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Implications of Hydrologic Data Assimilation in Improving
Suspended Sediment Load Estimation in Lake Tahoe, California

by

Marc Alan Leisenring

A thesis submittal in partial fulfillment of the
requirements for the degree of

Master of Science
in
Civil and Environmental Engineering

Thesis Committee:
Hamid Moradkhani, Chair
Robert Annear
Chris Berger
Dacian Daescu

Portland State University
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Abstract

Pursuant to the federal Clean Water Act (CWA), when a water body has been listed as impaired, Total Maximum Daily Loads (TMDLs) for the water quality constituents causing the impairment must be developed. A TMDL is the maximum daily mass flux of a pollutant that a waterbody can receive and still safely meet water quality standards. The development of a TMDL and demonstrating compliance with a TMDL requires pollutant load estimation. By definition, a pollutant load is the time integral product of flows and concentrations. Consequently, the accuracy of pollutant load estimation is highly dependent on the accuracy of runoff volume estimation. Runoff volume estimation requires the development of reasonable transfer functions to convert precipitation into runoff. In cold climates where a large proportion of precipitation falls as snow, the accumulation and ablation of snowpack must also be estimated.

Sequential data assimilation techniques that stochastically combine field measurements and model results can significantly improve the prediction skill of snowmelt and runoff models while also providing estimates of prediction uncertainty. Using the National Weather Service's SNOW-17 and the Sacramento Soil Moisture Accounting (SAC-SMA) models, this study evaluates particle filter based data assimilation algorithms to predict seasonal snow water equivalent (SWE) and runoff within a small watershed in the Lake Tahoe Basin located in California. A non-linear regression model is then used that predicts suspended sediment concentrations (SSC) based on runoff rate and time of year. Runoff volumes and SSC are finally combined to provide an estimate of the average annual sediment load from the watershed with estimates of prediction uncertainty.

For the period of simulation (10/1/1991 to 10/1/1996), the mean annual suspended sediment load is estimated to be 753 tonnes/yr with a 95% confidence interval about the mean of 626 to 956 tonnes/yr. The 95% prediction interval for any given year is estimated to range from approximately 86 to 2,940 tonnes/yr.

Dedication

With love and gratitude this thesis is dedicated to my beautiful wife, Koree Dianne Karr Leisenring, for her continuous support and patience throughout my extended academic career. I would also like to thank my parents, Robert and Randy Leisenring, for always believing in me and providing me a solid foundation in life, which has helped give me the self-confidence and determination to pursue a higher education and a professional engineering career.

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This work would not have been possible without the guidance and direction of Dr. Hamid Moradkhani who, through his extensive novel research, has provided a basis for applying data assimilation techniques within a hydrologic modeling framework. I would also like to acknowledge Dr. Roy Koch who was my first professor at PSU. His graduate class on applied environmental data analysis changed my entire perspective on the power and potential of statistical science to help understand complex environmental phenomena.

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Chapter 1 Introduction

Lake Tahoe is designated as an Outstanding National Resource Water (ONRW) due to its extraordinary clarity. However, since 1968 scientists have measured a decline in water clarity (as measured by Secchi disk depth) at the rate of approximately one foot per year. Consequently, the lake has been listed as “water quality limited” by the California Lahontan Regional Water Quality Control Board (Lahontan) and by the Nevada Department of Environmental Protection (NDEP). Under Section 303(d) of the federal Clean Water Act (CWA), a water body that is determined to be water quality limited is placed on the 303(d) list of impaired water bodies and a Total Maximum Daily Load (TMDL) for the pollutant causing the impairment must be developed. A TMDL is a calculation of the maximum amount of a pollutant that a waterbody can receive and still safely meet water quality standards. The CWA defines water quality standards to include (1) beneficial uses, (2) water quality criteria/objectives, and (3) application of an antidegradation objective (Lahontan RWQCB & Nevada DEP, 2010). The primary beneficial use relevant to lake clarity is non-contact water recreation and because Lake Tahoe is designated as an ONRW, the USEPA does not allow any degradation under the CWA’s antidegradation policy.

Once a TMDL has been established, an implementation plan must be developed to reduce the causes of impairment. The primary cause of impairment has been identified as increased loadings of fine particulates ($<16\text{ }\mu\text{m}$) (Lahontan RWQCB, 2010). Watershed development and anthropogenic activities are believed to be major contributors of fine particulates. As such, a TMDL for fine particulates has been established and various

stakeholders in the Tahoe Basin have been conducting monitoring, source assessments, and developing various models to assist with water quality management decisions in the Basin (Lahontan RWQCB & Nevada DEP, 2010).

Accurate estimation of pollutant loads is highly dependent on the prediction skill of surface runoff simulation. Much of the surface runoff in the Tahoe Basin is driven by snow accumulation and melt – two processes that are inherently difficult to predict particularly in the mountainous western United States where snowpack properties can be highly heterogeneous (Harr, 1981). Also, the steep topography, highly variable precipitation, and diverse geology make it difficult to estimate surface and groundwater interactions. Even with reasonably accurate estimates of surface runoff, pollutant load prediction is confounded by the complex physics and inherent randomness of pollutant mobilization and transport. Sequential hydrologic data assimilation within a stochastic modeling framework has the potential to significantly improve sediment load predictions. Moreover, the use of lumped, conceptual and empirical models that require a relatively small number of inputs may still be used to provide reasonably accurate results while providing estimates of prediction uncertainty.

1.1 Goals and Objectives

The goal of this research is to demonstrate how data assimilation using particle filtering combined with Monte Carlo methods can be used to estimate annual suspended sediment flux for the Ward Creek drainage basin in Lake Tahoe, California (Figure 1). The primary objectives are to:

1. Use the National Weather Service SNOW-17 model to estimate rainfall plus snowmelt and use Sacramento Soil Moisture Accounting (SAC-SMA) model to estimate stream flow.
2. Assimilate daily snow water equivalent (SWE) into SNOW-17 and daily stream flow data into SAC-SMA using the particle filter to produce an ensemble of stream flow estimates thereby providing estimates of prediction uncertainty.
3. Develop an empirical suspended sediment concentration (SSC) model that can be sequentially combined with uncertain stream flow estimates within a Monte Carlo modeling framework to predict average daily SSC concentrations with uncertainty bounds.
4. Compute the average annual SSC load with uncertainty bounds (prediction interval) to Lake Tahoe from the Ward Creek watershed using the ensemble estimates of flow and concentration.

With a hydraulic residence time of about 700 years (Goldman, 1988), long-term sediment loadings are more of a concern in Lake Tahoe than episodic mass loading events. As such, this study focuses on predicting average annual suspended sediment loads rather than individual mass loading events. While this study only evaluates a relatively short time period (5 years), the methods applied could be extended to the entire period of available data to provide more accurate estimates of annual sediment loads.

Figure 1. Ward Creek Watershed in Lake Tahoe, California.

1.2 Document Organization

Chapter 2 provides a brief background of watershed modeling and simulation of hydrologic processes including snow accumulation and melt, soil moisture accounting and runoff estimation, and stream flow routing. An overview of pollutant load estimation is then provided followed by a summary of sequential data assimilation using the Ensemble Kalman Filter (EnKF) and the particle filter (PF). Chapter 3 describes the study area and methods used in this research including the selected modeling approach, the data assimilation techniques utilized, and the performance evaluation methods. Chapter 4 summarizes and discusses the results. Chapter 5 provides conclusions and recommendations for future study.

Chapter 2 Background and Literature

2.1 Watershed Modeling

Watershed modeling can be broadly defined as a systematic approach for using spatial and temporal data, conceptual models, and statistical techniques to evaluate the hydrology, hydraulics, and/or water quality of a topographically-defined resource management area. The hydrologic processes often considered include interception, snow accumulation and melt, evapotranspiration, infiltration, runoff, interflow, and groundwater recharge. Hydrologic models are systems-based models that are designed through parameterization of one or more of these processes with respect to system inputs (e.g., precipitation, temperature, etc.), states (e.g., snow water equivalent, soil moisture storage, etc.), and outputs (e.g., stream flow). Figure 2 is a simple schematic of a system-based model.

Figure 2. Schematic Representation of a Systems-Based Model.

A hydrologic model may be classified into several general categories depending on how it accounts for the random, spatial, and temporal variation in hydrologic phenomena (Chow et al., 1988). For example, models may be classified as physically-based or empirical, deterministic or stochastic, lumped or distributed, and event-based or continuous. Most of these classifications represent a spectrum of model types as it is typically not practical to account for all sources of spatial and temporal variation as well

as observational and structural errors within a single watershed model. The choice of model depends on the modeling objectives and constraints (e.g., resources/expertise), and the availability of spatial and temporal data needed for model forcing, parameterization, and calibration. A brief summary of the different classes of models is provided below.

2.1.1 Physically-Based versus Empirical

Physically-based models are typically derived from the fundamental equations of mass, energy, and momentum conservation. Empirical models, such as regression models, are derived from statistical analyses and summary of data where the model structure and parameters may have little, if any, physical meaning. However, all physically-based models include some empirical equations or parameters because of the necessary generalization of some of the more complex processes, such as infiltration, interflow, evapotranspiration, or sediment transport.

2.1.2 Deterministic versus Stochastic

Deterministic models do not consider random variation – the same inputs and initial states will always result in the same output. Stochastic models, on the other hand, incorporate an element of uncertainty into at least one or more of the inputs, parameters, states, or outputs. This uncertainty may be used to reflect not only random inputs and processes, but also the error associated with data collection and the approximations of reality incorporated into the model structure (Chow et al., 1988). Thus, stochastic models are well suited for representing inherently random hydrologic systems.

2.1.3 Lumped versus Distributed

Lumped models use spatially-averaged parameters and variables such that computations are independent of the space dimensions. Distributed models divide the spatial domain into discrete points or elements such that model parameters and state variables are functions of the space dimensions. Lumped models can become pseudo-distributed by using the concept of hydrologic response units (HRUs) where each HRU represents a lumped system. For example, HRUs may be contiguous areas that are defined topographically or they may be lumped, non-contiguous areas defined by land use type.

2.1.4 Event-Based versus Continuous

Event-based models are designed to predict the response from a single storm event (e.g., design storm) while continuous models are designed to predict the response from many events. Continuous models rely on a longer time series of representative meteorological data that may extend over many storm events or years to produce a time series output for runoff, which can then be analyzed statistically to determine peak flow-frequencies or flow-duration probabilities, for example. In contrast, event-based methods normally require defining a set of antecedent conditions for the watershed and selecting a particular design storm event (e.g., 10-year, 24-hour) prior to simulation. The advantage of event-based simulation is that input requirements are normally simpler. The advantage of continuous simulation is that variations in runoff due to changing antecedent soil moisture or other watershed conditions can be directly accounted for and the output can be used to look at variability in runoff patterns with season, dry and wet years, differences in storm patterns, and other hydrologic variables.

2.2 Simulation of Hydrologic Processes

Hydrologic simulation generally includes translating precipitation into stream flow by accounting for the various processes that affect the timing and magnitude of discharges. In cold climates where the snow pack represents a significant component of the water balance, snow accumulation and ablation must first be accounted for. The melting of the snow pack plus rainfall contributes to soil moisture and groundwater storage, which in turn, contribute to direct runoff, shallow interflow, and stream channel base flow. A brief summary of these hydrologic processes and some of the common methods used to simulate them are provided below.

2.2.1 Snow Accumulation and Ablation

Several processes occur during the accumulation and ablation of a snowpack. Accumulation involves the buildup of freshly fallen snow followed by snowpack evolution or metamorphism. Metamorphism includes four primary mechanisms, each causing densification of the snowpack: 1) gravitational settling, 2) destructive metamorphism, 3) constructive metamorphism, and 4) melt metamorphism (Dingman, 2002). Gravitational settling involves the initial densification of the snowpack due to the weight of overlying snow. During destructive metamorphism individual snowflakes begin to become spherical as the small crystalline snowflake projections evaporate (sublimate). During constructive metamorphism, the condensation of water vapor within the snowpack forms ice bridges between snow grains causing additional increases in size. Melt metamorphism occurs when liquid water is formed at the surface and then refreezes at depth. The initial presence of liquid water in the snowpack causes small snow grains to melt and large snow grains to grow. As melting progresses the snowpack eventually

reaches its maximum liquid water holding capacity and snowmelt discharge begins. At this time the snowpack is typically vertically heterogeneous with several layers of different densities due to multiple snowfall and freeze/thaw events (Dingman, 2002).

The two primary approaches for simulating these snow processes include energy balance methods and temperature index methods. Energy balance methods explicitly simulate heat exchange processes and therefore require several inputs including incoming and reflected solar radiation, incoming longwave radiation, temperature, precipitation, relative humidity, and wind (Franz, 2006). Temperature index methods use air temperature as the sole index of heat exchange at the surface of the snow cover based on empirical relationships between air temperature and melt rates. Conditions where temperature may be a poor index of heat exchange include 1) warm temperatures with high humidity and high wind, 2) clear sky periods with aged snow surface and cold temperatures, and 3) calm wind periods with above normal air temperatures (Anderson, 1976). While energy balance methods can perform better under these conditions and typically require less calibration because many of their parameters are measureable quantities, calibrated temperature index models have been found to perform equally well for simulating snow water equivalent (SWE) for large river basins (Anderson, 1973; Franz, 2006). Due to the difficulty in accurately estimating the spatial variation in the input variables for an energy balance model, the temperature index method is still used by the National Weather Service River Forecast System (NWSRFS) (Anderson, 2006).

2.2.2 Runoff and Stream Flow

With estimates of rainfall and snowmelt quantities, storm event runoff and stream base flows may be estimated using a number of different empirical and physically-based models. Example empirical models for estimating runoff include the rational method and unit hydrograph models (Chow et al., 1988), curve number models (Lyon et al., 2004), regression equations (Driver & Tasker, 1990), and artificial neural networks (Govindaraju & Rao, 2000). Physically-based hydrologic models use precipitation data as the primary model input and predict storm water runoff rates based on parameters that are related to physical processes and states in the modeled watershed. These types of models utilize water balance concepts and can be generally classified as either infiltration excess overland flow or saturation excess overland flow. Infiltration excess overland flow, also known as Hortonian overland flow (Horton, 1933), occurs when the rainfall intensity exceeds the infiltration capacity of the land surface. This process occurs in urban and arid areas and during times of intense rainfall. Infiltration capacity is typically estimated using an infiltration model, such as Horton's equation, Philips equation, or the Green-Ampt equation (Chahinian et al., 2004; Chow et al., 1988).

