INCORPORATING UNCERTAINTY INTO PARAMETER ESTIMATION AND EVALUATING THE AGNPS MODEL WITH UNCERTAIN PARAMETERS

By

PENG YUE

Bachelor of Science
University of Tianjin
Tianjin, China
1985

Master of Science
University of Tianjin
Tianjin, China
1988

Submitted to the Faculty of the
Graduate College of the
Oklahoma State University
in partial fulfillment of
the requirements for
the Degree of
DOCTOR OF PHILOSOPHY
May, 1997

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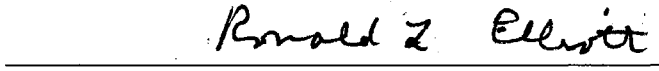
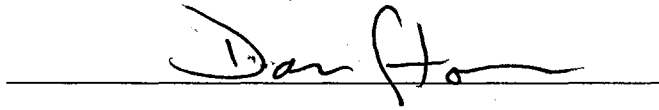
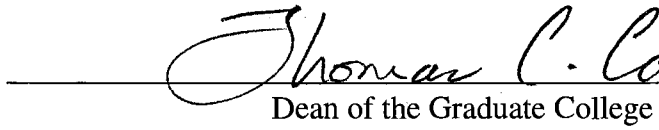
Thesis Approved:

Thesis Advisor







Dean of the Graduate College

ACKNOWLEDGMENTS

I wish to express my sincere appreciation to my major advisor, Regents Professor and Sarkey's Distinguished Professor Dr. C. T. Haan, for his advice, guidance and encouragement throughout the completion of my graduate program. His wealth of knowledge and his great patience contributed immeasurably to my research efforts. This appreciation is also extended to the remainder of the advisory committee, Dr. R. L. Elliott, Dr. Barry K. Moser and Dr. Daniel E. Storm, for their supportive advice and constructive comments.

I would also like to acknowledge my sincere gratitude to Dr. D. Edwards, Associate Professor at University of Kentucky, for providing me with the data for this study. These data were instrumental to this research. I am very grateful to Biosystems and Agricultural Engineering Department, OSU, for providing me with financial resources, which made my research possible.

Special thanks go to the friends and family members who came down with me during the course of the research. Finally, I am most grateful to my wife, Zhengping Yan, and my son, Spencer T. Yue, for their love, willingness to sacrifice and support.

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LIST OF SYMBOLS

$\underline{X}$ = The matrix named X.

$\underline{X}^T$ = The transpose of $\underline{X}$.

$\underline{X}^{-1}$ = The inverse of $\underline{X}$.

tr($\underline{X}$) = The trace of $\underline{X}$.

|$\underline{X}$| = The determinant of $\underline{X}$.

$\underline{\hat{X}}$ = Estimated values of $\underline{X}$.

$\underline{Y}$ = The observed values of a response modeled as some function f(*).

$\underline{\hat{Y}}$ = The values of $\underline{Y}$ as estimated by function f(*).

$\bar{Y}$ = The mean of Y.

C_v = The coefficient of variation.

$\underline{\Theta}$ = The random model parameters.

f($\underline{x}$, $\underline{\theta}$) = The function of the model input vector $\underline{x}$ and the parameter vector $\underline{\theta}$.

$\underline{e}$ = The residual vector, which is the difference between $\underline{Y}$ and $\underline{\hat{Y}}$.

$\underline{\eta}$ = Transformed residual vector.

$\underline{\beta}$ = The regression coefficients.

p($\underline{X}$, $\underline{\Theta}$) = The joint probability density function of random variables $\underline{X}$ and random parameters $\underline{\Theta}$.

p($\underline{\Theta}$) = The prior probability density function of the random parameters $\underline{\Theta}$.

p($\underline{\Theta}$ /$\underline{Y}$) = The posterior probability density function of the random parameters $\underline{\Theta}$.

$l(\underline{\Theta})$ = The likelihood function of the random parameters $\underline{\Theta}$.

μ_x , σ_x^2 = The expected mean and variance of random variable X.

$\bar{X}$, S_x^2 = The sample mean and variance of random variable X.

EXP() = The exponential operator.

$\prod_{i=1}^{n}$ = The product operator.

$\propto$ = The proportional operator.

$\underline{J}$ = The Jacobian matrix.

l_x = The lower confidence limit of random variable X.

u_x = The upper confidence limit of random variable X.

$N(\mu, \sigma^2)$ = Normally distributed with mean μ and variance σ^2.

CHAPTER I

INTRODUCTION

Hydrologic modeling has become commonplace. Virtually all hydrologic designs, more or less, are based on the results of applying a hydrologic model. Many hydrologic models, from simple regression to very complicated physically based models, have been developed to represent hydrologic systems. In applying a hydrologic model, no matter how simple or complex the model is, two important problems must be considered, parameter estimation or calibration and model evaluation. Traditionally, scientists hypothesize that there exists a set of "true" but unknown constants for input parameters in hydrologic modeling. This set of constants can be estimated by adjusting parameters in the model to make the model predictions agree with the corresponding observed data. With these estimated "true" parameters, most hydrologic models provide certain predictions. However, this approach ignores the fact that hydrologic processes such as rainfall, runoff, etc., are stochastic. Because any function of a random variable is itself a random variable (Haan, 1977), all hydrologic processes are to some degree uncertain. Therefore, even though particular predictions are given by a model, uncertainty is involved in these predictions because one can not be sure how good these predictions are.

Vicens et al. (1975) classified hydrologic uncertainty into three categories:

1. The inherent variability in natural processes;
2. Model uncertainty;
3. Parameter uncertainty.

The inherent variability in natural processes refers to variability in space and time of meteorologic events such as rainfall, temperature, sun radiation, etc. The observed data used in hydrologic design are only a small part of the population of these events. Uncertainty arises because samples used to calibrate hydrologic models may not characterize the population of hydrologic events very well. It can be expected that this kind of uncertainty will be reduced when the sample size gets larger.

Model uncertainty arises because one can not be sure that a specific hydrologic process is completely and correctly modeled. Even the most complex physically based model is still incomplete simply because the real world is too complicated to model exactly. Actually, all hydrologic models are to some degree parametric, empirical, and lumped (Haan, 1989). This may indicate that all hydrologic models have to some extent uncertainties. With a better understanding and description of the hydrologic process being modeled, model uncertainty may be reduced.

In calibrating a hydrologic model, it is customary to assume that all data used in calibration are observed correctly and to assume that all input uncertainties are in the parameters. Thus, for a given model, parameter uncertainty reflects incompleteness in the model, incomplete information and inadequate parameter estimation techniques (Haan,

1989). Different parameter estimation techniques will typically give different parameter estimates. There are many kinds of uncertainties involved in parameters. In practice parameters are often used to represent nearly all uncertainty in hydrologic modeling.

With an available model and observed data, we can not control the first and the second type of uncertainties, but we can control parameter uncertainty to an extent by using an appropriate estimation technique and identifying the uncertainty in input parameters. Conventional parameter estimation techniques such as Maximum Likelihood, Least Squares and Least Absolute Value, only provide point estimates. However, one is not sure how good these point estimates are. In other words, the uncertainty involved in these point estimates is unknown. Due to uncertainties in parameter estimation, it is impossible to determine exactly the true point estimates. We have to settle for the next best: a specification of the most likely range of point parameter estimates in the form of a probability density function (pdf). With uncertainty in parameters, model predictions must be uncertain. Eventually, the only certainty is uncertainty (Morgan and Henrion, 1992). Evaluating the performance of a model recognizing uncertainty in input parameters is essential if one wants to assign confidence limits to model predictions.

Objectives

The objectives of this study were to:

1. Evaluate the efficiency of the Bayesian methodology by comparing the point

estimates of input parameters by the Bayesian methodology with those by the Least Squares method.

2. Improve the method of analyzing uncertainty in the parameters of hydrologic models.

3. Evaluate model performance in a probabilistic manner by studying the impact of parameter uncertainty on model predictions when parameters are estimated using prior information, site-specific information, or posterior information.

General Procedure

The Agricultural Non-Point Source pollution model (AGNPS)(Young et al., 1987) was selected for this study. Curve Number (CN) and land slope values in AGNPS were estimated by the generalized least square approach for multiple model responses (minimizing the objective function $O=[\Sigma e_{1i}^2+\Sigma e_{2i}^2+\bullet\bullet\bullet]$, where the first subscript of e represents the model output being predicted, the second subscript of e represents the observation, and e is the error in the prediction). The same parameters in AGNPS were estimated by the Bayesian approach based on the same observed data. Comparisons were made to see if there was a significant difference between these two sets of parameters estimated from the different techniques.

The Least Squares parameter estimation is the most widely used and accepted method in hydrologic and water quality modeling. If the point estimates of input parameters by the Bayesian method are close to those by Least Squares, the Bayesian method may be considered as a good parameter estimation technique in hydrologic and

water quality modeling. Once the Bayesian methodology was proven effective, the Bayesian method was employed to determine the probability density functions of the model parameters CN and land slope.

With the distribution of the model parameters, the probability density function of the model predictions can be found by Monte Carlo simulation. Three conditions regarding parameter distributions were considered in generating pdfs for the model predictions: 1) prior information from published literature; 2) site specific information from observed data; and 3) posterior information by incorporating priori information into the site specific information. The 90% and 95% confidence intervals were placed on the pdfs of the model predictions for different types of parameter information. The width of the intervals is a measure of uncertainty in model predictions. If the observed data falls within the confidence intervals for some type of parameter information, the model predictions in the same case may be viewed as statistically acceptable and the input parameters may be considered to be estimated properly. The effects of incorporating prior information on the uncertainty of the model responses were studied.

CHAPTER II

LITERATURE REVIEW

Literature reviewed in support of this study included work which addressed parameter estimation, uncertainty analysis techniques and model evaluation. Accordingly, this chapter discusses four of the most commonly used parameter estimation criteria, namely, Least Squares, Absolute Value, Maximum Likelihood Function and Bayesian Determinant criteria. Model validation and some criteria for evaluating how well a model with the best estimated parameters can predict future events are discussed. Finally three methods of analyzing the impact of model input uncertainty on model output uncertainty, Sensitivity Analysis, First Order Analysis (FOA) and Monte Carlo Simulation (MCS), are presented.

Calibration of Hydrologic and Water Quality Models

Many hydrologic models have been developed to simulate hydrologic systems, groundwater systems, water quality systems and/or combinations of these systems. Some examples of such models are USLE (Universal Soil Loss Equation), ANSWERS (Areal Nonpoint Source Watershed Environmental Response Simulation), AGNPS (Agricultural Nonpoint Source pollution model). Any hydrologic model, no matter how simple or

complex it is, can generally be represented as (Haan, 1989)

$$\underline{O} = f(\underline{I}, \underline{P}, t) + \underline{e} \tag{1}$$

where $\underline{O}$ is an n×k matrix of hydrologic responses to be modeled, $\underline{f}$ is a collection of functional relationships, $\underline{I}$ is an n×m matrix of inputs, $\underline{P}$ is a vector of p parameters, t is time, $\underline{e}$ is an n×k matrix of errors, n is the number of data points, k is the number of responses, m is the number of inputs, and p is the number of parameters.

The inputs $\underline{I}$ are called variables or state variables by some authors (Troutman, 1985). It is not always clear how to distinguish $\underline{I}$ and $\underline{P}$. However, this is not of extreme importance. The fact we have classified all model input elements as either $\underline{I}$ or $\underline{P}$ does not necessarily mean we are going to calibrate the model by adjusting all the parameters. In practice only a few of the most sensitive parameters are estimated by calibration.

If we let $\underline{\hat{O}}$ represent the model predictions and $\underline{O}$ represent what actually occurs, then the error term $\underline{e}$ can be expressed as

$$\underline{e} = \underline{O} - \underline{\hat{O}} \tag{2}$$

$$\underline{\hat{O}} = f(\underline{I}, \underline{P}, t) \tag{3}$$

Parameters in the model are usually estimated by comparing the observed data with the model predictions based on an objective function related to error terms. This procedure

is called model calibration. However, not every parameter has to be estimated by model calibration. Some parameters may be directly estimated by measurement or from tables and/or charts, and some may be indirectly estimated by calculations based on measurements. Lacking measurement data, some parameters may have to be estimated based on personal experience or expert judgement.

Usually, hydrologic models have a large number of parameters. For instance, AGNPS has more than twenty parameters for each cell. If the watershed to be modeled is divided into ten cells, the total parameters will be more than two hundred. The more parameters a model has, the more difficult is the model calibration. It is almost impossible to calibrate a model by adjusting hundreds of parameters. In practice there are two cases when we do not need to estimate parameters by calibration. We do not calibrate the parameters when changing the parameter does not change the model responses very much. These parameters are often viewed as insensitive and are usually held constant in model calibration. We do not calibrate the parameters if we have independent knowledge about the values of these parameters.

It might be argued that calibration for a physically based model may not be necessary since the calibration lessens the extent to which the model may be characterized as physically based. However, "performing a calibration, provided it is done and interpreted correctly, does not make a model any less physically based ...", as Troutman (1985) pointed out, "Given that the model is well-behaved, ... it is a mathematical fact that the parameter estimates will tend to be close to the true parameter values." Once we accept the above statement, we may say that the degree of difference between the parameter estimates by calibration and the

physically based parameters may indicate the degree of physical significance of the model, provided that an appropriate calibration scheme is employed and that the calibration data are adequate and appropriate.

The most common parameter estimation schemes reported in water resources literature include:

1. Least squares
2. Minimization of absolute errors
3. Maximum likelihood estimation
4. Bayesian estimation

The function and efficiency of each method are different. Even for the same model and the same observed data, they may produce different sets of parameters. These methods, however, are not completely independent of each other. The relationship among them will be discussed later.

Least Squares

The Least Squares method is the most widely used parameter estimation method in hydrologic modeling. Least Squares is a straight forward method and is easy to use. It is most widely used in linear regression where it has proven to be an efficient and robust method. Least Squares produces model parameters that minimize the sum of the squares of the differences between model responses and the corresponding observed data. In the case of the linear regression model (Haan, 1977)

$$\underline{Y} = \underline{X}\underline{\beta} + \underline{\epsilon} \tag{4}$$

where $\underline{Y}$ is a n×1 vector of dependent variables, $\underline{X}$ is a n×p matrix of independent variables, $\underline{\beta}$ is a p×1 vector of regression coefficients (parameters) and $\underline{\epsilon}$ is a n×1 vector of errors. The least squares method for this model can be expressed as

$$\min_{\underline{\beta}}[OF] = \sum_{i=1}^{n} [Y_i - \underline{X}_i\underline{\beta}]^2 \tag{5}$$

where Y_i is the *i*th observed value of the dependent variable, and $\underline{X}_i$ is the *i*th row of the n×p matrix of independent variables. The best set of parameters is found by adjusting parameters ($\underline{\beta}$) until equation (5) is satisfied. Because a linear model using the least squares method insures that the sum of the errors between model predictions and the corresponding observed data is always equal to zero, least squares' parameter estimates are unbiased.

It is worth noting that no assumptions have been made to this point concerning the regression model. In order to use some well-developed theorems concerning hypothesis testing and confidence interval estimation, it is necessary to make the assumption that the $\underline{\epsilon}_i$ are identically and independently distributed as a normal distribution with a mean of zero and a variance of σ^2 (Haan, 1977). Based on this assumption, confidence intervals can be placed on both model predictions and model parameters.

When least squares is extended to nonlinear systems, the concept can be expressed in the form

$$\min_{p} OF = \sum_{i=1}^{n} [O_i - \hat{O}_i]^2 \qquad (6)$$

where O_i is the observed data, and $\hat{O}_i$ is the corresponding model predictions. Parameter estimation from equation (6) is called the ordinary least squares method (OLS). In nonlinear cases, the least squares method can not guarantee that the sum of the errors between model predictions and the corresponding observed data is equal to zero. In other words, parameter estimates from OLS may not necessarily be unbiased. Note that there are still no assumptions concerning the stochastic nature of the errors to be made up to this point. Similar to the linear case, in order to make statements about the optimization of the parameter estimates, some assumptions concerning the stochastic nature of the errors are necessary. The following assumptions have been made for OLS method, because under these assumptions, OLS becomes identical to the maximum likelihood method. This gives the OLS method more statistical meaning. These assumptions are:

1. The errors have a mean of zero.
2. The errors are statistically independent of each other.
3. The errors are identically distributed with a constant variance of σ^2.
4. The errors are normally distributed.

When the above assumptions are satisfied, the least squares estimate will have the properties of unbiasedness, minimum variance, and asymptotic efficiency. These assumptions should be tested after parameter optimization. Unfortunately, as Clarke (1973) and Sorooshian and Dracup (1980) pointed out, the least squares assumptions are particularly

strong and often are not satisfied by the errors of hydrologic models. If one or more assumptions are violated, some type of transformation of the model errors should be taken to correct the violations of the assumptions, and parameters should be reoptimized. This topic will be discussed later.

Using principles from OLS, some alternative methods have been developed such as the weighted least squares (WLS), also called generalized least squares (GLS) (e.g. Kuczera, 1982). For instance, in rainfall-runoff models more weight might be assigned to the larger runoff since hydrologic designs are usually controlled by peak flow. The objective function and the weighting factor used by U.S. Army Corps of Engineers are (Sorooshian and Dracup, 1980)

$$\min_{\underline{p}} OF = \underline{e}^T \underline{w}\, \underline{e} \tag{7}$$

$$w_i = \frac{O_i + \bar{O}}{2\bar{O}} \tag{8}$$

where $\underline{e}^T = (e_1, e_2, ..., e_n)$ is a vector of errors, w_i is an n×n specified weight diagonal matrix, $\bar{O}$ is the average of the runoff. This weighted least squares method will improve the reproduction of peak flow because more weight is placed on peak flow. However, placing emphasis on fitting the peak flows in the calibration phase may violate the assumption of homogeneous variance. Sorooshian and Dracup (1980) indicated the above weighted least squares scheme is in direct conflict with the principles of the maximum likelihood theory.

To this point the parameter estimation techniques discussed are only for one model output (one dependent variable). However, many hydrologic models have more outputs. GLS offers a promising approach for dealing with several outputs. For example, for rainfall-runoff modeling, the model outputs may be peak flow and runoff volume. Let $e_{11}, e_{12}, ..., e_{1n}$ represent the errors for peak flow and $e_{21}, e_{22}, ..., e_{2n}$ represent the errors for runoff volume. The vector of errors in equation (7) is substituted by

$$\underline{e}^T = [e_{11}, e_{21}, \cdots, e_{1n}, e_{2n}] \tag{9}$$

Kuczera (1982) employed GLS for calibration of a rainfall-runoff model where measurements on ground water elevation as well as runoff are available. He points out that the ground water data, if properly exploited, can lead to parameter estimates more stable than those using only precipitation-runoff data. This error structure can be extended to any number of available model outputs. Now if different weights are assigned to each of the model outputs, for instance, w_1 to peak flow and w_2 to runoff volume, equation (7) becomes

$$\min_{\underline{p}} OF = w_1 \sum_{i=1}^{n} e_{1i}^2 + w_2 \sum_{i=1}^{n} e_{2i}^2 \tag{10}$$

where w_1 and w_2 may be related to the importance of peak flow and runoff volume. In this study, this form of generalized least squares will be used as a comparison to the Bayesian determinant criteria.

Minimization of Absolute Errors

The minimization of absolute errors method (MAE) requires minimizing the sum of the absolute errors between model predictions and the corresponding observed data. It can be expressed in the form

$$\min_{\underline{p}} OF = \sum_{i=1}^{n} | O_i - \hat{O}_i | \qquad (11)$$

where O_i, $\hat{O}_i$ and $\underline{p}$ have the same meaning as in equation (6). Similar to the least squares method, MAE is a straight forward method. Also, under some assumptions it becomes identical to the maximum likelihood method. There are four primary assumptions for the MAE method. The first three assumptions for the least squares method still apply to the minimization of absolute errors. Only the fourth assumption is different. The assumptions for MAE are (Troutman, 1985):

1. The errors have a mean of zero.
2. The errors are statistically independent of each other.
3. The errors are identically distributed with a constant variance of σ^2.
4. The errors follow a double exponential distribution.

Troutman (1985) stated that if a model is correctly specified, in the sense that the probability distribution of errors is centered around zero for all events, parameter estimates obtained by least squares and those obtained by minimization of sum of absolute errors should tend to have the same values as the sample size grows larger. However, in reality no

model is perfect. In some circumstances, one method may be superior to the other. Troutman (1985) evaluated the least squares method and MAE method both with and without a logarithmic transform correction, and concluded that MAE optimization with a logarithmic transform seemed to give the best results for the validation period.

Maximum Likelihood Estimation

The maximum likelihood technique is probably the most general and widely used procedure for parameter estimation in the field of statistics (Troutman, 1985). What makes it different from other procedures such as OLS and MAE is that it first has to assume the structure of the errors e_1, e_2, ..., e_n. The idea behind the maximum likelihood estimation (MLE) method is that the errors are considered as random variables. Their joint probability distribution is $p_e(\underline{e}/\underline{p})$. Since the errors are assumed to be independently distributed, the joint probability distribution can be written as $p(e_1/\underline{p}).p(e_2/\underline{p})...p(e_n/\underline{p})$. This expression is known as the likelihood function. Maximum likelihood estimates are those values which maximize the likelihood function. Obviously, when different probability distributions are assigned to the errors, the likelihood function will be different. One typical set of assumptions about the errors is that the errors are assumed to be identically, independently and normally distributed with mean of zero and variance σ^2. Under this assumptions, the likelihood function is

$$L_n(\underline{p}, s^2) = \prod_{i=1}^{n} (2\pi s^2)^{-1/2} \exp\{-(2s^2)^{-1} e_i^2\} \qquad (12)$$

where s^2 is the sample estimate of error variance σ^2. Because taking logarithms is a monotonic operator, maximum likelihood estimates are not affected by one to one logarithmic transformations. The logarithm of the likelihood function is often used in parameter estimation. The log likelihood function corresponding to equation (12) is

$$\ln L_n(\underline{p}, s^2) = -\frac{n}{2}\ln(2\pi) - \frac{1}{2}\sum_{i=1}^{n}\ln s^2 - \frac{1}{2}\sum_{i=1}^{n} s^{-2} e_i^2 \qquad (13)$$

Parameter estimates are sought that maximize either equation (12) or (13).

Because the likelihood function depends explicitly on the assumptions regarding the error structure, it is more general and may be applied in situations where the error structure is more complicated. Beck and Arnold (1977) and Troutman (1985) demonstrate how the maximum likelihood method can be related to other parameter estimation techniques such as least squares, weighted least squares and minimization of absolute errors. Sorooshian and Dracup (1980) discussed the application of maximum likelihood estimation with correlated and heteroscedastic errors. Sorooshian (1981) evaluated MLE, OLS and WLS in a rainfall-runoff model and concluded that the MLE criterion which was formulated based on the heteroscedastic error assumption produced the best set of parameters compared to those of OLS and WLS.

Maximum likelihood estimation is also used with several dependent variables. Troutman (1985) described the application of the maximum likelihood method in a two dependent variables case. In order to apply the MLE procedure, the errors e_{1i} , e_{2i} (where the

first subscript 1 and 2 refer to two dependent variables, for example peak flow and runoff volume in rainfall-runoff modeling) are assumed to have a bivariate normal distribution with zero mean and a covariance matrix that is estimated along with the physical parameters. It may be shown that maximization of the likelihood function is equivalent to minimization of the following equation (Troutman, 1985)

$$W_n(\underline{p}) = \sum_{i=1}^{n} (O_{1i} - \hat{O}_{1i})^2 \cdot \sum_{i=1}^{n} (O_{2i} - \hat{O}_{2i})^2 - [\sum_{i=1}^{n} (O_{1i} - \hat{O}_{1i})(O_{2i} - \hat{O}_{2i})]^2 \qquad (14)$$

where O_{1i} and $\hat{O}_{1i}$ are the observed data and predicted value of peak flow, respectively, O_{2i} and $\hat{O}_{2i}$ are the observed data and predicted value of runoff volume, respectively. Let

$$e_{1i} = O_{1i} - \hat{O}_{1i}$$

$$e_{2i} = O_{2i} - \hat{O}_{2i}$$

Substituting these two expressions into equation (14) yields

$$W_n(\underline{p}) = \sum_{i=1}^{n} e_{1i}^2 \cdot \sum_{i=1}^{n} e_{2i}^2 - [\sum_{i=1}^{n} e_{1i} e_{2i}]^2 \qquad (15)$$

This turns out to be the same as the Bayesian determinant criteria when two model responses are concerned. The optimal parameters obtained by use of this procedure produced good predictions for both peak flow and runoff volume. While the parameters calibrated only based on one series of model responses, for example peak flow, produced good predictions for peak flow, they may give poor predictions for runoff volume, and *vice versa* (Yan, 1990).

Bayesian Estimation

As its name suggests, Bayesian parameter estimation is based on the form of Bayes' theorem. Consider a vector of observations $\underline{y}$ and a vector of parameters $\underline{p}$. The joint probability density function can be expressed as

$$f(\underline{y},\underline{p}) = f(\underline{y}/\underline{p})f(\underline{p}) = f(\underline{p}/\underline{y})f(\underline{y}) \tag{16}$$

By rearranging the terms in equation (16), a form of Bayes' theorem can be found as

$$f(\underline{p}/\underline{y}) = \frac{f(\underline{y}/\underline{p})f(\underline{p})}{f(\underline{y})} \tag{17}$$

Because the likelihood function $L(\underline{p}/\underline{y})$ is numerically equal to $f(\underline{y}/\underline{p})$, and because $f(\underline{y})$ is equal to the integral of $f(\underline{y}, \underline{p})$ with respect to $\underline{p}$ evaluated from negative infinity to infinity, equation (17) can be expressed in another form of Bayes' theorem by the relation

$$f(\underline{p}/\underline{y}) = \frac{L(\underline{p}/\underline{y})f(\underline{p})}{\int_{-\infty}^{\infty} L(\underline{p}/\underline{y})f(\underline{p})d\underline{p}} \tag{18}$$

where $f(\underline{p})$ can be viewed as the prior distribution of parameters, $L(\underline{p}/\underline{y})$ can be viewed as the site-specific information, and $f(\underline{p}/\underline{y})$ can be viewed as the posterior distribution of parameters. Therefore, Bayes' theorem provides a way to incorporate prior information into site-specific information to produce a posterior distribution which contains more information about

parameters so that it may be reasonable to believe that it would reduce uncertainty involved in parameter estimation. Prior distributions may come from literature, regional information, expert judgement and so on. Kuczera (1982) employed Bayes' theory to combine regional and site-specific information in order to estimate peak flows of desired recurrence intervals. In general, the incorporation of regional information reduces uncertainty in the estimation of peak flows. Wilson and Haan (1991) developed an approach in Bayesian format to combine information from a regional or national data base with site-specific information. The prior information in their approach comes from the regression equations of the national data base that is obtained as a part of WEPP (Water Erosion Prediction Project) (Wilson and Haan (1991). This approach is applied to estimate rill and interrill erodibility by Wilson et al. (1991) and Wilson and Haan (1992). Since parameters are represented by probability density functions, uncertainty in erosion parameters can be evaluated by examining the dispersion or spread in the probability density functions. They conclude that the proposed Bayesian approach worked very well resulting in stable and usually smaller spread in the pdfs. When simulation methodology is employed to evaluate the performance of models, the advantage of using parameter distributions with a smaller variance becomes obvious.

Site-specific information may come from the calibration of hydrologic models. However, the parameter estimation techniques discussed in previous sections, such as Least Squares and Maximum Likelihood Estimation, can only produce point estimates for parameters. Box and Draper (1965) and Box and Tiao (1973) proposed a Bayesian approach to characterize parameter uncertainty from several model responses in the form of probability density functions. Suppose the residuals for different model responses follow a multivariate

normal distribution, the pdf of parameters $\underline{p}$ given observations $\underline{y}$ can be expressed as

$$f(\underline{p}/\underline{y}) \propto |\underline{S(p)}|^{-n/2} \tag{19}$$

where n is the number of observations, and $\underline{S(p)}$ is a k×k matrix of residuals which is defined as $\underline{S(p)} = \underline{e}^T \underline{e}$.

$$\underline{e} = \begin{vmatrix} e_{11} & e_{12} & \cdots & e_{1k} \\ \vdots & \vdots & & \vdots \\ e_{n1} & e_{n2} & \cdots & e_{nk} \end{vmatrix} \tag{20}$$

where k is the number of model responses. Equation (19) is the joint probability density function of model parameters. The point estimates of parameters are sought that maximize equation (19), so it is the mode of the joint pdf. When there is only one model response being considered, the point estimate of the Bayesian approach will becomes the same as the least squares estimation. However, what makes the Bayesian approach better is that it provides a pdf for parameters not just point estimates.

Kuczera (1983) employed this approach in a rainfall-runoff model for one model response, with errors being possibly both correlated and heteroscedastic. Edwards (1988) applied this Bayesian approach to fifteen watersheds in the Washita River basin in southern-central Oklahoma to characterize the mean and variance of model parameters S (retention factor) and T_p (time to peak) for each watershed, which were used to develop the regional

relationship of S and T_p for ungaged catchments.

Up to this point the most widely used parameter estimation techniques have been reviewed. The common assumptions for these techniques are independence and constancy of variance. These two assumption are particularly strong and are often violated in hydrologic modeling as stated by Clarke (1973) and Sorooshian and Dracup (1980). If violation of the constancy of variance assumption is suspected, Box and Cox (1964) present the following general power transformation to achieve constant variance:

$$\begin{aligned} Y &= \frac{(y+K)^{\lambda} - 1}{\lambda} && \lambda \neq 0 \\ Y &= \log(y+K) && \lambda = 0 \end{aligned} \tag{21}$$

where Y is the transformed response, and λ and K are transformation parameters. The goal of such a transformation is to select appropriate transformation parameters so that the transformed response has a constant variance.

If violation of time independence is suspected, an autoregressive-moving average (ARMA) time series model can be used to correct this violation. A general ARMA(p,q) model is defined as (Haan, 1994)

$$y_t = \phi_1 y_{t-1} + \phi_2 y_{t-2} + \cdots + \phi_p y_{t-p} + a_t - \theta_1 a_{t-1} - \theta_2 a_{t-2} - \cdots - \theta_q a_{t-q} \tag{22}$$

where ϕ_1 , ϕ_2 , ..., ϕ_p are the pth order autoregressive parameters, θ_1 , θ_2 , ..., θ_q are the qth order moving average parameters, and a_t is white noise. In the context of hydrologic modeling, a lower order ARMA model such as ARMA(1, 0) or ARMA(1, 1) has been often

used (e.g. Sorooshian and Dracup, 1980, Troutman, 1983).

For the continuous daily mode rainfall-runoff model, the residuals are most likely correlated because large streamflow today may indicate large streamflow tomorrow. But for event based models, because of the way by which the model input and output observations are collected independently, there may be less correlation existing between observations. Therefore, for event based modeling, it may not be necessary to be concerned about correlation in residuals.

Validation of Hydrologic and Water Quality Models

Since hydrologic phenomena are too complicated to model exactly, there are currently no complete physical hydrologic and water quality models. Many models are developed based upon a limited data base in some range (time, location, scale, etc.), then expanded beyond the range in which they were developed. For instance, the Universal Soil Loss Equation (USLE) model was developed based upon a standard plot with a slope of 9% and a slope length of 72.6 feet. When it is expanded to a watershed scale or even basin scale, some assumptions or relations made in the model development may not hold firm so that the model may or may not give reasonable predictions in this situation. Supposing that scale is not a problem, a model may still perform quite differently for different size of events. For example, a rainfall-runoff model which is calibrated for peak flow in a wet period may produce good peak flow predictions for a wet period but poor peak flow predictions for a dry period, and *vice versa* (Troutman, 1985). Model validation is a process which helps users to build confidence in the ability of the model to make reliable predictions for the situation

in which the model is intended to be used.

Definition and Classification of Model Validation

In recent years "validation" has become an important subject in the field of hydrologic and water quality modeling. In spite of this fact, the term "validation" has come in use only very recently. Model validation addresses the question of whether or not a model adequately represents observed phenomena (Luis and McLaughlin, 1992). There exists no widely accepted definition of what constitutes "validation" (Pescatore, 1994). Many definitions of validation have been suggested in the published literature. For example, the International Atomic Energy Agency (IAEA) proposes the following definition for validation (Pescatore, 1994; Tim et al., 1995):

> "Validation is a process carried out by comparison of model predictions with independent field observations and experimental measurements. A model can not be considered validated until sufficient testing has been performed to ensure an acceptable level of predictive accuracy (note that the acceptable level of accuracy is judgmental and will vary depending on the specific problem or question to be addressed by the model)".

In a recent editorial in Advances in Water Resources, Hassanizadeh and Carrera (1992) provided an alternative definition as

> "the process of substantiating that a model possesses a satisfactory degree of accuracy and certainty within its entire domain of applicability and over the entire spatial and temporal scales for which the model is intended to be used".

From a different point of view, one may have a completely different interpretation about validation. Pescatore (1994) classifies the definitions of validation into three classes:

I. Purist view

The first class of definitions links validation to the desire to predict the physical world as faithfully as possible. The definition given by Hassanizadeh and Carrera belongs to this class. Based upon this point of view, Konikow (1992) argued that in any fashion, "ground-water models can not be validated. ... In any event, the accuracy of the prediction can not be assessed until after the predicted period of time has passed". Therefore, in this category, one may actually invalidate a model rather than validate.

II. Operational view

The second class of definitions suggests that validation is accomplished only when the results of "blind" tests (split sampling tests) have been predicted. A model is calibrated based upon one part of the observed data. The model is considered to be validated if it can reproduce the other part of the observed data with an acceptable accuracy.

Alot of hydrologic events, such as rainfall, runoff, etc., are assumed to be stochastic processes. They are usually assumed to have the same statistical properties over time. If a model is able to reproduce the observations which are not used in calibration with an acceptable accuracy, it should have the ability to give predictions in the future with the same accuracy. Validating a model by using part of the observed data which are used in model calibration is considered not to be sufficient

because it only demonstrates the ability of the model to reproduce the history used to calibrate the model.

III. A confidence building process

Since an absolute confidence in the ability of a model to predict reality over a long time period can not be guaranteed and even on a limited time scale "sufficient validation" entails subjective judgement, the definitions of validation have been modified as a process of building scientific and public confidence in the methods developed to produce predictions. In the sense of this approach, one may not know when a model is validated until it is judged to be acceptable by developers and the users after several iterations among them. A model which was considered valid may be invalidated at a later date.

Measures of Model Validation

The second definition of validation usually applies to hydrologic and water quality modeling. Almost all validations entail the comparison of model predictions with observations. The commonly used measure to assess a model's performance is goodness-of-fit. The American Society of Civil Engineers (1993) recommends some goodness-of-fit criteria to evaluate how well model predictions match the observed data being simulated. In addition to goodness-of-fit, validation can be measured through a linear regression of predictions against observed data. Flavelle et al. (1990) performed the linear regression in both the calibration and the validation phases.

1. Goodness-of-fit Criteria

For a single event model, deviation (percent error) of a model response from observed data is one goodness-of-fit criterion:

$$PE(\%) = \frac{\sum_{i=1}^{n} (O_i - \hat{O}_i)}{\bar{O}} \cdot 100 \tag{23}$$

where O_i is the observed data of the model response, $\hat{O}_i$ is the predicted value of model response, and $\bar{O}$ is the mean of the observed data. This simple test can be used to determine if the model predictions are biased. When PE is large, either positive or negative, the model predictions must be biased. When the percentage of PE is low, the model predictions may be unbiased but still leaving room for the possibility of being biased.

Another commonly used goodness-of-fit criterion is the sum of squared residuals (SSR) or mean square of deviation.

$$SSR = \sum_{i=1}^{n} (O_i - \hat{O}_i)^2 \tag{24}$$

This criterion is an overall measure of goodness-of-fit. The best fit (in a least squares sense) is that which minimizes equation (24). Therefore, the best fit parameters must be least squares estimates in this sense. However, Sorooshian and Dracup (1980) point out, the SSR, although a good test in curve fitting, is not necessarily a good indicator of the best model fit. In other words, a good model fit in calibration phase may not necessarily produce good

model predictions. The parameter set should give a good model fit in both the calibration and prediction phase.

Sorooshian et al. (1983) used both of the above criteria together with others to assess the effectiveness of three parameter estimation techniques, namely simple least squares, maximum likelihood for autocorrelated error case, as well as maximum likelihood for heteroscedastic error case.

Another goodness-of-fit criterion is the coefficient of determination, R^2, or the correlation coefficient between model predictions and observed data. The correlation coefficient is simply the square root of the coefficient of determination.

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (O_i - \hat{O}_i)^2}{\sum_{i=1}^{n} (O_i - \bar{O})^2} \tag{25}$$

The possible values for R^2 are from zero to one. A high value of R^2 indicates good results from a model, while a low value indicates poor, or even statistically insignificant results. The coefficent is a good measue of the degree of association between the observed and predicted values (Aitken, 1973). This relationship is good for linear models. Unfortunately, most hydrologic and water quality models are non-linear and the values from equation (25) may not necessarily be restricted to zero to one. In other words, this criterion may not apply to hydrologic and water quality models.

When there is more than one model response of concern, the Total Sum of Squared

Residuals (TSSR) can be used as a measure

$$TSSR = \sum_{i=1}^{n} e_{1i}^2 + \sum_{i=1}^{n} e_{2i}^2 + \cdots \quad (26)$$

where e_{1i} is the residual for the first model response, e_{2i} is the residual for the second model response, and so on. Since the units for different model responses could be quite different, it is better to use the normalized residuals which are the residuals divided by the mean of the corresponding model output.

Yan and Haan (1991) used an alternative criterion to evaluate multiobjective optimization against single objective optimization. The average of the square root of the normalized residual for each model output is calculated first, then an overall average of all concerned outputs is computed as a criterion to evaluate parameter estimation techniques.

In sum, many goodness-of-fit criteria are commonly used to test how well the model predictions match the corresponding observed data in both the calibration phase and the validation phase. They are simple and easy to use. When goodness-of-fit criteria are used to compare two calibration methods or two models, there are less subjective decisions involved than when they are used to validate a model because in the latter case the model users must determine under what conditions the model is considered to be validated.

2. Linear Regression Analysis

In this method, a simple linear regression of the model predictions versus the corresponding measured data is performed. Then the standard error of regression is

interpreted as the goodness-of-fit, and the slope and intercept are interpreted as the model bias (Flavelle, 1992).

If the model is perfect and the observed data are error free, the model predictions should be exactly the same as the corresponding measured data and the regression line must be a straight line with slope of one and intercept of zero. In reality, there is no such model and observed data usually contain some degree of measurement errors. The assumptions of unit slope and zero intercept can be tested using standard hypothesis tests. Specifically, the test of hypothesis concerning slope "b" and intercept "a" can be made by noting that $(a-\alpha_0)/S_a$ and $(b-\beta_0)/S_b$ both have t distributions with (n-2) degrees of freedom, where S_a is the standard error of the intercept and S_b is the standard error of the slope. The null hypothesis about the intercept, H_0: $\alpha=0$, and the alternative hypothesis, H_a: $\alpha \neq 0$, is tested by computing

$$t = (a-0)/S_a \tag{27}$$

The null hypothesis H_0 is rejected for a given significance level if the absolute value of t is greater than $t_{1-\alpha/2,\, n-2}$, otherwise H_0 is not rejected (intercept equal to zero). Similarly, the null hypothesis about slope, H_0: $\beta=1$, and the alternative hypothesis, H_a: $\beta \neq 1$, is tested by computing

$$t = (b-1)/S_b \tag{28}$$

The hypothesis H_0 is rejected if the absolute value of t is greater than $t_{1-\alpha/2,\, n-2}$, otherwise, H_0 is not rejected. Failing to reject both null hypotheses does not mean that the model is free

of biases, only that this analysis fails to identify model biases (Flavelle, 1992). If biases are identified in the model, the regression line will be off the equal value line having a slope of one and intercept of zero.

On the other hand, the standard deviation of the model predictions, y, at any value of measured data, x, can be used as a measure of the uncertainty of the model predictions. Confidence intervals can be placed on the regression line so that the uncertainty in the model predictions can be evaluated at a given level of confidence.

Simple linear regression is well known and the tools for performing linear regression are usually readily available. The results of the linear regression analysis can be presented graphically revealing a visual impression about how well the predictions match the observed data.

In addition to measures of goodness-of-fit and linear regression analysis, the residuals can be examined against observed data (or predictions) as a visual test to detect bias in model predictions (eg. Edwards and Haan, 1989). If the residuals are not randomly and equally distributed around zero as the value of observed data increases, the model is considered to have biases. If the residuals are consistently greater than zero the model tends to underestimate the observed events. If the residuals are consistently less than zero the model tends to overestimate the observed events.

Uncertainty Analysis

Traditionally, parameters in the context of hydrologic and water quality modeling are treated as a set of constants. For given model inputs, such as rainfall volume, model

predictions are fixed values also. However, parameters in hydrologic and water quality models should be considered as random variables. This idea has been discussed by many scientists (*e.g.* Haan, 1989; Barfield et al., 1989; Vicens et al., 1975; Beck, 1987). With uncertain parameters, a model must give uncertain predictions. It is usually not immediately obvious that uncertainty in parameters may significantly affect the model predictions. Uncertainty analysis is used to find out the impact of the uncertainty in parmaeters on the model predictions. Sensitivity analysis, First Order Analysis (FOA) and Monte Carlo Simulation (MCS) are the most widely used uncertainty analysis tools. In the case of one uncertain parameter, the output pdf may be determined directly from an analytical transformation procedure based on the model and the input parameter pdf. An example can be found in the work of Haan and Schulze (1987).

