{A.37})$$

$$\frac{\partial f_5}{\partial x_3^0} = c_1 \cdot z \cdot r_2 \cdot -(1. - P_f) \cdot dxr_3 \cdot c_2 f_5 +$$

$$(1. - P_{f3}) \cdot c_2 f_5 \cdot c_1 \cdot \varepsilon \cdot \Theta r \cdot r_2 \quad (\text{A.38})$$

$$\frac{\partial f_6}{\partial x_3^0} = \left(\left(\frac{2(x_6 - x_1)^2}{x_3^0} \right) \cdot r_1^{m_1} \cdot Px \right) + (u_e \cdot (1. - r_1) \cdot$$

$$\frac{x_6 - x_1}{(x_3^0 + x_1^0)^2} \cdot \left(\frac{2(x_6 - x_1)^2}{x_3^0} \right) \cdot$$

$$r_2^{m_2} \cdot r_1^{m_1} \cdot Px \quad (\text{A.39})$$

$$\begin{aligned}
 \frac{\partial f_7}{\partial x_3^1} = & \left(\frac{-2(x_6 - x_1)^2}{x_3^0{}^3} \right) \cdot Px \cdot r_1^{m_1} \cdot \beta_1 + \\
 & \left(\frac{2(x_6 - x_1)^2}{x_3^0{}^3} \right) \cdot r_2^{m_2} \cdot r_1^{m_1} \cdot Px \cdot \beta_1 \quad (A.40)
 \end{aligned}$$

Derivatives for LZFPM (x_4^0):

$$\frac{\partial f_1}{\partial x_4^0} = 0 \quad (\text{A.41})$$

$$\frac{\partial f_2}{\partial x_4^0} = -c_1 \cdot \varepsilon \cdot \Theta r \cdot r_2 + z \cdot r_2 \cdot (-d'_l) \quad (\text{A.42})$$

$$\frac{\partial f_3}{\partial x_4^0} = (c_1 \cdot \varepsilon \cdot \Theta r + z \cdot d'_l) \cdot P_{f3} \cdot r_2 \quad (\text{A.43})$$

$$\begin{aligned} \frac{\partial f_4}{\partial x_4^0} = & (c_1 \cdot z \cdot r_2 \cdot ((c_2 \cdot r_5 \cdot (-\frac{r_4}{x_4^0}) + \\ & r_4 \cdot (\frac{d'_l \cdot d''_l \cdot x_5^0}{C_1^2}) \cdot r_5) + \frac{r_4}{x_4^0}) + \\ & (c_2 \cdot r_5 \cdot r_4 - r_4 + 1.) \cdot ((c_1 \cdot \varepsilon \cdot \Theta r \cdot r_2) + \\ & z \cdot r_2 \cdot d'_l)) \cdot (1. - P_{f3}) \end{aligned} \quad (\text{A.44})$$

$$\frac{\partial f_5}{\partial x_4^0} = (c_1 \cdot z \cdot (1. - P_{f3}) \cdot ((\frac{-r_4}{x_4^0}) + c_2 \cdot r_5 \cdot$$

$$\frac{r_4}{x_4^0} - r_4 \cdot \frac{d'_l \cdot d''_l \cdot x_5^0}{C_1^2} \cdot r_5) + (1. - P_{f3}) \cdot$$

$$c_2 f_5 \cdot (c_1 \cdot \varepsilon \cdot \Theta r + z \cdot d'_l)) \cdot r_2 \quad (\text{A.45})$$

$$\frac{\partial f_6}{\partial x_4^0} = 0. \quad (\text{A.46})$$

$$\frac{\partial f_7}{\partial x_4^0} = 0. \quad (\text{A.47})$$

Derivatives for LZFSM (x_5^0):

$$\frac{\partial f_1}{\partial x_5^0} = 0. \quad (A.48)$$

$$\frac{\partial f_2}{\partial x_5^0} = -c_1 \cdot \varepsilon \cdot \Theta r \cdot r_2 + z \cdot r_2 \cdot (-d''_{\ell}) \quad (A.49)$$