Saturation excess overland flow occurs when the soil becomes saturated such that any additional precipitation causes runoff. This process is most applicable in humid areas and at locations where the depth to bedrock or the water table is shallow, such as near surface water bodies. This type of runoff is the main mechanism behind variable source area hydrology (Beven & Kirkby, 1979). The concept of variable source areas (VSAs) is based on the assumption that only saturated pervious and impervious areas contribute to direct runoff. With this approach the amount of water required before runoff from

pervious areas begins is equal to the porosity per unit area of the shallowest soils in the watershed, which are the zones fringing streams and creeks. Modeling the spatial extent and temporal fluctuation of a VSA is based on a water balance approach and depends on a number of hydrological and morphological factors like rainfall intensity, soil texture, water table depth, and topographic attributes of the terrain (Hernandez et al., 2003).

2.2.3 Flow Routing

Flow routing refers to a computational procedure of estimating the timing and magnitude of flows at a downgradient location based on a time series of flows at an upgradient location. In hydrologic flow routing (also called lumped flow routing) the flow is assumed to be only a function of time whereas in hydraulic flow routing (also called distributed flow routing) the flow is assumed to be a function of both time and space (Chow et al., 1988).

Hydrologic routing is simply based on the continuity equation applied to the hydrologic system:

$$\frac{dS}{dt} = Q_{in}(t) - Q_{out}(t) \quad (1)$$

Where $\frac{dS}{dt}$ is the change in storage, $Q_{in}(t)$ is the inflow at time t , and $Q_{out}(t)$ is the outflow at time t . This equation is solved using a storage function for the system. Hydrologic flow routing procedures differ in the specification of this storage function and the common methods include linear reservoir routing, level pool routing, and the Muskingum method. Linear reservoir routing assumes storage is a linear function of the outflow whereas level pool routing assumes that the storage is a nonlinear function of the

outflow (Chow et al., 1988). The Muskingum method assumes the storage is a linear function of both the inflow and outflow where the storage volume is represented as a combination of prism and wedge storages. The Nash cascade is a special case of linear reservoir routing where the storage in the system is represented as a series of identical reservoirs.

Hydraulic flow routing procedures utilize Newton's second law (momentum) in addition to continuity, which allow for flow rate and water level to both vary in space and time. The Saint-Venant equations are the set of partial differential equations that describe one-dimensional open channel flow. The numerical solution of the full Saint-Venant equations is referred to as dynamic wave routing. The dynamic wave model should be used when backwater effects are not negligible such as for mildly sloping and tidally or reservoir influenced river reaches (Chow et al., 1988).

During steady and uniform flow conditions, the inertial and pressure forces within the momentum equation can be neglected and the Saint-Venant equations reduce to the kinematic wave model. The kinematic wave model may be solved analytically or numerically. However, numerical schemes can better handle variations in channel properties and initial and boundary conditions (Chow et al., 1988). The Muskingum-Cunge method is a numerical solution of the kinematic wave model that is based on the Muskingum method where the model parameters are computed based on channel characteristics and the flow rate in the channel (Barry & Bajracharya, 1995; Cunge, 1969; Merkel, 2002). The analytical solution of the Muskingum-Cunge formula is:

$$Q_{out_t} = C1 \cdot Q_{in_t} + C2 \cdot Q_{in_{t-1}} + C3 \cdot Q_{out_{t-1}} + q_t \cdot dx \quad (2)$$

Where $Qout_t$ is the channel reach outflow at time t , Qin_t is channel reach inflow at time t , $Qout_{t-1}$ is channel reach outflow at the previous time step, and q_t is lateral inflow per unit length of channel dx at time t . C1, C2, and C3 are the Muskingum constants which are computed as follows:

$$C1 = \frac{(dt-2KX)}{C0} \quad (3)$$

$$C2 = \frac{(dt+2KX)}{C0} \quad (4)$$

$$C3 = \frac{(2K(1-X)-dt)}{C0} \quad (5)$$

$$C0 = 2K(1 - X) + dt \quad (6)$$

$$K = \frac{dx}{ck} \quad (7)$$

$$X = 0.5 \left(1 - \frac{Qin_t}{bb \cdot ck \cdot So \cdot dx} \right) \quad (8)$$

$$ck = \frac{5}{3} \left(\frac{y^{2/3} \cdot \sqrt{So}}{nn} \right) \quad (9)$$

$$y = \left(\frac{nn \cdot Qin_t}{bb \sqrt{So}} \right)^{3/5} \quad (10)$$

Where K is the travel time parameter (s), X is the unitless storage parameter, dt is the time step, ck is the flood wave celerity (m/s), So is longitudinal slope of the channel, y is the flow depth (m), nn is Manning's roughness coefficient, and bb is the bottom width (m).

2.3 Pollutant Load Estimation

The mass loading of any aqueous phase constituent is defined as:

$$M_T = \int_{t=0}^{t=T} M(t)dt = \int_{t=0}^{t=T} Q(t)C(t)dt \quad (11)$$

where M_T is the total mass load over a time period T , $M(t)$ is instantaneous mass flux at time t , $Q(t)$ is flow rate at time t , and $C(t)$ is constituent concentration at time t . The mass flux into Lake Tahoe from any particular tributary watershed is a function of the

various hydrologic pathways including overland flow, interflow, and in-stream routing. While interflow may be a major pathway for dissolved constituents such as nitrate, for suspended sediment, the mass flux associated with interflow is likely a minor transport mechanism as compared to the other two processes. Hence, the focus of this review is on non-point pollutant transport from surface sources.

2.3.1 Loads from Land Surfaces

Overland flow transport processes are responsible for the initial mobilization and entrainment of pollutants from land surfaces. Due to the complexity of these processes, empirical approaches are often employed (Fitzpatrick et al., 2001). Some common approaches include land use based methods, build-up / wash-off methods, and empirical soil loss equation methods.

Land Use Based Methods

Land use based methods utilize characteristic runoff concentrations for each land use within a watershed. This type of estimate usually does not account for variation in storm water pollutant concentrations with flow, but instead uses an average concentration obtained from monitoring runoff from relatively homogeneous land use areas. The advantage of this simple approach is that concentration estimates will always be within the range of observed values. Example loading models that utilize land use based concentrations include PLOAD (CH2M HILL, 2001) and the Source Loading and Management Model (SLAMM) (Voorhees & Pitt, 1997). The Pollutant Load Reduction Model (PLRM) is a Tahoe-specific modeling tool based on the U.S. EPA Storm Water

Management Model (SWMM) that also utilizes characteristic runoff concentrations (Northwest Hydraulic Consultants et al., 2010).

Build-Up / Wash-Off

Build-up / wash-off methods predict pollutant accumulation during dry periods and wash off during storm events. Pollutant accumulation within a watershed may be based upon parameters such as type of land use, season, atmospheric deposition rates, and watershed management practices. Wash-off is typically a function of parameters such as rainfall intensity, watershed slopes, and sediment particle sizes to estimate the mobility (i.e. entrainment and transport) and subsequent wash-off of pollutants. The Storm Water Management Model (SWMM) (Huber & Dickinson, 1988) and the Hydrologic Simulation Program – Fortran (HSPF) (Bicknell et al., 1997) are two commonly used watershed models that allow the use of build-up and wash-off functions for estimating pollutant loads from land areas.

Soil Erosion and Sediment Transport Methods

Soil erosion and transport methods are often based on the widely used Universal Soil Loss Equation (USLE) (Wischmeier & Smith, 1965) and variations thereof such as Modified Universal Soil Loss Equation [MUSLE] (Williams & Berndt, 1977) and the Revised Universal Soil Loss Equation [RUSLE] (Renard et al., 1997). USLE based models predict the erosion of topsoil based on soil erosion potential, rainfall or runoff erosion energy, runoff path length, slopes, cover, and erosion control practices. This type of method is most often applied to agricultural lands, construction sites, and other open space areas where sediment loss is of primary concern. USLE methods are typically not

used for urban areas where other pollutant entrainment processes are prevalent and impervious areas and landscaping prevent or reduce erosion. Example sediment load estimation models that utilize variations of USLE include RUSLE2 (USDA, 2011) and the Soil Water and Assessment Tool (SWAT), which is a watershed model that uses the SCS curve number method for estimating flow rates and the Modified Universal Soil Loss Equation (MUSLE) for estimating sediment loads (USDA & Texas A&M University, 2011).

2.3.2 In-Stream Transport Processes

If the water quality constituent is conservative (i.e., non-reactive) and the transport is assumed to be approximately steady over the period of analysis, then the mass flux from the watershed can be assumed to equal the overland flow mass flux. However, if the constituent is non-conservative or if the in-stream transport processes are unsteady during the period of analysis then mass flux at the watershed outlet will differ from the mass flux from overland flow processes. In-stream transport processes are often represented in receiving water quality models (Chapra, 1997; Fitzpatrick et al., 2001) and are fundamentally described by the mass balance equation:

$$\frac{\partial}{\partial t}VC = M_{in} - M_{out} \pm R \quad (12)$$

where V is the stream reach storage volume, C is the mass concentration, M_{in} is the mass flux into the reach, M_{out} is mass flux out of the reach, R is the mass increase or decrease due to reaction kinetics. Reaction kinetics describes the rate at which a substance reacts as a function of reactant concentrations (Chapra, 1997). For a single reactant and a constant volume, the general reaction formula is:

$$R = V \frac{dC}{dt} = -VkC^n \quad (13)$$

where k is reaction rate constant and n is the reaction order. A zero-order reaction ($n=0$) integrates to a linear decay function and a first-order reaction ($n=1$) integrates to an exponential decay function. While higher order reaction terms are possible (e.g., Borsuk & Stow 2000) the zero and first order reaction formulas are most often used in practice (Chapra, 1997).

For a conservative substance, such as suspended sediment, settling and resuspension may be described as a first order reaction where k is equal to the apparent settling velocity of the suspended particles divided by the average depth.

2.3.3 Regression Models

Regression models are empirical models that relate various explanatory variables to pollutant concentrations or loads. Regression models are often used when data and/or resources are unavailable to develop separate estimates of overland flow transport and in-stream transport (or it is deemed unnecessary based on the study objectives). Common explanatory variables for estimating suspended sediment concentration include watershed characteristics, stream flow, or field measured water quality parameters such as turbidity and specific conductivity (Christensen et al., 2000). Dana et al. (2004) evaluated the performance of various multivariate linear regression models for predicting suspended sediment loads in the Truckee River in California. The researchers found that the natural logarithm of suspended sediment concentration (SSC) could be best related to 2-hour lagged flow, turbidity, temperature, and specific conductivity. The U.S. Geological Survey's SPARROW model utilizes nonlinear regression models that predict the

logarithm of pollutant concentrations from various compound flow terms and time trend terms (Schwarz et al., 2006). Example compound flow terms are logarithms of flow and squared logarithms of flow and example time trend terms include the year fraction and various transformations thereof. Thus, a seven-parameter model could be formulated as:

$$\log C(t) = a + b \cdot \log Q + c \cdot (\log Q)^2 + d \cdot T_y + e \cdot T_y^2 + f \cdot \sin(2\pi T_y) + g \cdot \cos(2\pi T_y) \quad (14)$$

Where $\log C(t)$ is the logarithm of constituent concentration at time t , $\log Q$ is the logarithm of flow rate, T_y is the decimal fraction of the year, and a, b, c, d, e, f , and g are constants. The benefit of this equation is that it only requires the flow and the time of year to predict the concentration. After a reasonable regression model is developed for predicting pollutant concentration, daily load estimates can be computed as the product of concentration times flow.

2.4 Hydrologic Data Assimilation

Data assimilation techniques can be considered as either sequential or variational (Liang, 2004). In sequential data assimilation the states of the system as predicted by the model are updated whenever new observations are available. This approach assumes that observations can only influence future estimates. In variational data assimilation the states of the system at all points in time over the assimilation period are adjusted based on available observations. This approach assumes that observations can influence both future and past estimates. Within the hydrologic modeling community, sequential data assimilation appears to have gained more traction than variational data assimilation, as

discussed below, but that may change in the near future as these computationally intensive modeling techniques are more widely adopted.

Two types of sequential data assimilation methods were found in the hydrologic modeling literature: direct insertion and recursive Bayesian estimation. Direct insertion simply involves replacing model estimates with observations. While rules are sometimes applied to recognize uncertain measurement periods (e.g., Rodell & Houser, 2006), direct insertion methods assume that observations are perfect and model predictions should be ignored (Sun et al., 2004). Since measurements are known to be imperfect, this method can introduce substantial bias into the model estimates and is generally not recommended (Slater & Clark, 2006).

Recursive Bayesian estimation is a probabilistic approach for evolving state variables of a dynamic system using the transitional probability of the model process, $p(x_t|x_{1:t-1})$, and the conditional probability of the model estimates given observations, $p(x_t|y_{1:t-1})$. If the dynamic system can be assumed to follow a Markov process, the probability of predicting the true current state only depends on the probability of the previous state (i.e., the current state is conditionally independent of all earlier states) and the transitional probability can be reduced to: $p(x_t|x_{1:t-1}) = p(x_t|x_{t-1})$.

The states of the dynamic model are:

$$x_t^{i-} = f(x_{t-1}^{i+}, u_t^i, \theta) + \omega_t^i \quad (15)$$

where x_t^i is a vector of states for ensemble member i at time t , $f(\cdot)$ is a nonlinear dynamic operator, u_t^i is the forcing data, θ is a vector of parameters, and ω_t^i is the

system random noise. The negative and positive signs represent before and after the update of the state ensemble, respectively.