Sensitivity Analysis

Sensitivity analysis is a method to identify important input parameters for the model being used. The sensitivity with respect to one parameter is determined by changing this parameter by a small amount while other parameters are held constant at the most appropriate values for the particular condition being studied.

There are two types of sensitivity coefficients. One is called an absolute sensitivity coefficient or simply the sensitivity coefficient, S, and the other a relative sensitivity coefficient, S_r. The absolute sensitivity is given by

$$S = \frac{\partial O}{\partial I} \tag{29}$$

where O and I represent a particular model output and an input parameter respectively. S gives the absolute change in O for a unit change in I. The shortcoming of the absolute sensitivity coefficient is that its value depends on the units of O and I. This makes it difficult to compare the impacts of changes in different input parameters on particular model outputs. The relative sensitivity coefficient is introduced to overcome this problem.

$$S_r = \frac{\partial O}{\partial I}\frac{I}{O} \tag{30}$$

S_r gives the percentage change in O for a 1% change in I. The relative sensitivity coefficients are dimensionless.

Obviously for most hydrologic and water quality models, because analytic partial derivatives can not be obtained, sensitivity coefficients must be calculated numerically.

$$\frac{\partial O}{\partial I} = \frac{O_2 - O_1}{I_2 - I_1}, \qquad \frac{O}{I} = \frac{\bar{O}}{\bar{I}} = \frac{O_1 + O_2}{I_1 + I_2} \tag{31}$$

The importance of input parameters can be ranked on the basis of their relative sensitivity coefficients. Only the most sensitive parameters are retained for further uncertainty analysis.

First Order Analysis

The FOA is a simple method to assess the effect of uncertain model parameters on model predictions. The term "simple" here implies relatively easy to compute. It only requires estimates of the mean and the variance of model parameters, and also the covariance of parameters if they are correlated. To demonstrate the application of FOA, consider the generalized hydrologic model equation (3). Any model response $\hat{O}$ can be approximated by a Taylor series about the expected value of parameters $\underline{p}$

$$\hat{O} \approx f(\underline{I},\underline{\bar{p}},t)+\sum_{i=1}^{l} \frac{\partial f}{\partial p_i}|_{\underline{\bar{p}}}(p-p_i)+\frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l} \frac{\partial^2 f}{\partial p_i \partial p_j}|_{\underline{\bar{p}}}(p-p_i)(p-p_j)+\cdots \qquad (32)$$

where an overbar represents a mean value. Neglecting the second and higher order terms because they are small compared to the first two terms, and taking expectations on both sides, it follows that

$$E[\hat{O}] \approx f(\underline{I},\underline{\bar{p}},t) \qquad (33)$$

The variance of $\hat{O}$ can be found from the relation, $\mathrm{Var}(\hat{O}) = E(\hat{O}^2) - E^2(\hat{O})$, by noting that the expectation of $f(\underline{I}, \underline{\bar{p}}, t)$ is equal to itself and the expectation of $\sum_{i=1}^{l} \frac{\partial f}{\partial p_i}|_{\underline{\bar{p}}}(p-p_i)$ is equal to zero. The variance can be addressed as

$$Var(\hat{O}) \approx \sum_{i=1}^{l}\sum_{j=1}^{l} \frac{\partial f}{\partial p_i}\frac{\partial f}{\partial p_j}|_{\underline{\bar{p}}} E[(p_i-\bar{p}_i)(p_j-\bar{p}_j)] \qquad (34)$$

When the parameters are uncorrelated, the first order approximation of the variance of model output can be simplified as

$$Var(\hat{O}) \approx \sum_{i=1}^{l} (\frac{\partial f}{\partial p_i})^2 |_{\bar{p}} var(p_i) \qquad (35)$$

where the partial derivative term is the absolute sensitivity with respect to parameter p_i at the mean parameter value. This absolute sensitivity can be computed by numerical differentiation. Two ways to determine the variances of parameters are from model calibration using the Bayesian approach, and, as stated by Prasher et al. (1984), estimated from upper and lower bounds appropriate to the parameters.

When the model being used is linear with respect to parameters, the assumptions of first order analysis are perfectly satisfied. However, hydrologic models usually are nonlinear models. A FOA variance of model response becomes an approximation in the case of nonlinear models. FOA has been shown to produce good estimates of the mean and variance of a model response if the coefficient of variation of the input parameter is small and the response is nearly linear with respect to the parameter in the range of interest (Haan et al., 1995). Benjamin and Cornell (1970) point out that a widely used rule of thumb for determining if a FOA variance is valid is to restrict parameter coefficient of variation to less than 0.2 (Stevens, 1993). More details about the accuracy of FOA can be found in Stevens' work.

Monte Carlo Simulation

Monte Carlo Simulation (MCS) is a sampling method from the model parameter

space. MCS is widely used for characterizing the uncertainties of model output due to the parameter uncertainties. It requires a distribution for each parameter. When MCS is applied to assess the uncertainty on model outputs in hydrologic modeling, a set of parameters are sampled simultaneously from the multivariate distribution of parameters, then a model simulation with the sampled parameters' values is performed to produce estimates of model outputs. Since parameters are sampled at random, the simulated model outputs are random variables. Therefore, statistical methods can be applied to characterize the uncertainty of these outputs in the form of mean, variance, pdf and so on.

The accuracy of Monte Carlo simulation depends on the number of simulation runs. The number of simulation runs depends on both the cost of each model run and what accuracy needs to be achieved. Morgan and Henrion (1992) presented two methods to estimate the number of simulation runs for MCS. One method is based on the idea of uncertainty about the mean. To estimate the number of runs by this method, we have to make a small number of initial Monte Carlo runs. The mean and variance of model output are calculated from the results of these initial runs. Assume model outputs are normally distributed. Suppose we want to be sure with α confidence level that the confidence interval around the mean of the initial runs with width of w contains the real mean of model outputs. The number of simulation runs can be estimated by

(36)

where s is the standard deviation estimated from the initial runs and c is the deviation of the

standard normal deviate with probability α.

The other method for determining sample size is based on the precision of the estimated cumulative distribution. The number of simulation runs is estimated by the relation

$$n = p(1-p)\left(\frac{c}{\Delta p}\right)^2 \tag{37}$$

where p is the percentile of model output, c is the deviation of the standard normal deviate with probability α, and Δp is a half of the percentile interval width. Note that this estimate is completely independent of the input parameter distribution. This allows one to determine the number of model runs before any simulation is done.

Prabhu (1995) uses another approach to determine the sample size. MCS is done many times for different numbers of model runs, say, 100, 200, ..., and the mean of model response is calculated for each number of model runs and is plotted against the number of model runs. When the mean tends to be stable, it indicates that the number of model runs is adequate.

The Monte Carlo method is used by many authors in hydrologic modeling. It may be accurate enough when the number of model runs is large. Prabhu (1995) employed MCS to investigate uncertainty of model outputs by sampling at random eight parameters simultaneously. Stevens (1993) used MCS as a comparison method to analyze the accuracy of First Order analysis. Sorooshian (1981) employed MCS to generate runoff values with and without contaminated errors which were used as calibration data for comparing the power and the effectiveness of Maximum Likelihood against least squares.

CHAPTER III

THEORY

This research is mainly based upon present knowledge of two major subjects: Bayesian analysis of uncertainty and updating parameter distributions.

Bayesian Analysis of Uncertainty

Bayesian analysis is a relatively straightforward method of analyzing uncertainty in model parameters. Application of the method requires intensive calculations, especially when the number of parameters being analyzed increases. Perhaps this is the reason why Bayesian analysis of uncertainty was not widely used in the past years. With the development of computer techniques, higher speed computers are available so that less time will be consumed in the intensive calculations. The method of Bayesian analysis is built on the basis of Bayes' Theorem. Therefore, Bayes' Theorem is a good place to start the discussion of uncertainty analysis by Bayesian statistical theory.

Bayes' Theorem

Bayes' Theorem by itself is nothing more than a statement of relationships between

conditional probabilities. The application of Bayes' Theorem forms a major branch of statistical analysis, Bayesian statistical theory. The following is only the general framework of the theory.

Consider the joint probability density function, $p(\underline{X}, \underline{\Theta})$, where $\underline{X} = [x_1, x_2, \ldots x_n]^T$ is a vector of n random variables and $\underline{\Theta} = [\theta_1, \theta_2, \ldots \theta_k]^T$ is a vector of k parameters. Note that both $\underline{X}$ and $\underline{\Theta}$ are treated as random variables. The joint probability density function can be evaluated by the conditional pdf $p(\underline{X}/\underline{\Theta})$ and marginal pdf $p(\underline{\Theta})$ or by the conditional pdf $p(\underline{\Theta}/\underline{X})$ and marginal pdf $p(\underline{X})$ as:

$$p(\underline{X}, \underline{\Theta}) = p(\underline{X}/\underline{\Theta}) \cdot p(\underline{\Theta}) = p(\underline{\Theta}/\underline{X}) \cdot p(\underline{X}) \tag{38}$$

For a given set of values of $\underline{X}$, the conditional probability density function $p(\underline{\Theta}/\underline{X})$ can be obtained by rearranging terms as:

$$p(\underline{\Theta}/\underline{X}) = \frac{p(\underline{X}/\underline{\Theta}) \cdot p(\underline{\Theta})}{p(\underline{X})} \tag{39}$$

Equation (39) is a form of Bayes' Theorem.

In this equation, the expression $p(\underline{\Theta}/\underline{X})$ is known as the posterior probability density function of $\underline{\Theta}$ for given observed values of $\underline{X}$. The posterior pdf represents our beliefs about parameters after we have obtained the observed data. In the context of hydrologic and water quality modeling, the variable $\underline{X}$ could be runoff, sediment yield, or nutrient loss etc. The expression $p(\underline{\Theta})$ is known as the prior probability density function of the parameter vector

$\underline{\Theta}$ which represents the information one already knows before any data on $\underline{X}$ are collected. The expression $p(\underline{X}/\underline{\Theta})$ is the conditional probability density function of $\underline{X}$ given a known set of parameters $\underline{\Theta}$. However, we often want to think of it as a function of $\underline{\Theta}$ for given values of $\underline{X}$, because it could be more convenient for us to observe the values of variables $\underline{X}$ than to observe the values of parameters $\underline{\Theta}$. When the pdf $p(\underline{X}/\underline{\Theta})$ is regarded as a function of $\underline{\Theta}$, for given observed values of $\underline{X}$, it is called the likelihood function and is often denoted by the symbol $L(\underline{\Theta}/\underline{X})$ which is numerically equal to $p(\underline{X}/\underline{\Theta})$. Although the likelihood function has the same value as $p(\underline{X}/\underline{\Theta})$, it is not a pdf and does not have quite the same properties — for example, it does not necessarily sum to unity for all possible values of parameters $\underline{\Theta}$. The likelihood function represents the information known about the parameters $\underline{\Theta}$ from the observed values of $\underline{X}$.

The denominator in equation (39) can be evaluated using the definition of marginal distribution as:

$$p(\underline{X}) = \int_{-\infty}^{\infty} p(\underline{X}, \underline{\Theta})\, d\underline{\Theta} = \int_{-\infty}^{\infty} L(\underline{\Theta}/\underline{X}) p(\underline{\Theta})\, d\underline{\Theta} \tag{40}$$

where the integration is over k-dimensional real space.

Therefore, another form of Bayes' Theorem can be written as:

$$p(\underline{\Theta}/\underline{X}) = \frac{L(\underline{\Theta}/\underline{X}) p(\underline{\Theta})}{\int_{-\infty}^{\infty} L(\underline{\Theta}/\underline{X}) p(\underline{\Theta})\, d\underline{\Theta}} \tag{41}$$

For given values of $\underline{X}$, the denominator in equation (41) is a normalizing constant which is necessary to ensure that the posterior pdf $p(\underline{\Theta}/\underline{X})$ sums to unity. By dropping this constant, Bayes' Theorem can also be written as:

$$p(\underline{\Theta}/\underline{X}) \propto p(\underline{\Theta})\, L(\underline{\Theta}/\underline{X}) \tag{42}$$

which is probably the most commonly used form of Bayes' Theorem.

With above definitions of posterior information, prior information and likelihood function, we may think of Bayes' Theorem in the more memorable form

$$\textit{Posterior} \propto \textit{Prior} \times \textit{Likelihood}$$

Bayesian Analysis of Uncertainty

Any hydrological and water quality model can be defined by the relation

$$\underline{Y} = f(\underline{X}, \underline{\Theta}) + \underline{\epsilon} \tag{43}$$

where $\underline{Y}$ is an n×p matrix of observed responses, $\underline{X}$ is an n×m matrix of inputs (state variables), $\underline{\Theta}$ is a k×1 vector of model parameters, and $\underline{\epsilon}$ is an n×p matrix of residuals (differences between observed responses and the corresponding model predictions). Note that n is the number of the observed data sets, p is the number of model responses, m is the number of input variables, and k is the number of parameters.

When Bayesian techniques are used to estimate parameters for hydrological models,

parameters $\underline{\Theta}$ are treated as random variables rather than fixed values. Bayesian techniques will provide the estimation results in the form of a distribution. Then the point estimates of the parameters could be taken as the most probable values of the parameters $\underline{\Theta}$, in other words, the mode of the joint distribution of parameters is the point estimate of the parameters.

To begin the estimation of parameters, suppose that each set of observed responses $\underline{y}_i = (\underline{y}_{i1}, \ldots, \underline{y}_{in})^T$ (i = 1, 2, ..., p) is independent and that each set of the corresponding residuals $\underline{\epsilon}_i = (\underline{e}_{i1}, \underline{e}_{i2}, \ldots, \underline{e}_{in})^T$ (i = 1, 2, ..., n) is, for given $\underline{\Theta}$, a normal distribution with mean zero and the p×p covariance matrix of the residuals $\underline{\Sigma}$. Then the joint probability density function of the n set of residuals is given by

$$p(\underline{\epsilon}/\underline{\Sigma}, \underline{\Theta}) = \prod_{i=1}^{n} p(\underline{\epsilon}_i/\underline{\Sigma}, \underline{\Theta})$$

$$= (2\pi)^{-np/2} |\Sigma|^{-n/2} e^{-\frac{1}{2}\sum_{i=1}^{n} \underline{\epsilon}_i' \underline{\Sigma}^{-1} \underline{\epsilon}_i} \qquad (44)$$

Now let S(Θ) be a p×p nonnegative symmetric matrix

$$\underline{S}(\underline{\Theta}) = [S_{ij}(\theta_i, \theta_j)] \qquad (45)$$

where

$$S_{ij}(\theta_i, \theta_j) = \sum_{k=1}^{n} \epsilon_{ki}\epsilon_{kj} \tag{46}$$

Since $\underline{\epsilon}_i$ is a p×1 vector and $\underline{\Sigma}^{-1}$ is a p×p matrix, $\underline{\epsilon}_i'\underline{\Sigma}^{-1}\underline{\epsilon}_i$ will be a scalar. The sum of n scalars is equal to the trace of the sum of the n scalar entries on the matrix diagonal. The exponent in equation (44) can be expressed as

$$\sum_{i=1}^{n} \underline{\epsilon}_i'\underline{\Sigma}^{-1}\underline{\epsilon}_i = tr\left[\sum_{i=1}^{n} \underline{\epsilon}_i'\underline{\Sigma}^{-1}\underline{\epsilon}_i\right] = tr\left[\sum_{i=1}^{n} \underline{\Sigma}^{-1}\underline{\epsilon}_i\underline{\epsilon}_i'\right] \tag{47}$$

thus

$$\sum_{i=1}^{n} \underline{\epsilon}_i'\underline{\Sigma}^{-1}\underline{\epsilon}_i = tr\left[\underline{\Sigma}^{-1}\underline{S}(\underline{\Theta})\right] \tag{48}$$

where "tr" represents the trace of a matrix. Substituting equation (48) into equation (44) yields

$$p(\underline{\epsilon}/\underline{\Sigma}, \underline{\Theta}) = (2\pi)^{-np/2} |\Sigma|^{-n/2} e^{-\frac{1}{2}tr[\underline{\Sigma}^{-1}\underline{S}(\underline{\Theta})]} \tag{49}$$

Given the observed data $\underline{Y}$, the likelihood function of uncertain parameters ($\underline{\Theta}$, $\underline{\Sigma}$) can be written as

$$l(\underline{\Theta}, \underline{\Sigma}/\underline{Y}) \propto |\Sigma|^{-n/2} e^{-\frac{1}{2}tr\left[\underline{\Sigma}^{-1}\underline{S}(\underline{\Theta})\right]} \tag{50}$$

To clarify the notation, there is a need to emphasize that $\underline{Y}$ refers to the n×p matrix

of observed values

$$\underline{Y} = \begin{bmatrix} y_{11} & \cdots & y_{1i} & \cdots & y_{1p} \\ \vdots & & \vdots & & \vdots \\ y_{j1} & \cdots & y_{ji} & \cdots & y_{jp} \\ \vdots & & \vdots & & \vdots \\ y_{n1} & \cdots & y_{ni} & \cdots & y_{np} \end{bmatrix} = \left[\underline{y}_1, \cdots, \underline{y}_i, \cdots, \underline{y}_p\right] \tag{51}$$

where $\underline{y}_i=[y_{1i}, ..., y_{ni})^T$ is the vector of n observations corresponding to the *i*th model response. Similarly, $\underline{\epsilon}$ refers to the n×p matrix of residuals

$$\underline{\epsilon} = \begin{bmatrix} \epsilon_{11} & \cdots & \epsilon_{1i} & \cdots & \epsilon_{1p} \\ \vdots & & \vdots & & \vdots \\ \epsilon_{j1} & \cdots & \epsilon_{ji} & \cdots & \epsilon_{jp} \\ \vdots & & \vdots & & \vdots \\ \epsilon_{n1} & \cdots & \epsilon_{ni} & \cdots & \epsilon_{np} \end{bmatrix} = \left[\underline{\epsilon}_1, \cdots, \underline{\epsilon}_i, \cdots, \underline{\epsilon}_p\right] \tag{52}$$

Application of Bayes' theorem requires prior information regarding the parameters of interest. The prior information must generally be expressed as a probability density function. Correct specification of the prior probability density function is extremely important. It is easy to see from Bayes' Theorem that misspecification of the prior distribution would lead to doubtful results. To avoid misspecifying the prior distribution, vague prior information is often used. This means we have little idea about the probability density function of the parameters of interest so that the posterior probability density function of the parameters will be dominated only by likelihood or observed data.

To continue, a prior probability density function of the model parameters $\underline{\Theta}$ and the covariance matrix $\underline{\Sigma}$ must be specified. We may assume that $\underline{\Theta}$ and $\underline{\Sigma}$ are approximately independent, then we may write

$$p(\underline{\Theta}, \underline{\Sigma}) = p(\underline{\Theta})\, p(\underline{\Sigma}) \tag{53}$$

Then, the non-informative priors are used for both parameters $\underline{\Theta}$ and $\underline{\Sigma}$. The parameters $\underline{\Theta}$ are assumed to have a local uniform distribution:

$$p(\underline{\Theta}) \propto \textit{constant} \tag{54}$$

and the prior distribution of $\underline{\Sigma}$ is specified as

$$p(\underline{\Sigma}) \propto |\underline{\Sigma}|^{-(p+1)/2} \tag{55}$$

Therefore, the prior distribution of model parameters $\underline{\Theta}$ and covariance matrix $\underline{\Sigma}$ can be written as

$$p(\underline{\Theta}, \underline{\Sigma}) \propto |\underline{\Sigma}|^{-(p+1)/2} \tag{56}$$

By Bayes' Theorem, the posterior joint probability density function of parameters $\underline{\Theta}$ and covariance matrix $\underline{\Sigma}$ is proportional to the product of their prior probability density function and their likelihood function. Using equation (50) and equation (56), the joint posterior distribution of ($\underline{\Theta}$, $\underline{\Sigma}$) can be obtained as:

$$p(\underline{\theta}, \underline{\Sigma} / \underline{Y}) \propto |\Sigma|^{-(n+p+1)/2} e^{-\frac{1}{2} tr[\underline{\Sigma}^{-1} \underline{S}(\underline{\theta})]} \tag{57}$$

It is sometimes convenient to work with the elements of $\underline{\Sigma}^{-1}$ rather than the elements of $\underline{\Sigma}$

$$p(\underline{\Theta}, \underline{\Sigma}^{-1} / \underline{Y}) = p(\underline{\Theta}, \underline{\Sigma} / \underline{Y}) \left| \frac{\partial \underline{\Sigma}}{\partial \underline{\Sigma}^{-1}} \right| \tag{58}$$

where the last term in the above equation is the Jacobian of the transformation from the elements of $\underline{\Sigma}$ to the elements of $\underline{\Sigma}^{-1}$. It can be shown that (Box and Tiao, 1973)

$$\left| \frac{\partial \underline{\Sigma}}{\partial \underline{\Sigma}^{-1}} \right| = |\underline{\Sigma}|^{p+1} \tag{59}$$

Now it follows from equations (57) - (59) that the posterior probability density function of ($\underline{\Theta}$, $\underline{\Sigma}^{-1}$) is

$$p(\underline{\theta}, \underline{\Sigma}^{-1} / \underline{Y}) \propto |\Sigma|^{-(n-p-1)/2} e^{-\frac{1}{2} tr[\underline{\Sigma}^{-1} \underline{S}(\underline{\theta})]} \tag{60}$$

Since we are only interested in the distribution of model parameters $\underline{\Theta}$, the covariance term $\underline{\Sigma}^{-1}$ is a set of nuisance parameters. The marginal posterior distribution of model parameters $\underline{\Theta}$ can be found by integrating equation (60) with respect to $\underline{\Sigma}^{-1}$. By the use of the Wishart distribution, Box and Tiao (1973) provide a derivation of the marginal posterior probability density function of $\underline{\Theta}$, which ends up with a remarkably simple relationship:

$$p(\underline{\Theta} / \underline{Y}) \propto |\underline{S}(\underline{\Theta})|^{-n/2} \tag{61}$$

where $|\underline{S}(\underline{\Theta})|$ is the determinant of matrix $\underline{S}(\underline{\Theta})$.

The point estimates of parameters $\underline{\Theta}$ are those which maximize the joint posterior probability density function of model parameters $\underline{\Theta}$. From the Bayesian point of view, if we took $|\underline{S}(\underline{\Theta})|$ as a loss function, the Bayes decision function of $\underline{\Theta}$ is the one which minimizes $|\underline{S}(\underline{\Theta})|$. It is equivalent to maximizing $|\underline{S}(\underline{\Theta})|^{-n/2}$ because $\underline{S}(\underline{\Theta})$ is a non-negative symmetric matrix.

Since a non-informative prior distribution was used in the above derivation, the posterior probability density function of parameters $\underline{\Theta}$ could be viewed as a distribution obtained only from observed data. The marginal distribution of a specific model parameter can be found by integrating equation (61) with respect to other parameters.

Update of Parameter Distribution

For any hydrologic and water quality model, model users should have some degree of beliefs of model parameters based on literature or personal experiences even before any observations of the model responses are used to calibrate the model. For instance, one may estimate the value of curve number according to the hydrological soil group and land uses. In addition, one may already have calibration results of the model parameters from data available. When any new observed data come in, there is a need to update the estimation of the model parameters.

Again, prior information refers to the distribution of parameters estimated before the current data are available. The site specific information refers to the calibration distribution of the parameters in equation (61) from the current data. Bayes' Theorem is used to incorporate the prior information into the site specific information to produce the posterior information. In this study, we will only discuss how to combine the prior information and site specific information for the parameters with a normal distribution or a lognormal distribution.

Normal Distribution

Suppose that the prior distribution of a parameter θ is a normal distribution with mean of θ_0 and variance of φ_0^2, so that

$$\theta \sim N(\theta_0, \varphi_0^2)$$

and suppose also that we have an observation of x which is normally distributed with mean equal to the parameter of interest and variance of φ^2, that is

$$x \sim N(\theta, \varphi^2)$$

where θ_0, φ_0^2 and φ are known. Then the prior probability density function and the likelihood function can be written as:

$$p(\theta) = (2\pi\varphi_0)^{-\frac{1}{2}} exp[-\frac{1}{2}(\theta-\theta_0)^2/\varphi_0^2] \qquad (62)$$

$$L(\theta/x) = (2\pi\varphi)^{-\frac{1}{2}} exp[-\frac{1}{2}(x-\theta)/\varphi^2] \tag{63}$$

It follows from Bayes' Theorem and equations (62) - (63) that the posterior probability density function of θ is

$$\begin{aligned} p(\theta/x) &\propto p(\theta)L(\theta/x) \\ &\propto exp[-\frac{1}{2}\theta^2(\varphi_0^{-2}+\varphi^{-2}) + \theta(\theta_0/\varphi_0^2 + x/\varphi^2)] \end{aligned} \tag{64}$$

It can be seen that the posterior probability density function is also a normal distribution with mean θ_1 and variance φ_1^2 equal to

$$\begin{aligned} \theta_1 &= \varphi_1^2(\theta_0/\varphi_0^2 + x/\varphi^2) \\ \varphi_1^2 &= \frac{1}{\varphi_0^{-2} + \varphi^2} \end{aligned} \tag{65}$$

Now, if the calibrated probability density function is a normal distribution, we may assume that the mean and the variance of the normal distribution are equal to x and φ^2, respectively. Together with the prior mean θ_0 and variance of φ_0^2, the posterior distribution can be calculated by equation (65).

Note that the variance of the calibrated distribution was assumed to be the variance of $N(\theta, \varphi^2)$. The assumption of sample variance equal to the population variance may not

be completely true, but probably that is the best estimate we could give based on the available data.

Lognormal Distribution

The posterior probability density function of a parameter θ with lognormal distribution can be obtained from the relationship between the normal and lognormal distributions. If a random variable θ follows a lognormal distribution with mean of $\bar{\theta}$ and variance of S_θ^2, the variable Y

$$Y = \ln\theta \tag{66}$$

will follow a normal distribution with mean $\bar{Y}$ and variance S_y^2 equal to (Haan, 1977)

$$\begin{aligned} \bar{Y} &= \frac{1}{2}\ln[(\bar{\theta}^2/(C_v^2+1)] \\ S_y^2 &= \ln(C_v^2+1) \end{aligned} \tag{67}$$

where C_v is the coefficient of variation of the original variable θ ($C_v = S_\theta/\bar{\theta}$). By this transformation, a lognormal distribution can be changed to a normal distribution only by calculating the mean and the variance of the normal distribution.

Suppose now that both the prior distribution of θ and the likelihood function of θ given the data x are lognormally distributed. From the above transformation, both the prior distribution and likelihood can be transformed to corresponding normal distributions. Then it follows from the previous subsection that the posterior distribution of the transformed

variable, p(y/x), will also be a normal distribution with mean of μ_y and variance of σ_y^2, where μ_y and σ_y^2 could be determined by equation (65).

$$p(y/x) \sim N(\mu_y, \sigma_y^2) \tag{68}$$

Now, the posterior distribution of variable θ is

$$p(\theta/x) = p(y/x)\left|\frac{dy}{d\theta}\right| \tag{69}$$

where

$$\left|\frac{dy}{d\theta}\right| = \frac{1}{\theta} \tag{70}$$

and hence

$$p(\theta/x) = \frac{1}{\theta}p(y/x) \tag{71}$$

Therefore, the posterior probability density function of variable θ is a lognormal distribution with mean of μ_θ and variance of σ_θ^2, where

$$\begin{aligned} \mu_\theta &= exp[\mu_y + \sigma_y^2/2] \\ \sigma_\theta^2 &= \mu_\theta^2 [exp(\sigma_y^2) - 1] \end{aligned} \tag{72}$$

In summary, the posterior distribution of a lognormally distributed variable could be calculated in three steps:

1. Transform lognormally distributed prior distribution and likelihood function to normal distributions;
2. Find out the posterior distribution for the transformed variable y; and
3. Transform the posterior distribution of the transformed variable into the posterior distribution of the original variable.

CHAPTER IV

DESCRIPTIONS OF AGNPS MODEL AND EXPERIMENTAL DATA

Description of the AGNPS Model

The AGricultural Non-Point Sources pollution model (AGNPS) was selected as the event-based model to be used in this research. AGNPS is a computer simulation model developed by the Agricultural Research Service (ARS) in cooperation with the Minnesota Pollution Control Agency and the U. S. Department of Agriculture's Soil Conservation Service. The objectives of this model were to obtain uniform and accurate estimates of runoff quality with primary emphasis on sediment and nutrients to compare the effects of various conservation alternatives on implementation as part of the management practices of the watershed (Young et al, 1987).

The AGNPS model has three basic components: hydrology; erosion and sediment transport; and transport of nitrogen, phosphorus, and chemical oxygen demand. The model provides output on hydrology with estimates of both runoff volume and peak runoff. In the erosion and sediment transport portion of the AGNPS model, estimates of upland erosion, channel erosion, and sediment yield are provided. Along with these, in the last portion of the

model, calculations are made for estimating nitrogen (N), phosphorus (P), and chemical oxygen demand (COD) concentrations in the runoff and the sediment discharge for a single storm event for all points in an agricultural watershed. Table 4-2 lists the outputs of the AGNPS model at the outlet of the watershed or for any cells. The AGNPS model can be applied to agricultural watersheds ranging in size from a few hectares to upwards of 20,000 hectares (Young et al., 1989).

AGNPS is a single-event-based model intended to simulate sediment and nutrient transport primarily from agricultural watersheds. The model works on a cell basis. Cells are equally sized square areas subdividing the watersheds. In this model, runoff and upland erosion are calculated first, then the detached sediment is routed from cell to cell through the watershed to the outlet. Pollutants are routed in a stepwise fashion from the headwaters of the watershed to the outlet so that the flow at any point may be examined. Accuracy of the simulation results can theoretically be increased by reducing the cell size, but this will increase the time to run the model. It is worth noting, however, that more accuracy may not be obtained by reducing the cell size after the cell size has been reduced to some degree.

Input data for AGNPS can be classified into two categories: watershed data and cell data. Watershed data include information applicable to the entire watershed and to the storm event to be simulated. Cell data include physical information describing each of the cells as well as information based on the land practices in the cell. Table 4-1 lists the inputs for the AGNPS model (Young et al., 1989).

Table 4-1. Input Data File for AGNPS

Column #	Data
	Watershed Data
1	Watershed identification
2	Cell area (acres)
3	Total number of cells
4	Precipitation (inches)
5	Energy-intensity value
	Cell parameters
1	Cell number
2	Number of the cell into which it drains
3	SCS curve number
4	Average land slope (%)
5	Slope shape factor (uniform, convex, or concave)
6	Average field slope length (feet)
7	Average channel slope (%)
8	Average channel side slope (%)
9	Mannings roughness coefficient for the channel
10	Soil erodibility factor (K) from USLE
11	Cover and management factor (C) from USLE
12	Support practice factor (P) from USLE
13	Surface condition constant (factor based on land use)
14	Aspect (one of 8 possible directions indicating the principal drainage direction from the cell)
15	Soil texture (sand, silt, clay, peat)
16	Fertilization level (zero, low, medium, high)
17	Incorporation factor (% fertilizer left in top a cm of soil)
18	Point source indicator (indicates existence of a point source input within a cell)
19	Gully source level (estimate of amount, tons, or gully erosion in a cell)
20	Chemical oxygen demand factor
21	Impoundment factor (indicating presence of an impoundment terrace system within the cell)
22	Channel indicator (indicating existence of a defined channel within a cell)

Table 4-2. AGNPS Output at the Watershed Outlet Or for Any Cell

Hydrology Output Runoff volume (inches) Peak runoff rate (cfs) Fraction of runoff generated within the cell
Sediment Output Sediment yield (tons) Sediment concentration (ppm) Sediment particle size distribution Upland erosion (tons/acre) Amount of deposition (%) Sediment generated within the cell (tons) Enrichment ratios by particle size Delivery ratios by particle size
Chemical Output Nitrogen Sediment associated mass (pounds/acre) Concentration of soluble material (ppm) Mass of soluble material (pounds/acre) Phosphorus Sediment associated mass (pounds/acre) Concentration of soluble material (ppm) Mass of soluble material (pounds/acre) Chemical Oxygen Demand Concentration (ppm) Mass (pounds/acre)

Algorithms of the AGNPS Model

As stated in the previous section, the AGNPS model consists of three basic components, namely, hydrology, erosion and sediment transport, and chemical transport. An overview of the AGNPS model structure is given by Young et al. (1989; 1994). Most of the following content draws from these two sources. Haan et al. (1994) is the another source to write the following algorithms of the AGNPS model.

Hydrology

Runoff volume and peak flow rate are estimated in the hydrology portion of the model. Runoff volume is estimated by using the Soil Conservation Service (SCS) curve number (CN) method (Soil Conservation Service, 1972). This method was chosen in AGNPS because of its simplicity and widespread use. The well-known relationship is given by

$$Q = \frac{(P-0.2S)^2}{(P+0.8S)} \qquad P \geq 0.2S \qquad (73)$$

where Q = runoff volume (in.);

P = total precipitation (in.); and

S = retention parameter or maximum potential soil moisture storage.

Runoff will not occur until the total depth of precipitation is greater than 0.2S. The retention parameter S (in units of inches) is related to CN by

$$S = \frac{1000}{CN} - 10 \qquad (74)$$

The curve number CN depends upon land use, hydrologic soil group, soil type, and hydrologic soil condition. S is in inches. It can be changed to millimeters (mm) by multiplying by 25.4. However, Q, P and S must be in the same units.

Peak runoff rate for each cell is estimated using the following empirical relationship proposed by Smith and Williams (1980)

$$Q_P = 3.79 A^{0.7} CS^{0.16} (RO/25.4)^{(0.903 A^{0.017})} LW^{-0.19} \qquad (75)$$

where Q_P = peak flow rate (m^3/s);

A = drainage area (km^2);

CS = channel slope (m/km);

RO = runoff volume (mm); and

LW = the watershed length-width ratio, calculated by L^2/A where L is the watershed length.

Erosion and sediment transport

A modified form of the Universal Soil Loss Equation (USLE) is used to estimate upland erosion for single storms as follows

$$SL = (EI)\,KLSCP\,(SSF) \tag{76}$$

where SL = soil loss;

EI = the product of the storm total kinetic energy and maximum 30-minute intensity;

K = the soil erodibility factor, which is a measure of soil's resistance to the erosive powers of rainfall energy and runoff. Experimentally, soil erodibility is the soil loss per unit rainfall index on a standard erosion plot;

L = the slope length factor;

S = the slope steepness factor, which is used to predict the effect of slope gradient on soil loss;

C = the cover and management factor, which accounts for above-ground effects, surface effects, and below-surface effects;

P = the supporting practice factor, which is used to evaluate the effects of contour tillage, strip cropping, terracing, subsurface drainage, and dryland farm surface roughening;

SSF = a factor to adjust for slope shape within the cell.

After runoff and upland erosion are calculated, detached sediment is routed from cell to cell through the watershed to the outlet. The basic routing equation is derived from the steady-state continuity equation as

$$Q_S(x) = Q_S(O) + Q_{SL}(x/L_r) - \int_0^{\infty} D(x)\, w\, dx \qquad (77)$$

where $Q_S(x)$ is the sediment discharge at the downstream end of the channel reach, $Q_S(O)$ is the sediment discharge into the upstream end of the channel reach, Q_{SL} is the lateral sediment inflow rate, x is the downstream distance, L_r is the reach length, w is the channel width, and D(x) = the deposition rate.

Eroded soil and sediment yield are subdivided into five particle size classes, clay, silt, small aggregate, large aggregate, and sand. Sediment load for each of the five particle size classes leaving a cell can be calculated. For more details refer to Young et al. (1989).

Chemical transport

The chemical transport part of the model estimates transport of N, P, and COD throughout the watershed. Chemical transport calculations are divided into soluble and sediment adsorbed phases. Nutrient yield in the sediment absorbed phase is calculated using total sediment yield from a cell as given by

$$Nut_{sed} = (Nut_f)\, Q_s(x)\, E_R \qquad (78)$$

where Nut_{sed} is N or P transported by sediment, Nut_f is N or P content in the field soil, $Q_S(x)$ is sediment yield, and E_R is the enrichment ratio which is calculated from

$$E_R = 7.4 Q_s(x)^{-0.2} T_f \quad (79)$$

where T_f is an adjustment factor used to correct sediment-adsorbed nutrient enrichment ratio for sand and clay soils.

Soluble nutrient estimates consider the effects of nutrient levels in rainfall, fertilization, and leaching. The concentration of soluble nutrients in runoff is estimated by the equation given by

$$Nut_{sol} = C_{nut} Nut_{ext} Q \quad (80)$$

where Nut_{sol} is the concentration of soluble N or P in the runoff, C_{nut} is the mean concentration of soluble N or P at the soil surface during runoff, Nut_{ext} is an extraction coefficient of N and P for movement into runoff, and Q is the total runoff volume.

Experimental Data

Four small watersheds in Washington County, Arkansas, were chosen for this study. There are no special considerations in the selection of these watersheds except they had readily available data. Experimental data were provided by Dr. Edwards (Edwards et al., 1994). The following subsections describe the nature of the data.

The four watersheds used in this study are located in the Lincoln Lake basin in northwestern Arkansas, which is approximately 12 miles away from Fayetteville. The four

watersheds are RM, RU, WM and WU, respectively. All four watersheds are covered with 100% pasture. Table 4-3 summarizes some of the characteristics of the study watersheds. Figure 4-1 to Figure 4-4 are topographic maps for the four study watersheds (Edwards et al., 1994). Since AGNPS model is a cell based model, the divided cells for each watershed were superimposed onto the corresponding topographic map (Figures 4-1 to 4-4). The four watersheds were divided into one to seventeen cells depending on the shape of each watershed (see Table 4-3). Since all the four watershed are small and each watershed has only one type of soil and the same coverage, they were considered as homogeneous watersheds. For each watershed, the same parameters were assigned to each cell.

Data were collected in order to demonstrate the degree of water quality improvement that can accompany Best Management Practices (BMP) implementation. The Arkansas Soil and Water Conservation Commission (ASWCC) and US Environmental Protection Agency (USEPA) sponsored the monitoring. The watersheds, RM, RU, WM and WU, were monitored from September 1991 to April 1994. The observed data used in this study include rainfall, runoff and sediment yield for each watershed. There are about thirty events for eahc watershed. Table 4-5 to Table 4-8 contain all available data for each watershed. The first column in these tables is Antecedent Moisture Conditions (AMC) which is used to adjust Curve Number (CN) in the SCS runoff model (Equation (73)). The number of AMC is determined based upon the total rainfall amount in the five days preceding the given storm. Table 4-4 gives the particular standards to define AMC (Smedema and Rycroft, 1983). The application of AMC will be explained in detail in the next chapter.

Since AGNPS is an event based model, all data in Tables 4-5 to 4-8 were listed

randomly rather than chronologically to eliminate the effects of dry season and wet season or dry year and wet year. The random arrangement of the data was done in an Excel spread sheet. First of all, rainfall, runoff volume and sediment yield data were entered chronologically in three columns so that rainfall, runoff volume and sediment yield for one event were in the same row. Secondly, in another column, a set of random numbers (between 0 and 1) with a uniform distribution were generated. Thirdly, all data were sorted by the column containing random numbers.

Data in each table were split up. Half of the data was used for model calibration, and the other half of the data served for model evaluation purposes. Because the data were split up randomly, we could expect that the part of the data for model calibration should possess the same statistical properties as the part of the data for model validation.