$$\frac{\partial f_3}{\partial x_5^0} = (c_1 \cdot \varepsilon \cdot \Theta r \cdot r_2 + z \cdot r_2 \cdot d''_{\ell}) \cdot P_{f3} \quad (A.50)$$

$$\begin{aligned} \frac{\partial f_4}{\partial x_5^0} = & (1. - P_{f3}) \cdot r_2 \cdot (c_1 \cdot z \cdot (c_2 \cdot r_4 \cdot \\ & (-\frac{r_5}{x_5^0}) + r_5 \cdot (\frac{-d'_{\ell} \cdot d''_{\ell} \cdot x_4^0}{c_1^2}) \cdot r_4) + c_2 f_4 \cdot \\ & (c_1 \cdot \varepsilon \cdot \Theta r + z \cdot d''_{\ell})) \end{aligned} \quad (A.51)$$

$$\begin{aligned} \frac{\partial f_5}{\partial x_5^0} = & (c_1 \cdot z \cdot (1. - P_{f3}) \cdot (c_2 \cdot r_4 \cdot \frac{r_5}{x_5^0} + r_5 \cdot \\ & (\frac{-d'_{\ell} \cdot d''_{\ell} \cdot x_4^0}{c_1^2}) \cdot r_4) + ((1. - P_{f3}) \cdot \\ & c_2 f_5) \cdot (c_1 \cdot \varepsilon \cdot \Theta r + z \cdot d''_{\ell})) \cdot r_2 \end{aligned} \quad (A.52)$$

$$\frac{\partial f_6}{\partial x_5^0} = 0. \quad (A.53)$$

$$\frac{\partial f_7}{\partial x_5^0} = 0. \quad (A.54)$$

Derivatives for UZK (d_u):

$$\frac{\partial f_1}{\partial d_u} = 0. \quad (\text{A.55})$$

$$\frac{\partial f_2}{\partial d_u} = -x_2 \quad (\text{A.56})$$

$$\frac{\partial f_3}{\partial d_u} = 0. \quad (\text{A.57})$$

$$\frac{\partial f_4}{\partial d_u} = 0. \quad (\text{A.58})$$

$$\frac{\partial f_5}{\partial d_u} = 0. \quad (\text{A.59})$$

$$\frac{\partial f_6}{\partial d_u} = 0. \quad (\text{A.60})$$

$$\frac{\partial f_7}{\partial d_u} = x_2 \cdot (1. - \beta_1 - \beta_2) \quad (\text{A.61})$$

Derivatives for LZPK (d'_l):

$$\frac{\partial f_1}{\partial d'_l} = 0. \quad (A.62)$$

$$\frac{\partial f_2}{\partial d'_l} = -x_4^0 \cdot z \cdot r_2 \quad (A.63)$$

$$\frac{\partial f_3}{\partial d'_l} = z \cdot r_2 \cdot P_{f3} \cdot x_4^0 \quad (A.64)$$

$$\frac{\partial f_4}{\partial d'_l} = -x_4 + (x_4^0 \cdot z \cdot r_2 \cdot (1. - P_{f3}) \cdot r_4 \cdot r_5) -$$

$$x_4^0 \cdot z \cdot r_2 \cdot (1. - P_{f3}) \cdot r_4 +$$

$$x_4^0 \cdot z \cdot r_2 \cdot (1. - P_{f3}) \quad (A.65)$$

$$\frac{\partial f_5}{\partial d'_l} = x_4^0 \cdot z \cdot r_2 \cdot (1. - P_{f3}) \cdot r_4 \cdot (1. - r_5) \quad (A.66)$$

$$\frac{\partial f_6}{\partial d'_l} = 0. \quad (A.67)$$

$$\frac{\partial f_7}{\partial d'_l} = \left(\frac{x_4}{(1 + \mu)} \right) \cdot (1. - \beta_1 - \beta_2) \quad (A.68)$$