The predicted model states are passed through the observation operator, $h(\cdot)$, to predict the observation, $\tilde{y}_t^i$, with observational random noise, φ_t^i .

$$\tilde{y}_t^i = h(x_t^{i-}) + \varphi_t^i \quad (16)$$

Applying Bayes' Law with the Chapman-Kolmogorov equation, the posterior probability density can be computed as (Moradkhani, Hsu, Gupta, & Sorooshian, 2005b):

$$p(x_t|y_{1:t}) = \frac{p(y_t - \tilde{y}_t) \int p(x_t - x_{t-1}) p(x_t|y_{1:t-1}) dx_{t-1}}{\int p(y_t - \tilde{y}_t) [\int p(x_t - x_{t-1}) p(x_t|y_{1:t-1}) dx_{t-1}] dx_t} \quad (17)$$

Since Equation 17 usually cannot be solved analytically due to the high dimensionality and non-linearity of hydrologic models, discrete approximations of the posterior probability density using sequential Monte Carlo methods are typically used (Andreadis & Lettenmaier, 2006; Clark et al., 2008; Durand et al., 2008; Moradkhani et al., 2005a; Slater & Clark, 2006). The most commonly used methods in hydrology are Kalman filter based Monte Carlo simulation approaches, such as the ensemble Kalman filter (EnKF) and the square root Kalman filter (EnSRF). However, particle filter-based approaches are also gaining more attention within the hydrological modeling community (Moradkhani et al., 2005b; Weerts & El Serafy, 2006; van Delft et al., 2009).

2.4.1 Kalman Filter

Kalman filtering is a class of sequential data assimilation methods that estimate the state of a dynamic system using various data sources and their estimated uncertainties (Liang,

2004). The standard Kalman filter is used on linear dynamic systems and provides an optimal solution for the given parameter set and assumed uncertainties. The extended Kalman filter (EKF) can be used for nonlinear dynamic systems, but can only provide near-optimal estimates due to the use of a linear approximation (Dong et al., 2007). The ensemble Kalman filter (EnKF) utilizes statistical distributions to represent the model error and observation uncertainties to produce an ensemble of assimilations by randomly sampling from each distribution (Liang, 2004). The advantage of the EnKF over the extended Kalman filter is that it does not require the development of the linearized state-space formulation of the hydrological model (Clark et al., 2008).

The ensemble Kalman filter can be used to update the model states vector, x , at each time step for each ensemble member using the Kalman update equation:

$$x_t^{i+} = x_t^{i-} + K_t(y_t - \tilde{y}_t^i) \quad (18)$$

Where, x_t^{i+} is the posterior (i.e., updated) state vector at time t , x_t^{i-} is the prior state forecast vector, y_t is the observations vector, $\tilde{y}_t$ is the predicted observations vector defined in (16), K_t is the Kalman gain:

$$K_t = P_t^- H^T (H P_t^- H^T + R_t)^{-1} = C_{xy} (C_{yy} + R_t)^{-1} \quad (19)$$

Where $P_t^- H^T = C_{xy}$ is the covariance of the states with the predicted measurements, $H P_t^- H^T = C_{yy}$ is the variance of the predicted observations, and R_t is the variance of the observational error in (16). H is the linearized observation operator ($H = \frac{\partial h}{\partial x}$) to translate from model space to measurement space. The model states error covariance, P_t^- , can be computed directly from the ensemble deviations (e_t^-):

$$P_t^- = \frac{1}{N_{ens}} e_t^- e_t^{-T} \quad (20)$$

$$e_t^{i-} = x_t^{i-} - \frac{1}{N_{ens}} \sum_{i=1}^{N_{ens}} x_t^{i-} \quad (21)$$

Burgers et al. (1998) suggest that the variance of the ensemble will be too low and filter divergence may occur unless the observations are perturbed. Whitaker and Hamill (2002) disagree with this approach and actually state that perturbing the observations results in suboptimal filter behavior, particularly when a small ensemble is used. Consequently, they introduced the square root ensemble Kalman filter (EnSRF) that does not require perturbed observations and maintains the correct error covariance (Whitaker & Hamill, 2002). The EnSRF uses the traditional Kalman gain for updating the ensemble mean but uses a “reduced” Kalman gain to update deviations from the ensemble mean. While some researchers are utilizing the EnSRF formulation of the ensemble Kalman filters (e.g., Clark et al., 2008; Clark et al., 2006; Sun et al., 2008), others are still relying on the Burgers et al. (1998) method of perturbing observations without noting any problems with filter divergence (e.g., Andreadis & Lettenmaier, 2006; Durand & Margulis, 2008; Moradkhani et al., 2005a; Zhou et al., 2006).

2.4.2 Particle Filter

The Kalman filter is only exact when the dynamical model, $f(\cdot)$, and the measurement model, $h(\cdot)$, are both linear and the model and measurement errors, ω_t and φ_t , are both Gaussian. Since hydrologic models are typically nonlinear and the system dynamics do not preserve the shape of the prior probability density function, the posterior probability density is often non-Gaussian and cannot be adequately characterized by the first two moments. Particle filtering is an alternative to the Kalman-based filtering methods that does not require model linearity or Gaussian error distributions. The primary difference

between the particle filter and the ensemble Kalman filter is that instead of replacing the individual ensemble members, or “particles”, using an update equation only the weights associated with those particles are updated. The posterior density in Equation 17 above is then approximated as a discrete function (Arulampalam et al., 2002):

$$p(x_t|y_{1:t}) \approx \sum_{i=1}^{N_p} w_t^{i+} \delta(x_t - x_t^i) \quad (22)$$

Where N_p is the number of particles, w_t^{i+} is the posterior (updated) normalized weight of the i th particle, and δ is the Dirac delta function. As described in Moradkhani et al. (2005b), the normalized weights are approximated as:

$$w_t^{i+} = \frac{w_t^{i-} \cdot p(y_t|x_t^i)}{\sum_{i=1}^{N_p} w_t^{i-} \cdot p(y_t|x_t^i)} \quad (23)$$

Where $p(y_t|x_t^i)$ is the posterior likelihood, which may be approximated either parametrically or non-parametrically. Assuming Gaussian model error, the likelihood may be approximated as:

$$p(y_t|x_t^i) = \frac{1}{\sqrt{2\pi\hat{R}_t}} \cdot \exp\left[-\frac{(\varepsilon_{y_t}^i)^2}{2\hat{R}_t}\right] \quad (24)$$

where $\varepsilon_{y_t}^i = (y_t - \hat{y}_t^i)$ is the residual of particle i and $\hat{R}_t$ is the variance of the particles residual.

A non-parametric alternative to Equation 24 is an estimate of the likelihood based on the Kaplan-Meier estimate of the cumulative distribution function (CDF), also known as the empirical CDF (Kaplan & Meier, 1958). The empirical CDF, $F(\boldsymbol{\phi})$, is defined as the proportion of $\boldsymbol{\phi}$ less than or equal to ϕ_j . By letting $\boldsymbol{\phi}$ equal the square of the posterior

differences between observations and predictions, $\left(\varepsilon_{y_t}^i\right)^2$, the empirical likelihood function can be computed as the compliment of $F(\boldsymbol{\Phi})$:

$$p(y_t|x_t^i) = 1 - F(\boldsymbol{\Phi}_t) = 1 - \frac{1}{N_p} \cdot \sum_{i=1}^{N_p} I(\Phi_t^i \leq \boldsymbol{\Phi}_t) \quad (25)$$

where $I(\cdot)$ is a conditional identity function that is either 1 when the conditional statement is true or 0 when the conditional statement is false.

The advantages of estimating the likelihood using empirical probabilities is that the procedure is free of parametric distributional assumptions and values are constrained to the range of available posterior differences between the observations and predicted observations. Since the highest probabilities are assigned to the smallest absolute differences, the potential for sample degeneracy or the phenomena where all but one particle have negligible weight is reduced. The disadvantage of using empirical probabilities is that even larger sample sizes are needed to accurately predict densities near the tails of the distribution.

With all particle filters, resampling may be used to avoid the problem of degeneracy where all but one particle will have negligible weight. However, resampling can lead to sample impoverishment, or lack of particle diversity, especially when the process noise is low. Sampling Importance Resampling (SIR) is a resampling scheme that only retains particles with cumulative importance densities that are greater than a corresponding uniform cumulative density (Arulampalam et al., 2002). The SIR algorithm is as follows (Moradkhani et al., 2005b):

1. Estimate the cumulative probability vector using the normalized weights:

$$F(w) = \sum_{w_t^i \leq w_t} w_t^i$$

where $\mathbf{w}_t$ is a $1:N_p$ vector of normalized particle weights at time t such that $F(\mathbf{w}_t^{N_p}) = 1$.

2. Select particles with importance weights greater than uniform by comparing the particle weights CDF to the uniform CDF:

Set $i = 1$ and $j = 1$

While $j \leq N_p$

While $i \leq N_p$

If $F(\mathbf{w}_t^i) > \frac{j}{N_p}$, then $x_t^i = x_t^j$ and $j = j + 1$

Else $i = i + 1$

Loop i

Loop j

3. Set weights of all resampled particles equal to $1/N_p$

While the SIR scheme is simple to implement, it can be inefficient, sensitive to outliers, and can quickly suffer from sample impoverishment due to the resampling at every time step (Arulampalam et al., 2002; Pitt & Shephard, 1999).

As an alternative to the SIR method, Leisenring & Moradkhani (2011) describe weighted random resampling (WRR) where the probability of a particle being selected during resampling is equal to its normalized weight. An index variable is used to track particles during resampling as follows:

1. Estimate the cumulative probability vector using the normalized weights:

$$F(w) = \sum_{w_t^i \leq w_t} w_t^i$$

where $\mathbf{w}_t$ is a $1:N_p$ vector of normalized particle weights at time t such that $F(\mathbf{w}_t^{N_p}) = 1$.

4. Randomly sample N_p values from the uniform distribution between 0 and 1.

$$\mathbf{z} \sim U(0,1)$$

5. For each z_j value, identify its bin index, B_j , on F such that:

$$B_j = i \text{ when } F(w_t^{i-1}) \leq z_j \leq F(w_t^i) \text{ and } F(w_t^0) = 0$$

6. Resample particles as follows: $x_t^{i+} = x_t^{B_j}$

7. Set weights of all resampled particles equal to $1/N_p$

Note that similar to the SIR algorithm as discussed above, the WRR algorithm can also result in the same value being resampled more than once. However, instead of the particles with low importance weights being *selectively* discarded by comparing empirical probabilities to the uniform distribution, the particles with low importance weights are *randomly* discarded. Therefore, this latter approach retains greater particle diversity due to the random sampling, especially when the process noise is small.

In general, resampling should be avoided if the importance weights are not significantly different from uniform probabilities. Pham (2001) proposed using the entropy difference of the two probability distributions as a measure of the deviation from uniform distribution as follows:

$$Ep_t = \log(N_p) + \sum_{i=1}^{N_p} w_t^i \log(w_t^i) \quad (26)$$

where Ep_t is the entropy difference, N_p is the number of particles, and w_t^i is the importance weight of particle i . Resampling is computed only when Ep_t is greater than a prescribed threshold, Ep_{thresh} .

Chapter 3 Methods

3.1 Study Area

The Ward Creek watershed is located in Placer County, California on the northwest side of the Lake Tahoe Basin in the central Sierra Nevada mountain range near Tahoe City. Precipitation is highly variable and strongly orographic with mean annual depths ranging from less than 800 mm near the lakeshore at approximately 6,200 feet above mean sea level to over 2,000 mm at the basin rim, which is at over 8,000 foot elevation (Thodal, 1997). Approximately two-thirds of the annual precipitation in the Tahoe basin occurs as snow fall with the majority occurring between November and April (Desert Research Institute, 2011). Consequently, snowmelt and rain-on-snow events account for the majority of the observed stream flow. While evapotranspiration is limited during periods of snow cover, Leydecker and Melack (2000) estimated that approximately 36% of the average annual precipitation in watersheds of central and southern Sierra Nevada Mountains is lost to evaporation. Model predictions indicate that during periods of snow cover the evaporation is reduced to 10% of the evaporation loss that would occur without snow cover. Thus, snow cover is a critical component of the overall water balance.

A brief summary of the geophysical characteristics of the Ward Creek watershed is provided below.

3.1.1 Land Use and Soils

The Ward Creek watershed is primarily undeveloped with over 90% of the area consisting of coniferous and vegetated lands. The majority of the urban development occurs near the lakeshore and near the Alpine Meadows Ski Area located in the upper

part of the watershed. Classified primarily as a sandy loam texture class, the soils in the watershed consist of highly permeable decomposed granite and glacial sediments within the Ward Creek Valley with a large fraction of exposed bedrock at the higher elevations (Thodal, 1997).

3.1.2 USGS Monitoring Stations and Drainage Areas

The USGS maintains three stream flow stations within the Ward Creek watershed. The drainage areas for each gauge are delineated in Figure 3. At the most downstream end, the watershed is estimated to be 25.1 km² (9.7 sq. mi.) at USGS 10336676 (Ward Creek at Highway 89). The next upstream gauge (USGS 10336675) captures approximately 23 km² (8.8 sq. mi.), or 90% of the watershed area. The most upstream gauge captures approximately 12 km² (4.7 sq. mi.), or approximately 50% of the watershed area. Approximately 66% of the average annual precipitation is estimated to be discharged to the furthest downstream gauge (Thodal, 1997). The remaining precipitation is lost to evapotranspiration, deep percolation, or shallow interflow that bypasses the gauge.

Figure 3. Major Drainage Areas and Monitoring Stations of Ward Creek Watershed.

3.2 Modeling Approach

In the Tahoe Basin, a large fraction of total precipitation occurs as snow and drainage areas are highly pervious. Consequently, stream flow is highly sensitive to snow melt and antecedent soil moisture conditions; both of which are inherently difficult to predict. For this research, SNOW-17 is used to predict snow melt and SAC-SMA is used to predict base flow and direct runoff. The Muskingum-Cunge hydrologic routing procedure is then used to estimate stream flow at each of the USGS monitoring stations. Suspended sediment concentration (SSC) is finally computed using a multivariate

regression model. A 6-hour time step is used in the above computations and then, once a day when snow water equivalent (SWE) and daily average flow are available, sequential data assimilation via the particle filter is used to improve the rain plus snowmelt (RM) and stream flow predictions. The details of the modeling approach including the implementation of the particle filter follows.