Table 4-3. Summarized Characteristics of the Study Watersheds

watershed	Area (acres)	Soil	Curve Number	Average Slope (%)	Number of Cells
RM	1.41	Captina silt loam	61	2	7
RU	3.04	Fayetteville fine sandy loam	74	3	1
WM	3.61	Hector-Mountainburg stony fine sandy loam/Allegheny gravelly loam	79	4	17
WU	2.62	Linker loam	64	4	16

Table 4-4. Classification of the Antecedent Moisture Conditions (AMC)

AMC class	Total rainfall in the 5 days preceding the given storm	
	Dormant Season	Growing Season
I	< 12.5 mm	< 35 mm
II	12.5 ~ 27.5 mm	35 ~ 52.5 mm
III	> 27.5 mm	> 52.5 mm

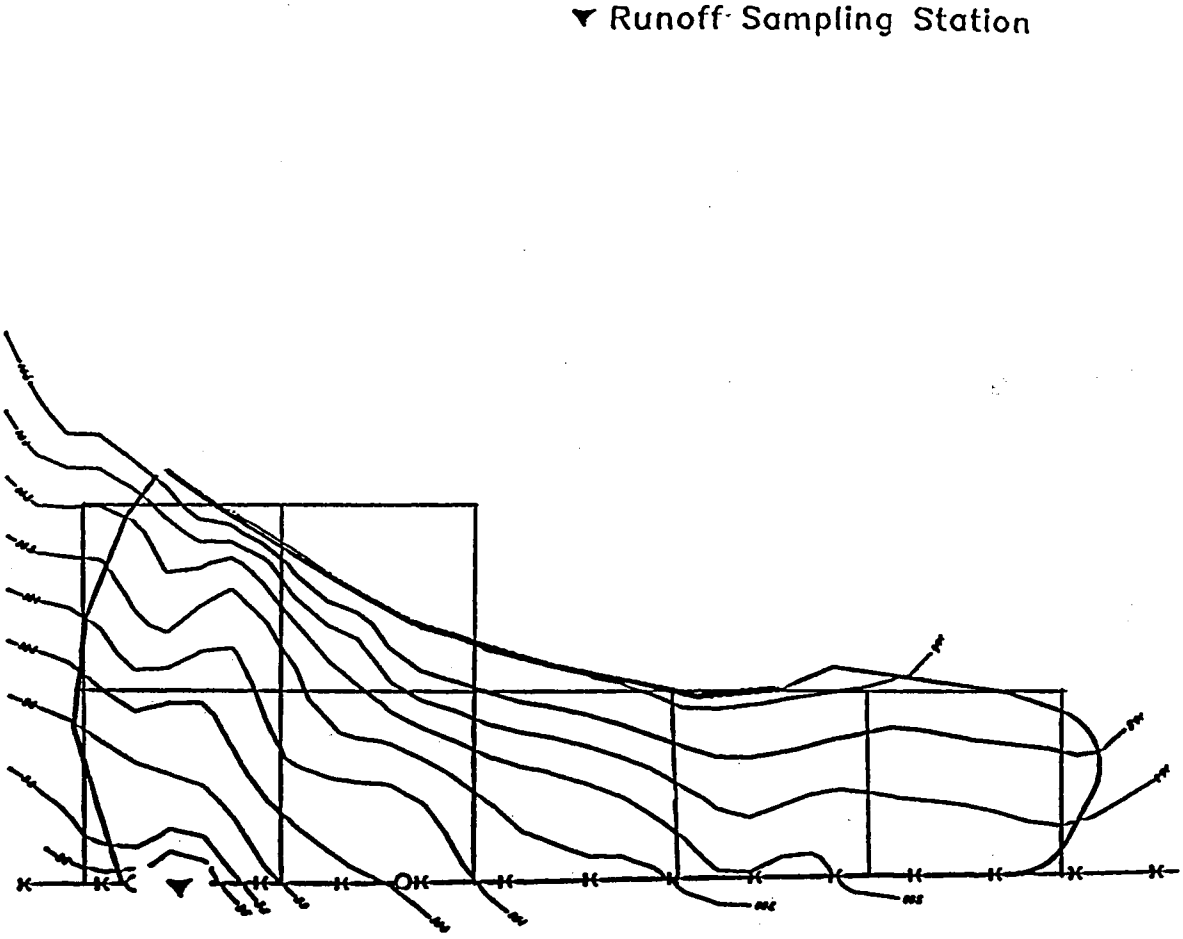

Figure 4-1. Topographic Map Of Watershed RM

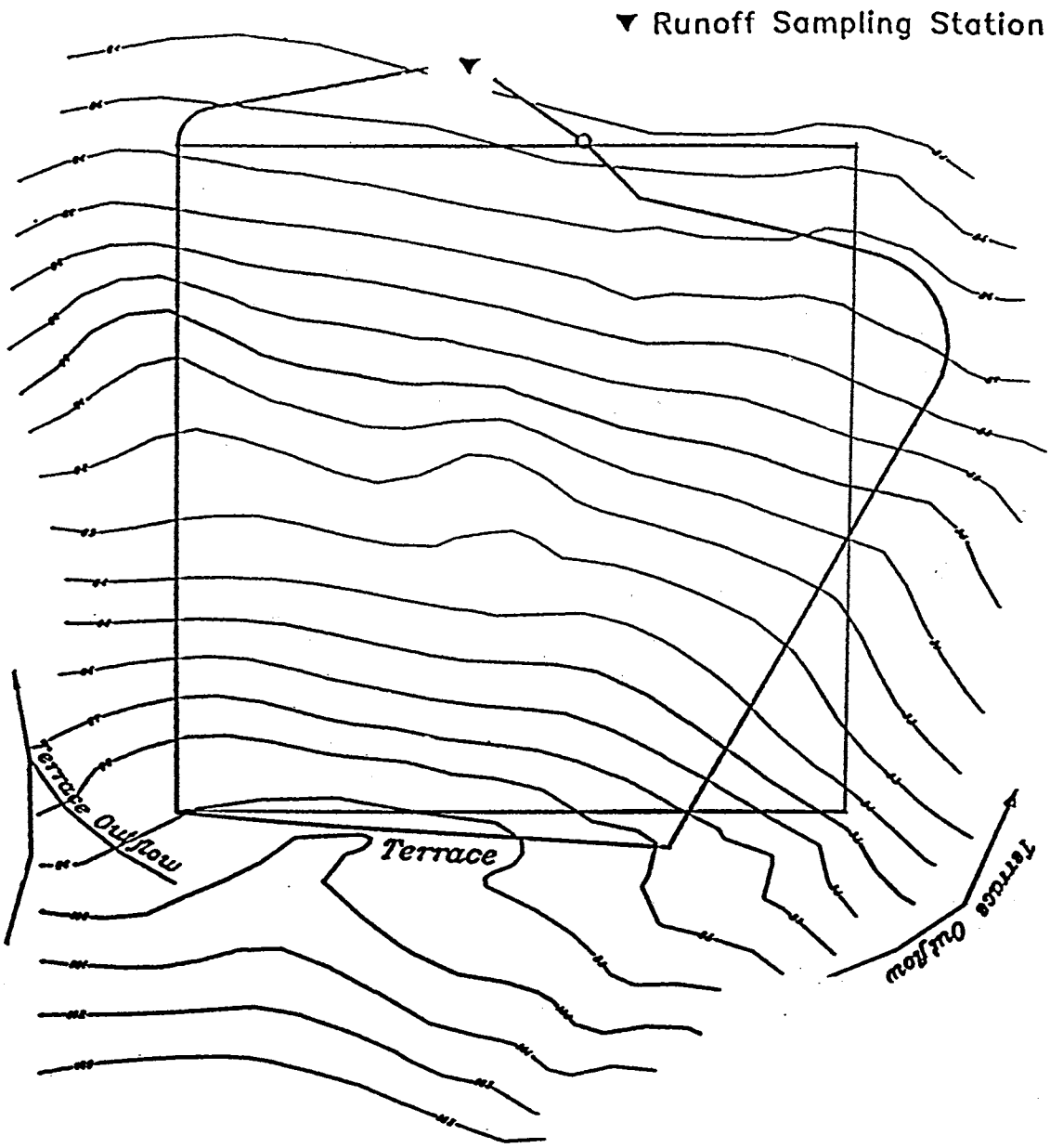

Figure 4-2. Topographic Map Of Watershed RU

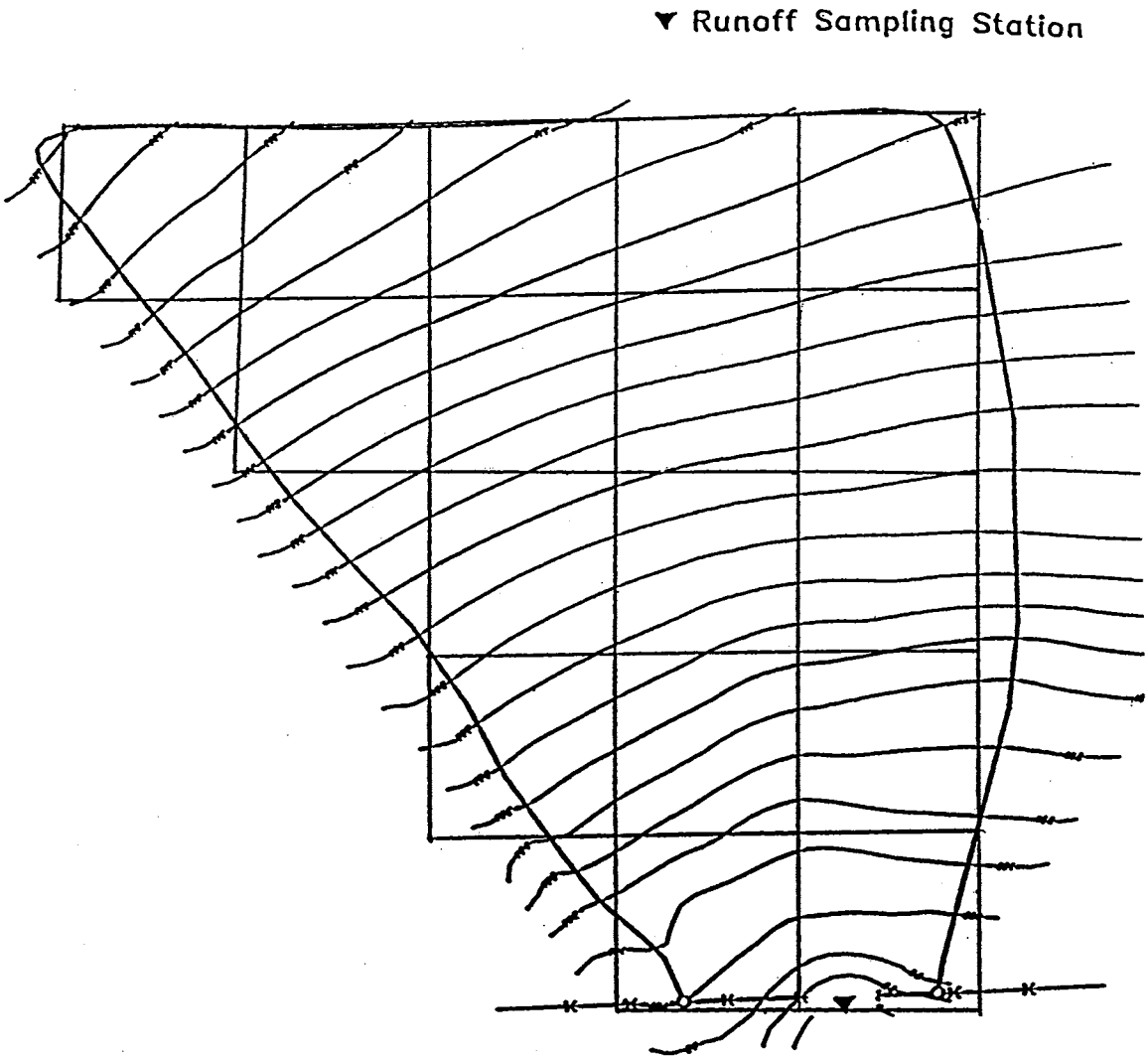

Figure 4-3. Topographic Map of Watershed WM

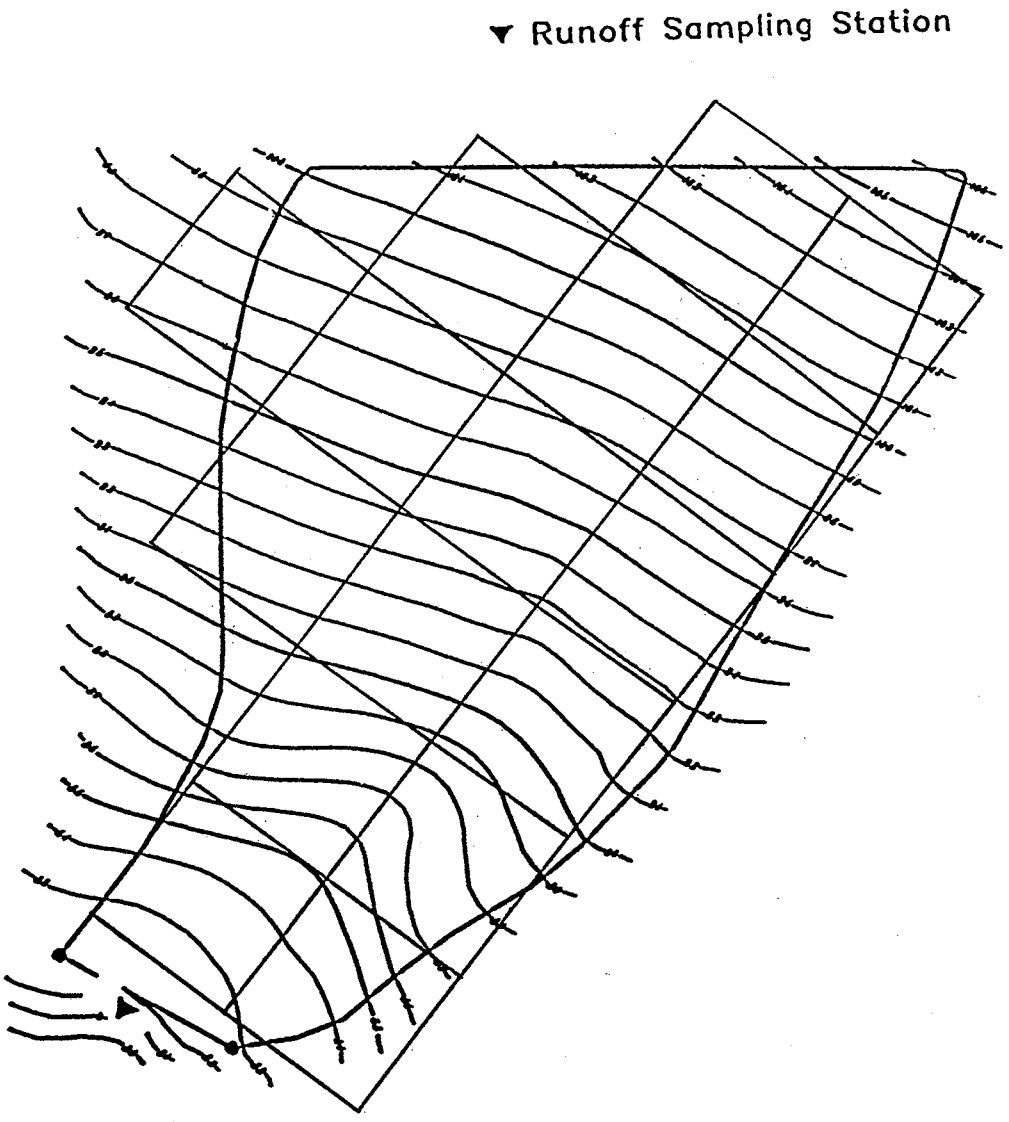

Figure 4-4. Topographic Map Of Watershed WU

Table 4-5. Observed Values for Watershed RM

Date	AMC	Rainfall (in)	Runoff (in)	Sediment Yield (lbs/ac)
06/06/92	1	1.47	0.02	0.14
05/17/92	2	0.76	0.03	0.94
09/21/92	1	3.37	0.54	2.32
07/05/92	1	1.26	0.04	0.33
10/26/91	3	2.25	0.17	27.52
11/14/93	3	0.64	0.10	0.70
05/10/93	3	1.57	0.09	0.16
07/30/93	1	2.32	0.21	0.67
05/09/93	1	2.03	0.16	0.69
11/16/93	3	1.07	0.08	1.03
12/12/91	1	0.41	0.00	0.00
11/11/92	1	1.77	0.01	0.23
04/14/93	1	1.00	0.01	0.18
01/04/93	1	1.44	0.14	7.54
12/15/92	3	2.00	0.50	2.83
09/14/93	2	1.34	0.08	0.40
03/03/93	1	0.86	0.04	0.95
05/11/92	1	2.26	0.07	1.82
11/12/92	3	0.90	0.07	2.96
08/04/92	3	1.88	0.09	0.16
06/25/93	2	2.38	0.35	2.49
04/04/93	2	1.08	0.03	0.14
11/14/93	3	0.63	0.14	2.57
04/15/93	3	1.89	0.49	1.89
09/15/93	3	2.68	0.30	1.02
10/14/92	1	1.80	0.01	1.22
10/16/93	1	1.45	0.04	0.24
10/17/93	3	0.49	0.07	0.52
01/26/94	1	0.84	0.02	0.82

Table 4-6. Observed Values for Watershed RU

Date	AMC	Rainfall (in)	Runoff (in)	Sediment Yield (lbs/ac)
06/25/93	2	2.38	1.06	5.52
05/09/93	1	2.03	1.03	8.63
04/15/93	3	1.89	0.62	5.21
11/16/93	3	1.07	0.65	0.88
10/24/91	1	2.49	0.01	0.08
04/04/93	1	1.11	0.07	0.36
12/03/93	2	0.53	0.17	0.65
05/28/92	1	1.28	0.06	0.11
09/21/92	1	3.51	1.51	52.65
11/11/92	1	1.77	0.28	1.58
05/10/93	3	1.57	1.22	2.21
09/14/93	2	1.34	0.08	0.60
12/12/91	1	0.47	0.34	4.54
03/19/93	2	0.90	0.11	1.49
10/31/91	3	1.04	0.18	0.12
12/14/92	3	1.93	0.69	2.19
09/15/93	3	2.68	0.66	2.54
10/26/91	3	2.25	0.65	15.45
15/11/92	1	2.26	0.25	0.34
11/14/93	1	2.69	1.43	1.94
03/26/94	1	1.51	0.02	0.07
01/26/94	1	0.84	0.11	1.79
01/04/93	2	1.44	0.98	27.29
02/04/92	3	1.92	0.70	2.69
04/14/93	1	1.00	0.03	0.15
02/24/93	1	3.37	0.01	0.15
06/06/92	1	1.47	0.67	1.21
12/09/92	1	1.25	0.48	1.52
11/16/93	3	1.07	0.43	0.49
11/12/92	3	1.11	0.60	5.30
12/16/92	3	2.01	0.69	1.25
07/05/92	1	1.74	0.19	1.38
10/16/93	1	1.94	1.00	2.49
07/16/92	1	1.88	0.01	0.06
07/30/92	1	2.32	0.70	9.35

Table 4-7. Observed Values for Watershed WM

Date	AMC	Rainfall (in)	Runoff (in)	Sediment Yield (lbs/ac)
04/14/93	1	0.69	0.01	0.15
10/31/91	3	1.37	0.76	2.58
01/04/93	1	0.95	0.06	0.64
10/26/91	3	2.32	1.23	86.33
10/28/91	3	1.42	0.65	4.42
10/24/91	1	3.57	0.04	0.32
12/15/92	3	4.64	2.67	13.9
09/15/93	3	3.22	0.75	2.72
10/20/93	3	1.02	0.21	0.19
11/24/93	3	0.54	0.05	0.15
05/09/93	3	1.95	0.87	0.79
11/19/91	3	0.48	0.05	0.09
11/11/92	1	2.10	0.05	0.25
08/06/92	3	0.71	0.27	0.12
08/05/92	3	2.04	0.69	2.97
11/16/91	3	1.12	0.61	0.69
09/15/93	3	2.84	1.80	2.45
04/15/93	2	2.08	0.68	1.72
05/08/93	1	2.84	0.45	1.32
07/30/92	2	3.76	1.13	117.18
12/09/92	1	1.50	0.07	0.32
11/16/93	3	1.18	0.28	0.51
12/12/91	1	0.71	0.01	0.20
10/16/93	1	1.20	0.05	0.12
06/06/92	2	1.61	0.62	2.81
11/12/92	3	0.59	0.03	0.95
03/26/94	1	1.87	0.01	0.02

Table 4-8. Observed Values for Watershed WU

Date	AMC	Rainfall (in)	Runoff (in)	Sediment Yield (lbs/ac)
03/26/94	1	1.87	0.00	0.00
09/24/93	1	1.32	0.03	0.21
11/16/93	1	0.94	0.04	1.91
12/09/92	1	1.50	0.03	0.86
06/25/93	2	2.17	0.31	4.63
08/05/92	3	0.71	0.03	0.42
12/15/92	3	1.97	0.44	3.98
04/15/93	2	2.08	0.34	3.85
01/09/93	2	0.85	0.09	6.70
10/19/93	2	0.77	0.01	0.25
06/06/92	2	1.61	0.14	1.05
10/14/92	1	1.52	0.01	0.03
10/28/91	3	0.64	0.02	0.08
11/14/93	2	0.54	0.02	0.22
05/09/93	3	0.44	0.01	0.20
07/30/93	2	3.76	0.77	41.84
11/12/92	3	0.59	0.05	0.54
08/04/92	3	2.04	0.27	2.02
10/26/91	3	0.53	0.01	0.03
05/10/93	3	1.15	0.30	1.49
11/17/91	3	0.83	0.09	0.92
11/11/92	1	2.10	0.02	0.10
09/13/93	3	3.22	0.66	5.83
10/24/91	1	3.57	0.11	1.37
10/26/91	3	1.79	0.14	18.92
04/04/93	1	1.15	0.04	0.67
05/02/93	2	0.68	0.06	1.94
03/19/93	1	0.95	0.00	0.00
12/14/92	3	2.30	0.65	26.20
10/31/91	3	1.19	0.13	0.53
10/16/93	3	0.56	0.04	1.10
01/20/93	3	0.94	0.04	0.80
06/02/92	2	1.15	0.00	0.00
05/08/93	1	2.84	0.55	14.65

CHAPTER V

ANALYSIS OF PARAMETRIC UNCERTAINTY AND PARAMETER ESTIMATION

The purpose of the analysis of parametric uncertainty was to determine the joint and marginal probability density functions of uncertain model parameters. At the same time while a joint probability density function of model parameters was calculated, the optimal model parameters were considered to be those corresponding to the mode of the joint distribution of model parameters. The joint pdf and the optimal parameters obtained in the way described above may be dubious without checking to see if the stochastic nature of the associated residuals satisfies the necessary assumptions. If the optimal parameters result in residuals which satisfy the necessary assumptions, the joint pdf of the model parameters may be regarded as the solution to equation (61); otherwise, a correction is required. The optimal values of the model parameters after the correction must be redetermined and the residuals rechecked until the assumptions about residuals are satisfied. Then marginal probability density functions for each parameter may be derived upon integration of the joint probability density function (Edwards, 1988).

The Bayesian parameter estimation technique provides not only point estimates but

probability density functions for model parameters. It is very difficult for us to verify how good the pdfs are. But the point estimates of parameters can be verified by comparing with the estimates from Least Squares. Once the point estimates of parameters based upon the Bayesian estimator are shown to be efficient, more credit will be added to the pdfs of the model parameters because the point estimates are simply the parameter estimates corresponding to the mode of the joint pdf of the parameters.

The model parameters were estimated by the Least Squares method using the same model and data. The residuals associated with the optimal parameters by Least Squares must be checked to see if the assumptions of Least Squares are valid. Least Squares is the most widely used and accepted parameter estimation technique. If the optimal parameters by the Bayesian technique are close to those by Least Squares, it may be a demonstration that the Bayesian parameter estimation technique is a good method to use in hydrologic and water quality modeling.

Model Parameterization

Hydrologic and water quality models usually contain many parameters. Estimating all parameters by calibration requires intensive work and may not be necessary because model performance is often controlled by fewer sensitive parameters. Once these most sensitive parameters are well estimated, a hydrologic and water quality model should produce fair predictions of the model responses of interest. Therefore, only the parameters to which the model performance was sensitive were considered to be uncertain, while the

other insensitive parameters were considered as fixed. The sensitivity of the model parameters can be determined by sensitivity analysis.

Prabhu (1995) did a complete sensitivity analysis for the parameters of the AGNPS model. The watershed used for his sensitivity analysis was WM which was one of the four watersheds in this study. The results of Prabhu's sensitivity analysis were directly applied to this study. As far as runoff volume was concerned, curve number was the only sensitive parameter. As far as sediment yields were concerned, the most sensitive parameter was land slope. The second most sensitive parameter was curve number. Therefore, it was decided that only curve number and land slope would be calibrated in this study. Both observed runoff volumes and sediment yields were used to calibrate these two parameters. It could be expected that the calibration results from both runoff and sediment yield should be better than the results from either runoff or sediment yield alone.

One may argue that there is no need to estimate land slope since land slope is a physical parameter which can be measured from a map directly. This is not completely true. If we look at the USLE model, equation (76), we will find that both the slope steepness factor (S) and the slope length factor (L) are related to the actual land slope. Their values are estimated from regression equations over many slopes. The calculated value of L or S for a specific land slope can be considered as an average value over many locations with the same land slope. But for a specific location, the values of L and S may need to be adjusted up or down to make the predicted sediment yields match the corresponding observed data. In the AGNPS model, we are not able to adjust the slope factor (S) and the slope length factor (L). Therefore, we should adjust the actual land slope to match the observed sediment

yields with the model predictions.

Parameter Estimation and Uncertainty Analysis

Least Squares Parameter Estimation Method

The general concept of the Least Squares method was discussed in the literature review and will not be repeated. Some special considerations are still worth mentioning.

When two model responses are concerned, the Least Squares method can be expressed as

$$\underset{\underline{\Theta}}{MIN\ OF} = \sum_{i=1}^{n} e_{1i}^2 + \sum_{i=1}^{n} e_{2i}^2 \tag{81}$$

where e_{1i} is the residual of runoff volume, e_{2i} is the residual of sediment yield, n is the number of rainfall events, and $\underline{\Theta}$ refers to curve number and land slope.

Problems may arise with equation (81) when the magnitude of the runoff volume and sediment yield are significantly different or when different units of runoff or sediment yield are used. Consider a situation that the magnitude of sediment yield is ten times bigger than that of runoff volume. Assume the relative accuracy of the model predictions for them is the same, for example within 5% of the observed data, then on average the residuals of runoff volume would be ten times less than the residuals of sediment yields. As a result, the sediment term in equation (81) will carry more weight than the runoff volume term. In other

words, the calibration results will be dominated by the residuals of sediment yield. The calibrated parameters in this situation may give model predictions on sediment yield with high accuracy and on runoff volume with low accuracy. Based on the same reason, one could imagine that the values of parameters to be calibrated may be different when different units are used, because the units would change the magnitude of runoff or sediment relative to each other.

If we desire to obtain the calibration parameters with which the AGNPS model would provide predictions of runoff volume and sediment yields with the same accuracy, the residuals in equation (81) have to be normalized. This can be done by having the actual residual divided by the mean of its observed data. That is

$$e = \frac{observed - predicted}{mean\ of\ observed} \tag{82}$$

When this definition of residual is applied to equation (81), an approximately equal weight will be put on runoff volume and sediment yields because the residuals of both runoff and sediment are relative residuals and are dimensionless. In this case, one could expect approximately the same accuracy for runoff and sediment, provided that the model is good and that the quality of the observed data for them is the same.

For one model response, no matter what residuals are used, the actual residuals or the relative residuals from equation (82), the Least Squares method will give the same calibration results.

When the constant variance assumptions of Least Squares are not satisfied, the square root transformation was selected for use in order to induce homoscedasticity in runoff volume and sediment yield residuals. This transformation is a member of the family of Box and Cox (1964) transformations presented in equation (21). In this case, the residuals in equation (81) are defined as:

$$\epsilon = \frac{\sqrt{observed} - \sqrt{predicted}}{mean\ of\ \sqrt{observed}} \tag{83}$$

Again, the residuals from the transformed model responses need to be rechecked. If the assumptions of Least Squares are still not satisfied, another member of the family of Box and Cox transformations may be applied.

Bayesian Parameter Estimation Method

Equation (61) in Chapter III is the Bayesian criterion for estimating the model parameters and analyzing uncertainty of the model parameters. But this equation was derived without consideration of relative residuals or transformation of the model responses. In order to use the Bayesian technique to analyze parameter uncertainty and to obtain the optimal parameter estimates, it must be proven that equation (61) still applies to the relative residuals of the model responses or transformed model responses. Edwards (1988) proves that equation (61) still holds for the transformed model responses. In the same fashion, it can be proven that equation (61) will also hold for the relative residuals of the model responses

and for the relative residuals of the transformed model responses.

Consider the model presented in Chapter III in equation (43), $\underline{Y} = f(\underline{X}, \underline{\Theta}) + \epsilon$, where the number of the model responses is equal to p=2. The residuals may be expressed as:

$$\epsilon_{1i} = y_{1i} - \hat{y}_{1i} = y_{1i} - f_1(\underline{X}, \underline{\Theta}) \tag{84}$$

$$\epsilon_{2i} = y_{2i} - \hat{y}_{2i} = y_{2i} - f_2(\underline{X}, \underline{\Theta}) \tag{85}$$

The relative residuals of the transformed model responses are defined as the difference between the square roots of the observations and the square root of the model predictions divided by the mean of the square roots of the observations.

$$\eta_{1i} = \frac{1}{a}\left(\sqrt{y_{1i}} - \sqrt{f_1(\underline{X}, \underline{\Theta})}\right) \tag{86}$$

$$\eta_{2i} = \frac{1}{b}\left(\sqrt{y_{2i}} - \sqrt{f_2(\underline{X}, \underline{\Theta})}\right) \tag{87}$$

where a and b are equal to the mean of the square root of the corresponding data.

Assume now that the η_{1i} are $N(0, \sigma_1^2)$ and the η_{2i} are $N(0, \sigma_2^2)$. Then (η_{1i}, η_{2i}) are $N(\underline{0}, \underline{\Sigma})$. Their joint probability density function may be written as

$$p(\underline{\eta}_i) = (2\pi)^{-1} |\underline{\Sigma}|^{-1/2} \exp\left[-\frac{1}{2}(\underline{\eta}_i^T \underline{\Sigma}^{-1} \underline{\eta}_i)\right] \tag{88}$$

where $\underline{\eta}_i = (\eta_{1i}, \eta_{2i})^T$. This probability density function may be related to that of the corresponding pair of observations, $\underline{y}_i = (\underline{y}_{1i}, \underline{y}_{2i})^T$, by the relation of

$$p(\underline{y}_i) = p(\underline{\eta}_i) |\underline{J}| \tag{89}$$

where $|\underline{J}|$ is the Jacobian of the transformation from $\underline{\eta}_i$ to $\underline{y}_i$.

$$|\underline{J}| = \begin{vmatrix} \frac{\partial \eta_{1i}}{\partial y_{1i}} & \frac{\partial \eta_{1i}}{\partial y_{2i}} \\ \frac{\partial \eta_{2i}}{\partial y_{1i}} & \frac{\partial \eta_{2i}}{\partial y_{2i}} \end{vmatrix} = \begin{vmatrix} \frac{1}{2a y_{1i}^{1/2}} & 0 \\ 0 & \frac{1}{2b y_{2i}^{1/2}} \end{vmatrix} = \frac{1}{4ab(y_{1i}y_{2i})^{1/2}} \tag{90}$$

It follows from equations (88) through (90) that the probability density function of $\underline{y}_i$ will be

$$p(\underline{y}_i) = |\underline{J}| (2\pi)^{-1} |\underline{\Sigma}|^{-1/2} \exp\left[-\frac{1}{2}(\underline{\eta}_i^T \underline{\Sigma}^{-1} \underline{\eta}_i)\right] \tag{91}$$

Now consider all pairs of observations, $\underline{y} = (\underline{y}_1, \underline{y}_2, \ldots \underline{y}_n)^T$, and suppose that the $\underline{y}_i$ are independent for all i. The probability density function of $\underline{y}$ is written as

$$p(\underline{y}) = g(\underline{y})(2\pi)^{-n}|\underline{\Sigma}|^{-n/2}\exp\left[\sum_{i=1}^{n}-\frac{1}{2}(\underline{\eta}_i^T\underline{\Sigma}^{-1}\underline{\eta}_i)\right] \tag{92}$$

where

$$g(\underline{y}) = \prod_{i=1}^{n}\frac{1}{4ab(y_{1i}y_{2i})^{1/2}} \tag{93}$$

Given a set of data, $\underline{y}$, the function $g(\underline{y})$ is a constant, and the residuals $\underline{\eta}_i$ are a function of the model parameters $\underline{\Theta}$. Then the probability density function of $\underline{y}$ is only a function of $\underline{\Sigma}$ and $\underline{\Theta}$. Therefore, the likelihood function of $\underline{\Sigma}$ and $\underline{\Theta}$ given the data $\underline{y}$ may be written as

$$L(\underline{\Sigma},\underline{\Theta}/\underline{y}) \propto |\underline{\Sigma}|^{-n/2}\exp\left[\sum_{i=1}^{n}-\frac{1}{2}(\underline{\eta}_i^T\underline{\Sigma}^{-1}\underline{\eta}_i)\right] \tag{94}$$

This likelihood function is identical to that used in Chapter III for derivation of the posterior probability density function. From this point, following exactly the same procedure as stated in chapter III, the posterior probability density function identical to equation (61) should be obtained. The only difference is that the elements of $\underline{S}(\underline{\Theta})$ are derived from the transformed residuals.

Procedures

The Least Squares method and the Bayesian method were two methods chosen for this study. For the purpose of comparison, curve number and land slope were calibrated under four conditions:

1). Curve number calibrated only from runoff volume;

2). Curve number and land slope calibrated only from sediment yields;

3). Curve number and land slope calibrated by the Least Squares method based upon both runoff volume and sediment yields; and

4). Curve number and land slope calibrated by the Bayesian technique based upon both runoff volume and sediment yields.

The calibration methods were not specified for conditions one and two because the Least Squares method and the Bayesian method will give the same estimates of model parameters for a single model output.

Suppose now that there are n rainfall events used for parameter estimation. Assume that the values of the other parameters of the AGNPS model are given. The procedures for parameter calibration for two conditions, one model response and two model responses, are given below:

Parameter calibration procedure for one model response:

1. Set upper and lower limits for curve number and land slope, and select proper increments for each of the two parameters.

2. Set the curve number and land slope equal to their lower limits in the AGNPS input data file.

3. For each rainfall event, update the rainfall amount in the AGNPS input data file. Then run the AGNPS model and record the residual of runoff volume or sediment yields. Repeat for all rainfall events.

4. Calculate the sum of the squared residuals.

5. Increase curve number or/and land slope by one increment. For every possible combination of curve number and land slope within their own upper and lower limits, repeat step 3 and step 4.

6. Find out the minimum value of the sum of the squared residuals for all possible combinations. The corresponding curve number and slope may be the calibrated results.

7. Check the necessary assumptions of residuals. If the assumptions are satisfied, the calibration results above are good. Otherwise, corrective action may be needed. Steps 2 to 6 have to be repeated and residuals rechecked.

Parameter calibration procedure for two model responses:

1. Set upper and lower limits for curve number and land slope, and select proper increments for each of the two parameters.

2. Set the curve number and land slope equal to their lower limits in the AGNPS input data file.

3. For each rainfall event, update the rainfall amount in the AGNPS input data file. Then run the AGNPS model and record the residual of runoff volume and the residual of sediment yields. Repeat for all rainfall events.

4. Calculate the sum of the squared residuals of runoff volume and the sum of the squared residuals of sediment yields. Then add them up to obtain the total residual sum of squares over both outputs, equation (81).

5. Calculate the determinant of $\underline{S}(\underline{\Theta})$ in equation (61).

6. Increase curve number or/and land slope by one increment. For every possible combination of curve number and land slope within their own upper and lower limits, repeat steps 3 to 5.

7. Find out the minimum of the values obtained in step 4 for all possible combinations of curve number and land slope. The corresponding curve number and slope will be the calibrated results by the Least Squares method.

8. Find out the maximum of the values obtained in step 5 for all possible combinations of curve number and land slope. The corresponding curve number and land slope will be the calibrated results by the Bayesian technique.

9. Check the necessary assumptions of residuals. If the assumptions are satisfied, the calibration results above are good. Otherwise, corrective action may be needed. Steps 2 through 8 have to be repeated and residuals rechecked.

10. The marginal distribution of curve number or slope can be obtained by integrating equation (61).

A C computer program was written to perform the procedures for both one model response and two model responses. This program will provide the calibration results of curve number and land slope for all four conditions listed in the beginning of this subsection.

The program will also provide the marginal distribution of the curve number and the marginal distribution of the land slope. The necessary assumptions of residuals need to be checked separately to confirm the calibration results by the program. The program was verified step by step through comparison of what the program does with what it should do. The source code of this program can be found in Appendix A.

Results and Discussions

Calibration of Parameters

The curve number and slope parameters were calibrated using the four conditions as stated above for all the four watersheds RU, RM, WM and WU. The point estimates of the parameters are shown in Tables 5-1 through 5-4. The model predictions and their associated residuals for each watershed are shown in Tables 5-5 through 5-8. When the parameters are estimated based upon one model response (either runoff volume or sediment yield), Least Squares and the Bayesian estimator will produce identical results. So the optimal methods were not specified in the tables. In order to make a judgement of how efficient the Bayesian estimator is, the sum of the squared errors (SSE) corresponding to the calibrated parameters were also shown in the tables. Note that both SSE of the runoff volume and SSE of the sediment yield were dimensionless so that they could be totaled. It is necessary to emphasize that the model residuals associated with the calibrated parameters need to be examined to see if the LS assumptions are satisfied.

Figures 5-1 through 5-8 are plots of residuals based upon the Bayesian estimator

against the corresponding rainfall amount for the four watersheds. It can be seen from Tables 5-1 through 5-4 that the calibrated parameters by Least Squares are either identical to or very close to those by the Bayesian estimator. If the residuals associated with the Bayesian estimator satisfy the Least Squares assumptions, the residuals related to the Least Squares method would probably satisfy the Least Squares assumptions too. Therefore, only the plots of residuals associated with the Bayesian estimator were presented.

On Figures 5-1 to 5-6, all residuals are distributed more or less around zero. The t test was employed to test the assumption of mean of zero. Table 5-9 shows that the null hypothesis of mean of zero was not rejected at the significance level of 0.05 for runoff residuals and sediment residuals in watersheds WM and WU, and for runoff residuals in watershed RU. The null hypothesis of mean of zero was rejected at the significance level of 0.05 for sediment residuals in watershed RU, but was not rejected at the significance level of 0.02. Therefore, the assumption of mean of zero may not be implausible for these three watersheds. Note that the t test can not be applied to any set of data which are not from a normal distribution. The normality of residuals will be tested later in this section. Figure 5-7 and Figure 5-8 (for watershed RM) indicate that the model predictions are completely biased since almost all residuals are greater than zero which means the AGNPS model underpredicts both runoff volume and sediment yields for watershed RM. It will also be shown later that the residuals for watershed RM are not normally distributed either. This will be explained subsequently.

Again, from Figures 5-1 to 5-6, there is a trend that the residuals are close to zero when the rainfall amount is small and that the residuals tend to increase when the rainfall

amount becomes larger. It means that the variances of the residuals increase slightly as rainfall amount increases. Strictly speaking, the assumption of homogeneous variance is violated. However, this phenomenon is not uncommon in hydrological and water quality modeling. Consider the situation that the residuals have a constant variance as rainfall amount becomes larger. One could expect that a heavy rainfall would generally produce a large runoff volume and sediment yield. Using the coefficient of variation (C_v) as a measure of accuracy of model predictions, one would expect the accuracy for small events to be lower than that for large events because the variances for all events, small or large, are identical. This may be desireable when prediction of large events is important, for example, flood forecasting. But in many cases, one may be interested only in predicting some events on an average basis. Consider now another situation in which the accuracy of the model predictions is identical for all size of events. Then the variances of the residuals will be small for small events and large for large events. Therefore, a slight increase of variances along with the size of the events may not be unacceptable in hydrological and water quality modeling.

The assumption of the normality of residuals was verified by plotting the residuals of runoff or sediment on a normal probability scale. This is a visual test. If residuals were perfectly normally distributed, the plot would be a straight line. Figures 5-9 through 5-14 are probability plots of residuals for watersheds RU, WM and WU. The distributions of the residuals of runoff volume and sediment yields may be approximated by normal distributions. Figures 5-15 and 5-16 indicate that the residuals of runoff volume for watershed RM may be normally distributed but the residuals of sediment yields for

watershed RM can not be normally distributed. Additionally, the Kolmogorov-Smirnov goodness-of-fit test was employed as a quantitative method to verify the assumption of the normality of residuals. The results are presented in Table 5-10. The null hypothesis of normally distributed residuals of runoff volume and sediment yields was not rejected at the 0.10 significant level for watersheds RU, WM and WU. For watershed RM, the null hypothesis of a normal distribution for the residuals of runoff volume was not rejected at the 0.10 significant level, but the null hypothesis of a normal distribution for the residuals of sediment yields was rejected even at the 0.05 significant level.

It can be concluded from the above discussion that the calibration results in Tables 5-1 through 5-3 for watersheds RU, WM and WU are valid. However, the estimates of the parameters for watershed RM in Table 5-4 can not be taken as the final calibration results since the Least Square's assumptions are not valid. It does not necessarily mean that the calibration techniques fail to work for watershed RM. It can be seen from Table 5-5 that the real cause of invalid Least Square's assumptions is the limitation of the output accuracy of the AGNPS model.

Table 5-8 provides the residuals and the predictions of runoff volume and sediment yields for watershed RM when the calibrated parameters are used in the AGNPS model. It can be seen that most model predictions are zero. For the predictions of sediment yields, there is only one, out of fifteen, non-zero value. The sediment yields of the AGNPS model is given in tons with two decimal place accuracy. When the unit of tons is changed to the unit of lbs/acre, 0.01 tons will be 14.29 lbs/ac for the watershed RM. Any values less than 0.005 tons would be output as zero by the AGNPS model. This is why most of the predicted

sediment yields are zero and the assumptions of the Least Squares method are not valid. Therefore, the AGNPS model may not be able to provide predictions for sediment yields accurately for the watershed RM. But this does not mean the AGNPS model is not an accurate model because most observations of sediment yields from the outlet of the watershed RM are less than 0.005 tons (7.15 lbs/ac). In addition, the amount of sediment yield of concern is usually much greater than 7.15 lbs/ac. In those cases, the AGNPS model would be a good model to use.