Derivatives for LZSK (d''_{ℓ}) :

$$\frac{\partial f_1}{\partial d''_{\ell}} = 0. \quad (\text{A.69})$$

$$\frac{\partial f_2}{\partial d''_{\ell}} = -x_5^0 \cdot z \cdot r_2 \quad (\text{A.70})$$

$$\frac{\partial f_3}{\partial d''_{\ell}} = z \cdot r_2 \cdot P_{f^3} \cdot x_5^0 \quad (\text{A.71})$$

$$\begin{aligned} \frac{\partial d_4}{\partial d''_{\ell}} = & -x_5^0 \cdot z \cdot r_2 \cdot (1. - P_{f^3}) \cdot r_4 + \\ & x_5^0 \cdot z \cdot r_2 \cdot (1. - P_{f^3}) \end{aligned} \quad (\text{A.72})$$

$$\frac{\partial f_5}{\partial d''_{\ell}} = -x_5 + x_5^0 \cdot z \cdot r_2 \cdot (1. - P_{f^3}) \cdot r_4 \quad (\text{A.73})$$

$$\frac{\partial f_6}{\partial d''_{\ell}} = 0. \quad (\text{A.74})$$

$$\frac{\partial f_7}{\partial d''_{\ell}} = \left(\frac{x_5}{(1 + \mu)} \right) \cdot (1. - \beta_1 - \beta_2) \quad (\text{A.75})$$

Derivatives for ZPERC (ϵ) :

$$\frac{\partial f_1}{\partial \epsilon} = 0. \quad (\text{A.76})$$

$$\frac{\partial f_2}{\partial \epsilon} = -c_1 \cdot y^\theta \cdot r_2 \quad (\text{A.77})$$

$$\frac{\partial f_3}{\partial \epsilon} = c_1 \cdot y^\theta \cdot r_2 \cdot P_{f3} \quad (\text{A.78})$$

$$\frac{\partial f_4}{\partial \epsilon} = c_1 \cdot y^\theta \cdot r_2 \cdot (1. - P_{f3}) \cdot c_2 f_4 \quad (\text{A.79})$$

$$\frac{\partial f_5}{\partial \epsilon} = c_1 \cdot y^\theta \cdot r_2 \cdot (1. - P_{f3}) \cdot c_2 f_5 \quad (\text{A.80})$$

$$\frac{\partial f_6}{\partial \epsilon} = 0. \quad (\text{A.81})$$

$$\frac{\partial f_7}{\partial \epsilon} = 0. \quad (\text{A.82})$$

Derivatives for REXP (θ) :

$$\frac{\partial f_1}{\partial \theta} = 0. \quad (\text{A.83})$$

$$\frac{\partial f_2}{\partial \theta} = -c_1 \cdot \varepsilon \cdot y^\theta \cdot r_2 \cdot \ln y \quad (\text{A.84})$$

$$\frac{\partial f_3}{\partial \theta} = (c_1 \cdot \varepsilon \cdot y^\theta) \cdot \ln y \cdot r_2 \cdot P_{f3} \quad (\text{A.85})$$

$$\begin{aligned} \frac{\partial f_4}{\partial \theta} = c_1 \cdot \varepsilon \cdot y^\theta \cdot \ln y \cdot r_2 \cdot \\ (1. - P_{f3}) \cdot c_2 f_4 \end{aligned} \quad (\text{A.86})$$

$$\frac{\partial f_5}{\partial \theta} = c_1 \cdot \varepsilon \cdot y^\theta \cdot \ln y \cdot r_2 \cdot (1. - P_{f3}) \cdot c_2 f_5 \quad (\text{A.87})$$

$$\frac{\partial f_6}{\partial \theta} = 0. \quad (\text{A.88})$$

$$\frac{\partial f_7}{\partial \theta} = 0. \quad (\text{A.89})$$

Derivatives for PFREE (P_f) :

$$\frac{\partial f_1}{\partial P_f} = 0. \quad (\text{A.90})$$

$$\frac{\partial f_2}{\partial P_f} = 0. \quad (\text{A.91})$$

$$\frac{\partial f_3}{\partial P_f} = -c_1 \cdot z \cdot r_2 \cdot (1. - r_3^{m_3}) \quad (\text{A.92})$$

