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Multiobjective calibration and sensitivity of a distributed land surface water and energy balance model

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Abstract. The feasibility of using spatially distributed information to improve the predictive ability of a spatially distributed land surface water and energy balance model (LSM) was explored at the U. S. Department of Agriculture Agricultural Research Service (USDA-ARS) Walnut Gulch Experimental Watershed in southeastern Arizona. The inclusion of spatially variable soil and vegetation information produced unrealistic simulations that were inconsistent with observations, which was likely an artifact of both discretely assigning a single set of parameters to a given area and inadequate knowledge of spatially varying parameter values. Because some of the model parameters were not measured or are abstract quantities a multiobjective least squares strategy was used to find catchment averaged parameter values that minimize the prediction error of latent heat flux, soil heat flux, and surface soil moisture. This resulted in a substantial improvement in the model's spatially distributed performance and yielded valuable insights into the interaction and optimal selection of model parameters.

1. Introduction

A land surface water and energy-balance model (LSM) [*Famiglietti and Wood*, 1994] was used to simulate the spatially distributed behavior of the U. S. Department of Agriculture Agricultural Research Service (USDA-ARS) Walnut Gulch Experimental Watershed (WGEW). This type of model generally has a large number of parameters that describe surface vegetation and soils that must be correctly specified to produce accurate water and energy balance simulations. Many of these parameters are physically realistic and observable; that is, they are dimensions or capacities which can be measured reliably. For these parameters, observed values can be used when available. Other parameters are not observable or are not physically realistic. Such parameters may well be conceptual representations of abstract watershed characteristics or empirical constants that can be used to optimize the simulation results on a trial-and-error basis to match the simulations to observations.

Two aspects add complexity to the problem of parameter specification in this study. First, because the surface conditions are spatially variable, the parameters might also be expected to vary spatially. Second, because the performance of the model is to be judged in terms of its ability to simultaneously predict the soil moisture states and the latent, sensible, and soil heat fluxes, the specification of parameters is a multiobjective calibration and evaluation process.

Many aspects of LSM calibration have been explored in other investigations. For example, *Sellers et al.* [1989] employed manual calibration of nine parameters in the simple biosphere (SiB) model to improve its comparison with field observations. *Franks and Beven* [1997] use a generalized likelihood uncertainty estimation approach to reduce the output uncertainty for the TOPUP model using First International Satellite Land Surface Climatology Project Field Experiment (FIFE) and Anglo-Brazilian Climate Observation Study (ABRACOS) observations. *Lettenmaier et al.* [1996] reported that in an intercomparison of various LSMs, those whose parameters were calibrated performed better than those without parameter calibration. For a review of conceptual hydrologic model calibration to observed data, see *Gupta et al.* [1998].

Automatic spatially distributed LSM calibration has been severely limited by the absence of adequate spatially variable hydrologic calibration data. Automatic calibration methods adjust LSM parameters to obtain a best fit of LSM predictions with observations. Therefore, to automatically obtain spatially distributed LSM parameters, spatially distributed observations of LSM predictions, such as soil moisture, surface heat fluxes, and runoff, must be available. Currently, distributed observations of LSM predictions are scarce, and when available, have relatively high uncertainty [*Franks et al.*, 1998]. Therefore spatially distributed LSM calibration has generally been limited to (1) specification of spatially variable parameters from soil, vegetation, or topographic maps derived from field surveys or remote sensing or (2) lumped or area-averaged calibration, where parameters are assumed to be constant over an area and are adjusted coincidentally to minimize error in streamflow [e.g. *Storck et al.* 1998]. An exception is a study by *Franks et al.* [1998], where distributed model parameterizations were first conditioned on lumped discharges and then further conditioned on distributed

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estimates of saturated areas estimated from remote sensing and topography using the weighting of estimates in a fuzzy set framework.

This paper consists of six sections. Section 2 describes the study site and the data set. Section 3 provides an overview of the LSM. The fourth section explores the hypothesis that the use of spatially distributed soils and vegetation information can help to improve the predictive ability of the LSM. Section 5 explores the hypothesis that a multiobjective parameter calibration method can be used to improve the estimates of nonobserved model parameters. The last section presents the conclusions and some final remarks.

2. Walnut Gulch and Monsoon `90 Observations

The Walnut Gulch Experimental Watershed (WGEW) is operated by the Southwest Watershed Research Center (SWRC) of the Agricultural Research Service, U.S. Department of Agriculture. The study catchment is a heavily instrumented area comprising the upper 148 km² of the Walnut Gulch drainage basin in an alluvial fan portion of the San Pedro River watershed in southeastern Arizona. Depth to ground water varies from 45 m at the lower end to 145 m in the center of the watershed. Soil types range from clays and silts to well-cemented boulder conglomerates [Kustas et al., 1992], with the surface soil textures being gravelly and sandy loams containing, on average, 30% rock and little organic matter. The mixed grass-brush rangeland vegetation ranges from 20 to 60% in coverage. This rangeland region receives 250 to 500 mm of precipitation annually, typically two thirds of it as convective precipitation during the summer monsoon season [Renard et al., 1993].