Probability Density Functions of Retention Parameter and Slope

Since the Least Square's assumptions were approximately satisfied for study watersheds RU, WM and WU, the marginal probability density functions of retention parameter and land slope were calculated by integrating Equation (61) and plotted just for these watersheds as shown on Figures 5-17 through 5-22. The dashed line represents the calibrated probability density function in these figures. Since none of these calibrated probability density functions follows exactly a known distribution, it will be difficult and very inconvenient to sample a value from such a distribution for use in an uncertainty analysis. It was decided that a known distribution would be used to approximate the calibrated probability density functions. A statistical software package, Bestfit (Palisade Corporation, 1993), was used to find the best approximation of a calibrated probability density function.

A lognormal distribution was chosen by Bestfit to approximate the calibrated probability density function of the retention parameter for watersheds RU, WM and WU.

For cases where the calibrated probability density function could not be approximated by a normal or lognormal distribution, only calibrated distributions were plotted. The distributions of land slope for watersheds RU and WM are such examples. In those cases, the mean and the standard deviation of the parameter were calculated based on its calibrated probability density function. Again, Bestfit was applied to do those calculations.

Comparison of Bayesian Estimator with Least Squares Technique

Tables 5-1 through 5-3 show the calibrated curve number and land slope for watersheds RU, WM and WU. Four sets of curve number and land slope were estimated, one set from runoff volume only, one set from sediment yields only, one set from both runoff volume and sediment yields by Least Squares technique, and another from both runoff volume and sediment yields by Bayesian estimator.

When the AGNPS model was calibrated only from runoff volume, land slope was not estimated by calibration because the curve number is the only sensitive parameter as far as runoff volume is concerned. The "real" land slope was selected as the value of land slope.

Four points could be made by observing the results in Tables 5-1 through 5-3:

1) The sum of squared errors (SSE) of runoff is the smallest when curve number was estimated by runoff volume alone, and the SSE of sediment yields is the smallest when the parameters were calibrated by sediment yields alone. However, the total SSE of either one may or may not be the smallest.

2) When the parameters were estimated by the Least Squares method based on both runoff volume and sediment yields, the SSE of runoff is equal to or very close to the smallest

SSE and the SSE of sediment yields is equal to or very close to the smallest SSE of sediment too. In addition, the total SSE is always the smallest.

3) The estimates of curve number by the Least Squares method based upon both runoff volume and sediment yields are equal to or very close to those based upon only runoff volume. Similarly, the estimates of land slope have this property too. This interesting property may be explained by the structure of the AGNPS model. The hydrologic model in AGNPS is independent from the Erosion and Sediment transport model. This indicates that a stepwise parameter estimation procedure could be applied. So curve number may be estimated only from runoff volume data and land slope may be estimated only from sediment yields. The estimates of the parameters by the stepwise procedure should be close to those by multipurpose objective function.

4) For the study watersheds WM and WU, the calibrated parameters by Least Squares are identical to those by Bayesian estimator. For watershed RU, the estimates of land slope by these two methods are the same, but the estimates of the curve number are a little different. If we compare the average of predicted runoff volume with the mean of observed runoff, we will find that the AGNPS model with the curve number estimated by the Least Squares method tends to underestimate the runoff while the model with the curve number estimated by Bayesian technique tends to overpredict runoff volume. The degree of the overprediction of runoff is less than that of the underprediction. Therefore, we may conclude that the Bayesian estimator is just as efficient as the Least Squares method and has the advantage of providing a probability density function for the estimate rather than simply a point estimate.

Table 5-1. Calibrated Parameters by Different Methods for Watershed RU

Optimization & criteria	Calibrated Curve Number	Calibrated Slope (%)	SSE * of Runoff	SSE of Sediment	Total SSE**
Runoff	82		14.7	316	330.7
Sediment	80	1	14.7	51.3	66.0
Runoff & Sediment (LS)	80	1	14.7	51.3	66.0
Runoff & Sediment (Bayesian)	86	1	16.6	59.2	75.8

* SSE = Sum of the squared errors

** Total SEE = column 4 + column 5

Table 5-2. Calibrated Parameters by Different Methods for Watershed WM

Optimization & criteria	Calibrated Curve Number	Calibrated Slope (%)	SSE * of Runoff	SSE of Sediment	Total SSE**
Runoff	72		1.5	31.3	32.8
Sediment	60	1	2.3	16.6	18.8
Runoff & Sediment (LS)	72	0	1.5	16.9	18.4
Runoff & Sediment (Bayesian)	72	0	1.5	16.9	18.4

* SSE = Sum of the squared errors

** Total SEE = column 4 + column 5

Table 5-3. Calibrated Parameters by Different Methods for Watershed WU

Optimization & criteria	Calibrated Curve Number	Calibrated Slope (%)	SSE * of Runoff	SSE of Sediment	Total SSE**
Runoff	66		4.7	13.0	17.7
Sediment	68	5	4.8	10.9	15.7
Runoff & Sediment (LS)	66	5	4.7	10.9	15.6
Runoff & Sediment (Bayesian)	66	5	4.7	10.9	15.6

* SSE = Sum of the squared errors

** Total SEE = column 4 + column 5

Table 5-4. Calibrated Parameters by Different Methods for Watershed RM

Optimization & criteria	Calibrated Curve Number	Calibrated Slope (%)	SSE * of Runoff	SSE of Sediment	Total SSE**
Runoff	52		25.1	27.3	52.5
Sediment	40	8	30.3	27.3	57.6
Runoff & Sediment (LS)	52	3	25.1	27.3	52.5
Runoff & Sediment (Bayesian)	50	3	25.3	27.3	52.6

* SSE = Sum of the squared errors

** Total SEE = column 4 + column 5

Table 5-5. Model Predictions and Residuals for Watershed RU

AMC	Rainfall (in)	Predicted Runoff (in)	Residuals* of Runoff (in)	Predicted Sediment Yields (lbs/ac)	Residuals of Sediment (lbs/ac)
2	2.38	1.15	-0.09	19.74	-14.22
1	2.03	0.31	0.72	6.58	2.05
3	1.89	1.21	-0.59	13.16	-8.95
3	1.07	0.51	0.14	6.58	-5.7
1	2.49	0.52	-0.51	13.16	-13.08
1	1.11	0.03	0.04	0	0.36
2	0.53	0.02	0.15	0	0.65
1	1.28	0.06	0	0	0.11
1	3.51	1.13	0.38	39.47	13.18
1	1.77	0.20	0.08	6.58	-5
3	1.57	0.93	0.29	13.16	-10.95
2	1.34	0.39	-0.31	6.58	-5.98
1	0.47	0	0.34	0	4.54
2	0.90	0.15	-0.04	0	1.49
3	1.04	0.48	-0.30	6.58	-6.46
3	1.93	1.25	-0.56	13.16	-10.97
3	2.68	1.95	-1.29	32.89	-30.35
3	2.25	1.55	-0.90	19.74	-4.29

* residuals = "observed" - "predicted"

Table 5-6. Model Predictions and Residuals for Watershed WM

AMC	Rainfall (in)	Predicted Runoff (in)	Residuals* of Runoff (in)	Predicted Sediment Yields (lbs/ac)	Residuals of Sediment (lbs/ac)
1	0.69	0	0.01	0	0.15
3	1.37	0.41	0.35	5.60	-3.02
1	0.95	0	0.36	0	0.64
3	2.32	1.10	0.13	11.20	75.13
3	1.42	0.44	0.21	5.60	-1.18
1	3.57	0.27	-0.23	5.60	-5.28
3	4.64	3.13	-0.46	28.01	-14.11
3	3.22	1.85	-1.10	16.81	-14.09
3	1.02	0.21	0	0	0.19
3	0.54	0.02	0.03	0	0.15
3	1.95	0.81	0.06	5.6	-4.81
3	0.48	0.01	0.04	0	0.09
1	2.10	0.01	0.04	0	0.25

* residuals = "observed" - "predicted"

Table 5-7. Model Predictions and Residuals for Watershed WU

AMC	Rainfall (in)	Predicted Runoff (in)	Residuals* of Runoff (in)	Predicted Sediment Yields (lbs/ac)	Residuals of Sediment (lbs/ac)
1	1.87	0	0	0	0
1	1.32	0	0.03	0	0.21
1	0.94	0	0.04	0	1.91
1	1.50	0	0.03	0	0.86
2	2.17	0.21	0.10	7.81	-3.18
3	0.71	0.03	0	0	0.42
3	1.97	0.63	-0.19	7.81	-3.83
2	2.08	0.18	0.16	7.81	-3.96
2	0.85	0	0.09	0	6.70
2	0.77	0	0.01	0	0.25
2	1.61	0.06	0.08	0	1.05
1	1.52	0	0.01	0	0.03
3	0.64	0.02	0	0	0.08
2	0.54	0	0.02	0	0.22
3	0.44	0	0.01	0	0.20
2	3.76	0.95	-0.18	23.44	18.40
3	0.59	0.01	0.04	0	0.54
3	2.04	0.68	-0.41	7.81	-5.79

* residuals = "observed" - "predicted"

Table 5-8. Model Predictions and Residuals for Watershed RM

AMC	Rainfall (in)	Predicted Runoff (in)	Residuals* of Runoff (in)	Predicted Sediment Yields (lbs/ac)	Residuals of Sediment (lbs/ac)
1	1.47	0	0.02	0	0.14
2	0.76	0	0.03	0	0.94
1	3.37	0	0.54	0	2.32
1	1.26	0	0.04	0	0.33
3	2.25	0.34	-0.17	14.29	13.23
3	0.64	0	0.10	0	0.70
3	1.57	0.10	-0.01	0	0.16
1	2.32	0	0.21	0	0.67
1	2.03	0	0.16	0	0.69
3	1.07	0.01	0.07	0	1.03
1	0.41	0	0	0	0
1	1.77	0	0.01	0	0.23
1	1.00	0	0.01	0	0.18
1	1.44	0	0.14	0	7.54
3	2.00	0.24	0.26	0	2.83

* residuals = "observed" - "predicted"

Table 5-9 T Test Results for Watersheds RU, WM and WU

	RU		WM		WU	
	Runoff	Sediment	Runoff	Sediment	Runoff	Sediment
# of Samples	18	18	13	13	18	18
Mean	-0.14	-5.20	0.045	0.035	0.07	0.42
Stdev	0.50	9.34	0.21	2.07	0.14	0.96
T value	1.17	2.36	0.22	0.06	2.08	1.88
Significance Level α	0.05	0.05 (0.02)	0.05	0.05	0.05	0.05
Table value ($t_{1-\alpha/2, n-1}$)	2.11	2.11 (2.57)	2.18	2.18	2.11	2.11
H_0: $\mu=0$	not rejected	rejected (not rejected)	not rejected	not rejected	not rejected	not rejected

Table 5-10 Tests of Normality by Kolmogrov-Smirnov

		Maximum Deviation	Significance level α	K-S Critical Values	H_0: Normally Distributed
RM	Runoff	0.166	0.10	0.304	not rejected
	Sediment	0.347	0.10 (0.05)	0.304 (0.338)	rejected
RU	Runoff	0.21	0.10	0.278	not rejected
	Sediment	0.11	0.10	0.278	not rejected
WM	Runoff	0.18	0.10	0.325	not rejected
	Sediment	0.28	0.10	0.325	not rejected
WU	Runoff	0.19	0.10	0.278	not rejected
	Sediment	0.10	0.10	0.278	not rejected