$$\frac{\partial f_4}{\partial P_f} = c_1 \cdot z \cdot r_2 \cdot (1. - r_3^{m_3}) \cdot c_2 f_4 \quad (\text{A.93})$$

$$\frac{\partial f_5}{\partial P_f} = c_1 \cdot z \cdot r_2 \cdot (1. - r_3^{m_3}) \cdot c_2 f_5 \quad (\text{A.94})$$

$$\frac{\partial f_6}{\partial P_f} = 0. \quad (\text{A.95})$$

$$\frac{\partial f_7}{\partial P_f} = 0. \quad (\text{A.96})$$

Derivatives for SIDE (μ) :

$$\frac{\partial f_1}{\partial \mu} = 0. \quad (\text{A.97})$$

$$\frac{\partial f_2}{\partial \mu} = 0. \quad (\text{A.98})$$

$$\frac{\partial f_3}{\partial \mu} = 0. \quad (\text{A.99})$$

$$\frac{\partial f_4}{\partial \mu} = 0. \quad (\text{A.100})$$

$$\frac{\partial f_5}{\partial \mu} = 0. \quad (\text{A.101})$$

$$\frac{\partial f_6}{\partial \mu} = 0. \quad (\text{A.102})$$

$$\frac{\partial f_7}{\partial \mu} = \frac{-c_1}{(1 + \mu)^2} \cdot (1. - \beta_1 - \beta_2) \quad (\text{A.103})$$

Derivatives for ADIMP (β_1) :

$$\frac{\partial f_1}{\partial \beta_1} = 0. \quad (\text{A.104})$$

$$\frac{\partial f_2}{\partial \beta_1} = 0. \quad (\text{A.105})$$

$$\frac{\partial f_3}{\partial \beta_1} = 0. \quad (\text{A.106})$$

$$\frac{\partial f_4}{\partial \beta_1} = 0. \quad (\text{A.107})$$

$$\frac{\partial f_5}{\partial \beta_1} = 0. \quad (\text{A.108})$$

$$\frac{\partial f_6}{\partial \beta_1} = 0. \quad (\text{A.109})$$

$$\frac{\partial f_7}{\partial \beta_1} = -(d_u \cdot x_2 + \frac{c_1}{(1 + \mu)}) + (\frac{x_6 - x_1}{x_3^0})^2 \cdot$$

$$Px \cdot r_1^{m_1} - Px \cdot r_1^{m_1} \cdot r_2^{m_2} + (1 - (\frac{x_6 - x_1}{x_3^0})^2) \cdot$$

$$r_2^{m_2} \cdot r_1^{m_1} \cdot Px \quad (\text{A.110})$$

Derivatives for PCTIM (β_2) :

$$\frac{\partial f_1}{\partial \beta_2} = 0. \quad (\text{A.111})$$

$$\frac{\partial f_2}{\partial \beta_2} = 0. \quad (\text{A.112})$$

$$\frac{\partial f_3}{\partial \beta_2} = 0. \quad (\text{A.113})$$

$$\frac{\partial f_4}{\partial \beta_2} = 0. \quad (\text{A.114})$$

$$\frac{\partial f_5}{\partial \beta_2} = 0. \quad (\text{A.115})$$

$$\frac{\partial f_6}{\partial \beta_2} = 0 \quad (\text{A.116})$$

$$\frac{\partial f_7}{\partial \beta_2} = -(d_u \cdot x_2 + \frac{c_1}{(1+\mu)}) + Px -$$

$$Px \cdot r_1^{m_1} \cdot r_2^{m_2} \quad (\text{A.117})$$

Derivatives for UZTWC (x_1) :

$$\frac{\partial f_1}{\partial x_1} = -m_1 \cdot mr_1 \cdot Px - u_e \cdot \left(\frac{1}{x_1^0}\right) \quad (A.118)$$

$$\frac{\partial f_2}{\partial x_1} = m_1 \cdot mr_1 \cdot Px \cdot (1 - r_2^{m_2}) \quad (A.119)$$

$$\frac{\partial f_3}{\partial x_1} = u_e \cdot \left(\frac{1}{x_1^0}\right) \cdot \left(\frac{x_3}{x_1^0 + x_3^0}\right) \quad (A.120)$$