3.2.1 SNOW-17 Model

Originally developed by Eric Anderson of the National Weather Service, SNOW-17 is a lumped parameter, temperature-index model that simulates the physical processes of a vertical column of snow (Anderson, 1973). Temperature and precipitation are the only forcing data needed to run the model. The main processes simulated by the model include:

- Form of precipitation (snow or rain),
- Accumulation of snow cover (temperature, liquid/frozen water content, density, etc.),
- Energy exchange at the snow-air interface,
- Internal state of snow cover,
- Transmission of liquid water through the snowpack, and
- Heat transfer at the soil-air interface

There are fourteen state variables and twelve model parameters including an eleven point areal depletion curve in the SNOW-17 model. The primary state variables include water and energy balance components of the snow pack, areal extent of snow cover, and snow depth and density. Figure 4 illustrates the conceptual model processes of SNOW-17.

Figure 4. SNOW-17 Model Flowchart (Anderson, 2006).

As illustrated by the figure, the model first determines whether precipitation is in the form of rain or snow by comparing the air temperature to the PXTEMP threshold parameter. The model then estimates the depth and density of new snow based on the quantity of precipitation and the air temperature. The quantity is based on the fraction of precipitation falling as snowfall and the assumed precipitation gage catch deficiency (SCF). If the air temperature is less than 0°C then the snowpack heat deficit, or negative heat storage (NEGHS), is reduced proportionally to the quantity of new snow. When the NEGHS is positive, no melt is simulated by the model. When NEGHS is negative, surface melt is simulated using an energy balance equation for rain-on-snow periods and a melt factor equation for non-rain periods.

Snowpack Heat Transfer

In addition to heat transfer associated with new snow, the model estimates snowpack heat transfer (expressed in terms of SWE¹) during three discrete conditions: rain-on-snow, non-rain melt, and no surface melt. During rain-on-snow, (1) the energy balance equation is used by assuming solar radiation is negligible because of overcast conditions, (2) incoming longwave radiation is equal to black body radiation at the air temperature, and (3) relative humidity is 90% (Anderson, 2006). Since wind speed is not a model input, a wind parameter (UADJ) is used to indicate the average wind speed function (millimeters/millibars) during rain-on-snow events.

During non-rain melt periods, SNOW-17 uses a simple melt factor approach where the quantity of melt is linearly proportional to the difference in air temperature and the base temperature parameter (MBASE), which is the temperature above when melt typically occurs. Recognizing that melt rates have seasonal variation due to solar irradiance, SNOW-17 uses a sinusoidal curve to vary the melt factor ($\text{mm}^\circ\text{C}^{-1}\text{hr}^{-1}$) between two user-supplied parameters (MFMIN and MFMAX), where MFMIN occurs on December 21st and MFMAX occurs on June 21st.

When the heat deficit of the snowpack is positive (i.e., pack temp $<0^\circ\text{C}$), no melt is simulated by the model. Changes to the heat deficit are estimated to be proportional to the thermal gradient in the upper layers of the snowpack. The gradient is computed as the difference between the air temperature and the antecedent temperature index (ATI), which is a time-weighted index of past air temperatures. The proportionality constant is

¹ Amount of heat required to melt or freeze 1 mm of ice or water at 0°C

called the negative melt factor, which varies according to the computed melt factor and the ratio of a user-supplied maximum negative melt factor (NMF) and MFMAX.

Internal Snowpack State Accounting

SNOW-17 tracks solid and liquid water content, total depth, and density of the snowpack. A snowpack is considered “ripe” when any additional melt or rainwater input will cause outflow (Anderson, 2006). The liquid water capacity, W_q , is computed as a function of the percent liquid water holding capacity parameter (PLWHC) and the ice portion of the total water equivalent. The liquid water at the snow surface, Q_w , is computed as the total melt plus rain. Excess liquid water is then calculated as Q_w plus W_q minus the heat deficit. Excess liquid water is then transmitted through the snowpack using a lag equation that varies according to the ratio of excess water to the total water equivalent of the snowpack.

At the end of the computational time step (6 hr), the average density of the snowpack is calculated using an empirical equation that estimates the changes in density due to compaction, destructive metamorphism, and liquid water melt metamorphism (Anderson, 2006). Depth is calculated as one-tenth the ratio of the ice water equivalent to the density. Snow covered area (SCA) is calculated using a user defined areal depletion curve (ADC) that relates fraction of snow cover to the mean aerial water equivalent fraction.

With the simulation of the above processes SNOW-17 predicts SWE, SCA, and rain plus melt (RM) at each time step. SWE and RM are expressed in millimeters and SCA is expressed as fraction of area covered (ranges from 0 to 1). Areal estimates may be

obtained by multiplying by a drainage area and these results may be used as input to hydrologic models that simulate surface runoff processes (infiltration, evapotranspiration, overland flow, etc.). In fact, the NWSRFS couples SNOW-17 with the Sacramento Soil Moisture Accounting Model (SAC-SMA) along with routing algorithms and reservoir regulation schemes to predict river flows (Laurine et al., 1996). Similarly, Khakbaz et al. (2008) implemented a semi-distributed version of SNOW-17 coupled with SAC-SMA to predict runoff response for several sub-basins of the East Fork Carson River watershed.

3.2.2 Sacramento Soil Moisture Accounting (SAC-SMA) Model

The SAC-SMA model is a lumped parameter, physically-based conceptual model that, as mentioned above, is currently a part of the National Weather Service River Forecast System (NWSRFS). It uses water balance accounting to track soil moisture during and between precipitation (or snow melt) events, which allows for both storm flows and base flows to be predicted continuously.

Storage Components

SAC-SMA conceptually represents the soil mantle as two distinct layers: an upper zone and a lower zone. The upper zone includes two storages, namely, the upper zone tension water storage and the upper zone free water storage. Tension water is the water absorbed to soil particles that can only be removed by evaporation or evapotranspiration. Free water is water within pore spaces that is not bound to soil particles and can be removed by vertical percolation to the lower zone or lateral percolation as interflow.

Similar to the upper zone, the lower zone storage also includes tension water and free water storage components, but the free water storage is divided into primary free water storage that drains slowly and a supplementary free water storage that drains more quickly. The different percolation rates from these two storages allow for a variety of baseflow recession curves to be estimated (Burnash & Ferral, 1996). Figure 5 illustrates the five soil moisture storage reservoirs of SAC-SMA.

Figure 5. Soil Moisture Storage Reservoirs in SAC-SMA.

Moisture Accounting and Flux Computations

SAC-SMA tracks the moisture in the upper and lower zone storages as a result of inflow and outflow fluxes. During rainfall and snow melt the upper zone tension water storage is completely filled before moisture becomes available to the other storages. After the upper zone tension water content reaches capacity, excess moisture immediately becomes available to the upper zone free water storage (i.e., instantaneous transfer of excess). If the upper zone free water storage is already saturated, the excess becomes surface runoff.

Water contained in the upper zone free water storage is lost to interflow and vertical percolation. Interflow is related linearly to the upper zone free water content:

$$IF_t = UZK \cdot UZFWC_t \quad (27)$$

where IF_t = interflow flux from upper zone free water storage at time t (mm/day), UZK = upper zone free water storage depletion coefficient (day^{-1}), $UZFWC_t$ = the upper zone free water content (mm).

Vertical percolation from the upper zone is computed based on the upper zone free water content and the lower zone percolation demand:

$$LZPD_t = PBASE \left[1 + ZPERC \left(\frac{\sum LZDEF_t}{\sum LZCAP} \right)^{REXP} \right] \quad (28)$$

where $LZPD_t$ = lower zone percolation demand at time t (mm/day), $PBASE$ = the percolation rate to the primary and supplemental free water storages when these storages are saturated (mm/day), $ZPERC$ = the ratio of maximum and minimum percolation rates (unitless), $\sum LZDEF_t$ = sum of lower zone deficiencies at time t (mm), $\sum LZCAP$ = sum of lower zone capacities (mm), $REXP$ = percolation curve shape parameter (unitless).

The sum of the lower zone deficiencies and capacities are computed as:

$$\sum LZDEF_t = (LZTWM - LZTWC_t) + (LZFPM - LZFPC_t) + (LZFSM - LZFSC_t)$$

$$\sum LZCAP = LZTWM + LZFPM + LZFSM$$

where $LZTWM$ = lower zone tension water capacity (mm), $LZTWC_t$ = lower zone tension water content at time t (mm), $LZFPM$ = lower zone primary free water capacity (mm), $LZFPC_t$ = lower zone primary free water content at time t (mm), $LZFSM$ = lower

zone supplemental free water capacity (mm), $LZFSC_t$ = lower zone supplemental free water content at time t (mm).

The actual percolation rate is then necessarily controlled by the supply of water available for percolation in the upper zone:

$$LZP_t = LZPD_t \left[\frac{UZFWC_t}{UZFWM} \right] \quad (29)$$

where LZP_t = lower zone percolation rate (mm/day), $LZPD_t$ = lower zone percolation demand (mm/day), $UZFWC_t$ = upper zone free water content (mm), $UZFWM$ = upper zone free water capacity (mm).

Lower zone free water supplies baseflow and groundwater recharge. Baseflow is computed as the sum of the fluxes from the primary and secondary free water storages:

$$BF_t = LZPK \cdot LZFPC_t + LZSK \cdot LZFSC_t \quad (30)$$

where BF_t = total baseflow flux from lower zone free water storage at time t (mm/day), $LZPK$ = lower zone free water primary storage depletion coefficient (day^{-1}), $LZFPC_t$ = the lower zone free water primary storage content (mm), $LZSK$ = lower zone free water supplemental storage depletion coefficient (day^{-1}), $LZFSC_t$ = the lower zone free water supplemental storage content (mm).

The total baseflow is divided into a channel component and a non-channel component where the non-channel component represents the loss to groundwater recharge or more generally subsurface discharge that bypasses the flow gauge.

$$BFCC_t = BF_t \left(\frac{1}{1+SIDE} \right) \quad (31)$$

where $BFCC_t$ = baseflow channel component at time t (mm/day), BF_t = total baseflow flux from lower zone free water storage at time t (mm/day), $SIDE$ = ratio of deep percolation to channel baseflow.

Figure 6 illustrates the five SAC-SMA storage components and how flux of water into and out of these components are related to stream flow (Burnash & Ferral, 1996).

Figure 1. Conceptual Illustration of the Sacramento Soil Moisture Accounting Model (Burnash & Ferral, 1996).

3.3 Snow Data Assimilation

SWE observations were sequentially assimilated into the SNOW-17 model using the particle filter with recognition that the differences between the true SWE and the predicted SWE are due to assumed errors in temperature and precipitation measurements as well as uncertainties in the underlying model structure. Based on previous research (Leisenring & Moradkhani, 2011), the particle filter was found to produce more robust estimates of SWE than the ensemble Kalman Filter. Also, it was found that the particle filter variant that used an empirical likelihood function (Equation 25) with weighted random resampling (EPF-WRR) provided comparable estimates as the more traditional Gaussian likelihood function with sampling important resampling (NPF-SIR) when ensemble sizes were large (i.e., $N \geq 1000$). Leveraging off of the previous research the EPF-WRR particle filter was used for SWE data assimilation in this study.

3.3.1 Forcing Data and SWE Observations

Daily snow water equivalent (SWE) data and hourly precipitation and temperature data were obtained for the National Resources Conservation Service (NRCS) Ward Creek #3 SNOTEL station for 1992-1996. To match the 6-hour time step used in the SNOW-17 model, the precipitation values were aggregated to 6 hour totals and hourly temperature values were aggregated to 6 hour averages. The model predicted SWE and RM every 6 hours and the end of the day (4 time steps), daily SWE observations were assimilated into the model using the particle filter as described below.

3.3.2 Ensemble Perturbation

To account for forcing data measurement error, temperature data were randomly varied using a fixed uniform error distribution assumption similar to Clark et al. (2008):

$$\tilde{T}_t^i = T_t - \gamma_T(1 - 2w_T^i) \quad w_T^i \sim U(0,1) \quad (32)$$

where $\tilde{T}_t^i$ is the temperature for particle i at time t , T_t is the measured temperature at time t , γ_T is a fixed temperature variance ($^{\circ}\text{C}$), and w_T^i is uniform random noise between zero and one for particle i .

Owing to multiplicative nature of precipitation and that zero or positive values are possible, the precipitation data were log-normally varied with a heteroscedastic assumption (i.e., the variance estimate was scaled by the magnitude) as follows:

$$\mu_{\ln P} = \ln \left[\frac{P_t^2}{\sqrt{P_t^2 + (\gamma_P \cdot P_t)^2}} \right] \quad (33)$$

$$\sigma_{\ln P} = \sqrt{\ln \left[\frac{(\gamma_P \cdot P_t)^2}{P_t^2} + 1 \right]} \quad (34)$$

$$\tilde{P}_t^i = \exp \left(\mu_{\ln P} + w_P^i \frac{\sigma_{\ln P}^2}{2} \right) \quad w_P^i \sim N(0,1) \quad (35)$$

where $\tilde{P}_t^i$ is the precipitation for particle i at time t , P_t is the measured precipitation at time t , γ_P is a variance scaling factor for precipitation data, and w_P^i is Gaussian white noise with mean of zero and standard deviation of one for particle i .

To account for model error and observation error, SWE predictions and SWE measurements were also perturbed using a lognormal error assumption since SWE is also bounded by zero. SWE predictions were perturbed to account for the model error and SWE observations were perturbed to account for measurement error.

The variance scaling factors, or hyper-parameters, used for all simulations are listed in Table 1.

Table 1. Hyper-parameters for Error Variance Estimation for SWE Assimilation.

Hyper-parameter	Value	Definition
γ_P	0.15	precipitation variance scale factor
γ_T	4.00	fixed temperature variance ($^{\circ}\text{C}$)
γ_S	0.10	SWE simulation variance scale factor
γ_M	0.10	SWE measurement variance scale factor

3.3.3 Rain Plus Melt Prediction

The primary output of SNOW-17 is the prediction of rain plus melt. The assimilation of SWE data into SNOW17 will improves estimates of SWE, which in turn, improves the estimates of rain plus melt.

Five years (1992-1996) of 6-hour precipitation and temperature data (N_{data}) and a fixed ensemble size (N_{ens}) of 1000 particles was used in the assimilation of SWE observations. When implementing the particle filter, the empirical likelihood cumulative distribution function defined in Equation 25 was used along with weighted random resampling with replacement (WRR) described in Section 2.4.2.