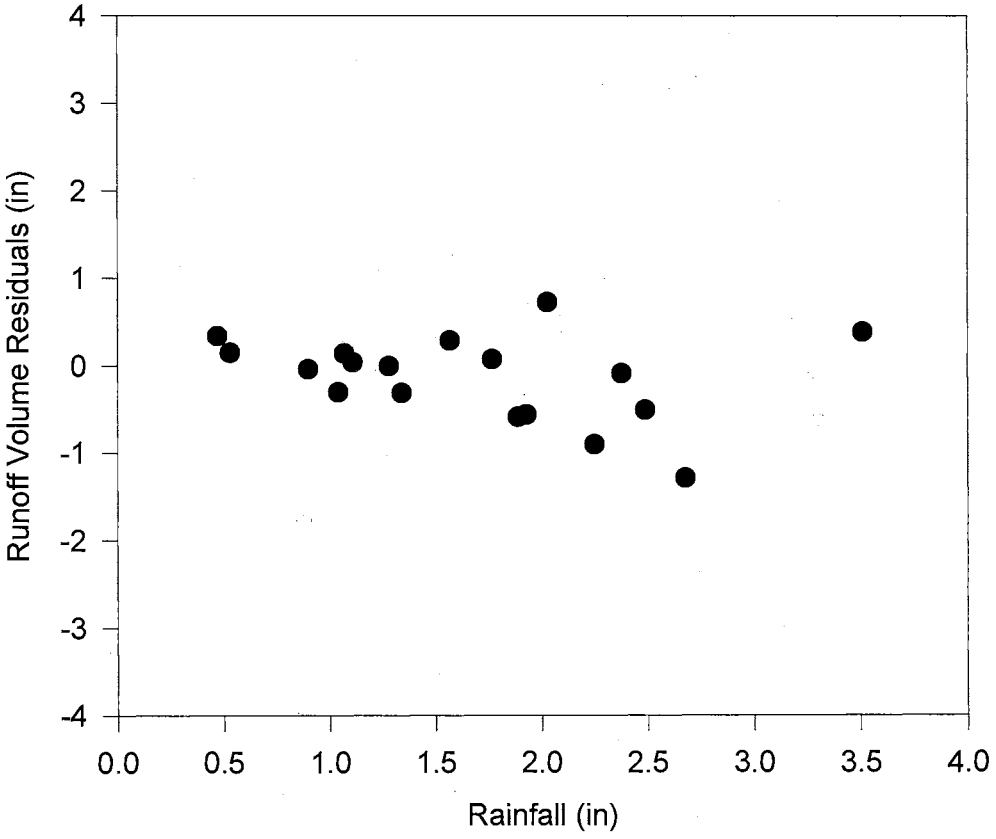

Figure 5-1. Runoff Volume Residual Plot for Watershed RU

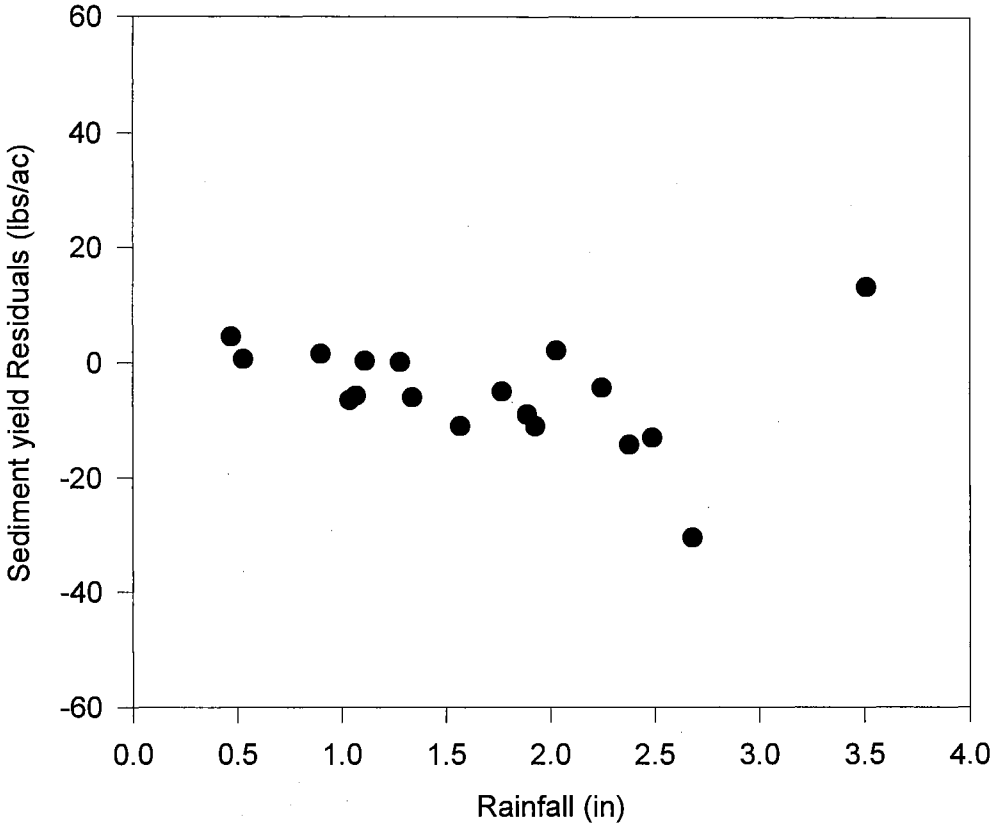

Figure 5-2. Sediment Yield Residual Plot for Watershed RU

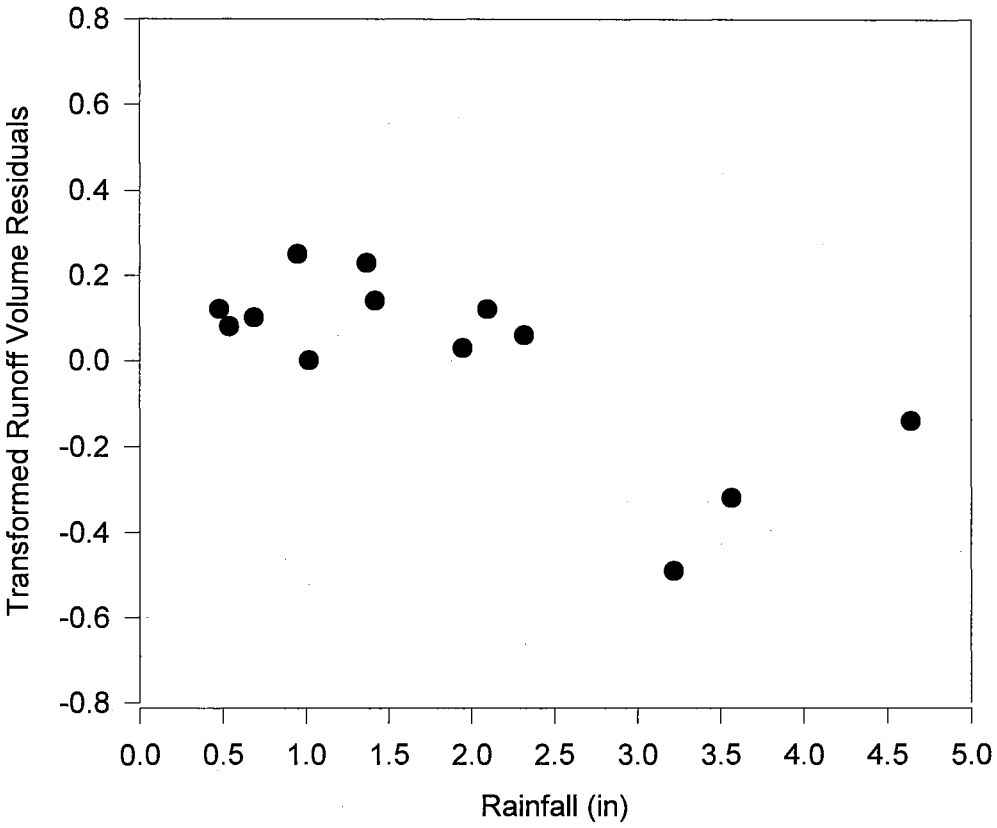

Figure 5-3. Transformed Runoff Volume Residual Plot for Watershed WM

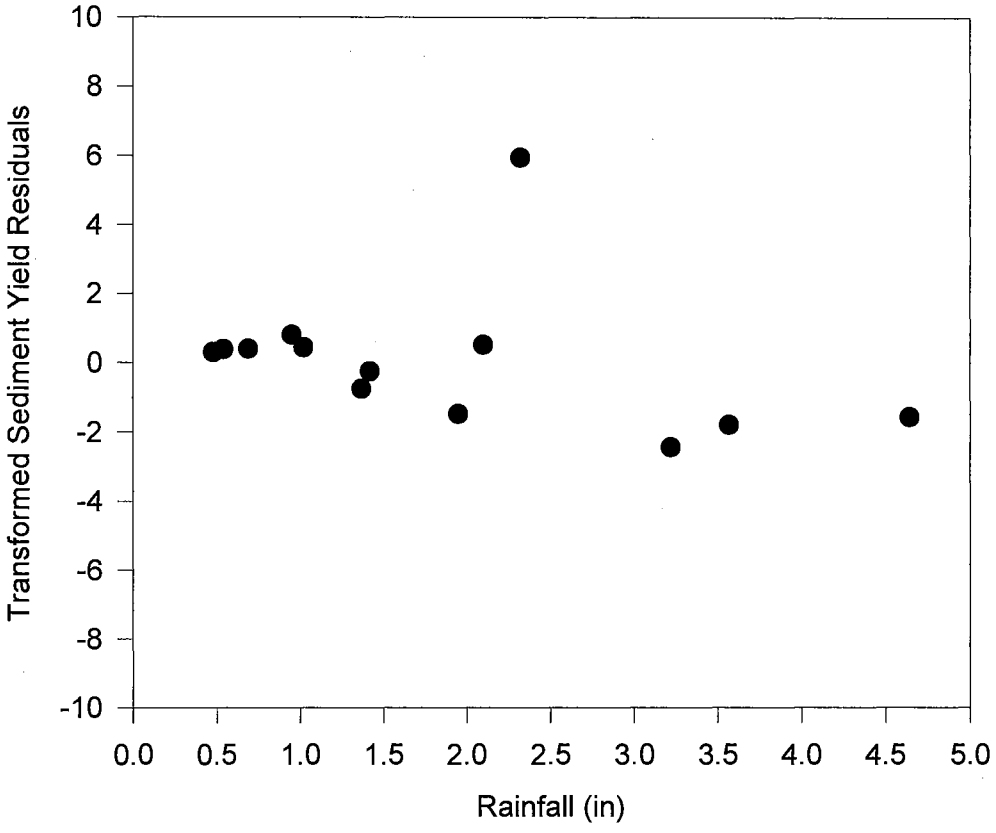

Figure 5-4. Transformed Sediment Yield Residual Plot for Watershed WM

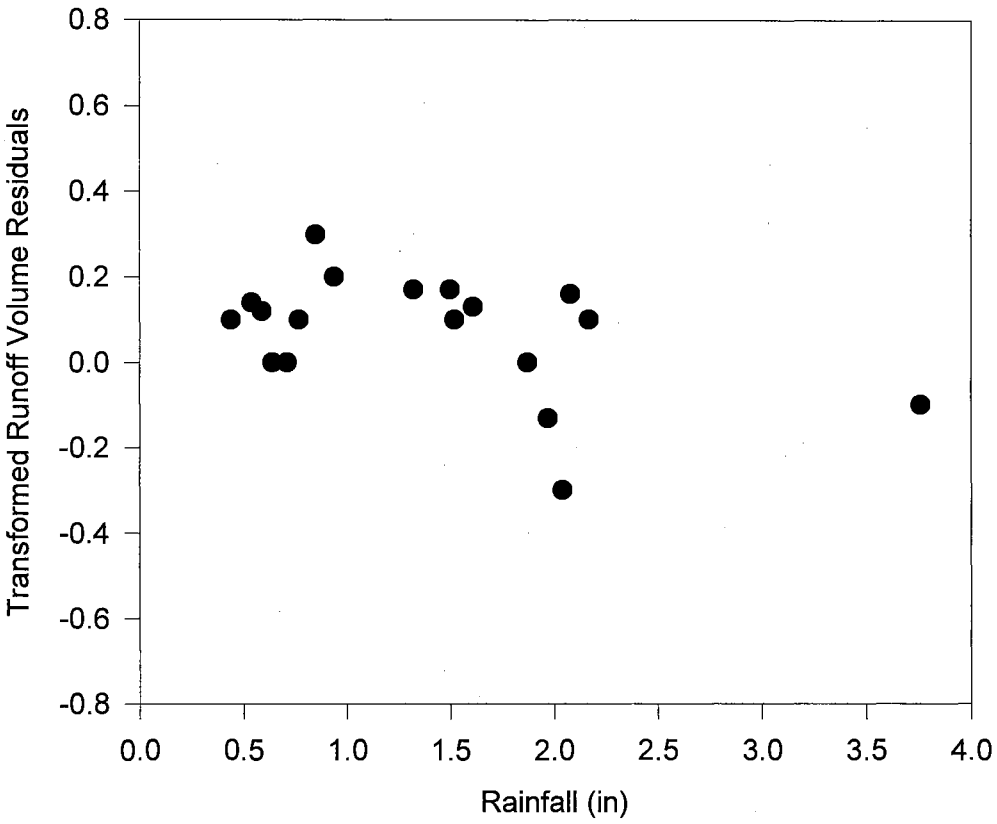

Figure 5-5. Transformed Runoff Volume Residual Plot for Watershed WU

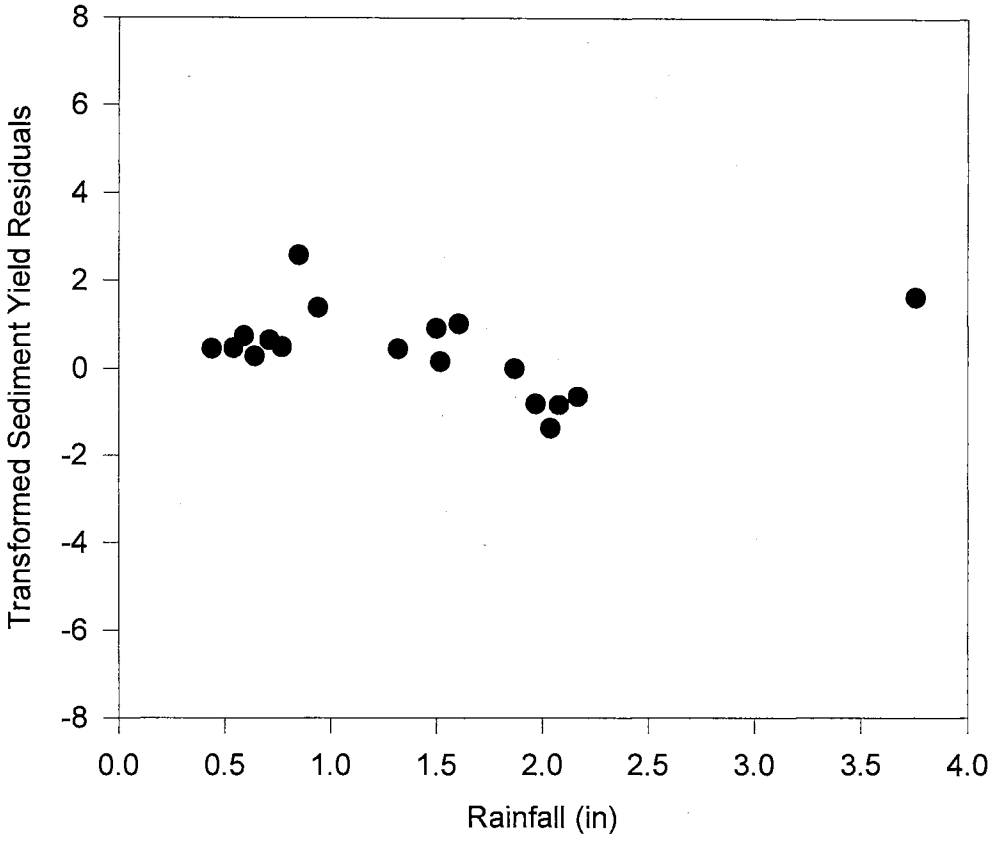

Figure 5-6. Transformed Sediment Yield Residual Plot for Watershed WU

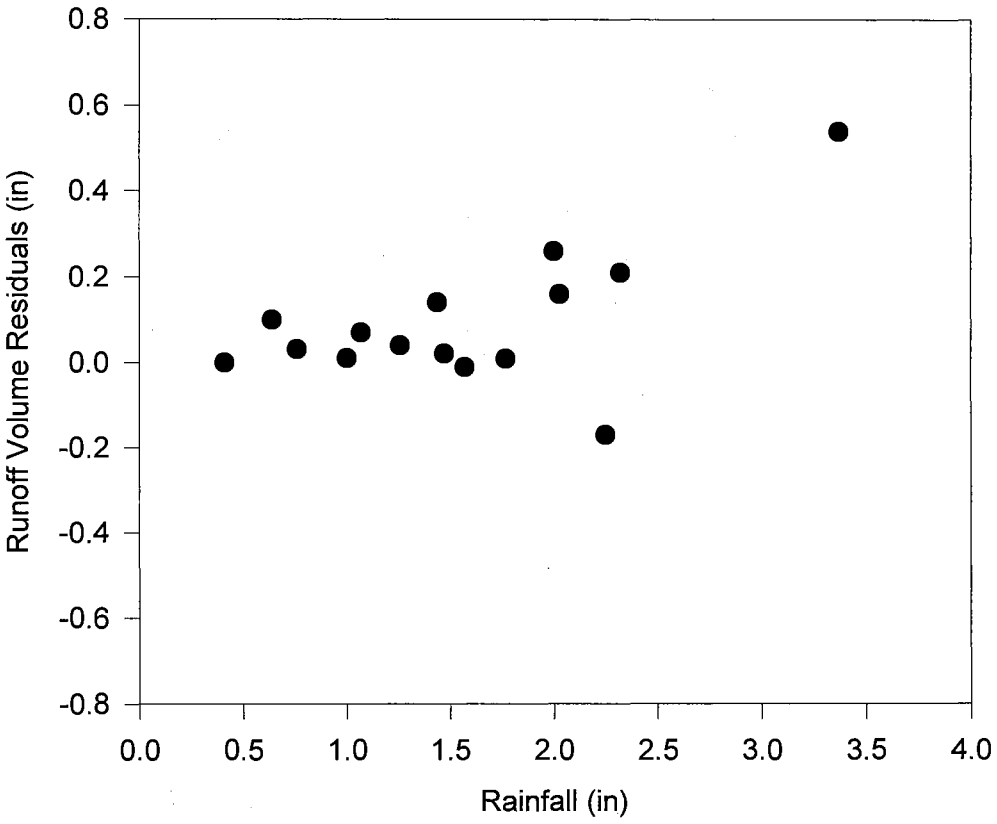

Figure 5-7. Runoff Volume Residual Plot for Watershed RM

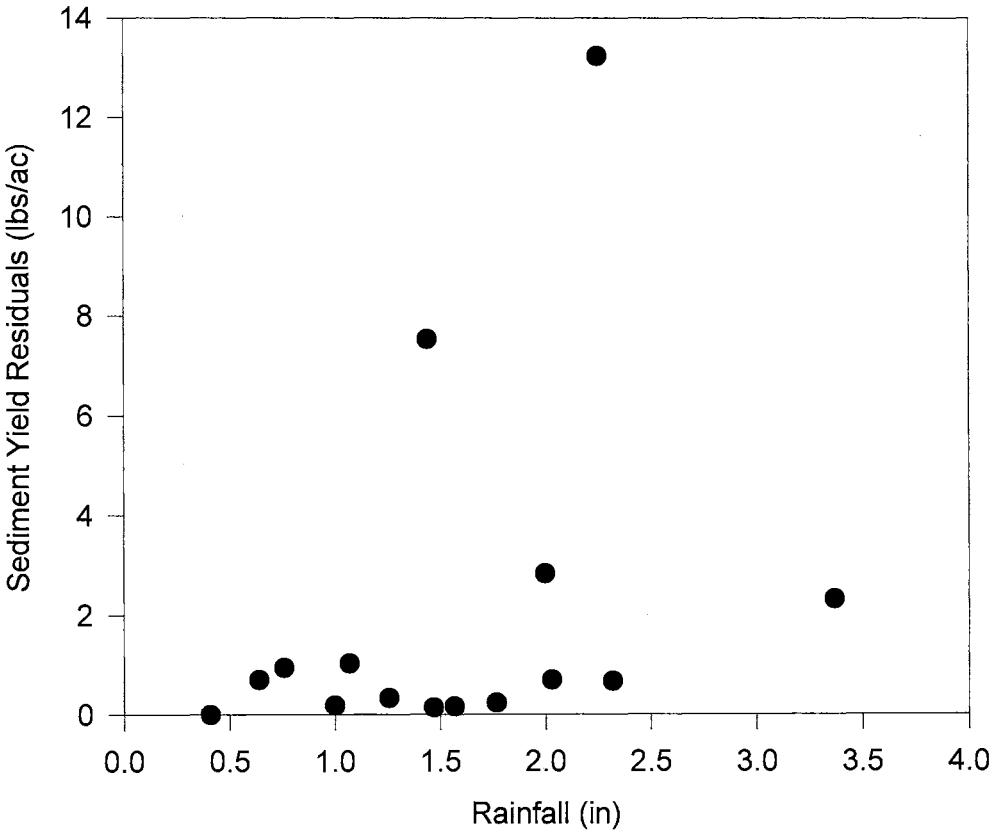

Figure 5-8. Sediment Yield Residual Plot for Watershed RM

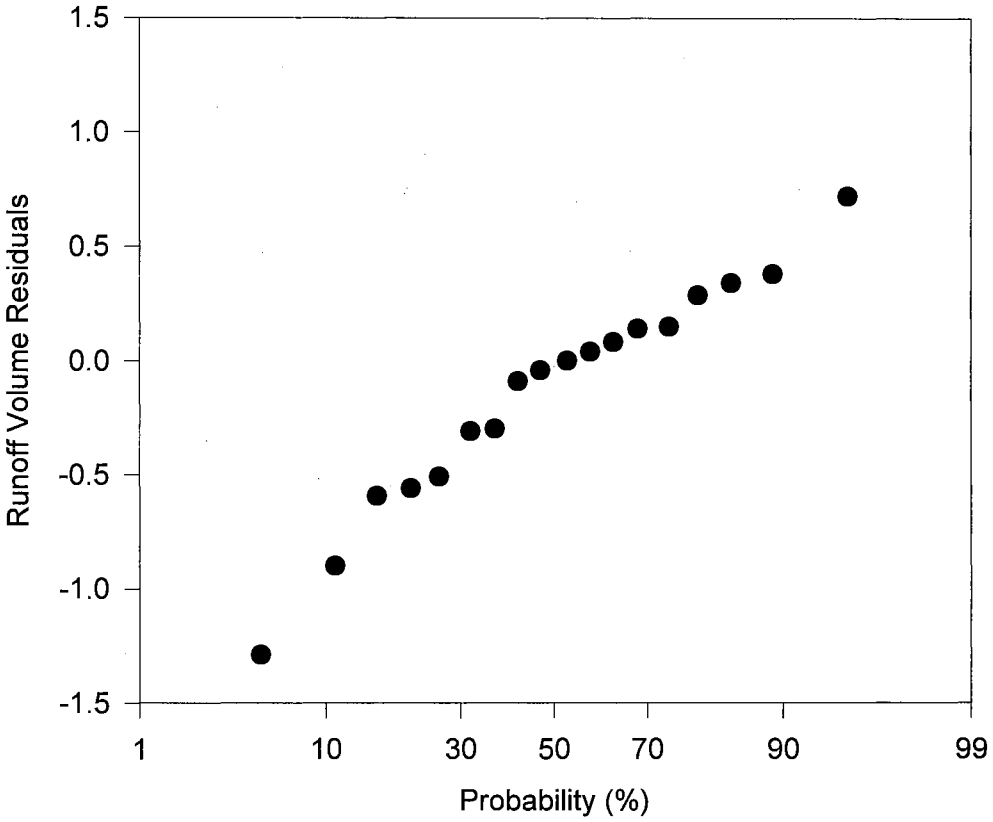

Figure 5-9. Probability Plot of Runoff Volume Residuals for Watershed RU

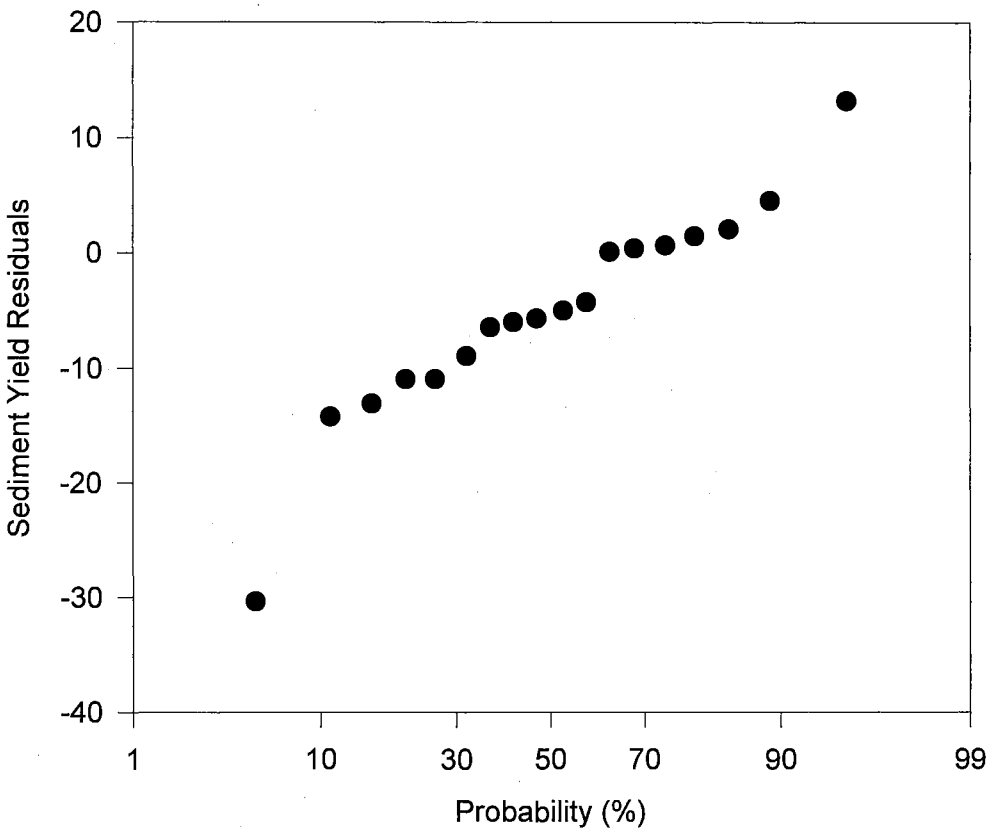

Figure 5-10. Probability Plot of Sediment Yield Residuals for Watershed RU

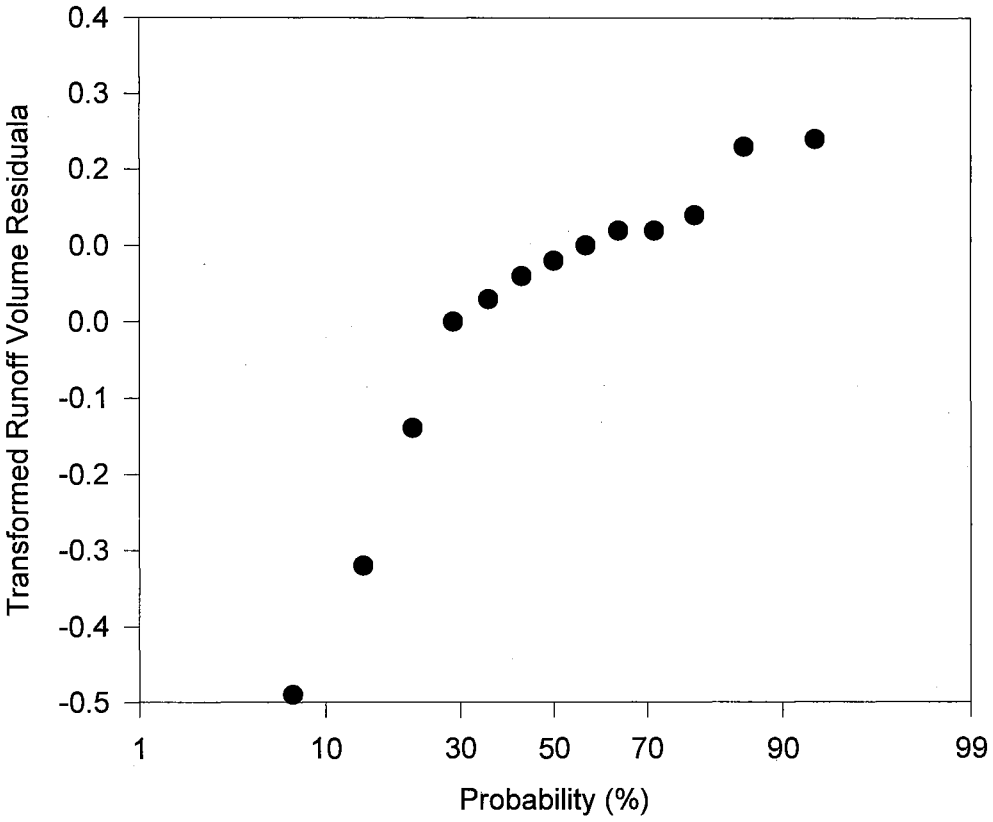

Figure 5-11. Probability Plot of Runoff Volume Residuals for Watershed WM

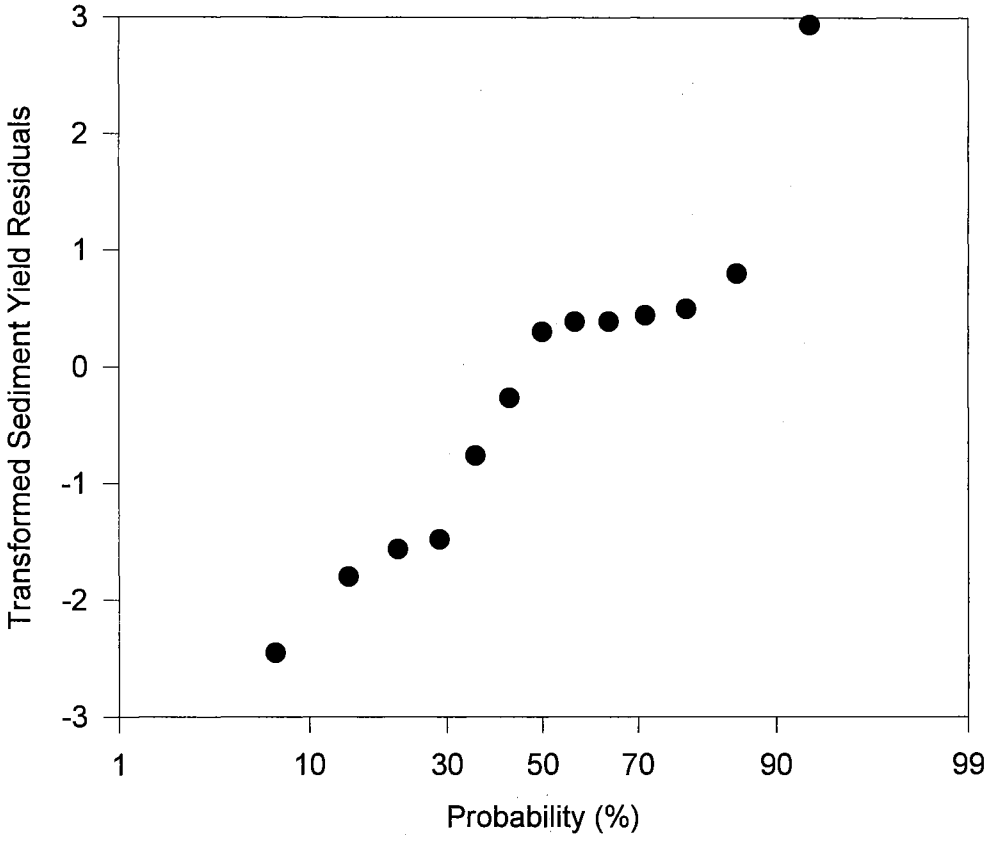

Figure 5-12. Probability Plot of Sediment Yield Residuals for Watershed WM

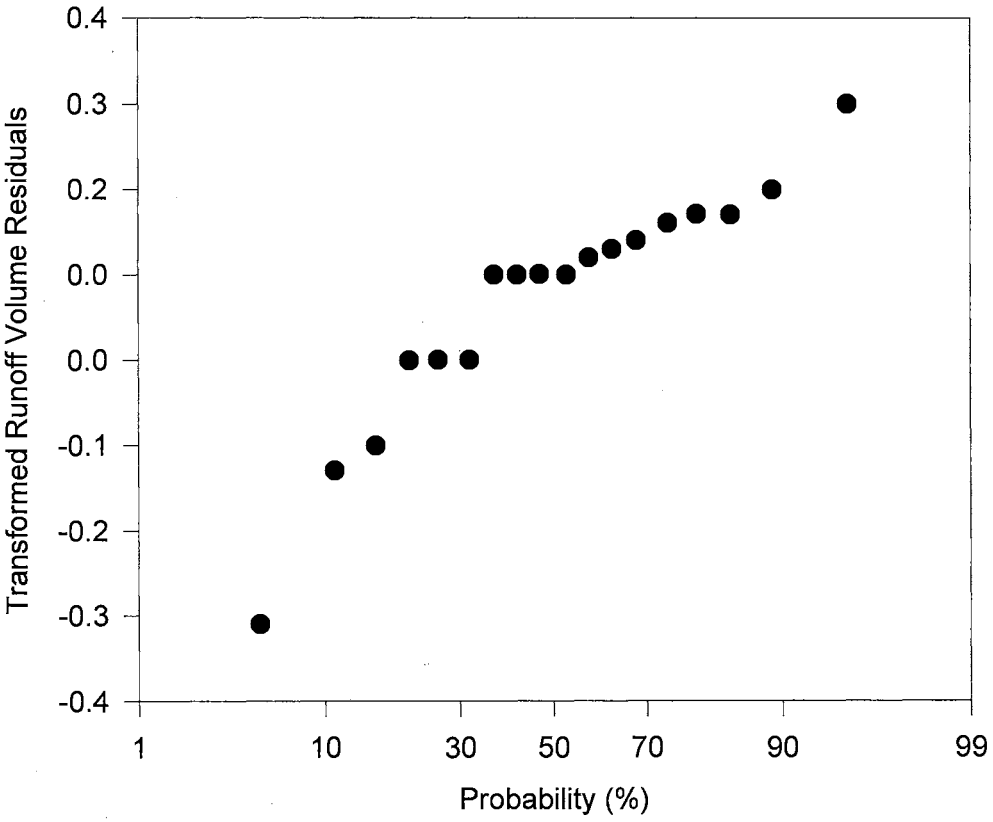

Figure 5-13. Probability Plot of Runoff Volume Residuals for Watershed WU

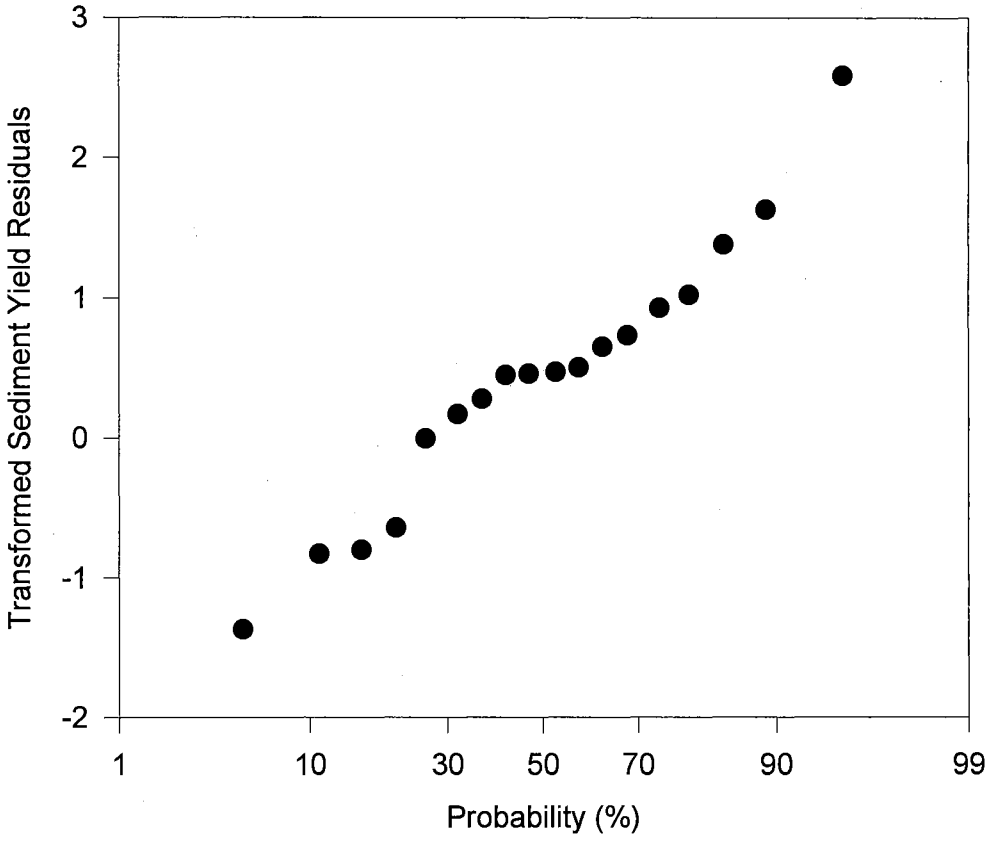

Figure 5-14. Probability Plot of Sediment Yield Residuals for Watershed WU

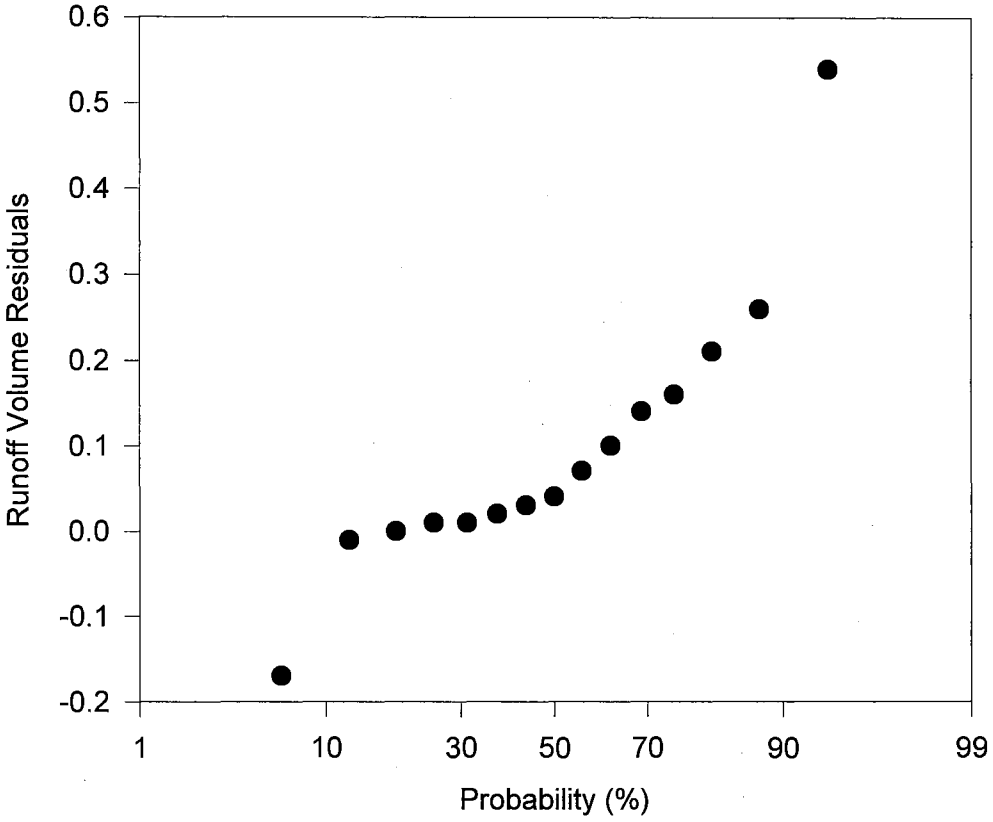

Figure 5-15. Probability Plot of Runoff Volume Residuals for Watershed RM

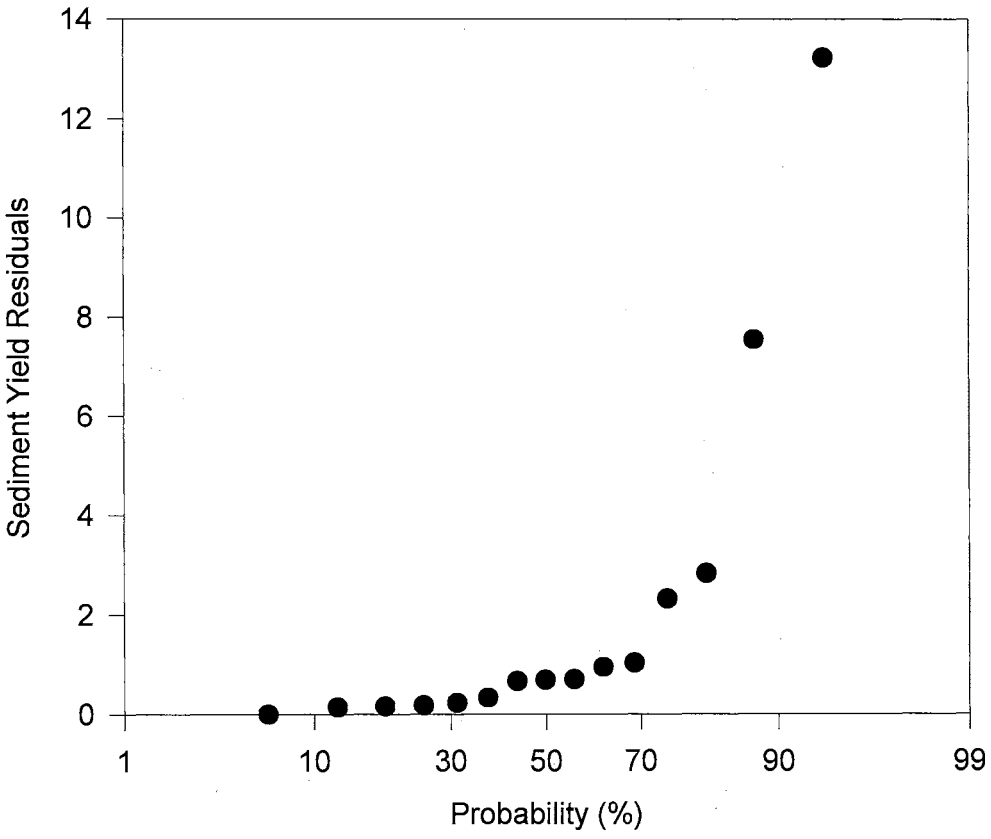

Figure 5-16. Probability Plot of Sediment Yield Residuals for Watershed RM

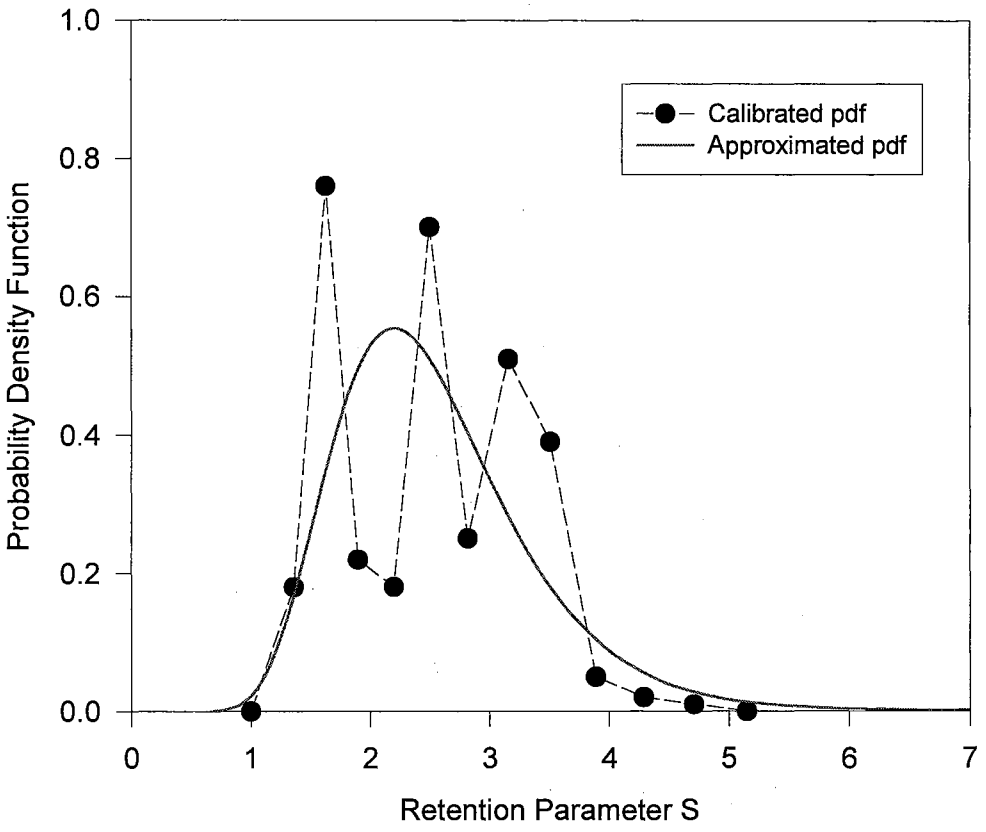

Figure 5-17. Distribution of Retention Parameter S for Watershed RU

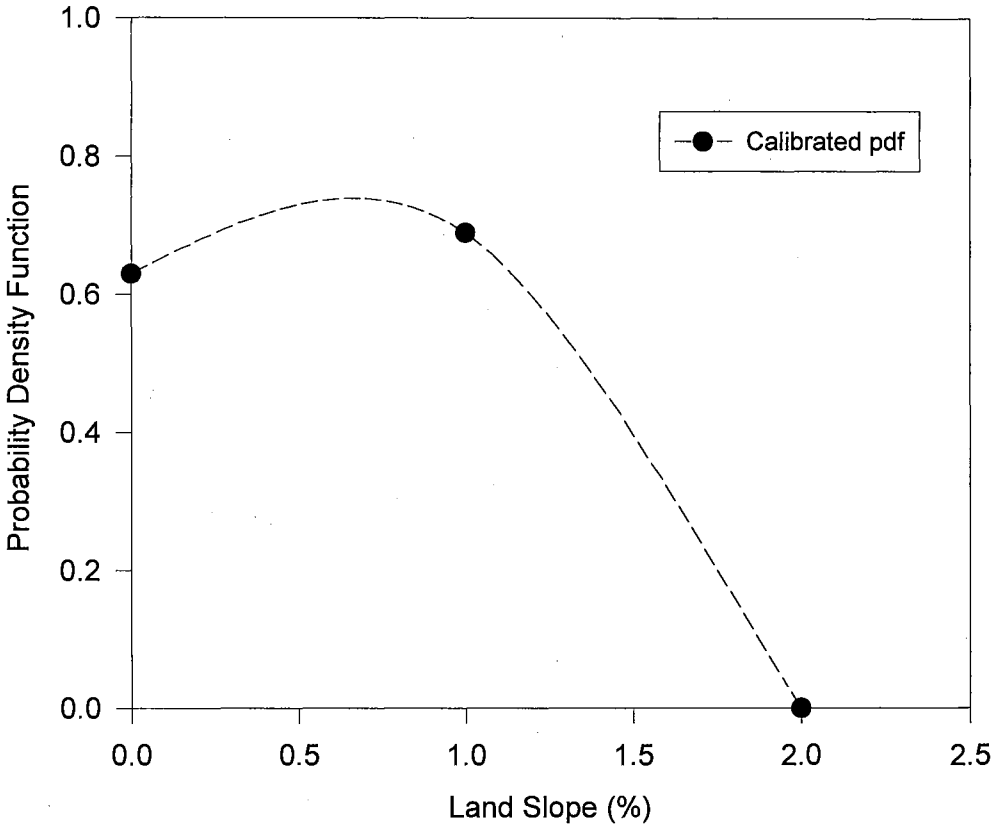

Figure 5-18. Distribution of Land Slope for Watershed RU

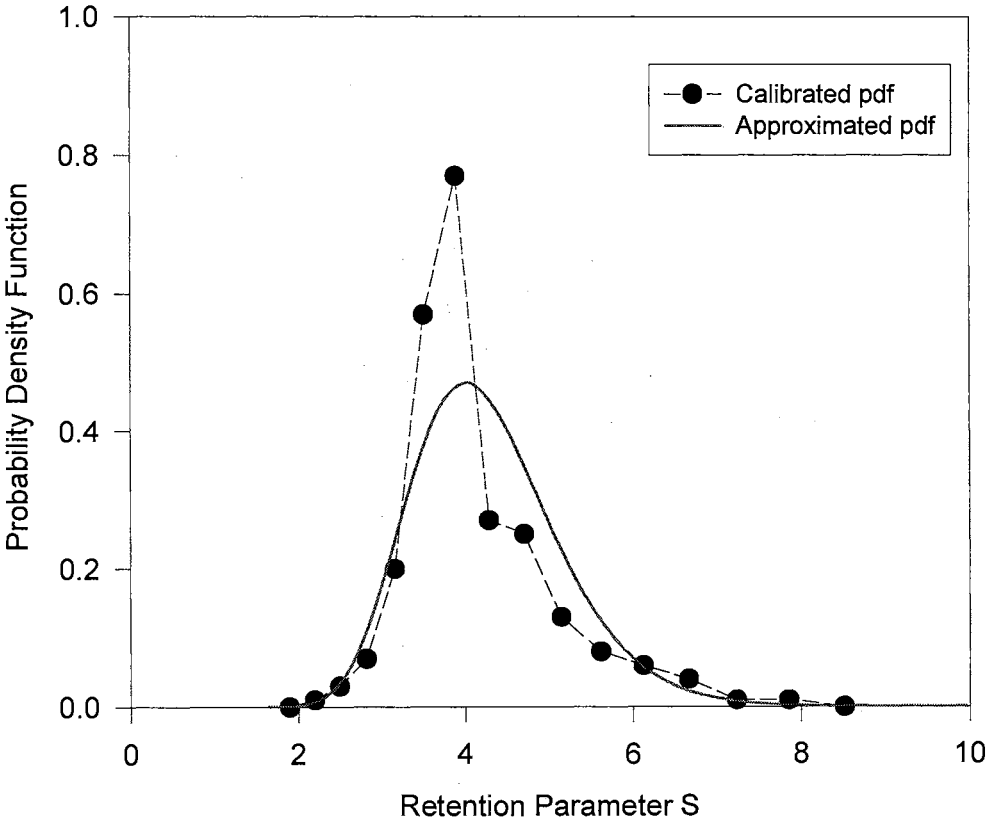

Figure 5-19. Distribution of Retention Parameter S for Watershed WM

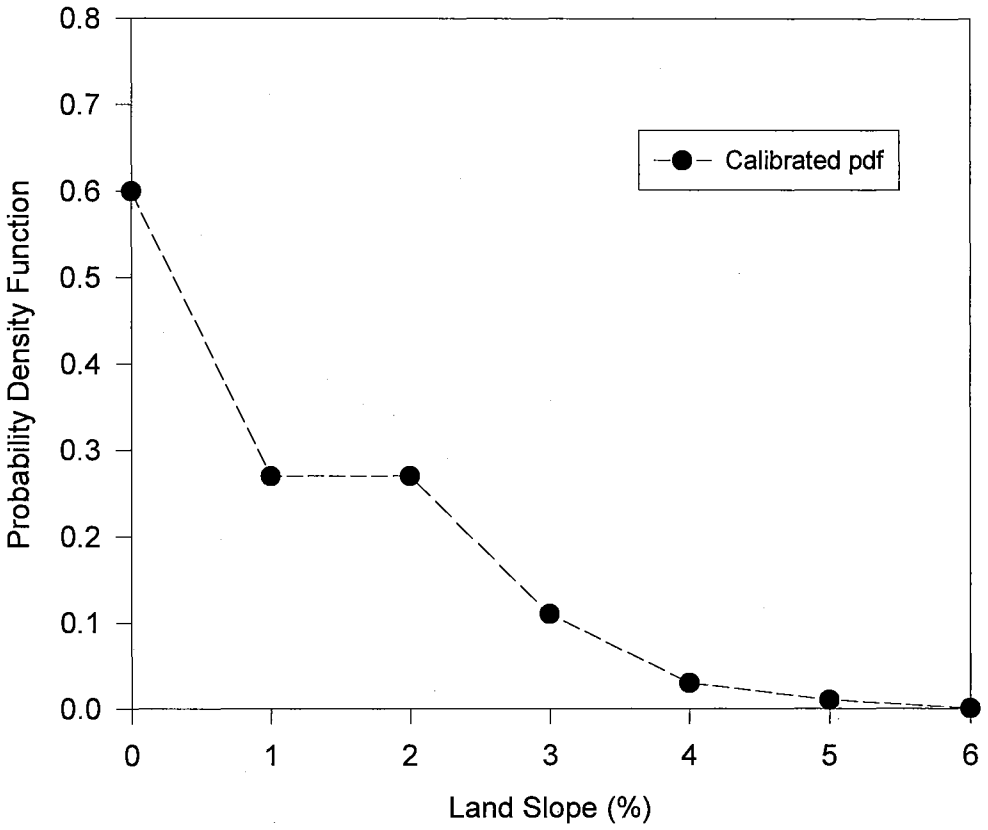

Figure 5-20. Distribution of Land Slope for Watershed WM

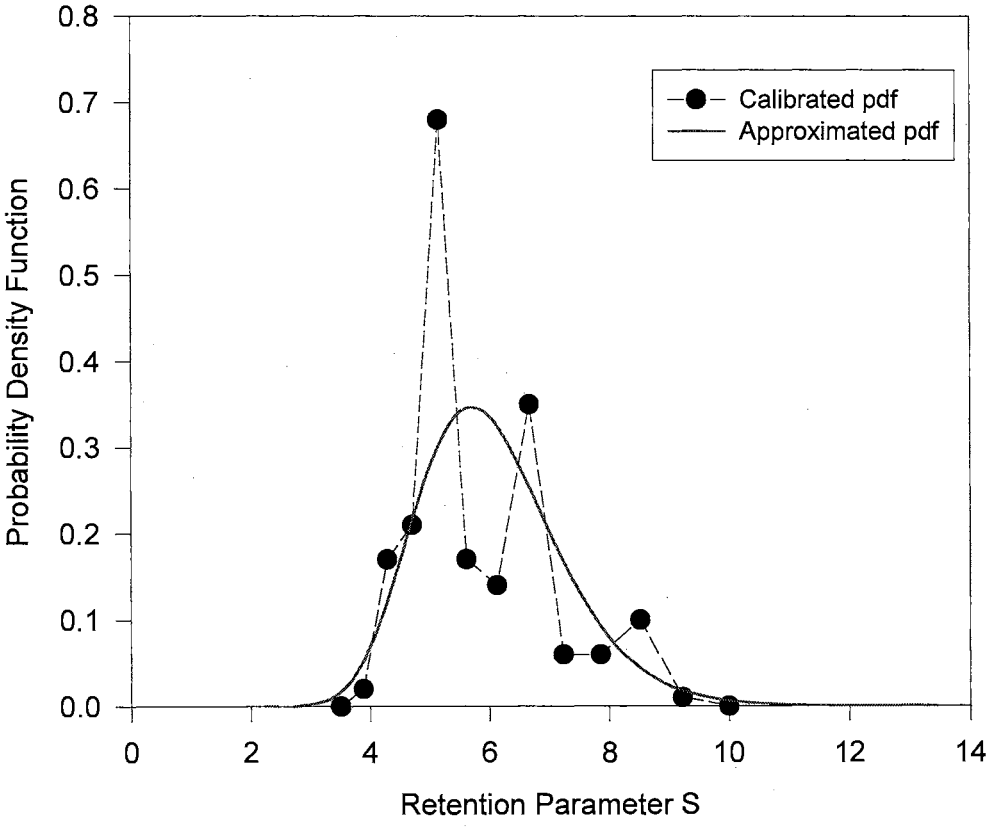

Figure 5-21. Distribution of Retention Parameter S for Watershed WU

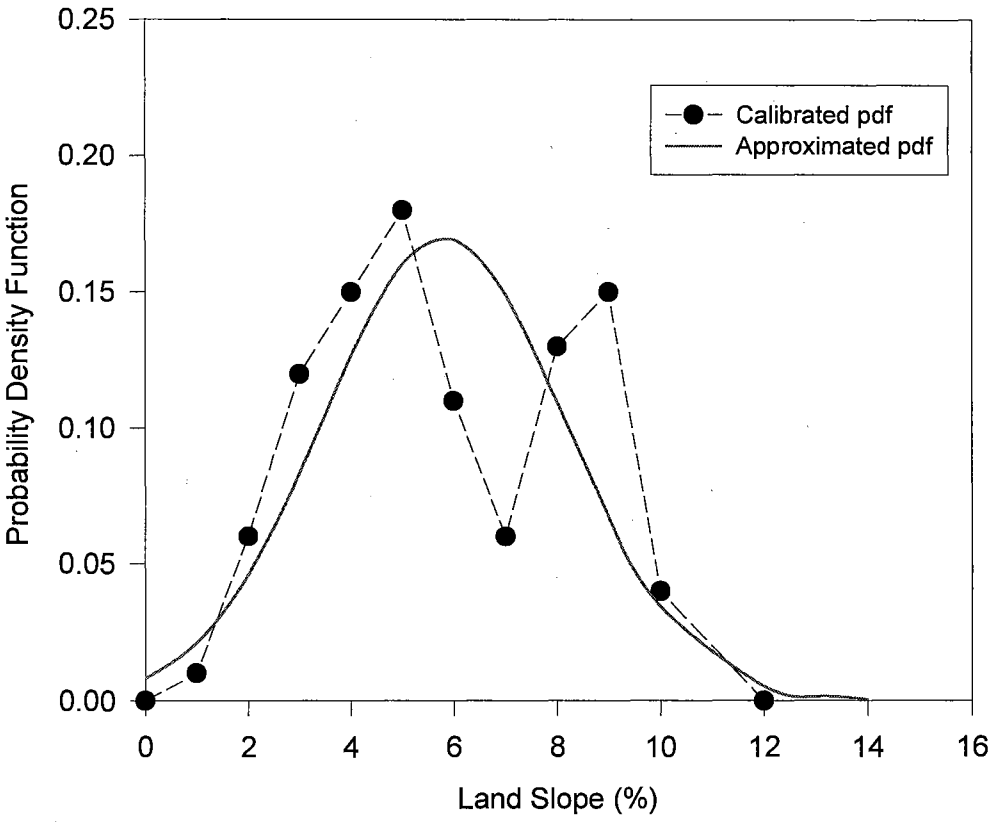

Figure 5-22. Distribution of Land Slope for Watershed WU

CHAPTER VI

INCORPORATING PRIOR INFORMATION INTO SITE-SPECIFIC INFORMATION AND EVALUATION OF AGNPS WITH UNCERTAIN PARAMETERS

The ultimate purpose of calibrating the parameters of a model is to make better use of the model to predict future events. However, the model with calibrated parameters may not be employed for predictions before it is validated. In this chapter, an effort will be made to evaluate the AGNPS model with uncertain curve number and land slope.

Evaluation of the AGNPS Model

The conventional method of validating a model is to check to see if the model with calibrated parameters could repeat the observations which are not used in the model calibration. A model would be considered validated if the model predictions match the corresponding observations. In this study, the calibrated parameters were considered to be uncertain. Instead of fixed values, the parameters were represented in the form of probability density functions. In this case, not only will the AGNPS model with point estimates of the calibrated parameters need to be validated, but also with all possible values of the calibrated

parameters. In other words, the input parameters for the AGNPS model need to be sampled by the Monte Carlo techniques from the calibrated or specified distributions, and the model is run for all sampled input parameters. Then the statistical characteristics of all possible model predictions are compared to the corresponding observations. Since the parameters were expressed in the form of a prior distribution, site specific distribution and posterior distribution, the AGNPS model was validated as described above for these three conditions separately. The prior distributions of parameters were obtained from literature; the site specific distributions were from the calibration of the AGNPS model; and the posterior distributions were the combinations of the prior distributions and the site specific distributions.

Since the model parameters were regarded as uncertain and were expressed in the form of probability density functions, the model responses must be random variables and may be described in the form of probability density functions also. The purpose of this study was trying to predict runoff volume and sediment yield on an average basis. The average of runoff volume and the average of sediment yield over many rainfall events would be considered as random variables and the distributions of them may be found by Monte Carlo simulations. Confidence intervals at some significance level can be then placed on the distribution of runoff or sediment yield. If the means of their observations fall into the corresponding intervals, it may be concluded that the model is validated at that significance level. Note that 90% confidence intervals mean that there is a 90% chance a model prediction would fall into the intervals. Here the model predictions were viewed as random variables. The AGNPS model with uncertain input parameters was evaluated over the data

from watersheds RU, WM and WU.

Procedures

Suppose that there are n rainfall events for the model evaluation that were not used in the model calibration. The distribution of the mean of simulated runoff volume and the distribution of the mean of simulated sediment yield may be found as follows:

1) Generate a random number from a lognormal distribution with specified mean and standard deviation for curve number, and for land slope.

2) Update curve number and land slope in the AGNPS input file with the generated values.

3) Run AGNPS for one rainfall event. Record the predicted runoff volume and sediment yield.

4) Repeat steps 1 through 3 for all rainfall events. Then calculate the mean of runoff volume and the mean of sediment yield.

5) Repeat steps 1 through 4 many times, say N times. Then there would be N values of the mean of runoff and N values of the mean of sediment. The determination of the number N will be described later in the subsection of Monte Carlo simulation.

6) Use the software Bestfit to analyze the two samples above separately. The distribution of the mean of runoff volume and the distribution of the mean of sediment yield can be obtained.

A C computer program was written to perform the procedure from step 1 to step 5. Step 6 has to be done manually. The random numbers generated by the program were checked to make sure that they follow the specified lognormal distribution with correct mean and variance. The source code of the program can be found in Appendix B.

Monte Carlo Simulation

Monte Carlo simulation is the most commonly used method for uncertainty analysis. The variance of the simulation results can be reduced simply by increasing the number of simulation runs. It is considered to be an accurate method compared to other uncertainty analysis methods, such as sensitivity analysis and First-Order analysis. Stevens (1993) employed Monte Carlo simulation as a standard comparison method to analyze the accuracy of First Order analysis. Now an important step of Monte Carlo Simulation is to determine an appropriate number of simulation runs so that the desired accuracy can be reached while keeping the simulation time as low as possible.

The number of simulation runs was decided by plotting the mean of the model response of interest against different numbers of simulation runs. The AGNPS model was run different numbers of times for a rainfall (3.76 inches) in watershed WM. The mean of runoff volume predictions and the mean of sediment yield predictions were plotted against the number of simulation runs as shown in Figure 6-1 and Figure 6-2. It can be seen that 200 simulation runs would be appropriate for runoff volume. However, the curve for sediment yields still oscillates a little bit when the number of simulation runs was 200. It was decided that it was safer to choose 400 runs because an increase of 200 simulation runs was

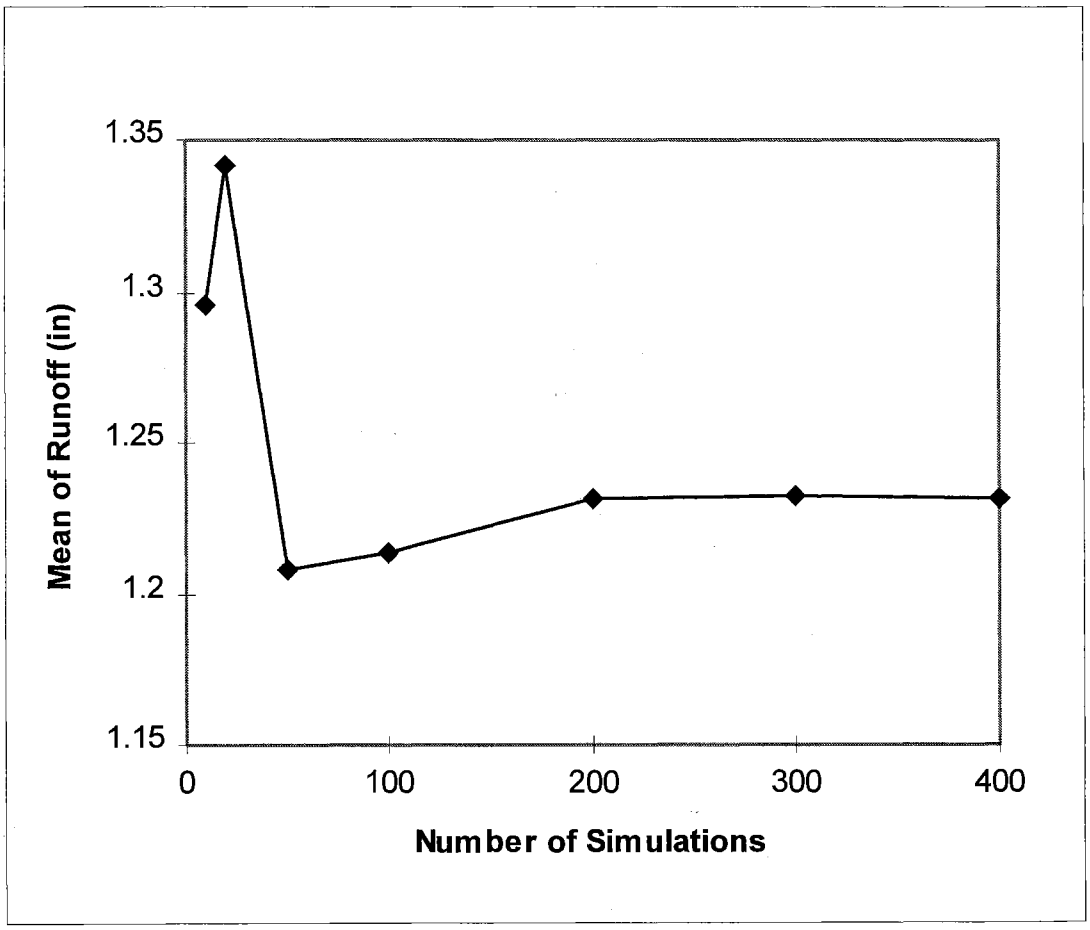

Figure 6-1 Determination of the number of simulation runs for runoff

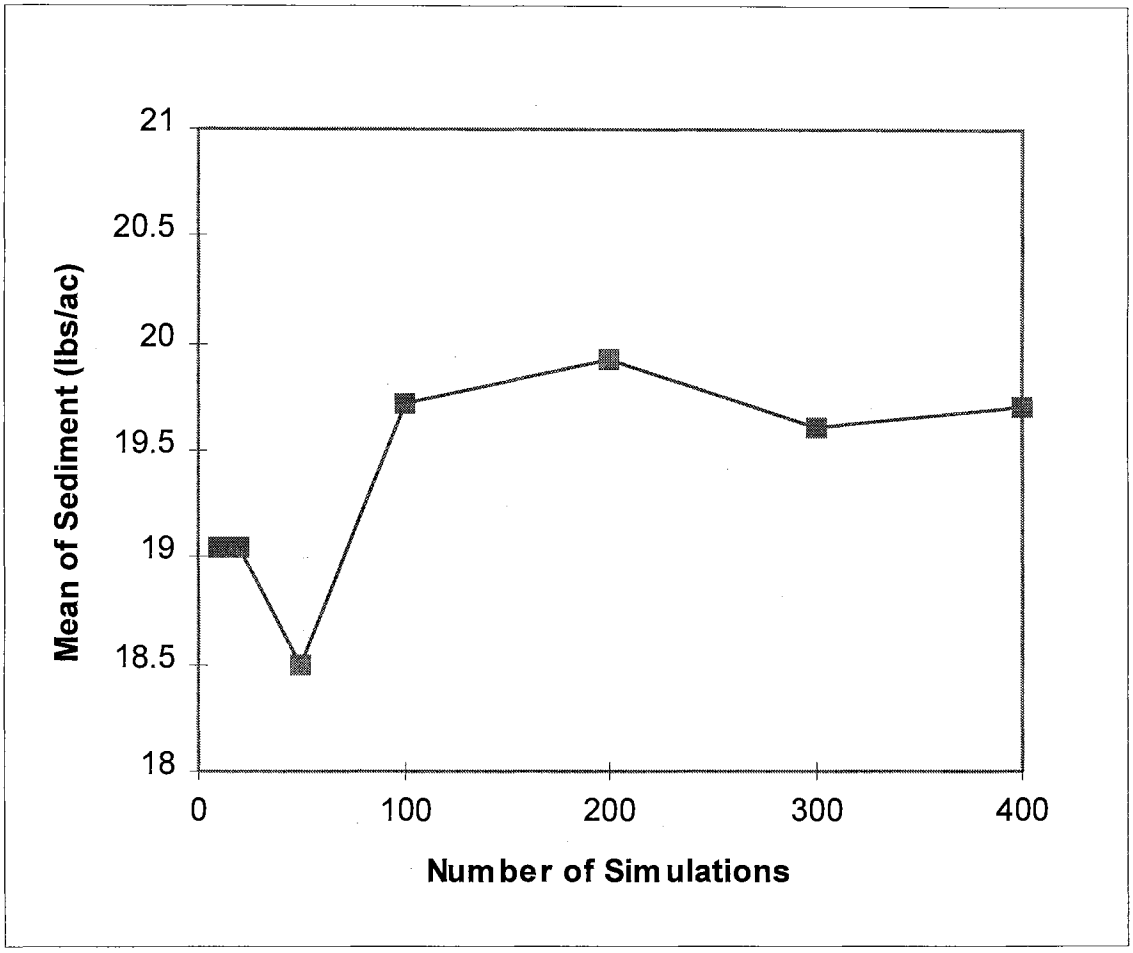

Figure 6-2 Determination of the number of simulation runs for sediment

affordable in this study, i.e. it takes only about four seconds to run the AGNPS model once. The same procedure was repeated for another rainfall event (4.64 inches) in watershed WM. Similar results, which are not presented here, were acquired.

The number of simulation runs may be related to the number of uncertain parameters, the degree of uncertainty in parameters and sensitivity of uncertain parameters. These factors are quite similar to one another for watersheds RU, WM and WU. Therefore, it was decided that 400 simulation runs were applied to all the three watersheds.