$$\frac{\partial f_4}{\partial x_1} = 0. \quad (A.121)$$

$$\frac{\partial f_5}{\partial x_1} = 0. \quad (A.122)$$

$$\frac{\partial f_6}{\partial x_1} = \left(1 - \left(\frac{x_6 - x_1}{x_3^0}\right)^2\right) \cdot mr_1 \cdot (1 - r_2^{m_2} \cdot Px) +$$

$$r_1^{m_1} \cdot (1 - r_1^{m_2}) \cdot Px \cdot \left(2 \cdot \frac{x_6 - x_1}{(x_3^0)^2}\right) +$$

$$\frac{u_e \cdot (1 - r_1)}{(x_3^0 + x_1^0)} + \left(\frac{x_6 - x_1}{x_3^0 + x_1^0}\right) \cdot \left(\frac{u_e}{x_1^0}\right) - \frac{u_e}{x_1^0} \quad (A.123)$$

$$\frac{\partial f_7}{\partial x_1} = \left(\frac{x_6 - x_1}{x_3^0}\right) \cdot Px \cdot mr_1 \cdot \beta_1 -$$

$$r_1^{m_1} \cdot \beta_1 \cdot 2 \cdot \left(\frac{x_6 - x_1}{(x_3^0)^2}\right) \cdot Px +$$

$$Px \cdot mr_1 \cdot r_2^{m_2} \cdot (1 - \beta_1 - \beta_2) +$$

$$\left(1 - \left(\frac{x_6 - x_1}{x_3^0}\right)^2\right) \cdot r_2^{m_2} \cdot mr_1 \cdot Px \cdot \beta_1 +$$

$$r_1^{m_1} \cdot Px \cdot \beta_1 \cdot 2 \cdot \left(\frac{x_6 - x_1}{(x_3^0)^2}\right) \cdot r_2^{m_2} \quad (A.124)$$

Derivatives for UZFWC (x_2) :

$$\frac{\partial f_1}{\partial x_2} = 0. \quad (A.125)$$

$$\frac{\partial f_2}{\partial x_2} = -r_1^{m_1} \cdot mr_2 \cdot Px - d_u - \frac{c_1 \cdot z}{x_2^0} \quad (A.126)$$

$$\frac{\partial f_3}{\partial x_2} = \frac{c_1 \cdot z}{x_2^0} \cdot P_{f_3} \quad (A.127)$$

$$\frac{\partial f_4}{\partial x_2} = \frac{c_1 \cdot z}{x_2^0} \cdot (1. - P_{f_3}) \cdot c_2 f_4 \quad (A.128)$$

$$\frac{\partial f_5}{\partial x_2} = \frac{c_1 \cdot z}{x_2^0} \cdot (1. - P_{f_3}) \cdot c_2 f_5 \quad (A.129)$$

$$\frac{\partial f_6}{\partial x_2} = \left(1. - \left(\frac{x_6 - x_1}{x_3^0}\right)^2\right) \cdot r_1^{m_1} \cdot (-mr_2) \cdot Px \quad (A.130)$$

$$\frac{\partial f_7}{\partial x_2} = d_u \cdot (1. - \beta_1 - \beta_2) + Px \cdot r_1^{m_1} \cdot mr_2 \cdot$$

$$(1. - \beta_1 - \beta_2) + \left(1. - \left(\frac{x_6 - x_1}{x_3^0}\right)^2\right) \cdot$$

$$mr_2 \cdot r_1^{m_1} \cdot Px \cdot \beta_1 \quad (A.131)$$

Derivatives for LZTWC (x_3) :

$$\frac{\partial f_1}{\partial x_3} = 0. \quad (\text{A.132})$$

$$\frac{\partial f_2}{\partial x_3} = c_1 \cdot r_1 \cdot \epsilon \cdot \theta \cdot y^{\theta-1} \cdot (x_3^0 + x_4^0 + x_5^0)^{-1} \quad (\text{A.133})$$

$$\frac{\partial f_3}{\partial x_3} = -c_1 \cdot z \cdot r_2 \cdot (1 - P_f) \cdot mr_3 +$$