The flow chart presented in Figure 7 summarizes the general steps of the data assimilation procedure. Note that the “t” subscript is intentionally omitted for simplicity. Resampling is only conducted when the entropy factor, Ep_t , in Equation 26 above is greater than $Ep_{thresh} = 0.05$.

Figure 7. Summary of SWE Data Assimilation Procedures.

3.3.4 Parameter Estimation

Traditional calibration methods typically rely on flow measurements at a single downstream location. As the number of catchments increase, the inverse problem of estimating parameters for each catchment based on measurements at a single location becomes more ill-posed. With dual state-parameter estimation, model parameters are not

specified for every catchment within a watershed. Instead, a parameter range is selected and the parameters values are allowed to evolve within this range by resampling based on the updated particle weights. However because the parameters do not vary with the dynamic model as the states do, the parameter ensemble may suffer from sample impoverishment during resampling. To avoid sample impoverishment and allow adequate parameter evolution, the parameters can be slightly perturbed by adding small Gaussian random noise as described by Moradkhani et al. (2005b). For this study, parameters were perturbed at every time step as follows:

$$\theta_t = \theta_t + \varepsilon_t \cdot \gamma_\theta \cdot \bar{\theta}_t \quad \varepsilon_t \sim N(0,1) \quad (36)$$

where θ_t is ensemble matrix of parameters at time t , ε_t is random Gaussian noise with mean of zero and standard deviation of one, γ_θ is the parameter variance scaling factor, and $\bar{\theta}_t$ is a vector of parameter means. After perturbation, kernel smoothing was applied to avoid over-dispersion of the parameter ensemble (Liu & West, 2001; Moradkhani et al., 2005a).

The parameters of SNOW-17 are only used during specific conditions. For example, the precipitation gauge deficiency factor, SCF, is only used during precipitation events and the melt factors, MFMIN and MFMAX, are only used during non-rain melt. If a parameter is updated during a time when it is not actively being used then the parameter ensemble may diverge from the “truth”. Therefore, prior to modifying parameters during data assimilation, specific conditional requirements should be met to reduce the possibility of sample divergence. Table 2 summarizes

the expected range of parameter values and the conditional requirements stipulated prior to parameter updating.

Table 2. Expected SNOW17 Parameter Ranges and Conditional Requirements for Parameter Modification.

Parameter	Expected Range	Conditional Requirement for Modification
MFMIN	0.05-0.6	Only update when non-rain melt is likely occurring: $P_t < 0$ and $SWE_t > 0$ and $T_t > MBASE = 0$
MFMAX	0.5-2.0	
SCF	0.8-2.0	Only during precipitation: $P_t > 0$
UADJ	0.02-0.20	Only when rain is likely falling on snow: $P_t > 0$ and $SWE_t > 0$ and $T_t > 0.5$
PXTEMP	0.5-4.0	Only when snow is likely falling: $P_t > 0$ and $T_t < 4.0$

The initial ensemble of parameter values were generated by uniformly sampling from the expected range of values shown in Table 2. Instead of using simple random sampling (SRS) where each parameter value is independently selected from a univariate uniform distribution, Latin Hypercube Sampling (LHS) was utilized to simultaneously select parameter values from the multivariate uniform distribution. The LHS results in a more uniform ensemble over all possible parameter permutations thereby reducing the sampling variance (McKay et al., 1979).

3.4 Flow Data Assimilation

The assimilation of flow data into SAC-SMA was conducted very similarly to the procedure used for assimilating SWE data into SNOW-17. In fact, the only difference with Figure 7 is the forcing data and the perturbation of the forcing data as described below.

3.4.1 Mean Areal Rain plus Melt

The rain plus melt estimates produced by SNOW17 described above are point estimates based on precipitation, temperature, and SWE at the Ward Creek SNOTEL station. Therefore, a procedure was developed to spatially distribute the rain plus melt and produce an estimate of the mean areal rain plus melt.

As part of the development of the Tahoe Pollutant Load Reduction Model (PLRM) (Northwest Hydraulic Consultants et al., 2010), methods for spatially adjusting precipitation and temperature data were developed. Hourly SNOTEL precipitation data were linearly adjusted based on the spatial distribution of monthly normal grids produced by the Parameter-elevation Regressions on Independent Slopes Model (PRISM) developed at Oregon State University (Oregon State University, 2011). Temperature adjustments were based on the Tahoe-specific lapse rate as developed by Tetra Tech (2007) for use in the Tahoe TMDL Watershed Model. Using the above methods, Northwest Hydraulic Consultants et al. (2010) distributed both precipitation and temperature hourly time series data to 800-meter grid cells, which are depicted as the analysis grid shown in Figure 8. As shown in the figure, the grid cell containing the Ward Creek SNOTEL station is Grid No. 29. Using this cell as the *base grid cell*, the following procedure was implemented to distribute the ensemble of rain plus melt (RM) estimates produced by SNOW17 with the particle filter.

1. Compute RM estimates for all grid cells in the watershed using SNOW17 without data assimilation.
2. Develop an ensemble of RM estimates at all other grid cell locations within the watershed using a proportional relationship:

$$\widetilde{RM}_{s,t}^i = \widetilde{RM}_{b,t}^i \frac{RM_{s,t}}{RM_{b,t}} \quad (37)$$

where $\widetilde{RM}_{s,t}^i$ is the adjusted rain plus melt for particle i at grid cell s at time step t , $\widetilde{RM}_{b,t}^i$ is the rain plus melt after SWE data assimilation for particle i at base grid cell at t , $RM_{s,t}$ is the rain plus melt estimate for particle i at grid cell s at time step t without data assimilation, and $RM_{b,t}$ is the unadjusted rain plus melt for particle i at base grid cell at time step t without data assimilation.

3. Compute the mean areal rain plus melt for the watershed:

$$\overline{RM}_t^i = \frac{1}{A_w} \sum_{s=1}^N A_s \cdot \widetilde{RM}_{s,t}^i \quad (38)$$

where $\overline{RM}_t^i$ is the mean areal rain plus melt for the watershed for particle i at time step t and A_w, A_s are the total drainage area and grid area, respectively.

Figure 8. Analysis Grid Used for Estimating Mean Areal Rain Plus Melt.

3.4.2 Ensemble Perturbation

Similar to the perturbation of the forcing data of SNOW17, SAC-SMA's forcing data were also perturbed. SAC-SMA is driven by RM and evapotranspiration estimates. While the ensemble of RM already reflects uncertainties associated with rainfall, temperature, and SNOW17 model structure errors, there are also errors associated with the computation of the mean areal RM. Therefore, each member of the mean areal RM ensemble was perturbed using a lognormal distribution with a heteroscedastic assumption:

$$\mu_{\ln RM} = \ln \left[\frac{RM_t^2}{\sqrt{RM_t^2 + (\gamma_{RM} \cdot RM_t)^2}} \right] \quad (39)$$

$$\sigma_{\ln RM} = \sqrt{\ln \left[\frac{(\gamma_{RM} \cdot RM_t)^2}{RM_t^2} + 1 \right]} \quad (40)$$

$$\widetilde{RM}_t^i = \exp \left(\mu_{\ln RM} + w_{RM}^i \frac{\sigma_{\ln RM}^2}{2} \right) \quad w_{RM}^i \sim N(0,1) \quad (41)$$

where $\widetilde{RM}_t^i$ is the mean areal rain plus melt for particle i at time t , RM_t is the SNOW17 predicted mean areal RM at time t , γ_{RM} is a variance scaling factor for RM, and w_{RM}^i is Gaussian white noise with mean of zero and standard deviation of one for particle i .

In addition to RM, SAC-SMA also requires potential evapotranspiration (PET) as an input. For this study, hourly PET data developed for the Ward Creek SNOTEL station as part of the Tahoe TMDL Watershed Model development (Tetra Tech, Inc., 2007) were used. These PET estimates are based on the Penman pan-evaporation method (Penman, 1948). The hourly PET data were aggregated to 6-hour totals to match the model time step and these values were lognormally perturbed to account for uncertainties associated with their derivation.

Finally, to account for model and measurement error, both the flow predictions and flow measurements were lognormally perturbed prior to assimilation.

3.4.3 State and Parameter Estimation

Similar to the procedure for estimating RM by assimilating SWE measurements into SNOW17, downstream flow was estimated by assimilating upstream flow measurements in SAC-SMA with the Muskingum-Cunge routing procedure. A plot of the flow measurements for the three USGS flow stations is provided Figure 9. As shown in the

figure, there does not appear to be a large lag in the flow rates at downstream stations as compared to upstream stations. Indeed, most of the peaks occur on the same day indicating that the time of concentration for this watershed is less than one day. However, since the SAC-SMA model time step is 6 hours, there may still be some benefit of utilizing the Muskingum-Cunge routing procedure and it provides a mechanism for sequentially routing the posterior ensemble of flows downstream.

Figure 10 summarizes the framework for sequentially applying data assimilation with SAC-SMA and the Muskingum-Cunge. As shown, SAC-SMA is used to predict a runoff ensemble, which is applied as lateral inflow to the Muskingum-Cunge model. The output from Muskingum-Cunge from an upstream reach is used as an input for the downstream reach. Because data assimilation occurs after routing flows, there is a feedback loop (dashed line) to the SAC-SMA model for updating states and parameters. Due to the strong correlation of flows between flow gauges as indicated in Figure 9, the sequential application of the particle filter allows for continued prediction skill improvement as flows are propagated downstream.

Figure 9. Daily Flow for Water Years 1992-1996 at the Ward Creek USGS Stations.

Figure 10. Framework for Sequential Data Assimilation with SAC-SMA for the Three Ward Creek Subwatersheds and Muskingum-Cunge River Routing of Flow Between USGS Stations.

SAC-SMA parameters were updated in the same manner as the SNOW17 parameters. However, no conditional requirements were used to determine whether parameters should be updated. Instead, the parameters were initialized using Latin Hypercube Sampling (LHS) across their entire expected ranges. As compared to standard uniform random sampling, LHS results in a more uniform ensemble over all possible parameter value combinations, thereby reducing the sampling variance (McKay et al., 1979). To ensure adequate “spin-up” of model parameters, LHS was used at every time step until the predicted flow reached a magnitude of the 20th percentile observed flow rate, which occurs in the spring of the first year of simulation. After this point the parameters were perturbed using Gaussian random noise at every time step according to Equation 37. The expected ranges for the SAC-SMA parameters used in this study are shown in Table 3. These ranges are based on the values reported in Zhang et al. (2011), except the range of percent impervious cover (PCTIM) was estimated based on the 30-meter, 2006 impervious surface cover from the National Land Cover Database (Fry et al., 2011).

Table 4 summarizes the Muskingum-Cunge river routing parameter ranges used in the data assimilation. As shown in the table only the bottom width and Manning’s roughness were allowed to evolve with the model. The average channel slope was estimated from available topographic information and the channel length increment was selected such that it would never be significantly smaller than the distance traveled by the flood wave during a single time step (Merkel, 2002). The variance scaling factor used to perturb forcing data, parameters, simulated flow, and observed flow are summarized in Table 5.

Table 3. Expected SAC-SMA Parameter Ranges Used for Parameter Modification.

Parameter	Expected Range	Description
UZW	10 – 300	Upper zone tension water capacity (mm)
UZFWM	5 – 150	Upper zone free water capacity (mm)
UZK	0.1 – 0.75	Interflow depletion rate (day^{-1})
PCTIM	0.005 – 0.05	Impervious cover fraction
ADIMP	0 – 0.2	Max additional impervious cover fraction due to saturation
ZPERC	5 – 350	Ratio of max and min percolation rates
REXP	1 – 5	Percolation curve shape parameter
LZW	10 – 500	Lower zone tension water capacity (mm)
LZFWM	5 – 400	Lower zone secondary free water capacity (mm)
LZFPM	10 – 1000	Lower zone primary free water capacity (mm)
LZSK	0.01 – 0.35	Depletion rate lower zone secondary (day^{-1})
LZPK	0.001 – 0.05	Depletion rate lower zone primary (day^{-1})
PREE	0 – 0.8	Percolation fraction that goes directly to lower zone

Table 4. Expected Muskingum-Cunge Parameter Ranges Used for Parameter Modification.

Parameter	Expected Range	Description
bb	5 – 50	Bottom width of channel (m)
nn	0.02 – 0.05	Manning's roughness coefficient
So*	0.05	Channel slope (m/m)
dx*	200	Channel increment (m)

* These parameters were kept constant

Table 5. Hyper-Parameters for Error Variance Estimation for Flow Assimilation.

Hyper-parameter	Value	Definition
γ_{RM}	0.15	rain plus melt variance scale factor
γ_{PE}	0.10	potential ET variance scale factor
$\gamma_{\theta 1}$	0.03	initial SAC-SMA parameter variance scale factor
$\gamma_{\theta 2}$	0.005	initial Muskingum-Cunge parameter variance scale factor
γ_Q	0.15	initial flow simulation variance scale factor
γ_M	0.10	flow measurement variance scale factor

3.4.4 Variable Variance Multiplier

A procedure was developed to dynamically adjust the spread of the state and parameter ensembles based on the prediction error of previous time steps. The state and parameter variance multipliers shown in Table 5 ($\gamma_{\theta 1}, \gamma_{\theta 2}, \gamma_Q$) were reduced when the absolute bias

was smaller than the outer 95th percent uncertainty bound and they were increased when the bias was larger than the outer 95th percent uncertainty bound.

The procedure was implemented after data assimilation as follows:

$$\hat{\varepsilon}_t = |\tilde{y}_t - y_t| \quad (42)$$

$$ub_t = \begin{cases} \tilde{y}_t - \tilde{y}_t^{L95} & \text{if } y_t < \tilde{y}_t \\ \tilde{y}_t^{U95} - \tilde{y}_t & \text{if } y_t > \tilde{y}_t \end{cases} \quad (43)$$

$$er_t = \frac{\hat{\varepsilon}_t}{ub_t} \quad (44)$$

where $\hat{\varepsilon}_t$ is the absolute value of the mean model error, y_t is the observation, $\tilde{y}_t$ is the mean predicted observation, ub_t is the partial uncertainty bound, $\tilde{y}_t^{L95}$ is the lower 95th percent uncertainty bound of the predicted observation, $\tilde{y}_t^{U95}$ is the upper 95th percent uncertainty bound of the predicted observation, and er_t is the ratio of the model error to the partial uncertainty bound. Figure 11 provides a conceptual illustration of the partial uncertainty bound and absolute value of the mean model error defined in the above equations.