Haan (1995) points out that two checks that should be incorporated into any Monte Carlo simulation are an examination of the correlation structure of the randomly generated parameter values and an examination of the probability density functions of the randomly generated parameter values. If the intent was to generate independent random variables but in fact a high degree of correlation ends up in the generated parameters, the output variance will be incorrectly estimated. If the probability density functions of the generated parameters are significantly different from the target probability density functions, the output uncertainty may also be incorrectly estimated. In this study, curve number and land slope were regarded as independent random variables. 400 curve numbers and land slopes were generated by the program mentioned in the previous subsection and the correlation matrix was found as follows:

$$\underline{\rho} = \begin{bmatrix} 1 & 0.01 \\ 0.01 & 1 \end{bmatrix}$$

It can be seen from the correlation matrix that the off-diagonal elements in the matrix are very close to zero. This indicates that correlation structure of the generated parameters matches statistically the target correlation structure (independent parameters). It was determined by the software Bestfit that both distributions of generated curve number and generated land slope match the target probability density functions approximately.

Distributions of the Model Parameters

Three types of information, prior information, site-specific information and posterior information, are described in this section. The prior information in this study was from Prabhu's thesis (1995) and was collected from a variety of literature sources. For example, the prior information on curve number was from Haan and Schulze (1987). The site-specific information was the calibration results from the previous chapter. And the posterior information was calculated using equations (65) through (72) in Chapter III based upon the prior and site-specific information.

The retention parameter S (S=1000/CN-10) was assumed to have a lognormal distribution and a coefficient of variation, C_v, of 0.5. Assuming the curve number estimated from tables for the existing soils and cover condition as the mean value, together with the value of C_v, the variance of S can be found. The land slope was assumed to have a coefficient of variation equal to 0.3, and the estimated land slope of a watershed was considered to be the mean of the land slope. The land slope was also assumed to be lognormally distributed. A lognormal distribution is often used to describe parameters in hydrologic and water quality models because it has a very nice property of being bounded

by zero.

Site-specific distributions of retention parameter and land slope were shown in Figures 5-17 through 5-22. For the convenience of Monte Carlo simulation, only the approximate probability density functions in these Figures were utilized. Figures 5-18, 5-20 and 5-22 suggest that land slope does not follow a lognormal distribution. However, land slope was assumed to be lognormally distributed for the Monte Carlo simulation in this study. Haan (1995) states that the order of expected value, variance and distributional shape is the order of priority in describing uncertain input parameters. Al-Issa (1995) investigated the effects of different distributions of input parameters on the model responses for AGNPS using the data from watershed WM and concluded that the type of distribution of the input parameters has a small effect on the uncertainties of the model responses. He also concluded that it is the variances of the input parameters that have a significant impact on the uncertainty of the model responses. Therefore, it may not be implausible to take a lognormal distribution as an approximation to the calibrated distribution of land slope, but the mean and the variance of the lognormal distribution were assigned to be identical to those of the calibrated distribution.

Since the prior and the site-specific distributions of the input parameters are lognormal, the posterior distributions of the input parameters are lognormal too. The mean and the standard deviation of the posterior distributions for retention parameter S were listed in Table 5-1, and the mean and the standard deviation of the posterior distributions for land slope were given in Table 5-2. It can be seen from the tables that the mean of the posterior distribution is always between the mean of the prior distribution and the mean of the site-

specific distribution, and that the coefficient of variation for the posterior distribution is always the smallest one among the prior, site-specific and posterior distributions. For a normal distribution, the mean of the posterior is actually a weighted average between the mean of the prior and the mean of the site-specific. As we know, if a variable $Y = \ln(X)$ follows a normal distribution, then X will follow a lognormal distribution. Since X and Y have a one-to-one monotonic relationship to each other, the mean of the posterior for a lognormal distribution must be between the means of its prior and its site-specific distribution.

For the convenience of comparison, the prior, site-specific and posterior distributions of retention parameter or land slope for each watershed were plotted on the same graph, as shown in Figures 6-3 through 6-8. Figures 6-3, 6-5 and 6-7 show that the posterior distribution of the retention parameter S is closer to the site-specific distribution than to the prior distribution. This suggests that the site-specific distribution of the retention parameter dominates the posterior. Figures 6-4, 6-6 and 6-8 show that the posterior distribution of the land slope is closer to the prior distribution than to the site-specific distribution, which indicates that the prior information is stronger than the site-specific information. It may not seem reasonable if the prior information is collected from literature. The information about parameters from literature should not be stronger than that from observed data. Otherwise, why waste money on observing data? But if the prior information is based upon the previous data and the site-specific information is from newly observed data, the prior information could be stronger the site-specific information.

Results and Discussions

Following the procedures described in the first subsection, the mean of the predicted runoff volume and the mean of the predicted sediment yield were simulated for different types of information (prior, site-specific or posterior) and for different watersheds (RU, WM or WU), respectively. These simulated means were analyzed using the software Bestfit to find the best fitting distributions. The frequency histograms and the best fitting distributions are shown in Figures 6-9 through 6-14 for watershed RU, in Figures 6-15 through 6-20 for watershed WM and in Figures 6-21 through 6-26 for watershed WU.

It can be seen from Figures 6-9 through 6-26 that the mean of runoff volume for all three watersheds was found to be normally distributed, and that the mean of sediment yield was found to be lognormally distributed for watersheds RU and WM and normally distributed for watershed WU.

Based upon the Central Limit Theorem, if a random variable X is made up of the sum of many small effects, then X might be expected to be normally distributed. One may expect that the mean of runoff volume and the mean of sediment yield follow a normal distribution because both of them can be viewed as a sum of n small random components where n is the number of rainfalls used in the model evaluation. The degree of uncertainty in those small components determines how large n needs to be for the sum to be approximated by a normal distribution. So it was not a surprise to see that the mean of runoff volume for all watersheds and the mean of sediment yield for watershed WU follow a normal distribution, and that the mean of sediment yield for watershed RU and WM follows a lognormal distribution. One can expect that they all can be approximated by a

normal distribution when the number of rainfall events used in the model evaluation becomes very large.

Confidence intervals were calculated for every distribution. For a normal distribution, the lower and upper confidence limits can be determined from

$$l_x = \bar{x} - z_{1-\alpha/2}\,\sigma_x$$
$$u_x = \bar{x} + z_{1-\alpha/2}\,\sigma_x \qquad (95)$$

where $z_{1-\alpha/2}$ is the value of Z from the standard normal distribution such that the area to the right of Z is $\alpha/2$ in percentage and x bar is the mean and σ_x is the standard deviation of the normal distribution.

For a lognormal distribution, the confidence intervals can be found in three steps:

1) Transform the lognormal distribution into a normal distribution based upon the relation Y=ln X, and calculate the mean and standard deviation of the normal distribution.

2) Use Equation (95) to calculate the confidential limits for the normal distribution.

3) The antilog of the confidence limits for the normal distribution will be the confidence limits for the lognormal distribution.

The 90% and 95% confidence intervals are given in Tables 6-3 and 6-4 for every distribution in each watershed. The width of confidence intervals in the tables may indicate to some extent the uncertain degree of the model predictions.

As shown in Figures 6-27 through 6-32, in order to make it easy to compare the

model responses for the prior, site-specific and posterior input parameters, the mean of runoff volume associated with them was plotted on one graph for each watershed, and the mean of sediment yield associated with them was plotted on one graph for each watershed. The corresponding confidence intervals were placed on the graphs. The mean of the observed values was also plotted on the graphs. Table 5-5 contains the values of the observed means for each watershed.

Figures 6-27, 6-29 and 6-31 show that the observed mean of runoff volume falls into the 90% confidence intervals of runoff predictions with prior, site-specific and posterior input parameters for every watershed. This does not mean all model predictions with the prior, site-specific and posterior input parameters are equally good because the interval width is different. For instance, the 90% interval width of runoff predictions with prior input parameters for watershed RU is 0.26 inches, 0.20 inches with site-specific input parameters and 0.16 inches with posterior input parameters. It can be seen from Table 6-3 that the order of interval width (from wide to narrow) for each watershed is the prior, the site-specific and the posterior runoff predictions. Obviously, the uncertainty involved in the posterior runoff predictions is the smallest and the uncertainty involved in the prior runoff predictions is the biggest. Therefore, as far as the confidence intervals are concerned, incorporating the prior information into the site-specific information does reduce the uncertainty in runoff predictions for each watershed. Again, Figures 6-27, 6-29 and 6-31 show that the distribution of posterior runoff predictions is closer to the distribution of site-specific runoff predictions for each watershed. This is because the site-specific information of retention parameter dominates the posterior information of retention parameter. Since the observed

mean of runoff volume falls into the confidence intervals of the prior runoff predictions, it may be concluded that the prior information of Curve Number is relevant.

It can be seen from Figure 6-28 that the observed mean of sediment yield falls only into the 90% confidence intervals of the site-specific sediment predictions for watershed RU. Figure 6-30 shows that the observed mean falls out of all 90% confidence intervals for watershed WM but within the 95% confidence intervals of the site-specific sediment predictions. Therefore, site-specific sediment predictions are probably plausible for watersheds RU and WM. The AGNPS model with the prior and posterior input parameters was not able to provide proper sediment predictions for watersheds RU and WM. Furthermore, the confidence intervals of the site-specific sediment predictions are the narrowest. The distribution of the posterior sediment predictions is closer to that of the prior sediment predictions for these two watersheds (Figures 6-28 and 6-30) because the prior distribution of land slope dominates the posterior. It may be concluded that the specification of prior information (both mean and coefficient of variation) about land slope was irrelevant for watersheds RU and WM.

From Figure 6-32 and Table 6-4, we can see that the observed mean of sediment yield for watershed WU falls into the 90% confidence intervals of the site-specific sediment predictions and falls into the 95% confidence intervals of both the prior and the site-specific sediment predictions. The means of the prior, site-specific and posterior sediment predictions are close to each other. The intervals of the prior sediment predictions are narrower than those of the site-specific sediment predictions, which results from stronger prior information about land slope. The intervals of the posterior sediment predictions are

the narrowest. It could probably be surmised that if the prior information of land slope had not been assumed so strong (to have a larger coefficient of variation instead) the intervals of the posterior sediment predictions would be wider to contain the observed mean of sediment yield. Therefore, we may conclude that the mean of land slope was properly estimated for the prior information of land slope in watershed WU but the coefficient of variation was specified too small.

Based upon the interval widths for both runoff predictions and sediment predictions, we can find that when the mean of the prior information about input parameters was properly specified the interval width of the posterior predictions is the smallest. This may be viewed as an indicator to see if the mean of the prior information is specified appropriately.

The observed mean of sediment yield falls into the 95% intervals of the site-specific sediment predictions and falls out of the 95% intervals of the posterior sediment predictions for all three watersheds. Thus, we can conclude that incorporating a misspecified prior into the site-specific information of input parameters will lead to worse or even false model predictions rather than reduce the uncertainty of the model predictions.

Table 6-1 Distribution of Retention Parameter for All Watersheds

Watersheds		Prior Distribution	Site-specific Distribution	Posterior Distribution
RU	Mean	3.51	2.47	2.67
	Stdev	1.76	0.78	0.70
	Cv	0.5	0.32	0.26
WM	Mean	2.66	4.06	3.68
	Stdev	1.33	0.80	0.66
	Cv	0.5	0.20	0.18
WU	Mean	5.63	5.73	5.55
	Stdev	2.81	1.08	0.97
	Cv	0.5	0.19	0.17

Table 6-2 Distribution of Land Slope for All Watersheds

Watersheds		Prior Distribution	Site-specific Distribution	Posterior Distribution
RU	Mean	3.00	0.52	2.36
	Stdev	0.90	0.50	0.66
	Cv	0.30	0.96	0.28
WM	Mean	4.00	1.02	3.39
	Stdev	1.20	1.16	0.97
	Cv	0.30	1.14	0.29
WU	Mean	4.00	5.80	4.46
	Stdev	1.20	2.35	1.06
	Cv	0.30	0.41	0.24

Table 6-3 Confidence Intervals on the Mean of Runoff Volume for All Watersheds

Watersheds		RU		WM		WU	
		90%	95%	90%	95%	90%	95%
Prior	lower	0.19	0.17	0.16	1.12	0.23	0.20
	upper	0.45	0.47	1.52	1.56	0.48	0.50
	width	0.26	0.30	0.36	0.44	0.25	0.30
Site-specific	lower	0.32	0.30	0.90	0.89	0.24	0.23
	upper	0.52	0.54	1.08	1.09	0.34	0.35
	width	0.20	0.24	0.18	0.20	0.10	0.12
Posterior	lower	0.30	0.29	0.97	0.96	0.25	0.25
	upper	0.46	0.47	1.13	1.14	0.35	0.36
	width	0.16	0.18	0.16	0.18	0.10	0.11

Table 6-4 Confidence Intervals on the Mean of Sediment Yield for All Watersheds

Watersheds		RU		WM		WU	
		90%	95%	90%	95%	90%	95%
Prior	lower	11.22	10.20	23.43	22.51	3.84	3.55
	upper	30.82	33.95	35.38	36.78	6.94	7.23
	width	19.60	23.75	11.95	14.27	3.10	3.68
Site-specific	lower	5.29	4.95	10.63	10.22	3.47	3.08
	upper	10.41	11.11	16.10	16.76	7.51	7.90
	width	5.12	6.16	5.47	6.54	4.04	4.82
Posterior	lower	12.44	11.75	19.34	18.75	4.04	3.80
	upper	22.51	23.83	26.74	27.58	6.50	6.74
	width	10.07	12.08	7.40	8.83	2.46	2.94

Table 6-5 Observed Mean of Runoff Volume and Sediment Yield for All Watersheds

	Watershed RU	Watershed WM	Watershed WU
Runoff Volume (in)	0.42	1.04	0.26
Sediment Yield (lbs/ac)	5.50	16.20	6.98

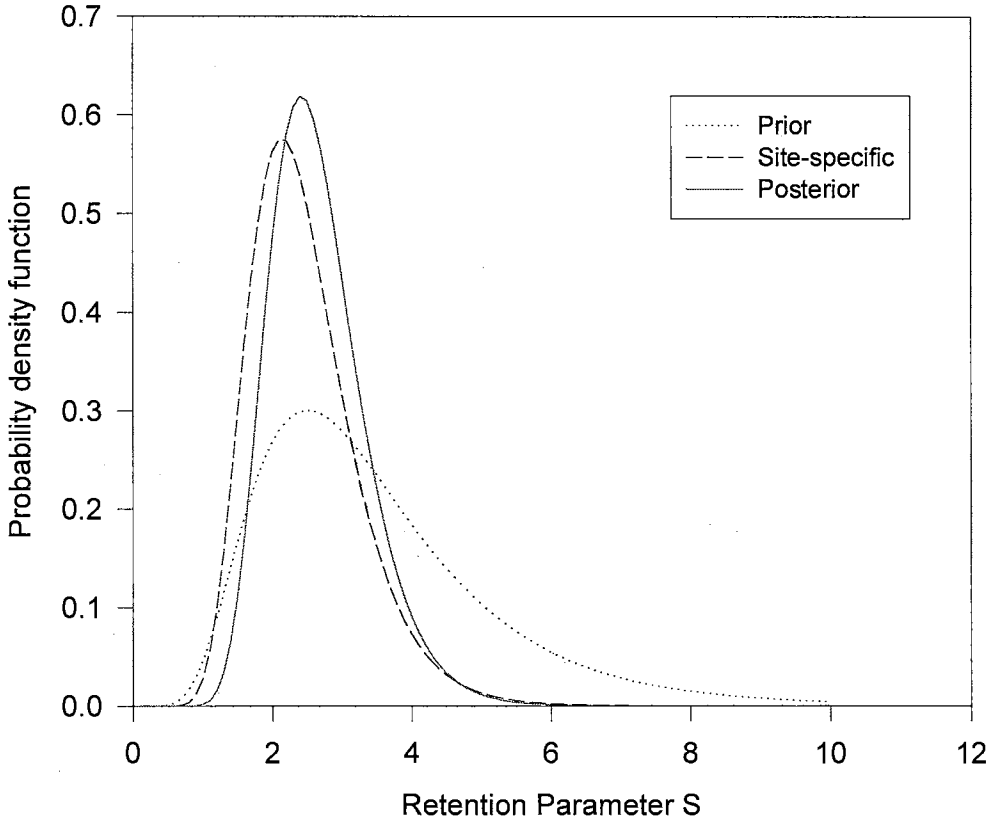

Figure 6-3 Prior, Site-specific and Posterior Distribution of Retention Parameter for Watershed RU

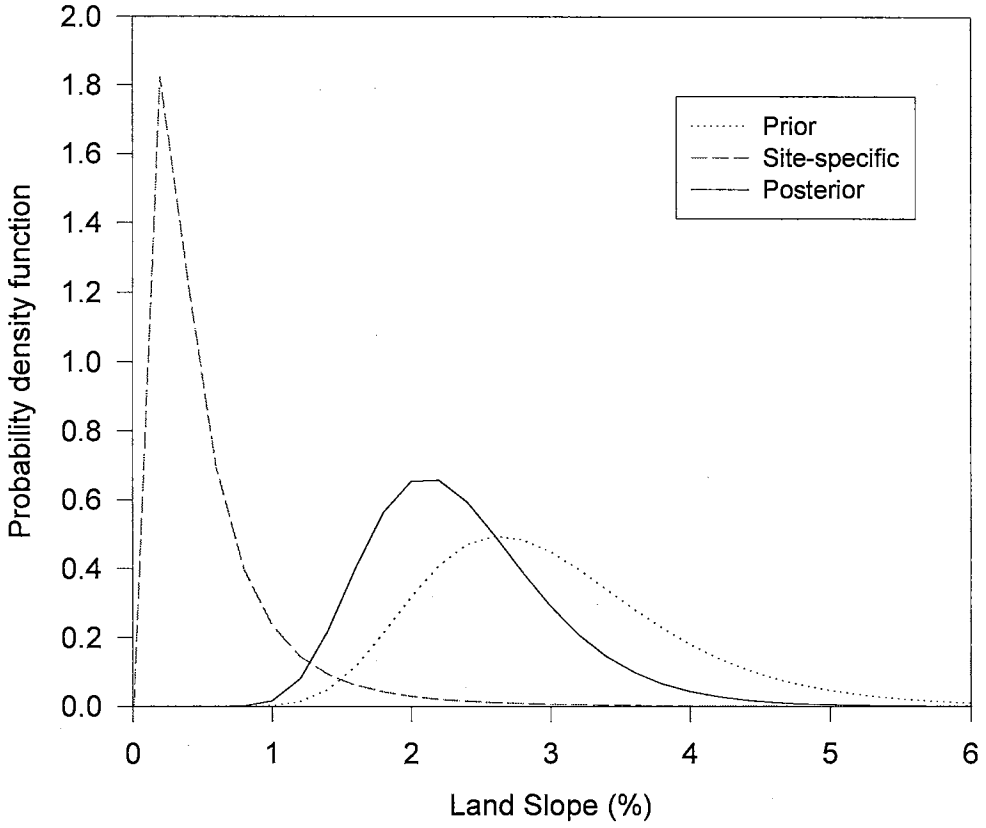

Figure 6-4 Prior, Site-specific and Posterior Distribution of Land Slope for Watershed RU

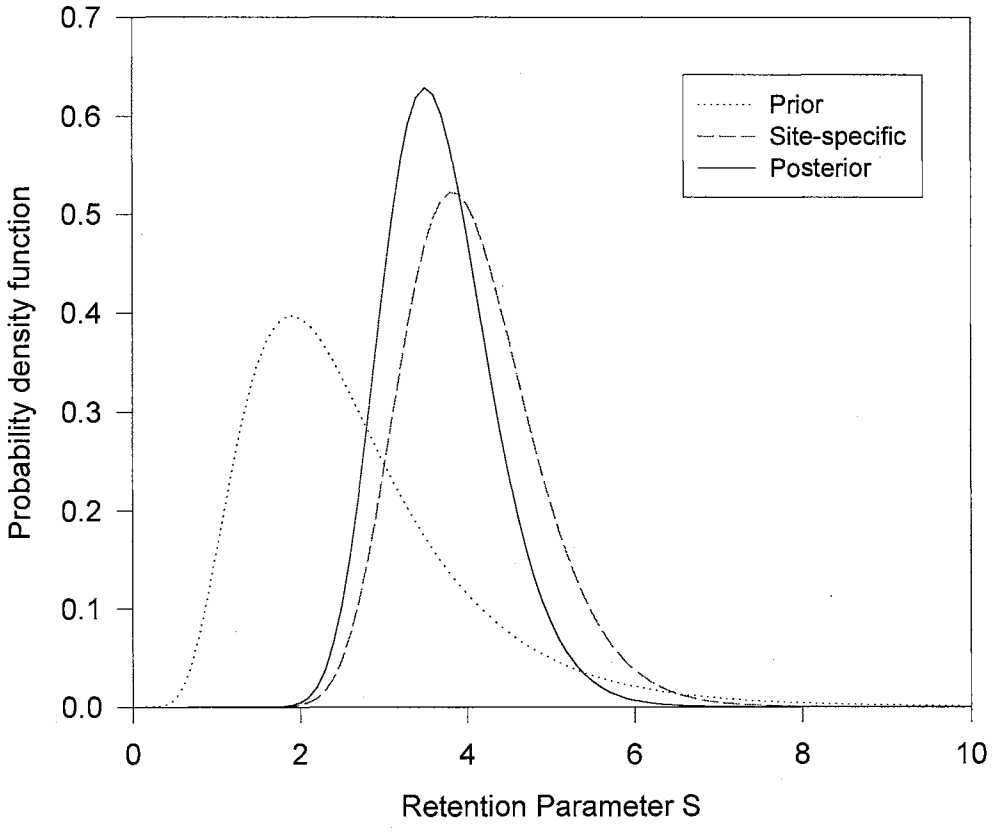

Figure 6-5 Prior, Site-specific and Posterior Distribution of Retention Parameter for Watershed WM

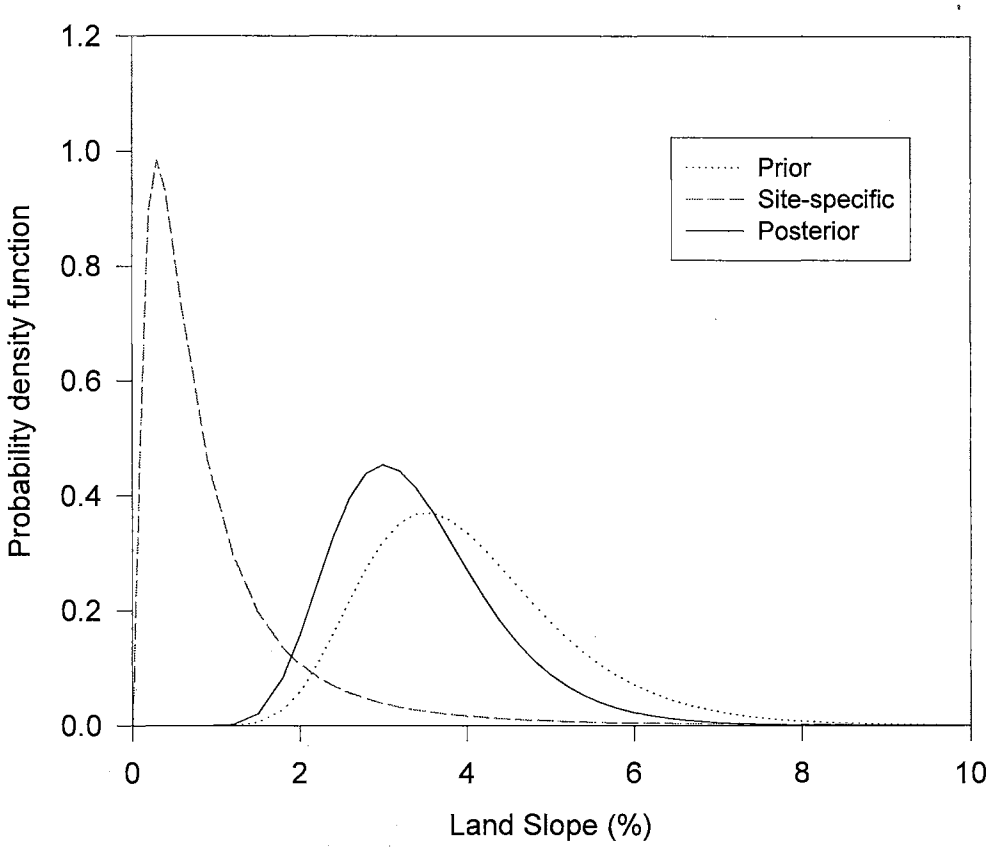

Figure 6-6 Prior, Site-specific and Posterior Distribution of Land Slope for Watershed WM

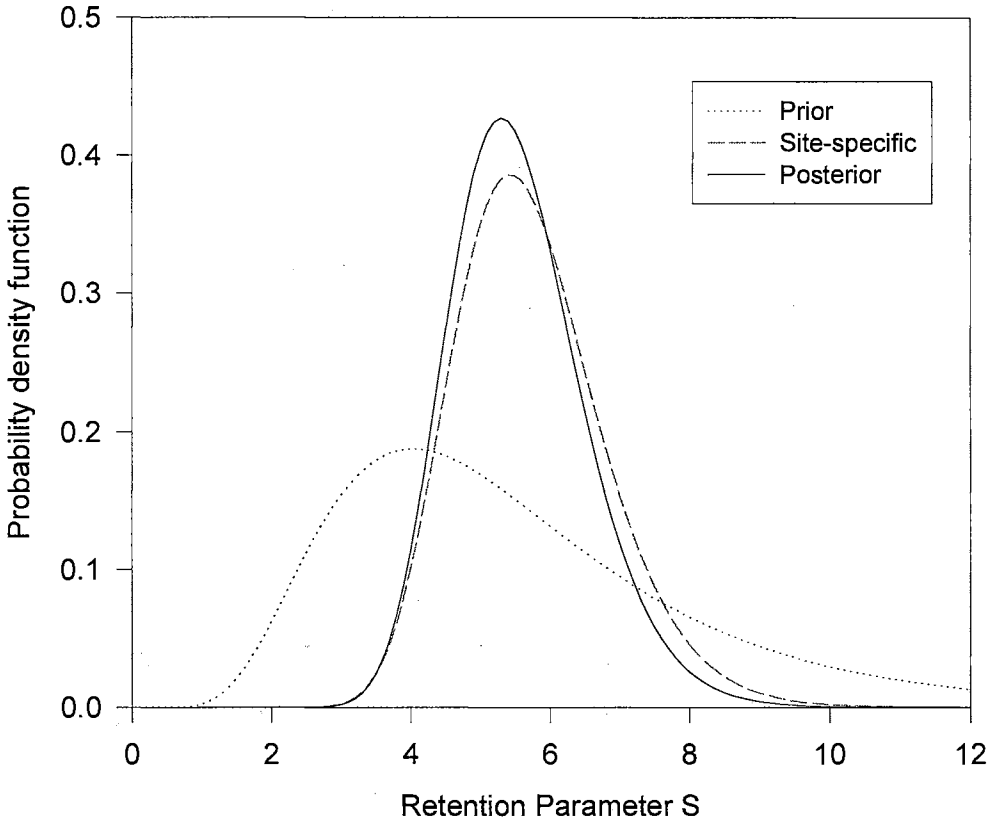

Figure 6-7 Prior, Site-specific and Posterior Distribution of Retention Parameter for Watershed WU

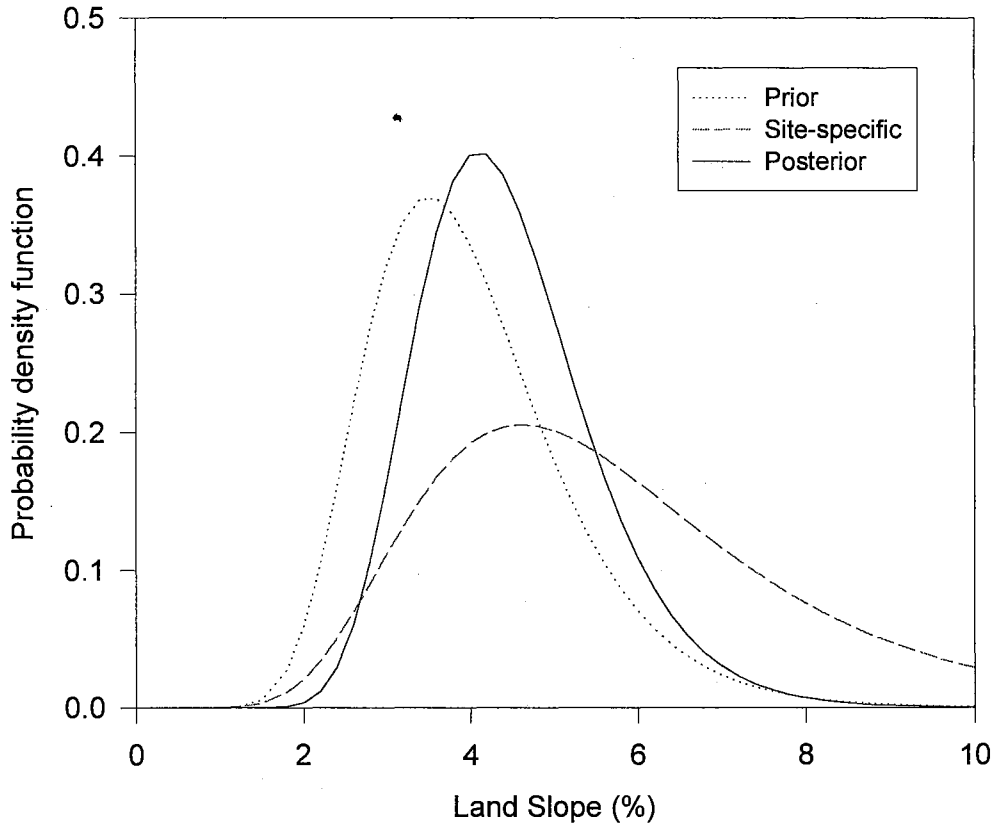

Figure 6-8 Prior, Site-specific and Posterior Distribution of

Land Slope for Watershed WU

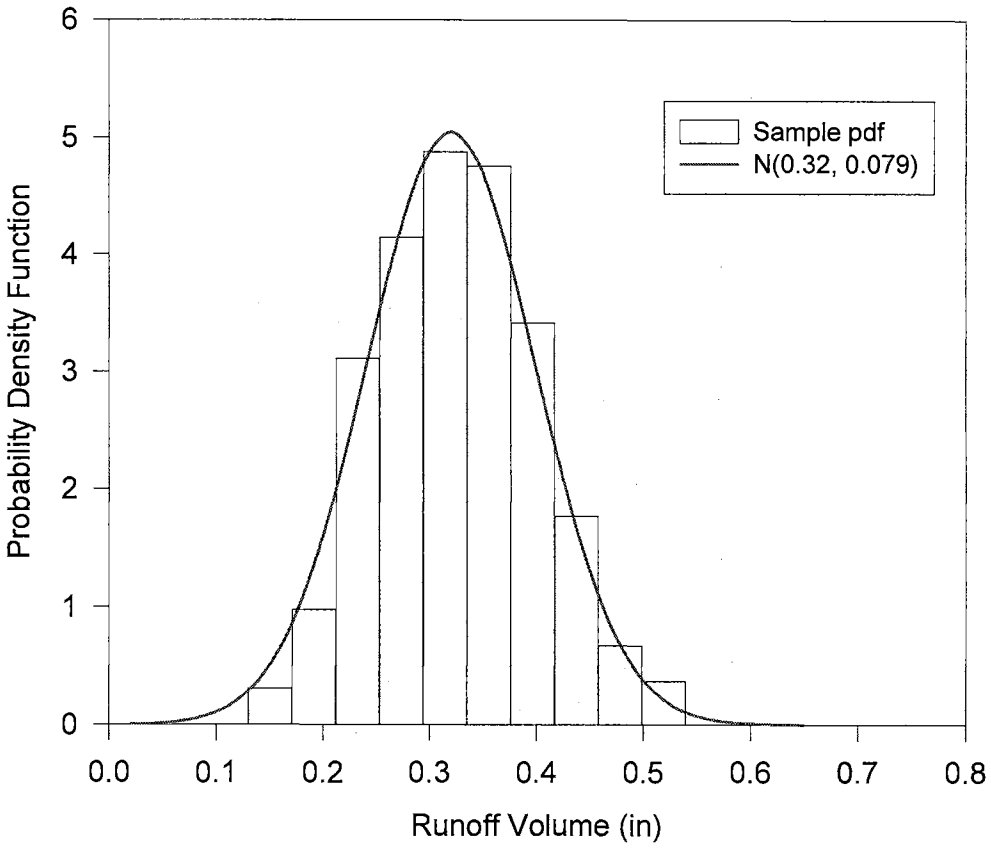

Figure 6-9 Distribution of the Mean of Runoff Volume Predictions with the Prior Input Parameters for Watershed RU

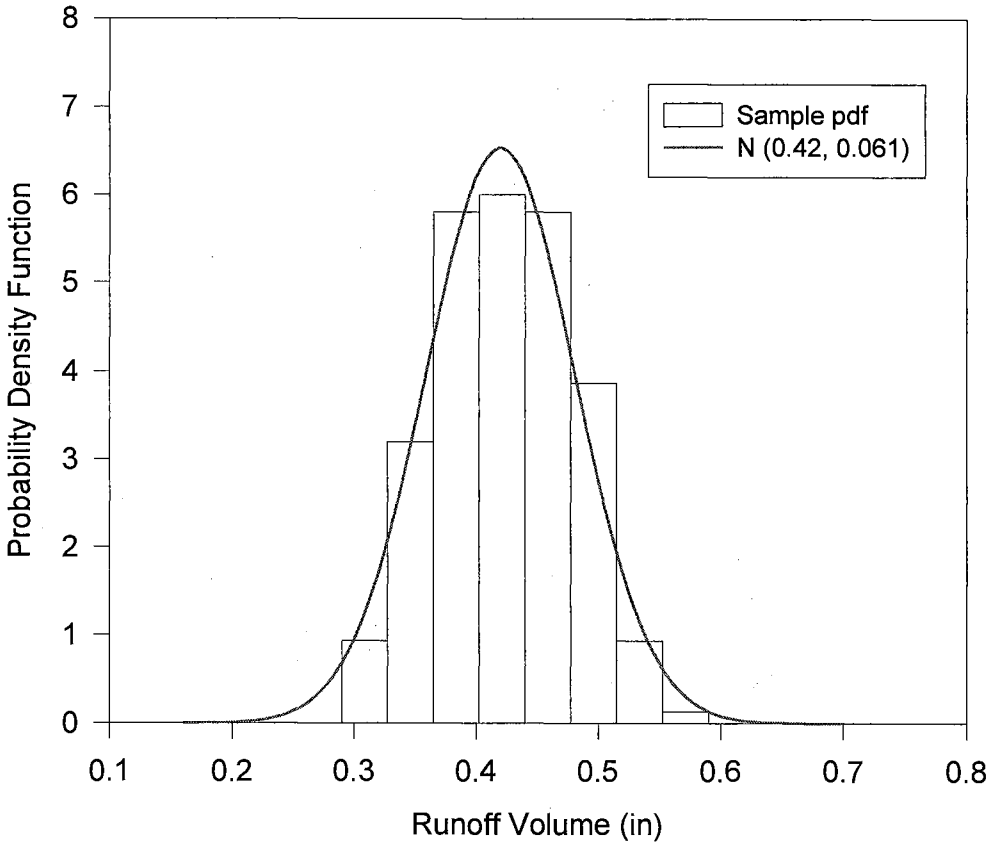

Figure 6-10 Distribution of the Mean of Runoff Volume Predictions with the Calibrated Input Parameters for Watershed RU

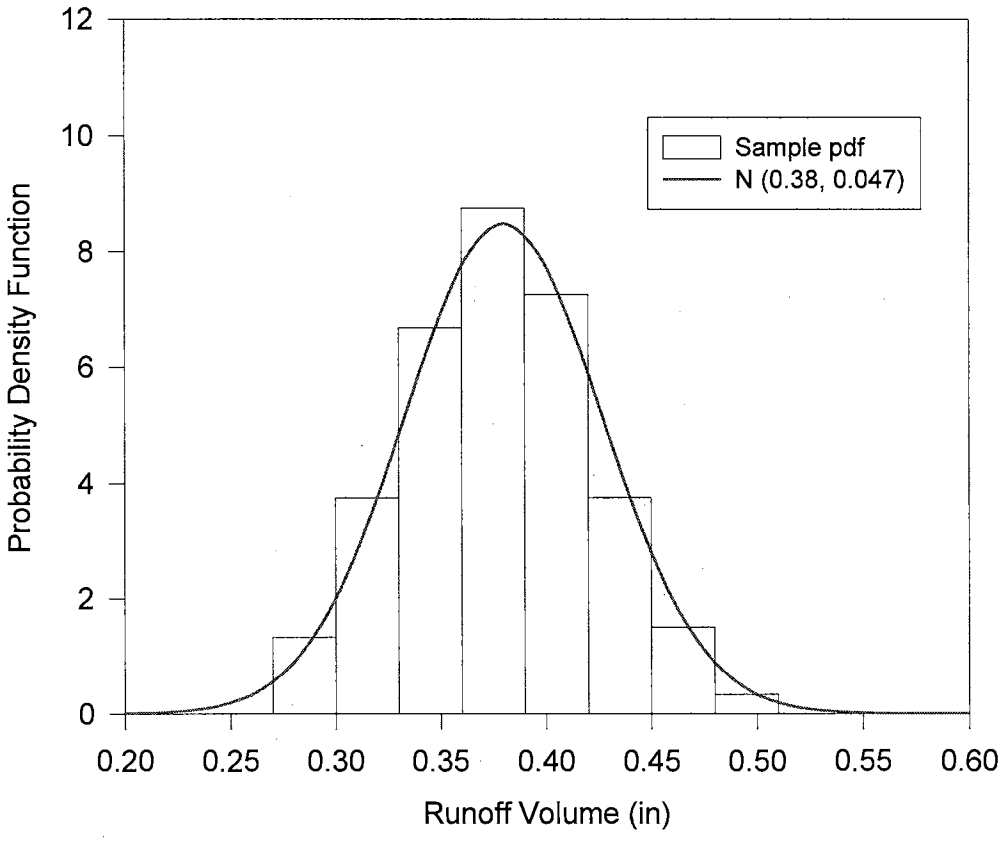

Figure 6-11 Distribution of the Mean of Runoff Volume Predictions with the Posterior Input Parameters for Watershed RU

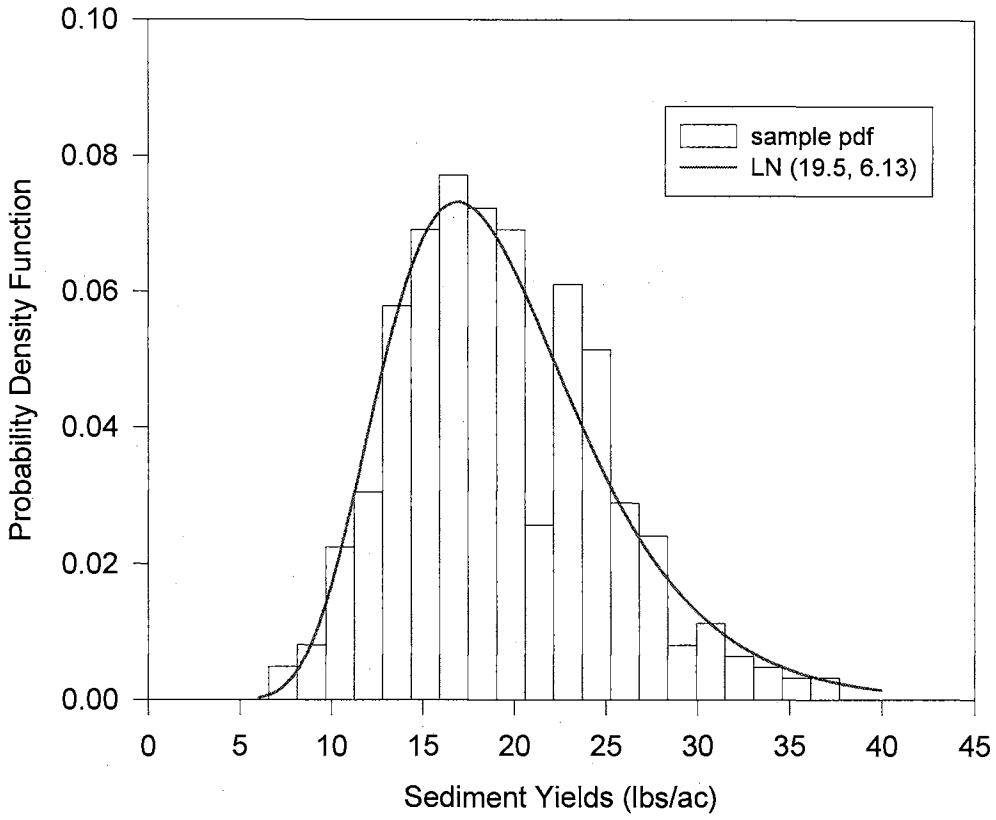

Figure 6-12 Distribution of the Mean of Sediment Yield Predictions with the Prior Input Parameters for Watershed RU