$$P_{f3} \cdot (-c_1 \cdot \epsilon \cdot \theta \cdot y^{\theta-1} \cdot r_2) \cdot (x_3^0 + x_4^0 + x_5^0)^{-1} -$$

$$u_e \cdot (1 - r_1) \cdot (x_1^0 + x_3^0)^{-1} \quad (\text{A.134})$$

$$\frac{\partial f_4}{\partial x_3} = (c_1 \cdot z \cdot r_2 \cdot (1 - P_f) \cdot mr_3 - (1 - P_{f3}) \cdot$$

$$(c_1 \cdot \epsilon \cdot \theta \cdot y^{\theta-1} \cdot r_2) \cdot$$

$$(x_3^0 + x_4^0 + x_5^0)^{-1}) \cdot c_2 f_4 \quad (\text{A.135})$$

$$\frac{\partial f_5}{\partial x_3} = (c_1 \cdot z \cdot (1 - P_f) \cdot mr_3 - c_1 \cdot \epsilon \cdot \theta \cdot y^{\theta-1} \cdot$$

$$(x_3^0 + x_4^0 + x_5^0)^{-1} \cdot (1 - P_{f3})) \cdot (r_2 \cdot c_2 f_5) \quad (\text{A.136})$$

$$\frac{\partial f_6}{\partial x_3} = 0. \quad (\text{A.137})$$

$$\frac{\partial f_7}{\partial x_3} = 0. \quad (\text{A.138})$$

Derivatives for LZFPC (x_4) :

$$\frac{\partial f_1}{\partial x_4} = 0. \quad (A.139)$$

$$\frac{\partial f_2}{\partial x_4} = c_1 \cdot r_2 \cdot \varepsilon \cdot \theta \cdot y^{\theta-1} \cdot (x_3^0 + x_4^0 + x_5^0)^{-1} \quad (A.140)$$

$$\frac{\partial f_3}{\partial x_4} = -c_1 \cdot \varepsilon \cdot \theta \cdot y^{\theta-1} \cdot r_2 \cdot$$

$$(x_3^0 + x_4^0 + x_5^0)^{-1} \cdot P_{f3} \quad (A.141)$$

$$\frac{\partial f_4}{\partial x_4} = -d'_l + (c_1 \cdot z \cdot (c_2 \cdot r_5 - 1.) \cdot x_4^0^{-1} -$$

$$c_2 f_4 \cdot c_1 \cdot \varepsilon \cdot \theta \cdot y^{\theta-1} \cdot (x_3^0 + x_4^0 + x_5^0)^{-1}) \cdot$$

$$r_2 \cdot (1. - P_{f3}) \quad (A.142)$$

$$\frac{\partial f_5}{\partial x_4} = (c_1 \cdot z \cdot (1. - c_2 \cdot r_5) \cdot x_4^0^{-1} -$$

$$c_1 \cdot \varepsilon \cdot \theta \cdot y^{\theta-1} \cdot (x_3^0 + x_4^0 + x_5^0)^{-1} \cdot$$

$$c_2 f_5 \cdot r_2 \cdot (1. - P_{f3}) \quad (A.143)$$

$$\frac{\partial f_6}{\partial x_4} = 0. \quad (A.144)$$

$$\frac{\partial f_7}{\partial x_4} = d'_l \cdot (1. + \mu)^{-1} \cdot (1. - \beta_1 - \beta_2) \quad (A.145)$$