Figure 11. Illustration of Partial Uncertainty Bound and Model Error Used to Compute Variable Variance Multipliers.

A moving average of er_t was then used in subsequent calculations to avoid excessive adjustment of the ensemble spread while still allowing for a relatively quick response when observations fall outside the prediction bound. To avoid over dispersion of the prediction ensemble, its magnitude was constrained to a value of 5 or less (i.e., variance multipliers could only be increased by 5 times their original values). This value was then used to vary the parameter variance scaling factor as follows:

$$\tilde{\gamma}_Q = \bar{er}_t \cdot \gamma_Q \quad (45)$$

$$\tilde{\gamma}_\theta = \bar{er}_t \cdot \gamma_{\theta 1} \quad (46)$$

where $\tilde{\gamma}_Q$ and $\tilde{\gamma}_\theta$ are the updated variance multipliers of the simulated states and model parameters, respectively, and $\bar{er}_t$ is the previous 2 day moving average of er_t .

3.4.5 Bias Correction

Data assimilation procedures typically assume that forecast errors are random variables with a zero mean. Consequently, as the model error increases the variance of the state ensemble must also increase. However, if a model produces a systematic bias due to structural insufficiencies or due to forcing data measurement bias, then precision is being sacrificed in an attempt to maintain prediction accuracy. If the bias can be estimated, the model forecast can be corrected prior to updating with the particle filter. Dee and da Silva (1996) present an approach for on-line forecast bias estimation as part of atmospheric data assimilation using the ensemble Kalman filter. The premise of the approach is that a systematic bias can be detected by computing the time average of the forecast error. This time average, or lagged moving average, can then be used to adjust the state ensemble prior to updating.

Pendergrass and Elmore (2004) evaluated two bias correction methods including lagged average and lagged linear regression to correct ensembles produced by various atmospheric forecast models. With the lagged average bias correction, the lag can be of any length because it is simply the average bias of the previous forecasts. However, with the lagged linear regression, the lag must be at least 2 time steps to fit a linear line and a longer period (≥ 3 time steps) is needed for meaningful least squares analysis. Forecasts corrected with the lagged linear regression method were found to produce less biased ensembles, particularly when the lag period increased. However, they tended to increase the variance more than the lagged average method (Pendergrass & Elmore, 2004).

For this study, the lagged average bias correction method was investigated as described below. Assuming observations are unbiased, the trajectory of the forecast bias can be tracked with a moving average of the model error computed after updating with the particle filter:

$$\varepsilon_t = \bar{x}_t^+ - h^{-1}(y_t) \quad (47)$$

where ε_t is the model error after updating, $\bar{x}_t^+$ is the state ensemble mean after updating, y_t is the unbiased observation, and $h^{-1}(\cdot)$ is the inverse of the observation operator.

If the observation operator cannot be readily inverted, then this procedure may not be feasible. Fortunately for this study the observation operator is a unit scalar because flow is both directly predicted and observed such that $\bar{x}_t^+ = h^{-1}(\bar{y}_t) = \bar{y}_t$ and $h^{-1}(y_t) = y_t + \varphi_t$ where φ_t is the observational random noise. Therefore, the forecast error in Equation 48 is simply $\varepsilon_t = \bar{y}_t - y_t - \varphi_t$ and the time-averaged forecast bias can be written as:

$$b_t = \frac{1}{T} \sum_{k=t-T}^{k=t} (\varepsilon_k) \quad (48)$$

where b_t is the time-averaged bias over previous time period T . Each member of the forecast ensemble is then adjusted with the time-averaged bias of the previous time step:

$$\tilde{x}_t^{i-} = x_t^{i-} - b_{t-1} \quad (49)$$

where $\tilde{x}_t^{i-}$ is the adjusted state forecast vector for particle i , x_t^{i-} is the state forecast vector for particle i , and b_{t-1} is the time-averaged bias of the previous time step. A two day lag period was utilized because review of the historical stream flow hydrograph indicates that longer lag periods would often miss the more episodic peak flow events. A shorter lag period (i.e., 1 day) would over-fit the observations.

3.4.6 Stochastic Load Estimation

To estimate suspended sediment concentration (SSC), a multivariate regression model was developed based on the approach of Schwarz et al. (2006) as discussed in Section 2.3.3. With this approach the predictor variables include logarithms of flow and various time trend terms. SSC measurements were obtained for the middle flow gauge (10336675) and the method of least squares was used to predict model parameters. The final best fit regression model is as follows:

$$\log C_t = 0.62 + 0.85 \log Q_t + 0.05 (\log Q_t)^2 + 9.58 T_y - 9.67 T_y^2 - 0.32 \sin(2\pi T_y) + 1.53 \cos(2\pi T_y) + \varepsilon_t \quad \varepsilon_t \sim N(0, 0.85) \quad (50)$$

Where $\log C_t$ is the logarithm of constituent concentration at time t , $\log Q_t$ is the logarithm of flow rate, T_y is the decimal fraction of the year, ε_t is the Gaussian model error with mean of zero and standard deviation equal to the regression model standard error (SE=0.85).

Figure 12 summarizes the results of the regression analysis including the 95% confidence and the 95% prediction intervals about the regression line. The confidence interval provides an indication of how well the average suspended sediment concentration can be estimated and the prediction interval provides an indication of how well individual values can be estimated. As shown in the figure, the coefficient of determination (R^2) is 0.52, indicating the regression model accounts for slightly more than 50% of the variation in logSSC. While the prediction interval is quite wide, the regression is statistically significant with a non-zero slope and intercept.

Figure 14 shows the residuals versus the observed logSSC with a histogram overlain with a Gaussian probability distribution function. Figure 14 is a normal quantile plot with Shapiro-Wilkes normality test results. Both the histogram and quantile plot indicate that the residuals are approximately Gaussian. While a normality test results indicates the residuals may not arise from a Gaussian distribution (i.e., $p < 0.05$), the plots indicate that the only a handful of data points near the tails of the distribution are not well represented. The data set includes zero SSC values, which may be due to undetectable quantities. The presence of non-detects or outliers introduced by random mass loading events may bias the distribution. Based on this assessment the regression equation with the lognormal transformations of flow and SSC is considered accurate enough for the purposes of this study. Future research may provide refinements to the regression equation.

Figure 12. Suspended Sediment Concentration Regression Model Fit Results.

Figure 13. Regression Model Residuals vs. LogSSC Observations.

Figure 14. Normal Probability Plot of Residuals.

Using the regression model, SSC was estimated for each member of the predicted flow ensemble at each daily time step at which flow was predicted. An ensemble of suspended sediment load was then computed from the product of daily average flow and concentration:

$$M_t^i = (86.4)Q_t^i C_t^i \quad (51)$$

where M_t^i is the daily mass flux of suspended sediment (kg/day) for particle i at time step t , Q_t^i is the daily average flow rate (m^3/s), and C_t^i is the associated suspended sediment concentration (mg/L). The constant 86.4 is for unit conversion from $\text{m}^3\text{-mg/L-s}$ to kg/day.

Chapter 4 Results and Discussion

Several performance metrics were used to evaluate the data assimilation methods described above, including the root mean square error (RMSE), percent bias (BIAS), the Nash-Sutcliffe efficiency (NSE), the ranked probability skill score (RPSS), the exceedance ratio (ER), and the normalized root mean square error ratio (NRR). The first three metrics provide indication of the mean prediction performance while the last three metrics provide an indication of the ensemble prediction performance. These metrics are defined and described in Appendix A. The results of assimilating SWE data into SNOW-17 and flow data into SAC-SMA to provide estimates of suspended sediment loads are presented and discussed below.

4.1 Snow Water Equivalent Assimilation

Prior to data assimilation, the five most sensitive parameters of the SNOW-17 model were estimated as to obtain a reasonably good agreement between predicted and observed SWE for the study location. These parameters included: (1) PXTEMP ($^{\circ}\text{C}$) – the dividing temperature between snow and rain; (2) SCF – the precipitation gage catch efficiency; (3) MFMAX – the maximum value of the seasonally varying non-rain melt factor occurring on June 21st; (4) MFMIN – the minimum value of the seasonally varying non-rain melt factor occurring on December 21st; and (5) UADJ (mm/mb/6 hr) – the wind speed function of the energy balance equation used during rain-on-snow periods. The Shuffled Complex Evolution, University of Arizona (SCE-UA) algorithm developed by Duan et al. (1992) was used to automate the estimation of these five parameters. The SCE-UA is a global optimization algorithm that performs a multi-start, controlled random search of the feasible parameter space using the “simplex” local search procedure of Nelder and

Mead (1965). However, instead of each simplex evolving independently the SCE-UA algorithm includes a periodic step where all of the points are shuffled and reassigned to ensure information sharing (Duan et al., 1992). Figure 15 shows the predicted versus observed SWE after model calibration. As indicated in the figure, SNOW-17 does a reasonable job of predicting snow accumulation and ablation even without data assimilation, but is underpredicting the peaks particularly during the two drier years.

Figure 15. SWE Prediction at SNOTEL Station without Data Assimilation.

As described previously in Section 3.3, SWE data were assimilated into SNOW17 using the empirical particle filter with weighted random resampling (EPF-WRR). Table 6 summarizes the performance statistics with and without EPF-WRR data assimilation. Figure 16 includes time series plots of SWE and percent snow covered area (SCA) after data assimilation.

Table 6. SWE Prediction Performance with Data Assimilation using Particle Filter.

	RMSE (mm)	BIAS (%)	NSE	RPSS (%)	ER95 (%)	NRR
w/o DA	123.48	-3.39	0.97	n/a	n/a	n/a
EPF-WRR	23.29	-0.16	1.00	97.41	2.24	0.75

As shown in Table 6, the particle filter (EPF-WRR) significantly improved the SWE predictions as compared to the predictions produced by the calibrated model without data assimilation (w/o DA). The mean ensemble predictions follow the observations closely as indicated by the very low percent bias and Nash-Sutcliffe efficiency of 1.00. Similarly, the prediction ensemble is exceptional with a ranked probability skill score (RPSS) of 97% and an exceedance ratio of 2%. The NRR less than 1 indicates that the ensemble may have slightly too much spread – smaller error variance multipliers (Table 1) could have been used. The primary reason for the superb performance is that the SWE observations occur at the exact location as the precipitation and temperature observations (at the SNOTEL station). With areal averaging (as discussed below) and the assumptions used to spatially distribute RM, the accuracy of hydrologic response is much lower than indicated by these intermediate estimates of SWE.

Figure 17 illustrates the evolution of SNOW17 parameters during data assimilation. As indicated all of the parameters converge to a reasonably narrow range with only minor variation in the average values after the initial year spin up period. Table 7 summarizes the fixed parameter estimates from the SCE-UA global optimization algorithm along with the median parameter estimates from the EPF-WRR for the period of simulation. These latter estimates are the parameter values for which 50% of the instantaneous ensemble means are above and 50% of the instantaneous ensemble means are below. The

evolution of parameter values during data assimilation as compared to the static SCE-UA calibrated values are illustrated in Figure 17. As indicated by the 95% prediction intervals, most of the parameters quickly converge to a relatively narrow range that often contains the original calibrated values. The primary exceptions are PXTEMP, which defines the dividing temperature between snow and rain, and SCF, which is the rain gage catch efficiency factor. Both of these parameters can affect the volume of snowfall and therefore are likely correlated and thus will be sensitive to each other's magnitude.

Table 7. SNOW17 Period of Simulation Median Parameter Estimates.

	PXTEMP	SCF	UADJ	MFMAX	MFMIN
SCE-UA	0.94	1.10	0.11	0.97	0.50
EPF-WRR	1.70	0.97	0.12	1.11	0.20

Figure 16. SWE Data Assimilation using the EPF-WRR Particle Filter. (a) Predicted and Observed SWE. (b) Mean Predict Snow Covered Area (SCA).

Figure 17. Evolution of SNOW-17 Parameters during Data Assimilation (10/1/1991 to 9/30/1996).

Figure 18 compares SNOW-17 RM estimates before and after areal averaging compared to stream flow observations at the upper USGS flow gauge. As shown, several of the RM peaks do not match well with the observed flow peaks. For example, the highest peak in RM occurs during the one of the driest years simulated (Water Year 3: 1994). While this phenomenon is possible, especially if the RM occurs when the soil moisture is low thereby permitting more water to soak into the ground, the lack of close agreement

indicates that the method used to distribute the RM and then compute the mean areal RM described in Section 3.4 could use some improvement.

Figure 18. Rain plus Melt (RM) Prediction Compared to Average Daily Flow. (a) RM Prediction for the SNOTEL station, (b) Areal Average RM for the Watershed (c) Average Daily Flow at USGS Gauge 10336674.

4.2 Flow Data Assimilation

Similar to SWE data assimilation, the empirical likelihood particle filter with weighted random resampling (EPF-WRR) was utilized for flow data assimilation. However, since

flow data are available at three flow gauges, data assimilation was performed sequentially using the Muskingum-Cunge routing procedure beginning with the most upstream flow gauge and ending with the most downstream flow gauge (see Figure 10).

As a baseline for comparison, the SCE-UA global optimization algorithm was used to estimate SAC-SMA parameters given the areal average rain plus melt estimates for the entire Ward Creek watershed shown in Figure 17c. Figure 19 is a comparison plot of observed flows to predictions after calibration, but before data assimilation. As indicated in the figure, the model is under-estimating the rising and receding limbs of seasonal stream flow and misses many of the short-duration peak flow rates.

Figure 19. Flow Prediction without Data Assimilation.

Nine different data assimilation scenarios were investigated based on whether parameters were estimated, whether variable variance multipliers were utilized, whether bias correction was used, and whether the Muskingum-Cunge flow routing procedure was used (see Section 3.4). Table 8 summarizes the nine data assimilation scenarios. Scenario 9 is identical to Scenario 8 except instead of sequentially applying flow data assimilation for the upper, middle, and lower watersheds as illustrated in Figure 10, the entire Ward Creek watershed was modeled as a single lumped drainage area and only the downstream flow data were assimilated into the model.