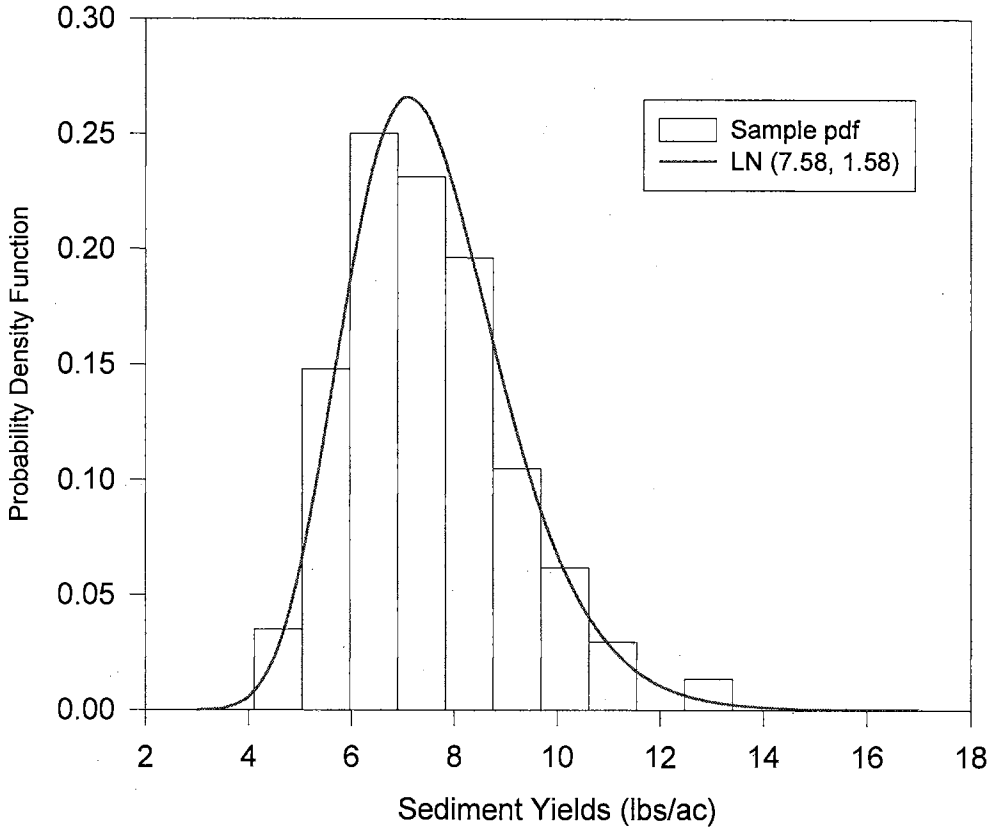

Figure 6-13 Distribution of the Mean of Sediment Yield Predictions with the Calibrated Input Parameters for Watershed RU

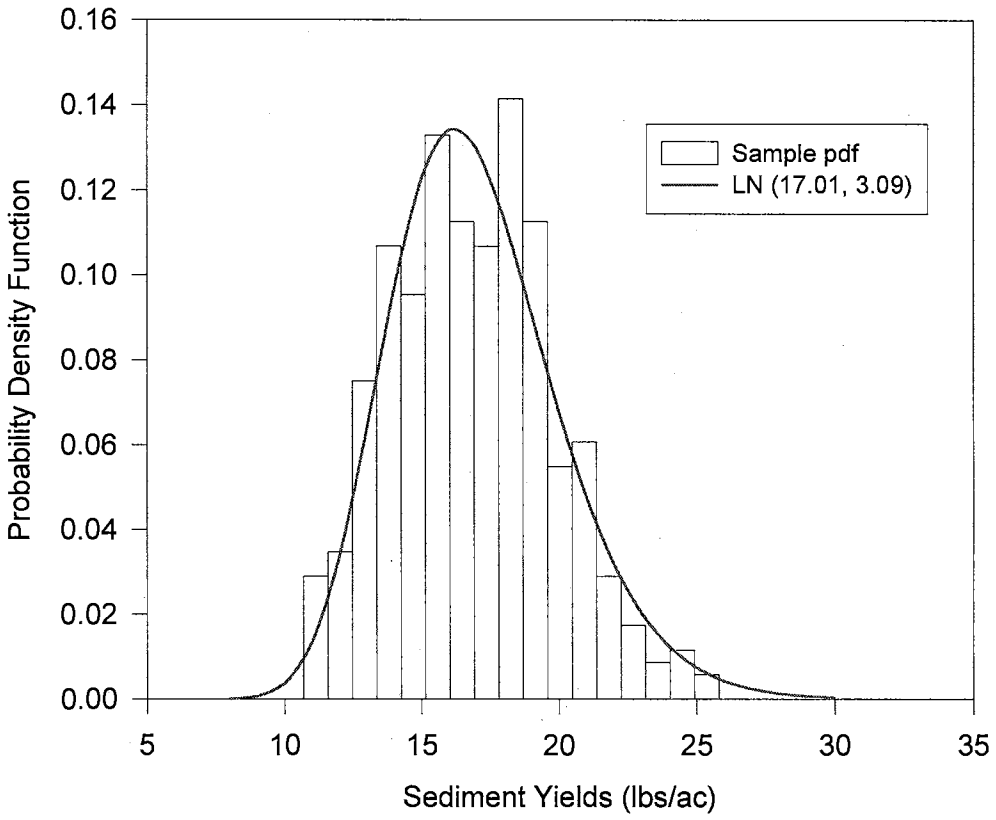

Figure 6-14 Distribution of the Mean of Sediment Yield Predictions with the Posterior Input Parameters for Watershed RU

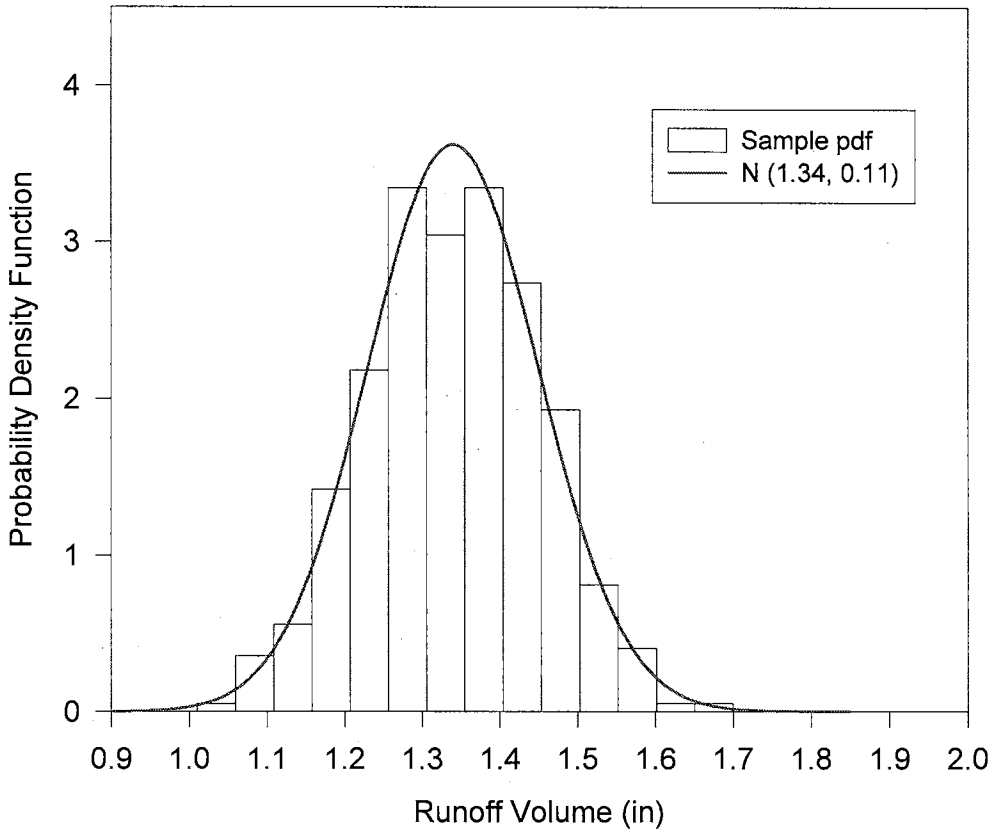

Figure 6-15 Distribution of the Mean of Runoff Volume Predictions with the Prior Input Parameters for Watershed WM

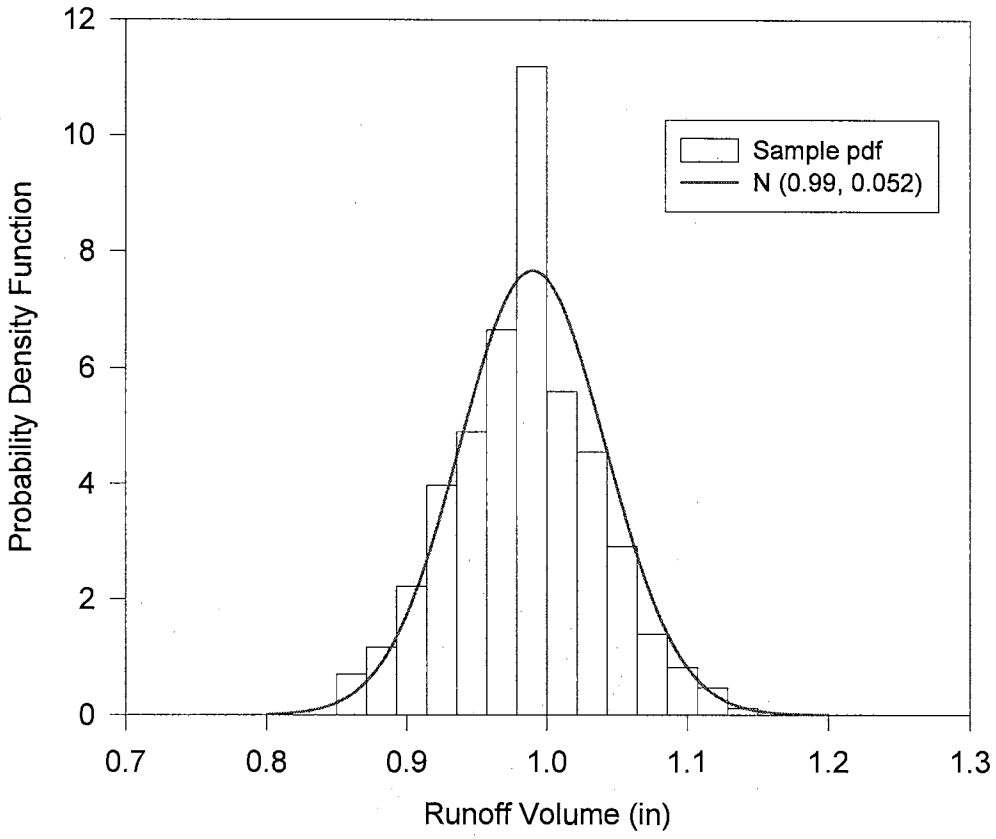

Figure 6-16 Distribution of the Mean of Runoff Volume Predictions with the Calibrated Input Parameters for Watershed WM

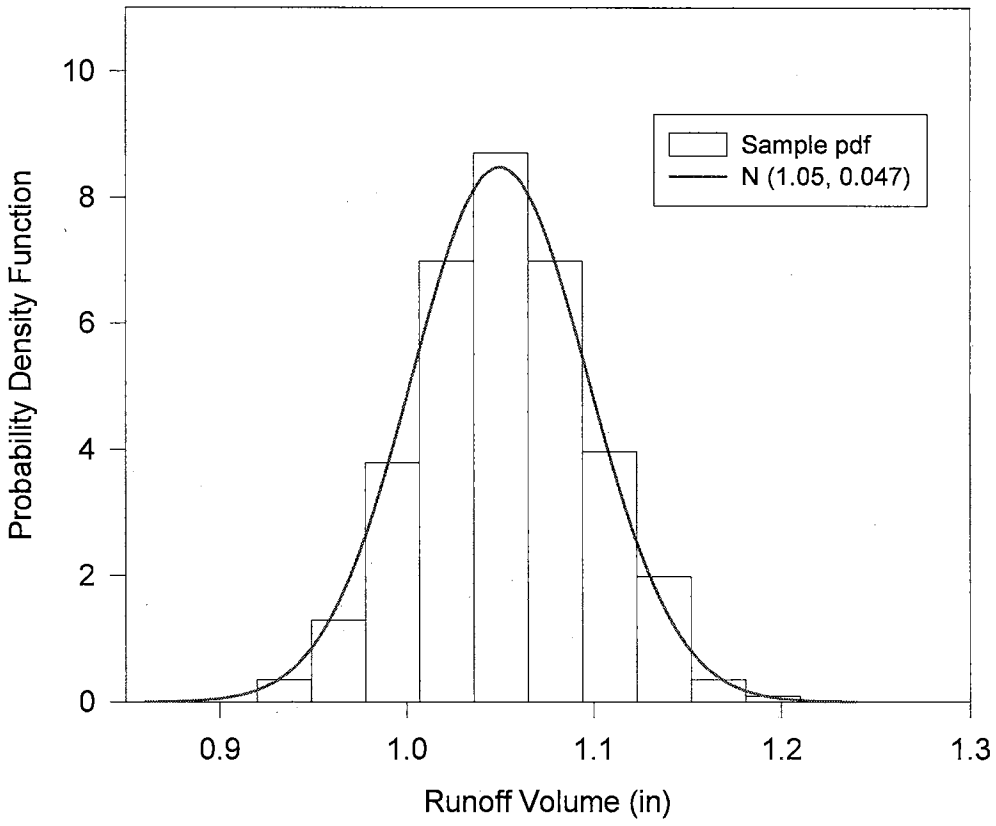

Figure 6-17 Distribution of the Mean of Runoff Volume Predictions with the Posterior Input Parameters for Watershed WM

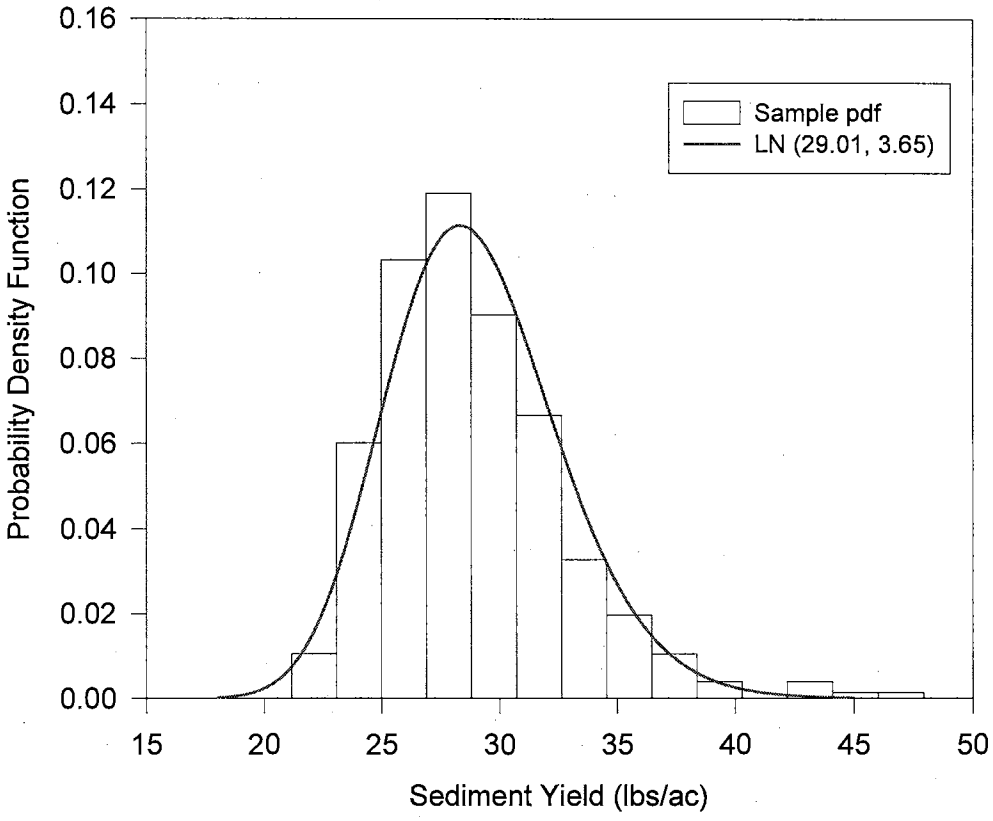

Figure 6-18 Distribution of the Mean of Sediment Yield Predictions with the Prior Input Parameters for Watershed WM

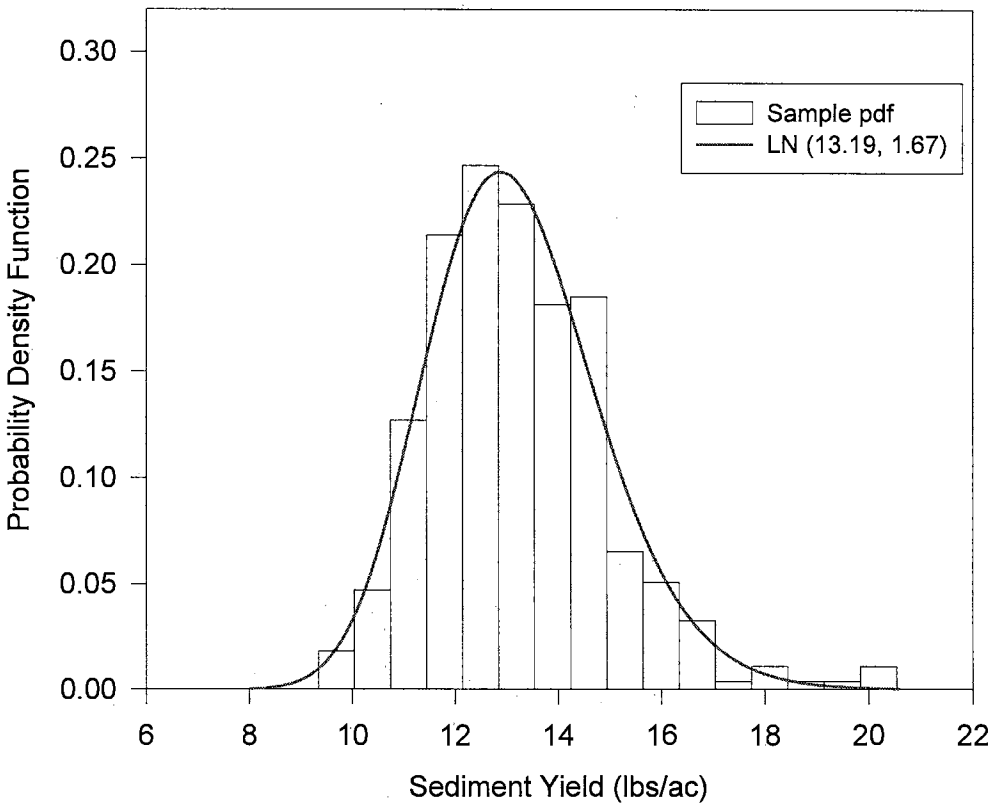

Figure 6-19 Distribution of the Mean of Sediment Yield Predictions with the Calibrated Input Parameters for Watershed WM

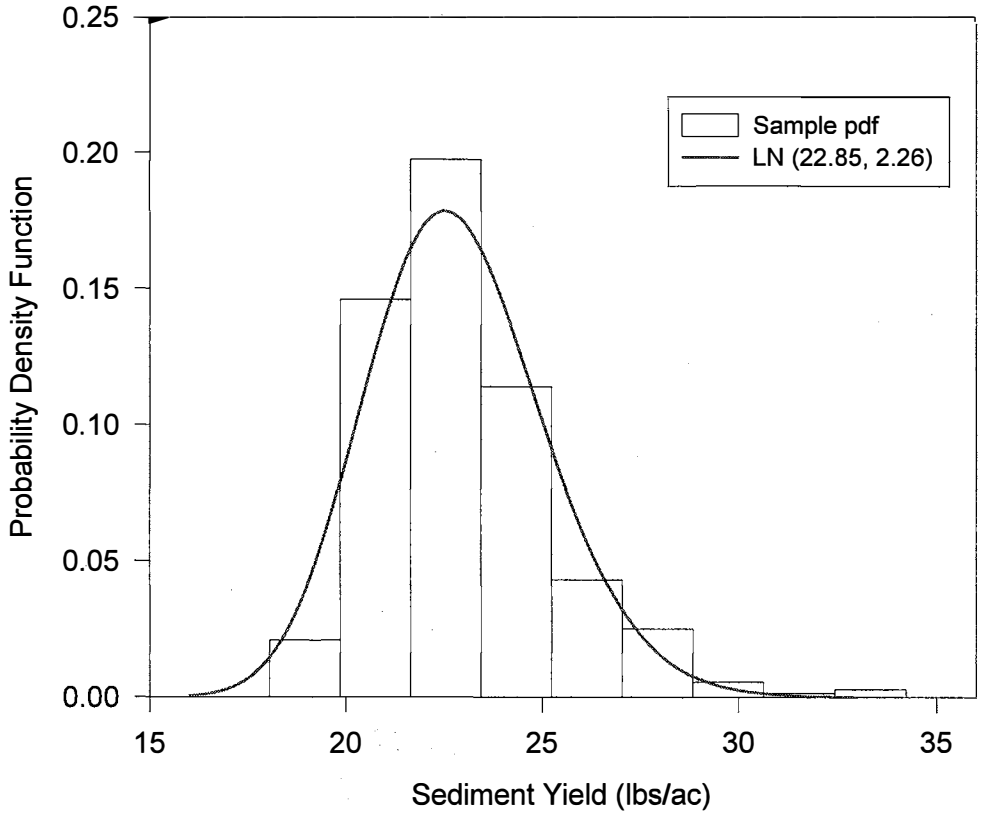

Figure 6-20 Distribution of the Mean of Sediment Yield Predictions with the Posterior Input Parameters for Watershed WM

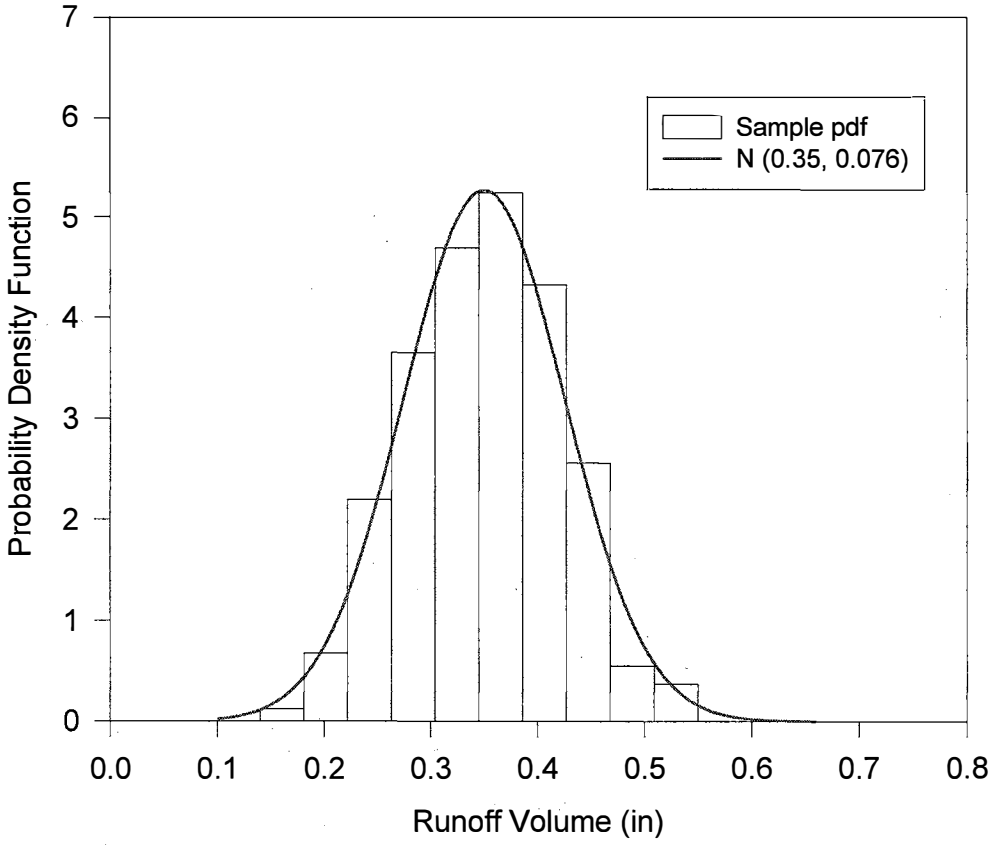

Figure 6-21 Distribution of the Mean of Runoff Volume Predictions with the Prior Input Parameters for Watershed WU

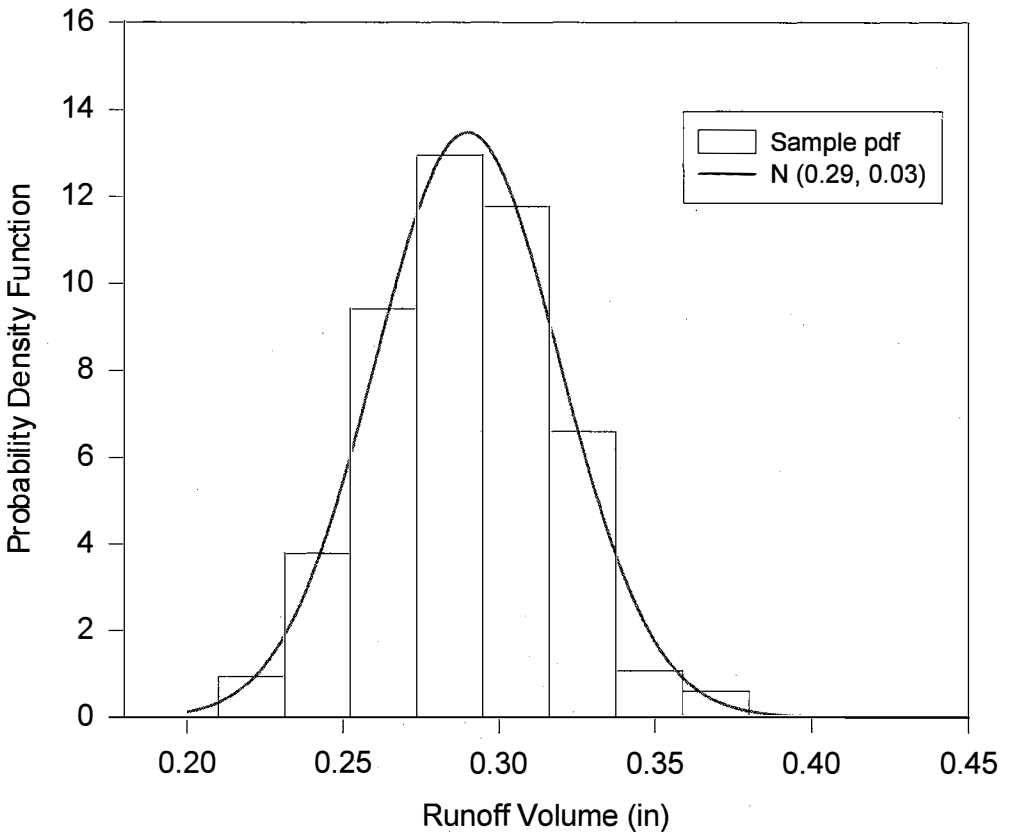

Figure 6-22 Distribution of the Mean of Runoff Volume Predictions with the Calibrated Input Parameters for Watershed WU

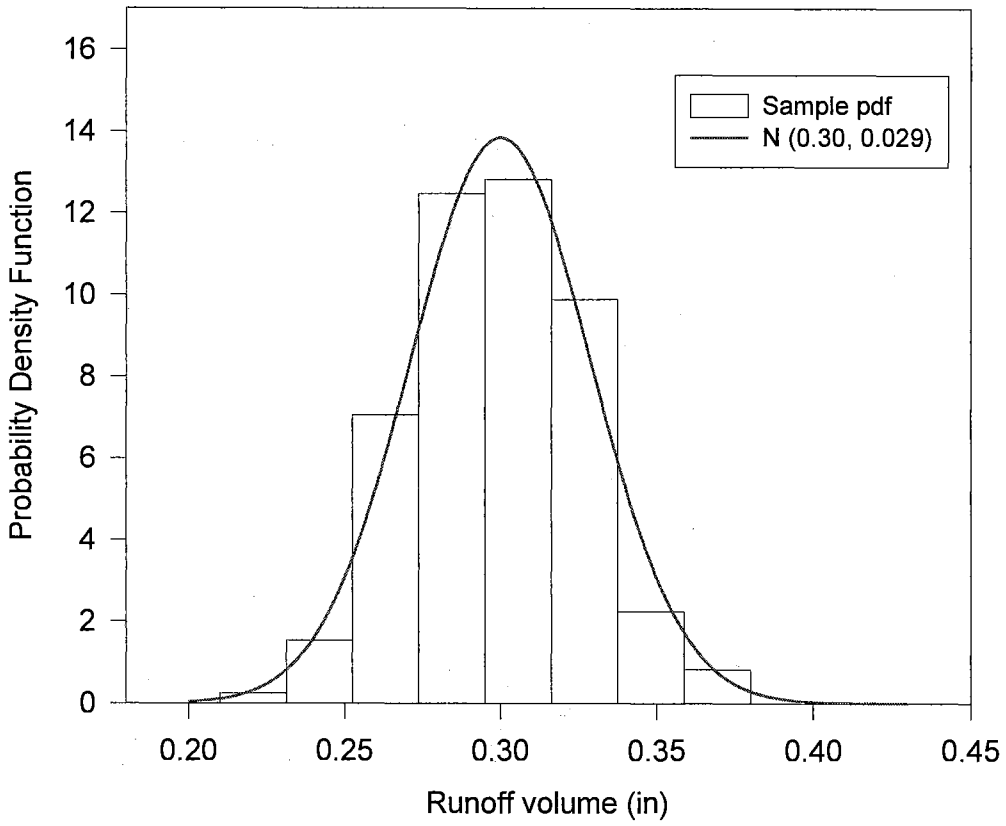

Figure 6-23 Distribution of the Mean of Runoff Volume Predictions with the Posterior Input Parameters for Watershed WU

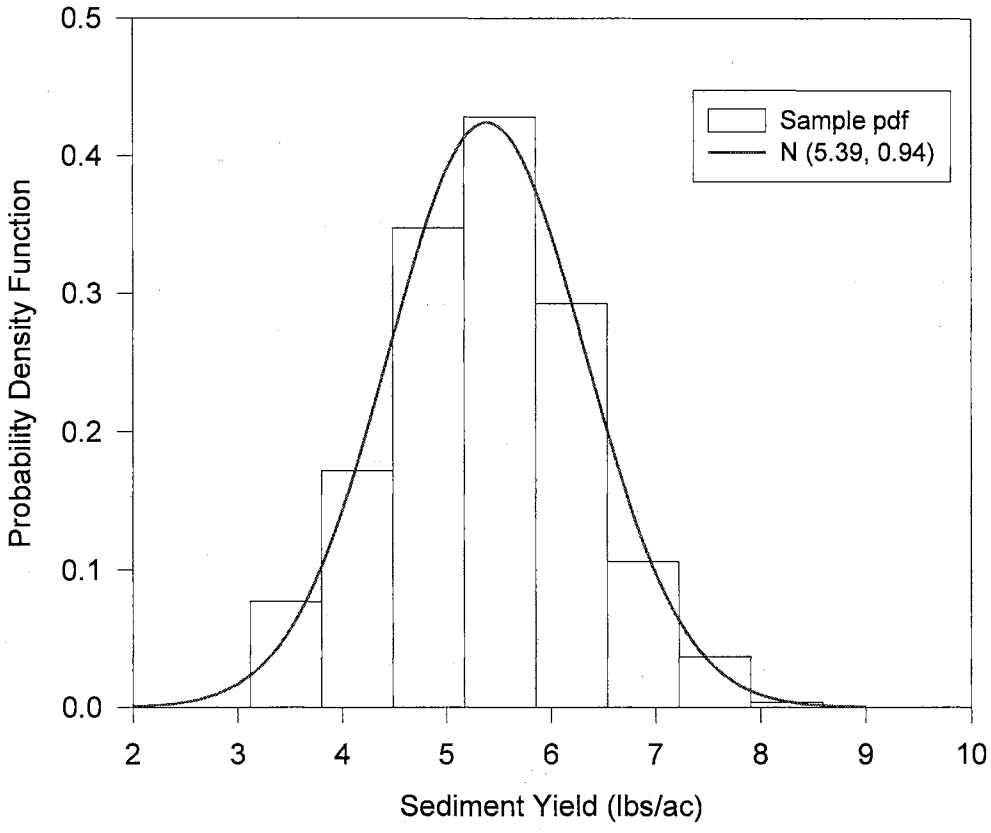

Figure 6-24 Distribution of the Mean of Sediment Yield Predictions with the Prior Input Parameters for Watershed WU

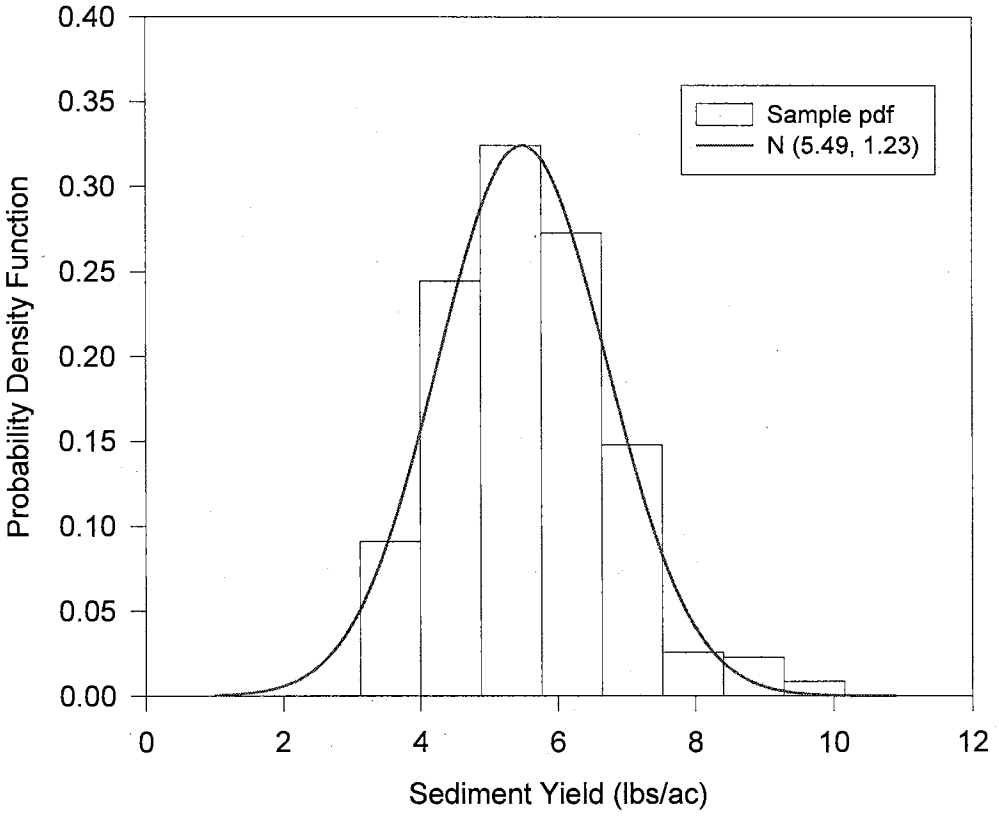

Figure 6-25 Distribution of the Mean of Sediment Yield Predictions with the Calibrated Input Parameters for Watershed WU

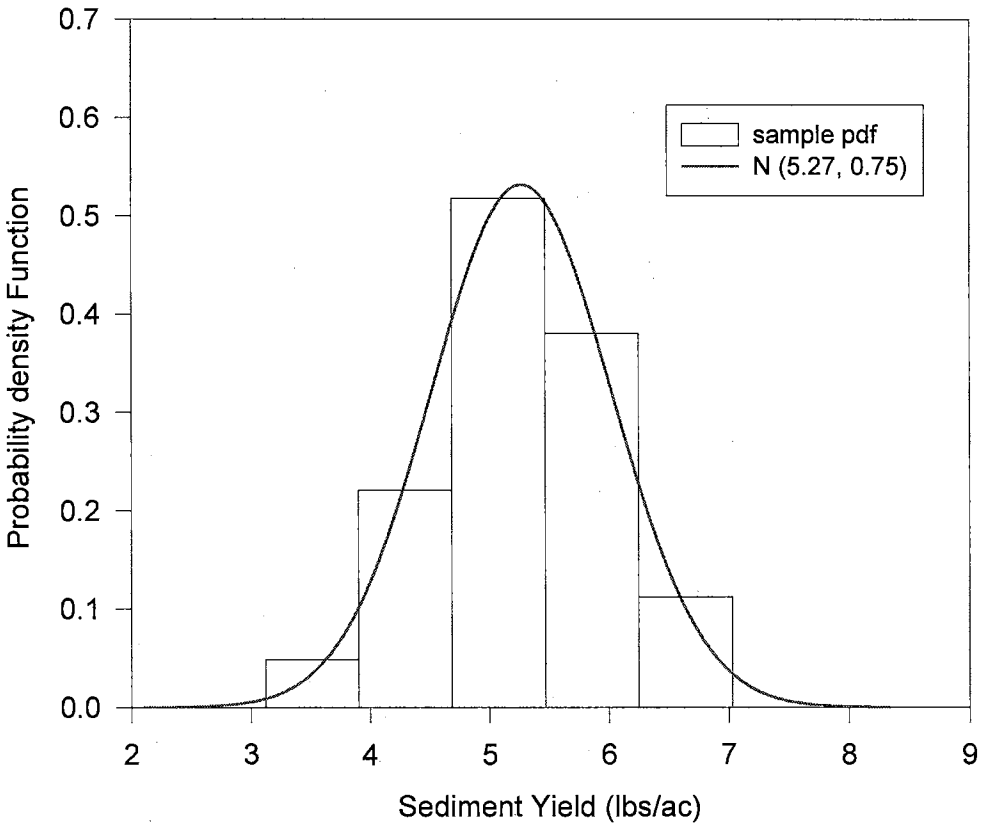

Figure 6-26 Distribution of the Mean of Sediment Yield Predictions with the Posterior Input Parameters for Watershed WU

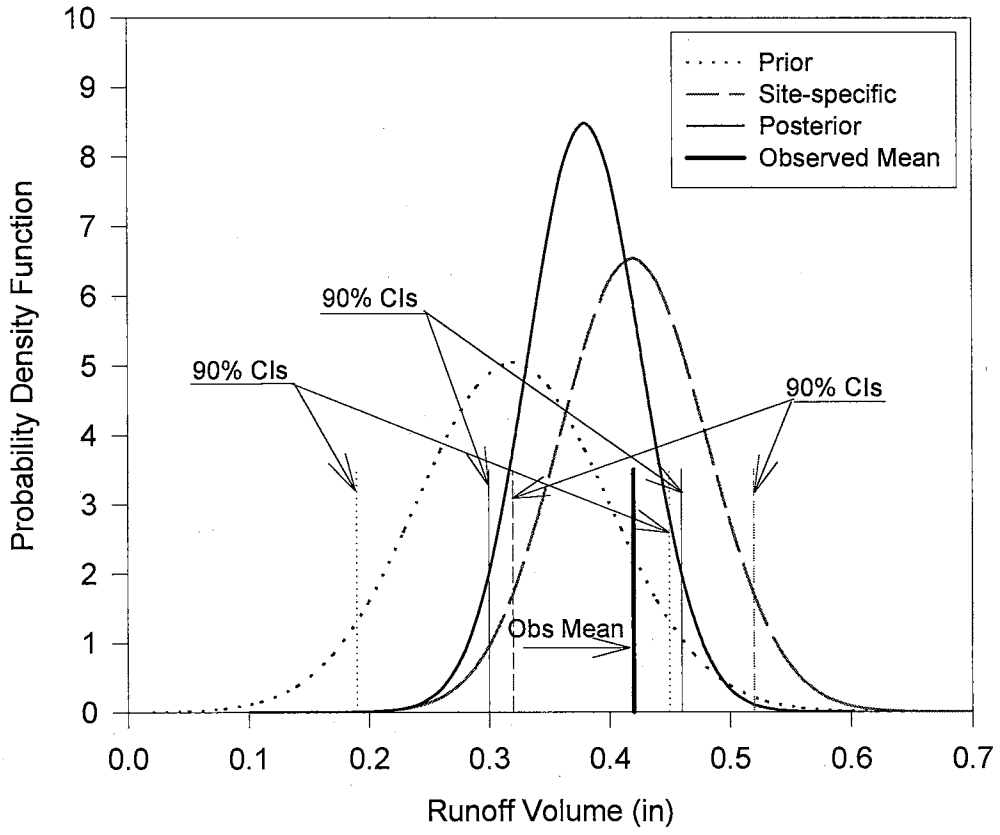

Figure 6-27 Comparison of the Observed Mean of Runoff Volume with the Predicted Mean for Watershed RU