Derivatives for LZFSC (x_5) :

$$\frac{\partial f_1}{\partial x_5} = 0. \quad (A.146)$$

$$\frac{\partial f_2}{\partial x_5} = c_1 \cdot r_2 \cdot \varepsilon \cdot \theta \cdot y^{\theta-1} \cdot (x_3^0 + x_4^0 + x_5^0)^{-1} \quad (A.147)$$

$$\frac{\partial f_3}{\partial x_5} = -c_1 \cdot \varepsilon \cdot \theta \cdot y^{\theta-1} \cdot r_2 \cdot$$

$$(x_3^0 + x_4^0 + x_5^0)^{-1} \cdot P_{f3} \quad (A.148)$$

$$\frac{\partial f_4}{\partial x_5} = (c_1 \cdot z \cdot (c_2 \cdot x_5^{0-1} \cdot r_4) - c_2 f_4 \cdot$$

$$c_1 \cdot \varepsilon \cdot \theta \cdot y^{\theta-1} \cdot (x_3^0 + x_4^0 + x_5^0)^{-1}) \cdot$$

$$r_2 \cdot (1. - P_{f3}) \quad (A.149)$$

$$\frac{\partial f_5}{\partial x_5} = -d_{\ell}'' + (c_1 \cdot z \cdot (-c_2) \cdot x_5^{0-1} \cdot r_4 -$$

$$c_1 \cdot \varepsilon \cdot \theta \cdot y^{\theta-1} \cdot (x_3^0 + x_4^0 + x_5^0)^{-1} \cdot$$

$$c_2 f_5 \cdot r_2 \cdot (1. - P_{f3}) \quad (A.150)$$

$$\frac{\partial f_6}{\partial x_5} = 0. \quad (A.151)$$

$$\frac{\partial f_7}{\partial x_5} = d_{\ell}'' \cdot (1. + \mu)^{-1} \cdot (1. - \beta_1 - \beta_2) \quad (A.152)$$

Derivatives for ADIMC (x_6) :

$$\frac{\partial f_1}{\partial x_6} = 0. \quad (\text{A.153})$$

$$\frac{\partial f_2}{\partial x_6} = 0. \quad (\text{A.154})$$

$$\frac{\partial f_3}{\partial x_6} = 0. \quad (\text{A.155})$$

$$\frac{\partial f_4}{\partial x_6} = 0. \quad (\text{A.156})$$

$$\frac{\partial f_5}{\partial x_6} = 0. \quad (\text{A.157})$$

$$\frac{\partial f_6}{\partial x_6} = (-2. \cdot \frac{x_6 - x_1}{(x_3^0)^2}) \cdot r_1^{m_1} \cdot (1. - r_2^{m_2}) \cdot$$

$$Px - u_e \cdot (1. - r_1) \cdot (x_3^0 + x_1^0)^{-1} \quad (\text{A.158})$$

$$\frac{\partial f_7}{\partial x_6} = (2. \cdot (\frac{x_6 - x_1}{(x_3^0)^2}) \cdot Px \cdot r_1^{m_1} \cdot \beta_1) \cdot$$

$$(1. - r_2^{m_2}) \quad (\text{A.159})$$

Derivatives for Px:

$$\frac{\partial f_1}{\partial Px} = 1. - r_1^{m_1} \quad (A.160)$$

$$\frac{\partial f_2}{\partial Px} = r_1^{m_1} \cdot (1. - r_2^{m_2}) \quad (A.161)$$

$$\frac{\partial f_3}{\partial Px} = 0. \quad (A.162)$$

$$\frac{\partial f_4}{\partial Px} = 0. \quad (A.163)$$

$$\frac{\partial f_5}{\partial Px} = 0. \quad (A.164)$$

$$\frac{\partial f_6}{\partial Px} = \left(1. - \left(\frac{x_6 - x_1}{x_3^0}\right)^2 \cdot r_1^{m_1}\right) - \left(1. - \left(\frac{x_6 - x_1}{x_3^0}\right)^2\right) \cdot$$

$$r_2^{m_2} \cdot r_1^{m_1} \quad (A.165)$$

$$\frac{\partial f_7}{\partial Px} = \beta_2 + \left(\frac{x_6 - x_1}{x_3^0}\right)^2 \cdot r_1^{m_1} \cdot \beta_1 +$$

$$r_1^{m_1} \cdot r_2^{m_2} \cdot (1. - \beta_1 - \beta_2) +$$

$$\left(1. - \left(\frac{x_6 - x_1}{x_3^0}\right)^2\right) \cdot r_2^{m_2} \cdot r_1^{m_1} \cdot \beta_1 \quad (A.166)$$

(Continued from inside front cover)

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