Table 8. Summary of Flow Data Assimilation Scenarios.

	Scenario No.								
Assimilation Condition	1	2	3	4	5	6	7	8	9
Parameter Estimation		X		X	X	X	X	X	X
Variable Variance Multiplier for States			X	X			X	X	X
Variable Variance Multiplier for Parameters					X	X		X	X
Bias Correction			X			X	X	X	X
Upstream Flow Routing	X	X	X	X	X	X	X	X	

Performance statistics for the model before and after data assimilation are shown in Table 9. Before data assimilation the model has a high negative bias (BIAS = -46%) and low Nash-Sutcliffe Efficiency (NSE = 0.64). Scenario 1, which does not include parameter estimation, variable variance multipliers, or bias correction, shows improved performance in the percent bias, but only a slight increase in NSE. Also, the ensemble performance is not great with an RPSS of only 67% and exceedance ratio of nearly 70%.

Scenario 2, which simply includes the addition of dynamic parameter estimation shows slight improvement with the bias reducing to -18% and the RPSS increasing to 82%.

Scenario 3, which includes bias correction and a variable variance multiplier for model states, but no parameter estimation, shows significant improvement over Scenario 2.

Scenario 4, which includes parameter estimation and a variable variance multiplier on model states, but no bias correction, shows no improvement in any of the performance metrics. In fact, the percent bias is higher than Scenarios 1 and 2 indicating that dynamic parameter estimation with variable variance multiplier on model states is causing the model to more severely under-predict discharge volumes. Scenario 5 with parameter estimation and a variable variance multiplier for parameters, but no bias correction shows improvement over Scenario 4. However, compared Scenario 3, which included bias correction, Scenario 5 only shows improvement in the exceedance ratio (ER95), indicating the ensemble is containing a higher percentage of the observations.

Scenario 6, which includes parameter estimation, a variable variance multiplier of model parameters, and bias correction, shows improvement for all of the ensemble performance metrics, but the RMSE and NSE are slightly lower and the percent bias is slightly higher than they were for Scenario 3. Scenarios 7 and 8 also perform very well. Scenario 7, which includes parameter estimation, a variable variance multiplier for model states, and bias correction, has the lowest RMSE and highest NSE. Scenario 8, which includes all of the methods, has nearly identical values for RPSS, ER95 and NRR as Scenario 7. However, the mean flow predictions as indicated by RMSE, BIAS, and NSE are not quite as good as Scenario 7.

Scenario 9, which is identical to Scenario 8 except for instead of using the distributed flow routing the entire watershed was modeled as a lumped system. The simulation

results indicate that the distributed flow routing using Muskingum-Cunge procedure provides some benefit, but primarily only in the percent bias estimate. For larger watersheds where the time of concentration is much greater than the model time step (6 hours in this study), implementing this procedure is expected to be more beneficial.

All of the scenarios have NRR values greater than 1 indicating that the particle ensembles have too little spread. The NRR may have been reduced by increasing the error variance scale factors (a.k.a. hyperparameters) shown in Table 5. The use of variable variance multipliers for model states and parameters appear to contribute to a slight reduction in the NRR, but not significantly. The model forcing hyperparameters may need to be increased to provide a larger impact on the NRR results, but this would likely increase the RMSE. Future research is needed in estimating optimum values for all of the data assimilation parameters.

Table 9. Performance Statistics for Data Assimilation Scenarios at Downstream Station (Sta676).

Scenario No.	RMSE (cms)	BIAS (%)	NSE	RPSS (%)	ER95 (%)	NRR
w/o DA	0.989	-46.24	0.638	n/a	n/a	n/a
1	0.901	-20.0	0.699	66.9	69.9	1.39
2	0.835	-17.9	0.742	81.3	44.1	1.38
3	0.522	-6.0	0.899	90.8	47.8	1.32
4	0.866	-25.4	0.722	80.9	51.8	1.38
5	0.782	-12.3	0.774	88.6	32.4	1.37
6	0.533	-7.6	0.895	93.7	19.0	1.34
7	0.507	-4.9	0.905	93.2	26.9	1.31
8	0.518	-6.7	0.901	93.2	26.8	1.32
9	0.529	-12.9	0.897	92.7	26.2	1.26

As discussed above, the scenarios with bias correction and parameter estimation (Scenarios 6, 7, and 8) improve flow predictions as compared to the scenario with parameter estimation only (Scenario 2) as well as the scenarios with variable variance multipliers plus parameter estimation (Scenarios 4 and 5). The scenario without parameter estimation, but with variable variance multiplier and bias correction (Scenario 3) also shows promise with comparable performance statistics for all metrics except ER95. Figures 19 through 22 include predicted versus observed flow for Scenarios 2, 3, 6, 7, and 8, respectively. The upper plot in each figure is a time series plot and the lower plot is a cumulative non-exceedance plot.

As shown in Figure 20, Scenario 2 provides significant improvement to flow predictions as compared to the results with no data assimilation (Figure 19). However, the model still tends to over-predict dry years (1992, 1994) and under-predict wet years (1993, 1995, 1996). Also, many of the peak flow rates are either under-predicted or completely missed and the frequency of flows less than about 0.001 cms is much higher than observed.

Scenario 3 (Figure 21) is a significant improvement with reasonable estimates of flow for most of the years of simulation and predictions that approximately match the non-exceedance frequencies for the mid-range to high flow rates. However, the model tends to over-predict the frequency of the lower flow rates.

Significant improvements are shown in Figure 22 and Figure 23 for Scenarios 6 and 7, respectively. Both scenarios include prediction intervals that contain most of the observations and the flow frequencies are better matched as compared to Scenarios 2 and

3 with better peak flow matching during both wet (1993, 1995, 1996) and dry years (1992, 1994).

The plots for Scenario 8 (Figure 24) are virtually the same as for Scenario 7. As shown in the non-exceedance plot, the observations fall within the 95% prediction interval for the entire range of flows except for very low flow rates where the rating curve developed for flow station may not be reliable.

Note that all of the non-exceedance plots show that the model predictions do not match the very low flows observed at the monitoring station. One possible cause of this may be due to inaccurate flow measurements at low stages in the river. The model indicates there may be a long base flow recession after the spring melt ends, but the flow gauge may not be able to accurately measure such low flows. Indeed, very few daily average flows are recorded below 0.01 cfs, while the model estimates that lower flows are possible.

Figure 20. Predicted vs. Observed Flow at Lower Station (Sta676) after Scenario 2 Data Assimilation (i.e., with parameter estimation, but without variable variance multipliers or bias correction). (a) Time series comparison of flows. (b) Cumulative non-exceedance frequency comparison of flows.

Figure 21. Predicted vs. Observed Flow at Lower Station (Sta676) after Scenario 3 Data Assimilation (i.e., no parameter estimation, but with variable variance multipliers on states and bias correction). (a) Time series comparison of flows. (b) Cumulative non-exceedance frequency comparison of flows.

Figure 22. Predicted vs. Observed Flow at Lower Station (Sta676) after Scenario 6 Data Assimilation (i.e., with parameter estimation, a variable variance multiplier on model parameters, and bias correction). (a) Time series comparison of flows. (b) Cumulative non-exceedance frequency comparison of flows.

Figure 23. Predicted vs. Observed Flow at Lower Station (Sta676) after Scenario 7 Data Assimilation (i.e., with parameter estimation, a variable variance multiplier on model states, and bias correction). (a) Time series comparison of flows. (b) Cumulative non-exceedance frequency comparison of flows.

Figure 24. Predicted vs. Observed Flow at Lower Station (Sta676) after Scenario 8 Data Assimilation (i.e., with parameter estimation, variable variance multipliers on both states and parameters, and bias correction). (a) Time series comparison of flows. (b) Cumulative non-exceedance frequency comparison of flows.

As discussed above in Section 3.4, several parameters of SAC-SMA and the Muskingum-Cunge routing routine were allowed to evolve during data assimilation. Recall that routing only applies for the middle and lower reaches because the upper reach has only lateral inflows. For the Muskingum-Cunge routine, the average bottom width (bb) and Manning's roughness coefficient (nn) were considered variable because these parameters are known to change with flow depth (Chow et al., 1988). Figures 24 through 26 are time series plots of the thirteen SAC-SMA parameters and two Muskingum-Cunge parameters that were allowed to evolve for the upper, middle, and lower watersheds, respectively, for the best performing scenario (Scenario 7).

As shown in the figures, the 95% prediction intervals for most of the parameters quickly reduce to a narrow range after the initial startup period. However, some of the parameters tend to maintain wide prediction intervals and vary more rapidly depending on the watershed simulated. As shown in (Figure 25), most of the SAC-SMA parameters for the upper watershed vary within a relatively narrow range, whereas the SAC-SMA parameters for the middle watershed (Figure 26) and lower watershed (Figure 27) show wider prediction intervals. Runoff estimates are inherently more sensitive to parameter perturbation for the upper watershed because there are no other upstream flows – only lateral inflows and Muskingum-Cunge routing is not used. For the middle and lower watersheds, the SAC-SMA parameters can only partially influence the flow rates. The lower watershed is the least sensitive to SAC-SMA parameters as indicated by the wider confidence intervals for nearly all parameters (i.e., the SAC-SMA parameter values have less influence on the model results). However, the Manning's channel roughness used in

the Muskingum-Cunge routine is more sensitive for this lower watershed because this parameter can directly impact the magnitude of flow rates.

As shown in the figures, many of the parameters do not converge towards or hover around the calibrated SCE-UA values for the entire watershed. Part of this non-convergence may be due to different physical properties among the subwatersheds as compared to the entire watershed, along with too short of a simulation. However, the high dimensionality of the model and the strong correlation of some of the parameters also likely contribute to these parameters not evolving towards a narrower range. A much longer period of simulation or multivariate sampling that accounts for the co-variability of the model parameters may be required before parameter convergence begins to occur.

While future research is needed to evaluate the sensitivity of the assumption of independent parameters when applying data assimilation techniques, fixed model parameters are not explicitly required to predict the central tendency and variability of stream flow. In fact, fixed model parameters are only needed if the model is to be applied without data assimilation for periods when flow observations are unavailable. Also, a wider flow prediction interval is produced by accounting for parameter uncertainty (i.e., letting them evolve rather than remain fixed) as evidenced by the lower exceedance ratios (ER95) for the scenarios with parameter estimation as compared to the scenarios without parameter estimation (for example, Scenario 7 versus Scenario 3 in Table 8).

Figure 25. Evolution of Parameters for Upper Watershed (Sta674) for Scenario 7.

Figure 26. Evolution of Parameters for Middle Watershed (Sta675) for Scenario 7.

Figure 27. Evolution of Parameters for Lower Watershed (Sta676) for Scenario 7.

4.3 Load Prediction

Figure 28 is a time series plot of daily average suspended sediment concentrations (SSC) compared to grab sample observations. The percent of the SSC observations that fall within the prediction interval is 82%. While this value is lower than desired, it is important to recognize some of the major sources of uncertainty and variation in the SSC observations. Episodic mass loading events (e.g., landslides, bank erosion, etc.) are completely random occurrences that cannot be predicted accurately in time or space. Also, as discussed in Section 3.4.6, one source of the SSC variation (and the related low R^2 for the regression equation) is that SSC measurements are collected as instantaneous grab samples while the flow predictions are daily averages. Given the stochastic nature of sediment transport, instantaneous grab samples are expected to have much higher variability than daily averages.

Figure 28. Suspended Sediment Concentration Prediction.

The total suspended sediment load for the period of simulation is approximately 3,765 tonnes, or a mean annual load of about 753 tonnes/yr with a 95% confidence interval about the mean of 626 to 956 tonnes/yr. The 95% prediction interval for any given year is estimated to range from approximately 86 to 2,940 tonnes/yr. Boxplots of annual suspended sediment load for each year of simulation are provided in Figure 29. These plots show the wide year-to-year variability of the load estimates from the watershed. The middle line is the median annual load, edges of the boxes are the 25th and 75th percentiles, the whiskers extend to the most extreme data points not considered outliers, and outliers are plotted individually as red crosses. As indicated, there is high variability in the estimated suspended sediment load for every year with the inter-quartile ranges

spanning a half an order of magnitude. However, there are clear differences between the drier years (1992 and 1994) and the wetter years (1993, 1995, and 1996), which indicates that a longer period of simulation may be needed to adequately characterize the true average annual sediment loading for this watershed.

Figure 29. Boxplots of Annual Suspended Sediment Load Predictions for Each Year of Simulation.

The estimate of the mean annual sediment load predicted in this study is lower, but the estimated prediction interval brackets loads estimates computed by others. Based on regression analysis and two different computational methods, Tetra Tech (2007) estimated that the mean annual load for Ward Creek ranged from 1,084 to 2,952 tonnes/year. However, the period of record used to compute the mean annual load

differed and there are some notable differences in the estimation methods and the underlying assumptions. For example, the regression model used by Tetra Tech (2007) is a simple power function with flow as the only explanatory variable. Analysis of residuals (e.g., normality, homoscedasticity, etc.) was not performed to evaluate the appropriateness of the regression function. Also, daily flows were regressed against instantaneous sediment yield, which was computed as the product of instantaneous sediment concentration and the average daily flow for the sample date. The correlation is spurious (at least a portion of it) because the dependent variable (e.g., sediment yield) is computed using the independent variable (e.g. average daily flow). Also, the method assumes that the instantaneous sediment concentration is representative of a daily average concentration, which in many cases is likely a poor assumption. For this study, the flow recorded at the time of the sediment measurement was used to develop the regression equation. The upper bound of the suspended sediment load prediction interval estimated in this study overlaps the lower bound of the range predicted by Tetra Tech (2007) indicating that the estimates are not significantly different when predicting the load for any given year.

Chapter 5 Summary and Conclusions

The SNOW-17 model was successfully coupled with the SAC-SMA model to predict rainfall and snowmelt runoff from the 25 square kilometer Ward Creek drainage basin in Lake Tahoe, California. SNOW-17 is a semi-physically based, temperature index model that predicts snow accumulation and ablation for a vertical column of snow using precipitation and temperature inputs. SAC-SMA is a physically-based watershed model that predicts soil moisture and runoff from rain plus snowmelt inputs. Both models are deterministic, lumped-parameter, continuous simulation models. A summary of methods and results is provided below along with recommendations for future research.