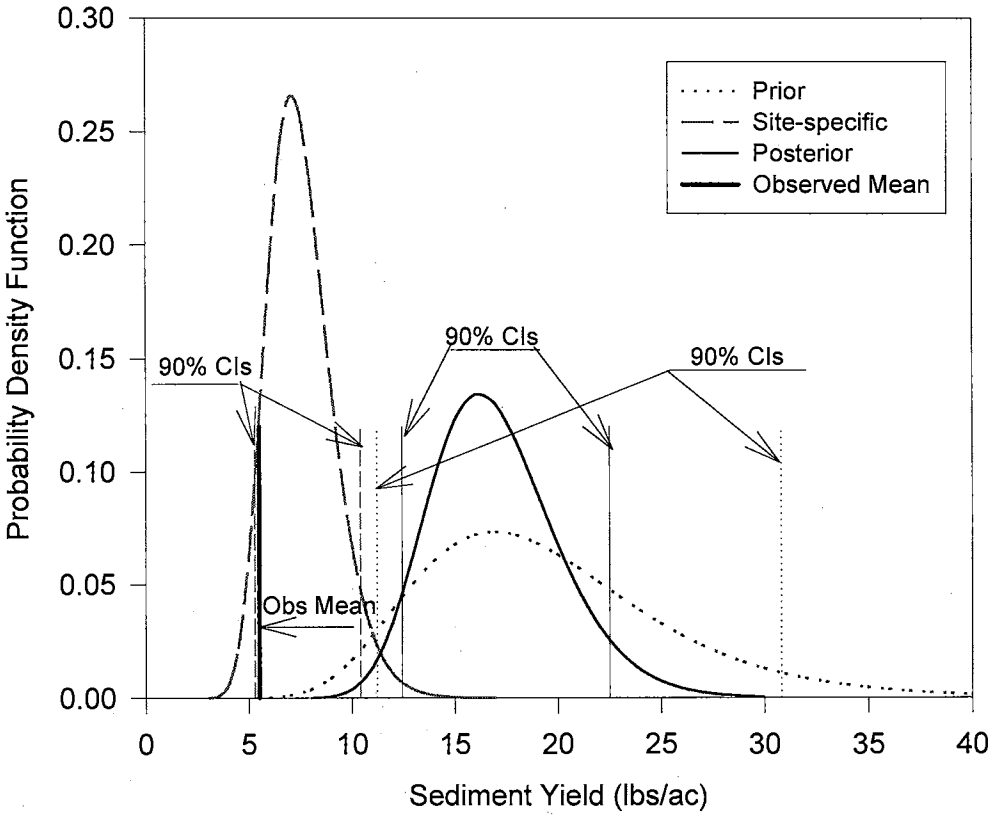

Figure 6-28 Comparison of the Observed Mean of Sediment Yield with the Predicted Mean for Watershed RU

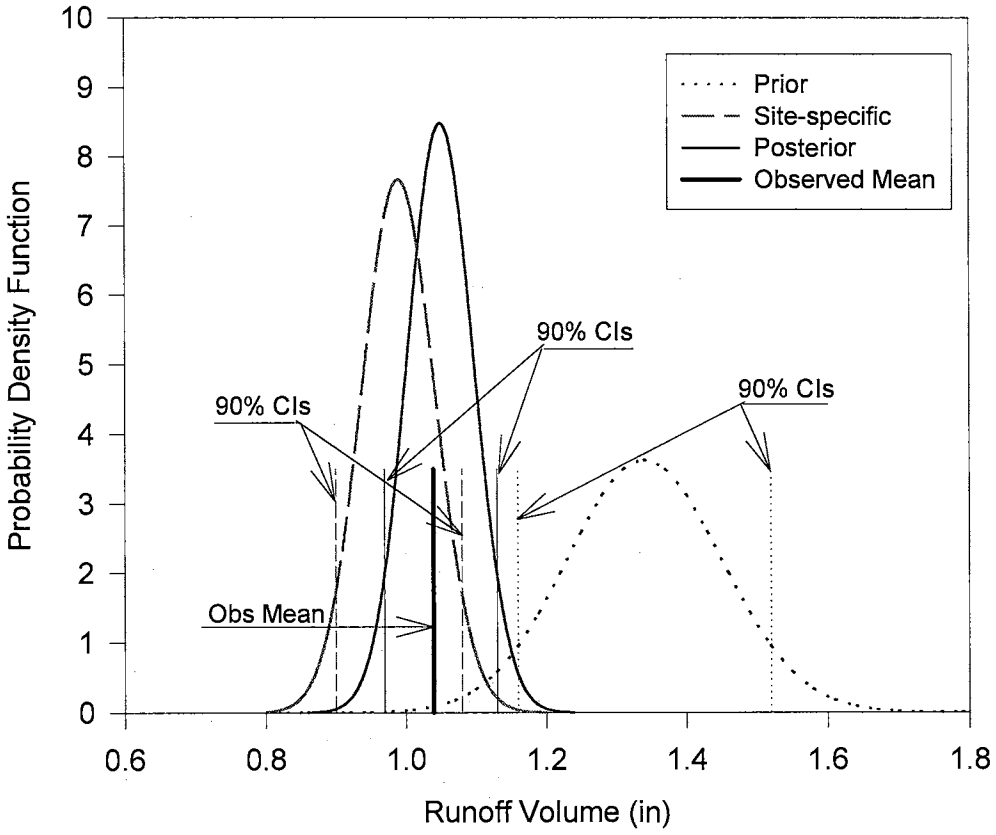

Figure 6-29 Comparison of the Observed Mean of Runoff Volume with the Predicted Mean for Watershed WM

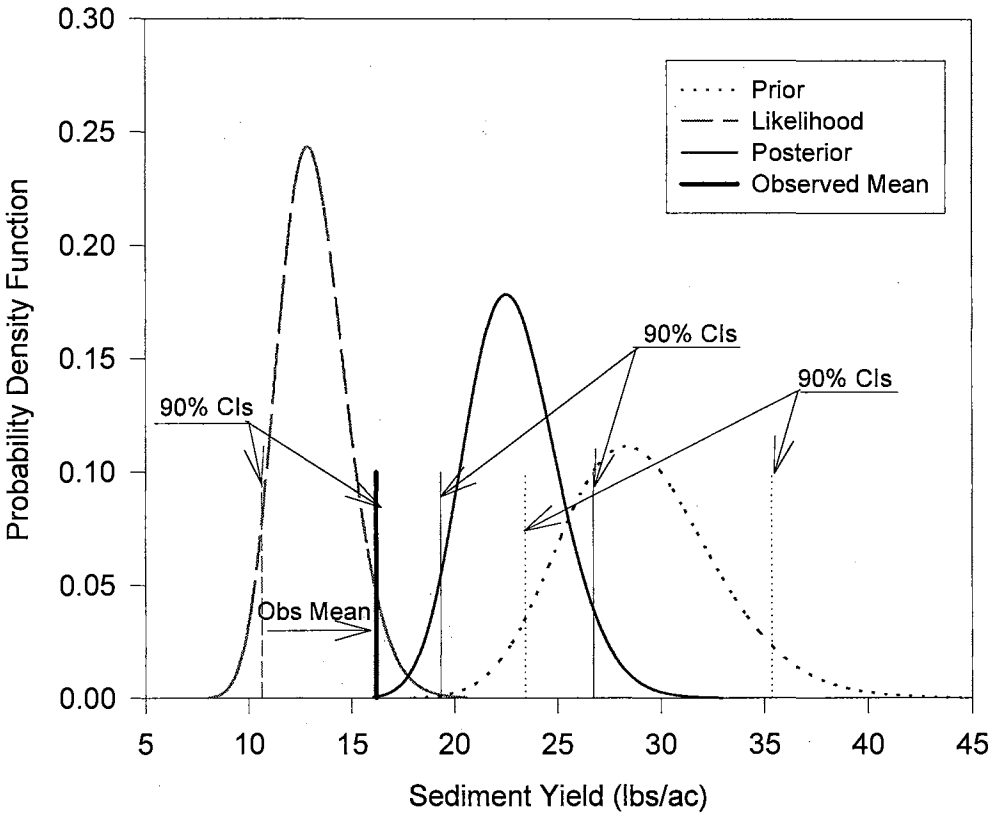

Figure 6-30 Comparison of the Observed Mean of Sediment Yield with the Predicted Mean for Watershed WM

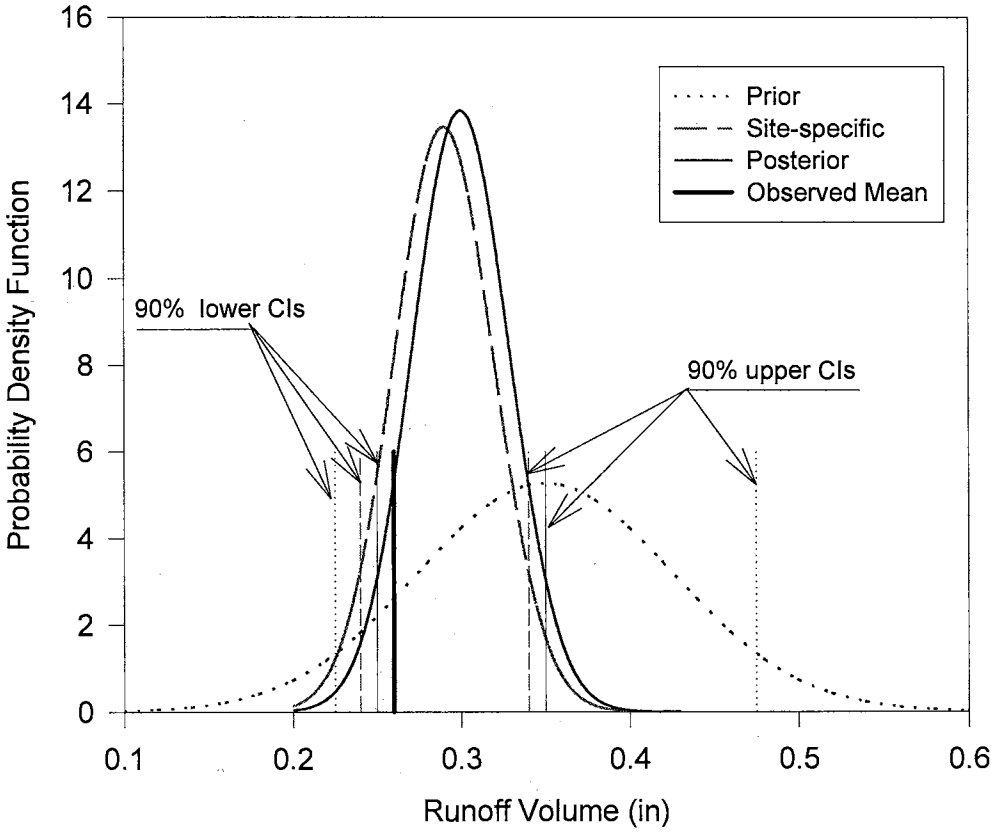

Figure 6-31 Comparison of the Observed Mean of Runoff Volume with the Predicted Mean for Watershed WU

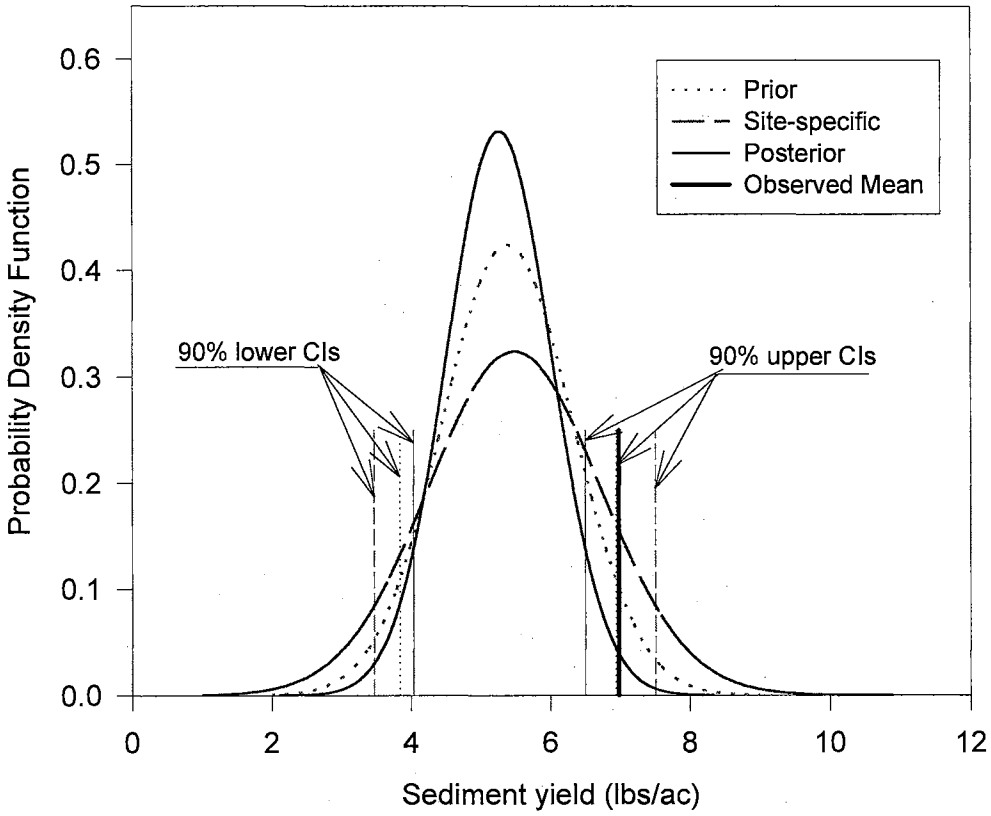

Figure 6-32 Comparison of the Observed Mean of Sediment Yield with the Predicted Mean for Watershed WU

CHAPTER VII

SUMMARY AND CONCLUSIONS

Summary

This dissertation has presented two important aspects in uncertainty analysis for hydrologic and water quality modeling: estimating the uncertainty of input model parameters in the calibration phase and evaluating the model performance with uncertain input parameters. It has also presented the development of the methodology incorporating the prior information into the site-specific information to produce the posterior information for any input parameter. The AGNPS model was used in this study to illustrate the method of uncertainty analysis and updating uncertain input parameters. Data used in this study were from four small watersheds in Arkansas.

Calibration and evaluation are two important aspects of hydrologic and water quality modeling. There are many methods to calibrate a model. All these traditional calibration techniques assume that there exists a "true" fixed value for each input parameter and only a point estimate for each input parameter is provided. However, the model parameters should be considered as random variables. One estimate is not enough to capture the statistical properties of a random variable. Bayesian estimation can furnish not only a point

estimate for each input parameter but also a marginal distribution for each input parameter. The Least Squares method is the most widely used and accepted method not just because of its simplicity but its efficiency as well. The point estimates of input parameters by Bayesian estimation were compared with those by Least Squares to test the efficiency of Bayesian estimation.

A very important procedure in model calibration, which is often ignored, is the verification of the Least Squares assumptions. Once the Least Squares assumptions are proven valid, the calibration results could be taken as the final calibration results. The Least Squares assumptions were checked for the calibration results by Bayesian estimation. Then marginal distributions of S and land slope were taken as the site-specific information for S and land slope.

The prior information about S and land slope was from the values reported in literature. The prior information was incorporated into the site-specific information to produce the posterior information about S and land slope. The performance of the AGNPS model was evaluated for these three types of information about S and land slope, respectively. Since input parameters were assumed as random variables, the model responses were random variables too and were expressed in the form of probability density functions. Confidence intervals were placed on the mean of runoff predictions and sediment predictions for different types of information about S and land slope. If the observed mean falls into the confidence intervals for the prior, site-specific or posterior information about S and land slope, the model predictions in the same case may be termed as statistically acceptable.

It is reasonable for one to expect that better model predictions should be obtained when more information is used to estimate input parameters of the model. An effort was made to see whether the uncertainty of model predictions was reduced by incorporating the prior information with the site-specific information.

Conclusions

Based upon the results of this study, the following conclusions can be drawn:

1) The point estimates of S and land slope by Least Squares are identical to or very close to those by Bayesian estimation for all watersheds used in this study. Therefore, Bayesian estimation is just as effective as Least Squares. However, in addition to point estimates of S and land slope, Bayesian estimation has the advantage of providing probability density functions for S and land slope as well.

2) The observed means of runoff volume and sediment yield fall into all the corresponding 95% confidence intervals of the site-specific predictions for all study watersheds. This proves from another point of view that Bayesian estimation can give good estimates for model parameters.

3) The prior information for retention parameter S is properly specified. The uncertainty in the runoff predictions of the AGNPS model is reduced by combining this prior information with the site-specific information of S for all three watersheds used in the model evaluation.

4) When the prior information is mis-specified, such as land slope in this study, incorporating the prior into the site-specific information will not reduce the

uncertainty in model predictions but will lead to worse or false model predictions. Therefore, more caution needs to be taken in specifying the prior information for a parameter. If one is not sure that the prior information is good for the specific use, it is better to use the site-specific information alone to give model predictions.

Recommendations for Further Research

The following topics are suggested for further research:

1) The procedure and methodology for uncertainty analysis elucidated in this dissertation should be applied to other hydrologic and water quality models to see if consistent results are obtained.

2) The risk associated with the uncertainty of model predictions should be studied further.

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APPENDIX

APPENDIX A

COMPUTER PROGRAM TO CALIBRATE AGNPS

BY BOTH LEAST SQAURES AND BAYESIAN ESTIMATION

```
/*****************************************************************
```

This program is writen to execute the AGNPS model for different rainfall events and adjusted slope and curve number. What this program does is:

1) Read rainfall depth and sediment yield and runoff from a data file called rainsed.dat.

2) For each possible combination of slope and curve number, update a input data file for AGNPS model for each rainfall event, Then run AGNPS model for all combinations of slope and curve number and rainfall events.

3) Record simulated sediment yield and runoff volume and compare them with measured values, calculate and record errors between simlulated values and measured values.

4) Find the least sum of squared errors and corresponding slope and cover factor under three conditions: runoff alone, sediment alone and the sum of runoff and sediment.

5) Find the calibrated slope and curve number based on Bayesian estimator. Then calculate the marginal distributions of slope and Curve number, respectively.

```
*****************************************************************/


#include <stdio.h>
#include <process.h>
#include <math.h>
#include <io.h>

#define ncell 7 /* # of cells */

#define N 31  /* # of rainfalls used in calibration */

#define  SN 11  /* number of increment of slope  */
#define  deltas  1.0  /* increment of slope */
#define  slpmin  0.0  /* minimum value of slope  */

#define  NC  25  /* # of the increment of CN */
#define  deltac 2 /* increment of CN */
#define  cnmin 40  /* minimum value of CN */
```

```
#define trans 0 /* transformation factor-- 0 or 1
                    0 = no transformation
                    1 = square root transformation */


/* sed[] - observed sediment discharge
   runoff[] - observed runoff volume
   rain[] - rainfall depth
   slp[] - slope
   curve[] - curve number
   sederr[][][] - sediment discharge errors
   rverr[][][] - runoff volume errors
   serr1[][] - sum of the squared errors of sediment discharge
   serr2[][] - sum of the squared errors of runoff volume
   serr12[][] - sum of the production of the sediment error
                    and runoff volume error
   sum[][] = serr1[][] + serr2[][]
   bayes[][] = the determinant of |S(x)|
   slpdist[] - marginal distribution of slope
   cndist[] - marginal distribution of CN     */


main()
 {

    int  i, j, k, m, n, curve[NC];
    int  amc[N];  /* amc - antecedent moisture condition */
    float  slp[SN];
    float  rain[N], sed[N], runoff[N];
    float energy[N], S, C;
    float serr1[SN][NC], serr2[SN][NC], serr12[SN][NC],
          sum[SN][NC];
    double slpdist[SN], cndist[NC];
    double bayes[SN][NC], power;

    int  CN, length, COD;
    float  eng, duration, rainfall, nitro;
    float  manning, kft, cft, pft, scc, msed, mrv;
    float  cn, rv, sederr[N], area, areac, e;
    float  ropk, tss, tp, rverr[N];
    char  type[16], command[20], string[66], f[8], g[8];
    int  a, b, c, d;
```

```
FILE *ifp; /* open the rainfall data file for reading. */
FILE *temp, *fp, *ofp;

ifp = fopen("rainsed.dat", "r");


/*  Initiate all arrays to zero  */

for(i=0; i<N; i++) {
  amc[i]=0;
  rain[i]=0.0;
  sed[i]=0.0;
  runoff[i]=0.0;
  energy[i]=0.0;
  sederr[i]=0.0;
  rverr[i]=0.0;
}

for(i=0; i<NC; i++) {
  curve[i]=0;
}

for(i=0; i<SN; i++) {
      slp[i]=0.0;
      for(j=0; j<NC; j++) {

      serr1[i][j]=0.0;
      serr2[i][j]=0.0;
      serr12[i][j]=0.0;
      sum[i][j]=0.0;
      bayes[i][j]=0.0;

      }
}


for(i=0;i<N;i++) {
       fscanf(ifp, "%d%f%f%f",
                  &amc[i],&rain[i],&runoff[i],&sed[i]);

        /*-----------------------------------------------------------------
            Calculate the rainfall energy for each rainfall.
        -----------------------------------------------------------------*/
```

```
        energy[i] = 17.90 * pow(rain[i], 2.0619);
        energy[i] = energy[i] / pow(24.0, 0.4134);

      printf("%4d%8.2f%8.2f%8.2f%8.2f\n", amc[i], rain[i],
            energy[i], runoff[i], sed[i]);
      }

fclose(ifp);

putchar('\n\n');


 msed = 0;
 mrv = 0;

 for(k=0; k<N; k++) {

     if(trans == 1) {
       sed[k] = pow(sed[k], 0.5);
       runoff[k] = pow(runoff[k], 0.5);
      }

       msed += sed[k]/N;
       mrv += runoff[k]/N;

 }
```

```
/* ++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
```

The following part of the program updatas the input data file for AGNPS (input.dat) for every rainfall event and all possible combinations of slope and Curve number. Run AGNPS model and record sediment yield and runoff volume loading for each run.

```
++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++*/


 ofp = fopen("cnslp.out","w");
 fprintf(ofp,
```

```
" Slope CN    Sum    Bayes   sederr    rverr\n\n");
fclose(ofp);

for(i=0; i<SN; i++) {
     slp[i] = i*deltas + slpmin;

     for(j=0; j<NC; j++) {
       curve[j]=j*deltac + cnmin;

       for(k=0; k<N; k++)  {

        ifp = fopen("input.dat", "r");
        temp = fopen("temp.dat", "w");


        for(m=0; m<=5; m++) {

            fgets(string, 65, ifp);
            fputs(string, temp);
        }

        fputc('\n', temp);

        /* updata the file input.dat */

        fscanf(ifp, "%s%f%f%f%f\n",
            type, &eng, &duration, &rainfall, &nitro);


      /* update energy value and rainfall value */

       fprintf(temp, "%16s%8.2f%8.1f%8.2f%8.2f\n",
            type,energy[k],duration,rain[k],nitro);


       /* update curve number */

       for(m=0; m<ncell; m++) {

            fscanf(ifp, "%d%s%d%s%d%d%f%d",
              &a,&f,&b,&g,&c,&CN,&e,&d);
```

```
/*-------------------------------------------------
      Calculate CN for different amc.
 -------------------------------------------------*/

switch (amc[k]) {

    case 1:  /* antecedent moisture condition I */
      cn = (4.2*curve[j])/(10 - 0.058*curve[j]);
      CN = cn + 0.5;
      break;

    case 2:  /* antecedent moisture condition II */
      CN = curve[j];
      break;

    case 3:  /* antecedent moisture condition III */
      cn = (23*curve[j])/(10 + 0.13*curve[j]);
      CN = cn + 0.5;
      break;

    default:
      printf("\nERROR: Unexpected rainfall type\n");
      printf("antecedent moisture condition: %d\n",
              amc[k]);
      exit(0);
    }


    fprintf(temp,"%8d%8s%8d%8s%8d%8d%8.1f%8d\n",
            a,f,b,g,c,CN,slp[i],d);


    fscanf(ifp, "%d%f%f%f%f%f%d",
      &length,&manning,&kft,&cft,&pft,&scc,&COD);

    fprintf(temp,"%16d%8.3f%8.2f%8.4f%8.2f%8.2f%8d",
        length,manning,kft,cft,pft,scc,COD);


    for(n=0; n<9; n++) {
    /*no fertilizer application, otherwise, k<10.*/

        fgets(string, 65, ifp);
```

```
            fputs(string,temp);
          }
        }

        printf("\n\nCN = %d     %d\n", CN, amc[k]);
        printf("slope = %5.2f      Curve # =%4d",
             slp[i], curve[j]);
        printf("     storm # = %3d\n", k);


      fclose(ifp);
      fclose(temp);

/* ------------------------------------------------------------------------------

   Run AGNPS model and calculate and record the following results:

    1) land slope (%);
    2) curve number;
    3) rainfall depth (in);
    4) simulated sediment discharge;
    5) simulated runoff volume;
    6) residuals which are the difference between simulated values and
      measured values;

   ------------------------------------------------------------------------------*/


      sprintf(command,"agrun %s", "temp.dat 0 0 0");
      printf("%s\n", command);
      system(command);


      putchar('\n');

   /* pick up interested results from the output file
     of AGNPS model.  */

     ifp = fopen("temp.nps", "r");

     for(m=0; m<4; m++) {
```

```
        fgets(string, 65, ifp);
    }

    fscanf(ifp, "%f%f%f%f%d%s%f%f%f",
          &area,&areac,&rainfall,&eng,&a,&g,
          &rv,&ropk,&tss);


    printf("%5.2f  %5.2f  %5.2f  %5.2f\n",
          rainfall, rv, ropk, tss);


    /*-------------------------------------------------------
            residual is defined as
        "measured value" - "simulated value"
    -------------------------------------------------------*/

    tss=tss*2000.0/area;

    if(trans == 1) {
      tss=pow(tss, 0.5);
      rv=pow(rv, 0.5);
    }

    sederr[k] = sed[k] - tss;
    rverr[k] = runoff[k] - rv;

    sederr[k] = sederr[k]/msed;
    rverr[k] = rverr[k]/mrv;


    printf("%4.1f  %4d  %4.2f  %8.2f %8.2f %8.2f %8.2f\n",
          slp[i],curve[j],rain[k],rv,rverr[k],
          tss,sederr[k]);


    fclose(ifp);

  }


ofp=fopen("cnslp.out","a"); /* "a" -- append */
```

```
        for(k=0; k<N; k++) {

          serr1[i][j] += sederr[k]*sederr[k];
          serr2[i][j] += rverr[k] * rverr[k];
          serr12[i][j] += sederr[k]*rverr[k];

        }

          sum[i][j] = serr1[i][j] + serr2[i][j];

          bayes[i][j] = (double)(serr1[i][j]*serr2[i][j]);
          bayes[i][j] +=(double)(-serr12[i][j]*serr12[i][j]);
          power = (double)(-N/2.0);
          bayes[i][j] = pow(bayes[i][j], power);


          fprintf(ofp,
                "%4.1f %4d  %6.2e %6.2e %6.2e %6.2e\n",
                 slp[i], curve[j],sum[i][j],bayes[i][j],
                 serr1[i][j],serr2[i][j]);


          fclose(ofp);


    }
        ofp = fopen("cnslp.out", "a");
        fputc('\n', ofp);
        fclose(ofp);

}
```

```
/* ------------------------------------------------------------------------------------

        1) Find the minimum value of "sum" and corresponding slope and
        CN, if there are more than one minimum value, record how many
        there have.

        2) Find the maximum value of "bayes" and correspinding slope and
        CN, check to see if there are more than one maximum.

------------------------------------------------------------------------------------*/


ofp = fopen("cnslp.out", "a");

S = slpmin;
CN = cnmin;
m = 0;
tss = sum[0][0];

for(i=0; i<SN; i++) {

    for(j=0; j<NC; j++) {

      if(sum[i][j] == tss){
          m += 1;
          S = slpmin + i*deltas;
          CN = cnmin + j*deltac;
      }

      if(i == 0) {
       if(j == 0)
          m = 0;
      }

      if(sum[i][j] < tss) {
          tss = sum[i][j];
          S = slpmin + i*deltas;
          CN = cnmin + j*deltac;
          m = 0;
      }
    }
  }
```

```
    fprintf(ofp,"\n LS error: %6.2e  S=%4.1f  CN=%4d\n",
            tss, S, CN);
    fprintf(ofp, " # of LS error: %2d\n\n", m+1);


S = slpmin;
CN = cnmin;
m = 0;
tss = serr1[0][0];

for(i=0; i<SN; i++) {

     for(j=0; j<NC; j++) {

       if(serr1[i][j] == tss){
            m += 1;
            S = slpmin + i*deltas;
            CN = cnmin + j*deltac;
       }

       if(i == 0) {
        if(j == 0)
            m = 0;
       }

       if(serr1[i][j] < tss) {
            tss = serr1[i][j];
            S = slpmin + i*deltas;
            CN = cnmin + j*deltac;
            m = 0;
       }
     }
    }

    fprintf(ofp,"\n LS error(sediment): %6.2e  S=%4.1f  CN=%4d\n",
            tss, S, CN);
    fprintf(ofp, " # of LS error: %2d\n\n", m+1);



S = slpmin;
CN = cnmin;
m = 0;
```

```
tss = serr2[0][0];

for(i=0; i<SN; i++) {

    for(j=0; j<NC; j++) {

      if(serr2[i][j] == tss){
          m += 1;
          S = slpmin + i*deltas;
          CN = cnmin + j*deltac;
      }

      if(i == 0) {
       if(j == 0)
          m = 0;
      }

      if(serr2[i][j] < tss) {
          tss = serr2[i][j];
          S = slpmin + i*deltas;
          CN = cnmin + j*deltac;
          m = 0;
      }
    }
  }

  fprintf(ofp,"\n LS error(runoff): %6.2e  S=%4.1f  CN=%4d\n",
          tss, S, CN);
  fprintf(ofp, " # of LS error: %2d\n\n", m+1);



S = slpmin;
CN = cnmin;
m = 0;
power = bayes[0][0];

for(i=0; i<SN; i++) {

    for(j=0; j<NC; j++) {

      if(bayes[i][j] == power){
          m += 1;
```

```
        S = slpmin + i*deltas;
        CN = cnmin + j*deltac;
    }

    if(i == 0) {
      if(j == 0)
        m = 0;
    }

    if(bayes[i][j] > power) {
        power = bayes[i][j];
        S = slpmin + i*deltas;
        CN = cnmin + j*deltac;
        m = 0;
    }
  }
}

fprintf(ofp,"\n Bayes error: %6.2e  S=%4.1f  CN=%4d\n",
        power, S, CN);
fprintf(ofp, " # of Bayes error: %2d\n\n", m+1);


/* ----------------------------------------------------------------

      Calculate the marginal distribution of slope

 ----------------------------------------------------------------*/

 for(i=0; i<SN; i++) {
   slp[i] = i*deltas + slpmin;
   slpdist[i] = 0.0;

   for(j=0; j<NC-1; j++) {

        CN = cnmin + j*deltac;
        S = 1000.0/CN - 10.0;
        S += -(1000.0/(CN+deltac) - 10.0);

     slpdist[i]+=S*(bayes[i][j]+bayes[i][j+1])/2;
   }
 }
```

```
power = 0.0;  /* the area under the pdf slpdist[i] */

for(i=0; i<SN-1; i++) {
  power += deltas*(slpdist[i]+slpdist[i+1])/2.0;
}

fprintf(ofp,"\n Slope   distribuion\n");

for(i=0; i<SN; i++) {

  slpdist[i] = slpdist[i]/power;

  fprintf(ofp," %5.2f    %8.2f\n",slp[i],slpdist[i]);

}


/* ------------------------------------------------------------

     Calculate the marginal distribution of CN

------------------------------------------------------------*/

for(i=0; i<NC; i++) {
  curve[i] = i*deltac + cnmin;
  cndist[i] = 0.0;

  for(j=0; j<SN-1; j++) {

    cndist[i]+=deltas*(bayes[j][i]+bayes[j+1][i])/2.0;
  }
}

power = 0; /* the area under the pdf cndist[j] */
for(i=0; i<NC-1; i++) {

  CN = cnmin + i*deltac;
  S = 1000.0/CN - 10.0;
  S += -(1000.0/(CN+deltac) - 10.0);

 power += S*(cndist[i]+cndist[i+1])/2.0;
}
```

```
        fprintf(ofp,"\n  CN    S   distribuion\n");

        for(i=0; i<NC; i++) {

          cndist[i] = cndist[i]/power;
          CN = cnmin + i*deltac;
          S = 1000.0/CN - 10.0;

          fprintf(ofp," %4d   %5.2f   %6.2f\n",
                          CN, S, cndist[i]);

        }


       fclose(ofp);


    return 0;
}
```

APPENDIX B

COMPUTER PROGRAM FOR MONTE CARLO SIMULATION

```
/*****************************************************************

      This program was designed to perform Monte Carlosimulation on AGNPS
      model under following conditions:

        1). Curve number with specified lognormal distribution
        2). Slope with specified lognormal distribution

      Requirements to run this programm:

        a. "input.dat" for AGNPS model
        b. "paramt.dat" to specify rainfall, mean and standard deviation for CN
           and Slope.
        c. define # of simulation and # of rainfall events

*****************************************************************/



#include <stdio.h>
#include <process.h>
#include <math.h>
#include <io.h>

#define ncell 1 /* # of cells */

#define NSIMU 400  /* # of simulations */

#define N  8  /* # of rainfall */

float stdnorm(void);
float lognorm(float, float);

main()
 {

   int  i, j, k, m, amc[N];
   float  slp, rain[N], sed, runoff, energy[N];
   float cnbar, scn, slpbar, sslp, S;

   int  CN, length, COD, cn;
   float  eng, duration, rainfall, nitro;
   float  manning, kft, cft, pft, scc;
```

```
float  rv, area, areac, e;
float  ropk, tss, tp;
char  type[16], command[20], string[66], f[8], g[8];
int  a, b, c, d;


FILE *ifp;
FILE *temp, *ofp;

ifp = fopen("paramt.dat", "r");

for(i=0; i<N; i++)    /* initialaze all arrays */
{
 amc[i] = 0;
 rain[i] = 0;
 energy[i] = 0;
}


 fscanf(ifp, "%d%f%f%f%f%f\n",
        &amc[0],&rain[0],&cnbar,&scn,&slpbar,&sslp);

 printf("%4d%8.2f%8.2f%8.2f%8.2f%8.2f\n",
         amc[0],rain[0],cnbar,scn,slpbar,sslp);

 if(N>1)
 {
      for(m=1; m<N; m++)
      {
       fscanf(ifp,"%d%f\n",&amc[m],&rain[m]);
       printf("%4d%8.2f\n",amc[m],rain[m]);
      }
 }

 fclose(ifp);

 putchar('\n');
```

```
    /*-----------------------------------------------------------------
        Calculate the rainfall energy for each rainfall.
    -----------------------------------------------------------------*/

    for(i=0; i<N; i++)
    {
     energy[i] = 17.90 * pow(rain[i], 2.0619);
      energy[i] = energy[i] / pow(24.0, 0.4134);

      printf("%4d%8.2f%8.2f\n",amc[i],rain[i],energy[i]);
    }


  putchar('\n\n');


/* ------------------------------------------------------------------------------------------

    The following part of the program updatas the input data file for AGNPS.

  ------------------------------------------------------------------------------------------*/


  ofp = fopen("simu.out","w");
  fprintf(ofp,
   " Slope   S    CN   runoff  sediment\n\n");
  fclose(ofp);


 for(m=0; m<N; m++)
 {

  for(i=0; i<NSIMU; i++)
  {

     /*-----------------------------------------------------------------
         generate random numbers for CN and slp with
         specified lognormal distribution.
     -----------------------------------------------------------------*/

      S = lognorm(cnbar,scn);
      CN = (int)(1000.0/(S+10.0));
```

```
slp = lognorm(slpbar,sslp);


 /*-----------------------------------------------------------
         calculate CN for different amc.
  -----------------------------------------------------------*/

 switch (amc[m]) {

  case 1:  /* antecedent moisture condition I */
       cn = (int)((4.2*CN)/(10 - 0.058*CN));
       break;

  case 2:  /* antecedent moisture condition II */
       cn = CN;
       break;

  case 3:  /* antecedent moisture condition III */
       cn = (int)((23.0*CN/(10.0 + 0.13*CN)));
       break;

  default:
       printf("\nERROR: Unexpected rainfall type\n");
       printf("antecedent moisture condition: %d\n",
              amc[m]);
       exit(0);
 }

 printf("\nCN = %3d  slope = %5.2f  simu# = %4d\n",
       CN, slp, i+1);


 ifp = fopen("input.dat", "r");
 temp = fopen("temp.dat", "w");


for(j=0; j<=5; j++) {

  fgets(string, 65, ifp);
  fputs(string, temp);
}

 fputc('\n', temp);
```

```
/* update energy value and rainfall value */

 fscanf(ifp, "%s%f%f%f%f\n",
    type, &eng, &duration, &rainfall, &nitro);

 fprintf(temp, "%16s%8.2f%8.1f%8.2f%8.2f\n",
         type,energy[m],duration,rain[m],nitro);


/* update curve number and slope factor */

 for(k=0; k<ncell; k++) {

    fscanf(ifp, "%d%s%d%s%d%d%f%d",
             &a,&f,&b,&g,&c,&COD,&e,&d);


    fprintf(temp,"%8d%8s%8d%8s%8d%8d%8.1f%8d\n",
                 a,f,b,g,c,cn,slp,d);


    fscanf(ifp, "%d%f%f%f%f%f%d",
          &length,&manning,&kft,&cft,&pft,&scc,&COD);

    fprintf(temp,"%16d%8.3f%8.2f%8.4f%8.2f%8.2f%8d",
             length,manning,kft,cft,pft,scc,COD);


    for(j=0; j<9; j++) {
  /*no fertilizer application, otherwise, k<10.*/

          fgets(string, 65, ifp);
          fputs(string,temp);
    }
 }


   fclose(ifp);
   fclose(temp);
```

```
/* ------------------------------------------------------------------------------------

        run AGNPS model and calculate and record the  following results:

        1) land slope (%);
        2) curve number;
        3) simulated sediment discharge;
        4) simulated runoff volume;

--- ------------------------------------------------------------------------------------*/


          sprintf(command,"agrun %s", "temp.dat 0 0 0");
          printf("%s\n", command);
          system(command);


          putchar('\n');

        /* pick up interested results from the output file
          of AGNPS model.  */

          ifp = fopen("temp.nps", "r");
          ofp = fopen("simu.out", "a");

          for(j=0; j<4; j++) {
                fgets(string, 65, ifp);
          }

           fscanf(ifp, "%f%f%f%f%d%s%f%f%f",
                 &area,&areac,&rainfall,&eng,&a,&g,
                 &rv,&ropk,&tss);


          tss=tss*2000.0/area;

          printf("%5.1f  %3d  %5.2f  %6.2f\n",
                  slp,CN,rv,tss);

          fprintf(ofp,"%5.1f  %5.2f  %3d  %5.2f  %6.2f\n",
                  slp,S,CN,rv,tss);
```

```
        fclose(ifp);
        fclose(ofp);

    }

    ofp = fopen("simu.out","a");
    fprintf(ofp, "\n");
    fclose(ofp);

  }
    return 0;
}


/*-----------------------------------------------------------------------------------------
     This function generates numbers with standard normal distribution, z(0,1)
-----------------------------------------------------------------------------------------*/

float stdnorm(void)
{
  float R, v1, v2, z;
  do
  {
    v1 = 2.0*rand()/32767.0 - 1.0;
    v2 = 2.0*rand()/32767.0 - 1.0;
    R = v1*v1 + v2*v2;
  }
  while(R>1.0);
  z = sqrt(-2.0*log(R)/R);
  z *= v1;
  return z;

}

/*-----------------------------------------------------------------------------------------
   This function generates numbers with a log-normal distribution with mean of mu
   and variance of sigma
-----------------------------------------------------------------------------------------*/

float lognorm(float mu, float sigma)
{
  float Cv, y, ybar, Sy, x;
```

```
 Cv = sigma/mu;

 ybar = 0.5*log(mu*mu/(Cv*Cv + 1.0));
 Sy = sqrt(log(Cv*Cv + 1.0));

 y = ybar + Sy*stdnorm(); /* normal distribution */

 x = exp(y);  /* lognormal distribution */

 return x;

}
```

2

VITA

Peng Yue

Candidate for the Degree of

Doctor of Philosophy

Thesis: INCORPORATING UNCERTAINTY INTO PARAMETER ESTIMATION AND EVALUATING THE AGNPS MODEL WITH UNCERTAIN PARAMETERS

Major Field: Biosystems Engineering

Biographical:

Education: Graduated from Qujing First High School, Yunnan, P.R. China in 1981; received Bachelor of Civil Engineering degree from Tianjin University, P.R. China in July 1985; received Master of Science degree in Civil Engineering from Tianjin University, P.R. China in February 1988; completed the requirements for the Doctor of Philosophy degree with a major in Biosystems Engineering at Oklahoma State University in May 1997.

Experience: Employed by Kunming Hydroelectric Investigation and Design Institute, P. R. China as a civil engineer from 1988 to 1993; employed by Oklahoma State University, Department of Biosystems and Agricultural Engineering as a graduate research assistant from 1993 to present.

Professional Memberships: American Society of Agricultural Engineering and Survey; Alpha Epsilon Honors Society, Oklahoma State University Chapter.