5.1 Summary of Methods

To account for the spatial variability of precipitation and snowmelt, a procedure was developed to distribute RM estimates from SNOW-17 across three major drainage areas of the Ward Creek watershed (referred to herein as the Upper, Middle, Lower watersheds). Precipitation data were distributed using monthly normal precipitation grids produced by the PRISM mapping system (Oregon State University, 2011) and temperature data were distributed based on a Tahoe-specific lapse rate (Tetra Tech, Inc., 2007). Areal average estimates of RM were produced for each watershed and used as inputs to the SAC-SMA model. The Muskingum-Cunge (MC) river routing procedure (Cunge, 1969) was then used to route flows downstream from the upper reach to the lower reach.

To improve snowmelt and stream flow predictions, snow water equivalent (SWE) and stream flow observations were sequentially assimilated into SNOW-17 and SAC-SMA,

respectively, using the particle filter. Particle filtering is a Bayesian-based approach for stochastically evolving model states by weighted resampling from an ensemble of model realizations (i.e., particles). Particle weights are estimated from the posterior likelihood of predicting the observations while assuming that both model states and measurements are uncertain. An importance sampling scheme was utilized in this study based on an empirical likelihood function with weighted random resampling (EPF-WRR) as described in Leisenring and Moradkhani (2011). In addition to utilizing the particle filter to estimate model states, model parameters were allowed to evolve dynamically using the procedure described by Moradkhani et al. (2005a).

The implementation of the particle filter requires *a priori* estimates of errors associated with forcing data, model parameters, model predictions, and observations. Errors are expressed in terms of hyperparameters, which are unitless variance multipliers. A procedure was developed to scale the variance multipliers for model parameters and predictions based on the accuracy of the mean predictions relative to ensemble spread. In addition, an online bias correction algorithm based on the lagged average bias was developed to detect and correct for systematic bias in model forecasts prior to updating with the particle filter.

A nonlinear regression equation was developed to predict suspended sediment concentration (SSC) from flow rate predictions and time of year. While the coefficient of determination (R^2) indicated that the regression model only accounts for about half of the variation in SSC, the model parameters were found to be statistically significant and the prediction residuals were approximately Gaussian. The regression model with the

estimate of the standard error was then used to estimate the suspended sediment load and prediction uncertainty for each member of the predicted flow ensemble for every daily time step at which flow was predicted.

5.2 Summary of Results

Snow water equivalent (SWE) data were sequentially assimilated into SNOW-17 using the dual state-parameter particle filter with empirical likelihood and weighted random resampling. For the period of simulation (water years 1992-1996) estimates of SWE were exceptional with a mean percent bias of less than 1%, a Nash-Sutcliffe efficiency (NSE) of 1.00, a ranked probability skill score (RPSS) of 97%, and an exceedance ratio (ER95) of 2%. However, these results are only intermediate estimates of SWE at the SNOTEL station where both precipitation and temperature measurements were taken. After spatially distributing rain plus melt and assimilating flow data into SAC-SMA with Muskingum-Cunge routing, hydrologic response predictions are less favorable. For example, flow predictions after dual state-parameter estimation at the most downstream USGS gauging station resulted in a percent bias of -18%, a NSE of 0.74, an RPSS of 81%, and an ER95 of 44% (see Scenario 2 in Table 9). Significant improvements to the prediction ensemble were found with the implementation of the variable variance multiplier and bias correction procedures. For example, both Scenarios 7 and 8 in Table 9 show RPSS values of 93% and ER95 values of 27%. In addition, the root mean square errors (RMSE) were lower (0.51 cms compared to 0.84 cms) and Nash-Sutcliffe Efficiencies (NSE) were higher (0.9 compared to 0.74) indicating an overall improvement to the mean model predictions.

An ensemble of suspended sediment concentrations (SSCs) was predicted from the ensemble of flow predictions and the non-linear regression model. The results indicate that about 82% of the SSC observations fell within the 95% prediction interval. Based on the 5 years of simulation, the resulting average annual load to Lake Tahoe from the Ward Creek watershed was estimated to be 753 tonnes/year with any given year predicted to be between 86 to 2,940 tonnes/year.

5.3 Recommendations for Future Research

During the course of this study, several areas of additional research were identified as summarized below.

- Spatially Distributing Rain plus Melt. This study developed a simple procedure for distributing rain plus melt estimates across the Ward Creek watershed, but the robustness of the approach was not fully evaluated. Additional research is needed to assess other methods of distributing rain plus melt. For example, one approach may include developing an approach to first distribute snow water equivalent observations to the spatial grid and then run the particle filter on each grid cell. Another approach could include incorporating SWE observations from the Advanced Microwave Scanning Radiometer – Earth Observing System (AMSR-E). Preprocessed daily (AE_DySno), 5-day (AE_5DSno), and monthly (AE_MoSno) SWE data are provided by the National Snow and Ice Data Center (NSIDC) (http://nsidc.org/data/docs/daac/ae_swe_ease-grids.gd.html).
- Multivariate Analysis. A parameter that evolves, but does not converge to a narrow range indicates that the parameter may be dependent on the model states

(i.e., non-stationary) or is dependent on other parameters that are evolving. If states and/or parameters are dependent (and several are suspected to be), then multivariate sampling using Markov Chain Monte Carlo (MCMC) or alternative method may improve estimates of posterior densities. Alternative methods may include holding some parameters fixed while allowing others to vary and then alternating. For example, the parameters that primarily affect volume could be allowed to vary while holding the parameters that affect timing fixed and then vice versa.

- State-Parameter Correlation. Utilizing the results from multiple model realizations with dual state-parameter estimates another area of potential research would be to investigate the cross-correlation of parameter values with model states. Parameter-state regression models could then be developed to allow parameters to vary even without data assimilation.
- State-Bias Correlation. Another related area of research would be to evaluate how the prediction bias changes with model states. Correlation functions between model states and the prediction bias could then be developed to provide estimates of bias whether or not observations are available.
- Hyperparameter Tuning. Several hyperparameters are used during data assimilation to approximate the error variance of model states, parameters, forcing data, and observations. While a procedure was developed to vary the hyperparameters for model states and parameters through the use of variable variance multipliers, additional research is needed. Estimation of appropriate

values for the other hyperparameters may improve ensemble predictions. The Normalized Root Mean Square Error Ratio (NRR) could be used as a tuning metric for the other hyperparameters (Moradkhani et al., 2006)

- SSC Regression Model. Improvements to the regression model may be possible. For example, additional data may be collected and analyzed and the existing data could be more thoroughly reviewed for quality and the identification of potential outliers. Also, additional explanatory variables could be incorporated into the model, such as moving averages of flow, rainfall intensity, air temperature, or various geophysical properties of the watershed. Finally, alternative methods to regression could be explored, such as the artificial neural networks or fuzzy logic.
- SSC Data Assimilation. Data assimilation techniques described in this study could be applied to the SSC regression model whenever SSC measurements become available. Regression parameters could be allowed to vary based on the uncertainty associated with those parameters as determined from the analysis of variance. The data assimilation algorithm would need to account for the irregular spacing of SSC measurements.

5.4 Concluding Remarks

The particle filtering approach described and implemented in this study can be used to significantly improve watershed model predictions of flow and suspended sediment load for the existing condition of the watershed. The approach also provides a mechanism for evaluating the uncertainty associated model estimates. Daily measurements of SWE and flow were needed for this data assimilation procedure. Therefore, this approach may not

be very applicable for estimating potential future runoff volumes and loads after implementing best management practices (BMPs) in the watershed. Example BMPs include sedimentation basins, infiltration basins, constructed wetlands, bioretention areas, and other structural and non-structural (e.g., street sweeping) measures used to reduce the volume and improve the quality of stormwater runoff. Estimating the quantity and quality of watershed discharges for some future condition is a challenge for any modeling effort because there are no data available to calibrate such a condition.

By quantifying the uncertainty associated with the existing condition, as well as the uncertainty associated with implementing similar BMPs in other locations, the potential uncertainty associated with the future condition may be inferred through the use of Monte Carlo simulation. For example, by analyzing BMP performance data a statistical model could be developed to account for suspended sediment concentration reductions. This statistical model could then be coupled with a conceptual model of BMP hydrology and hydraulics (e.g., infiltration, detention storage, etc.) to estimate load reductions associated with BMP implementation. Therefore, while this study focused on implementing data assimilation for the existing condition, the prediction ensemble of daily average flow and sediment load could be reanalyzed in the context of future conditions by propagating each particle through a BMP performance algorithm that accounts for the uncertainty associated with load reductions.

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Appendix A. Performance Metrics

The standard metrics of root mean square error (RMSE), percent bias (BIAS), and the Nash-Sutcliffe efficiency (NSE) were used to compare the mean predictions to observations. To evaluate the ensemble performance, the ranked probability skill score (RPSS) and the normalized root mean square error ratio (NRR) were computed. The RPSS indicates how much better the model estimates probabilities for multiple thresholds (M_k) than using the climatological average alone (NWS, 2006; Wilks, 2006). The daily mean computed over the simulation period was chosen as the climatological average and the thresholds were based on observation percentiles listed in Table A1.

Table A1. SWE observation percentiles forused for RPSS thresholds.

Percentile, k	1%	5%	10%	25%	50%	75%	90%	95%	99%
SWE (mm), M_k	15.2	58.4	76.7	213.4	624.8	937.3	1176	1290	1354
Flow1 (cms), M_k	0.0003	0.001	0.011	0.023	0.079	0.510	1.557	2.435	4.163
Flow2 (cms), M_k	0.0096	0.014	0.021	0.051	0.122	0.814	2.396	3.912	5.818
Flow3 (cms), M_k	0.0021	0.009	0.023	0.051	0.142	0.864	2.577	3.831	6.145

Percentile were computed after excluding all zero values from the SWE and flow records. SWE is based on the snow water equivalent observations at the Ward Creek SNOTEL station. Flow1 is the flow rates at the upper watershed station 674, Flow2 is the flow rate at the middle watershed station 675, and Flow3 is the flow rates at the lower watershed station 676.

The NRR is a normalized measure of ensemble dispersion relative to the deviation of the ensemble mean (Anderson, 2002; Moradkhani et al., 2005a). A value greater than 1 indicates that the ensemble has too little spread relative to the predicted mean and a value less than 1 has too much spread. Another measure of ensemble spread is the exceedance ratio (ER). The ER_k is the proportion of observations that fall outside of the k^{th} ensemble percentile during the entire analysis period (Moradkhani et al., 2006). For this study, the 95th percentile exceedance threshold was selected for the ER. The performance metrics used in this study are described below and equations are given in Table A2.

Root Mean Square Error (RMSE): A measure of accuracy.

- Range: 0 to ∞
- Perfect score: 0

Percent Bias (%BIAS): A measure of precision.

- Range: -100% to 100%
- Perfect score: 0

Nash-Sutcliffe Efficiency (NSE): A measure of accuracy.

- Range: $-\infty$ to 1
- Perfect score: 1
- $NSE < 0$, observed mean is better than model predictions

Rank Probability Skill Score (RPSS): A measure of ensemble accuracy.

- Range: $-\infty$ to 1
- Perfect score: 1 (or 100%)
- $RPSS = 0$, model prediction is no better than observed mean
- $RPSS < 0$, observed mean is better than model predictions

Normalized Root Mean Square Error Ratio (NRR): A normalized measure of ensemble dispersion.

- Range: 0 to ∞
- Perfect score: 1
- $NRR < 1$, too much spread
- $NRR > 1$, too little spread

95th Percentile Exceedance Ratio (ER95): Measure of the ensemble dispersion (spread of the prediction quantiles)

- Range: 0 to 100%
- Perfect score: 0%

Table A2. Summary of performance metrics used in this study.

Performance Measure	Equation
Root Mean Square Error (RMSE)	$\sqrt{\frac{1}{N_{data}} \sum_{t=1}^{N_{data}} (\overline{yp}_t - y_t)^2}$
Percent Bias (%BIAS)	$\left(\frac{\sum_{i=1}^{N_{data}} (\overline{yp}_t - y_t)}{\sum_{i=1}^{N_{data}} y_t} \right) \cdot 100$
Nash-Sutcliffe Efficiency (NSE) ¹	$1 - \frac{\sum_{t=1}^{N_{data}} (\overline{yp}_t - y_t)^2}{\sum_{t=1}^{N_{data}} (\overline{yp}_t - \bar{y}_t)^2}$
Rank Probability Skill Score (RPSS) ²	$RPS_t = \sum_{k=1}^K [F_t^k - O_t^k]^2$ <p>F_t^k: forecast probability at time t for threshold M_k</p> $F_t^k = \frac{1}{N_{ens}} \sum_{i=1}^{N_{ens}} I(yp_t^i < M_k)$ <p>I is an identify function that is 1 if true and 0 if false</p> <p>O_t^k: observed probability at time t for threshold M_k</p> $O_t^k = I(\bar{y}_t < M_k)$ $RPSS = 1 - \frac{\overline{RPS}}{\overline{RPS}_{climatology}}$ $\overline{RPS}_{climatology} = \frac{1}{N_{data}} \sum_{t=1}^{N_{data}} \sum_{j=1}^K [O_t^k - \bar{O}]^2$
Normalized Root Mean Square Error Ratio (NRR) ³	$\frac{\sqrt{\frac{1}{N_{data}} \sum_{t=1}^{N_{data}} (\overline{yp}_t - y_t)^2}}{\frac{1}{N_{ens}} \left\{ \sum_{i=1}^{N_{ens}} \sqrt{\frac{1}{N_{data}} \left[\sum_{t=1}^{N_{data}} (yp_t^i - y_t)^2 \right]} \right\} \sqrt{\frac{N_{ens} + 1}{2N_{ens}}}}$
95 th Percentile Exceedance Ratio (ER95) ⁴	$\frac{1}{N_{data}} \sum_{t=1}^{N_{data}} I(P_{95,t} > y_t) \times 100\%$ <p>Percent of the observations exceeding the 95th percentile of the ensemble at time t ($P_{95,t}$)</p>

¹ Adapted from Nash and Sutcliffe (1970); daily mean is used for the observation.

² NWS (2006); Wilks (2006)

³ Anderson 2002; Moradkhani et al., 2005a

⁴ Moradkhani et al., 2006