Eighty-five recording rain gauges, 11 primary watershed runoff-measuring flumes, and micrometeorological observations make the WGEW a valuable research location. During the Monsoon `90 experiment (July 23 through August 10, 1990), extensive remote-sensing observations were made, while eight micrometeorological energy flux (Metflux) instruments provided continuous measurement of local meteorological conditions and the surface energy balance [Kustas and Goodrich, 1994].

Precipitation is the most important spatial forcing variable in semiarid regions because of its highly variable, convective nature; thus much effort was devoted to deriving spatially distributed precipitation data sets for the Monsoon `90 experiment. A multiquadric-biharmonic interpolation algorithm [Syed, 1994] was used to produce spatially distributed precipitation values for the entire model domain from the available rain gauge data. All other meteorological forcing was assumed to be spatially constant and derived from averaging observations at the eight Metflux stations in place during the experiment. A spatial averaged soil moisture profile was derived from several in situ profile observations [Schmugge et al., 1994] and used to initialize the LSM on July 22 (Table 1).

3. Land Surface Model

The land surface water and energy balance model (LSM) [Famiglietti and Wood, 1994] simulates land surface runoff, energy fluxes, and soil moisture dynamics in three layers. This LSM is designed to predict diurnal dynamics of the water and energy fluxes at the land surface and local vertical recharge to the water table. It incorporates simple representations of atmospheric forcing, vertical soil moisture transport, plant-controlled transpiration, interception, evaporation, infiltration, surface runoff, and sensible and ground heat fluxes. The LSM incorporates a diurnal cycle and is driven with standard meteorological data with an hourly time step, this being considered sufficient to resolve the dynamics of the land-atmosphere interaction.

4. Use of Spatially Distributed Soils and Vegetation Information

This section examines the hypothesis that the use of spatially distributed soils and vegetation information can help to improve the predictive ability of the LSM. The LSM was used to simulate the land surface water and energy dynamics in a spatially distributed manner for the entire WGEW at a 40 m resolution. Predictions were made hourly from July 22 to August 15, or day of year (DOY) 204 to 228, of 1990. LSM parameter estimates were first specified by using catchment-averaged parameter values based largely on observations. Next, spatially distributed values for the parameters were derived from geographic information system's (GIS) maps.

4.1. Spatially Constant Parameters

Spatially constant parameters for the LSM were specified primarily on the basis of observations made during Monsoon `90 [Daughtry et al., 1991; Kustas et al., 1992, 1994a, 1994b, 1994c; Stannard et al., 1994; Moran et al., 1994a, 1994b; Humes et al., 1994a, 1994b; Weltz et al., 1994; Menenti and Ritchie, 1994; Hipps et al., 1994; Spangler, 1969]. The albedo of dry soil was specified by adopting the parameters suggested by Dickinson et al. [1993]. Soil profile temperatures measured in three trenches at the Lucky Hills and Kendall sites were analyzed and modeled to determine the temperature diurnal damping depth. The saturation soil moisture was assumed to be close to the porosity calculated from bulk density measurements. The surface saturated hydraulic conductivity was based on porosity using the Kozeny-Carmen equation with a coarse fraction correction, following Rawls et al. [1993]. The depth of the surface zone was specified equal to the maximum reported L band microwave penetration depth [Jackson, 1993] to aid compatibility with remote sensing data. Because of the deep water table at Walnut Gulch, surface processes show no sensitivity to the LSM water table parameters, so these were assigned to arbitrary values. The vegetation stress soil moisture parameter was assumed to be halfway between the saturated and residual soil moisture values, while the wilting point was assumed to be equal to the value of residual soil moisture because desert vegetation rarely wilts. The soil moisture at which evapotranspiration reaches the potential rate was assumed to be 10% below saturation, this being the approximate ratio suggested by Sellers et al. [1986]. Values for albedo of dry vegetation for semiarid areas were obtained from Dickinson et al. [1993], and the albedo of wet vegetation was assumed to be 5% lower than that for dry vegetation. The stomatal resistance, root activity factor, root density, root resistivity, and critical leaf water potential were not measured; indeed, because many of these parameters were not observable quantities, estimates were used.

Table 1. Catchment-Averaged LSM Parameters for Walnut Gulch, Based on Observations, GIS Coverage, and Multiobjective Calibration[a]

Parameter	Source	Observed	GIS	Calibrated
Vegetation parameters				
vegetation height, m	*Humes et al.* [1994a]	(0.22)		
leaf area index	*Daughtry et al.* [1991]	1.275	(1.31)	
minimum stomatal resistance, s m^{-1}	*Chow et al.* [1988]	40	267	(574)
initial water storage in canopy, m	assumed dry at start of simulation	(0)		
unstressed transpiration soil moisture, %	assumed halfway between θ_s and θ_r	(20)		
wilting point soil moisture, %	assumed θ_r (cacti rarely wilt)	(1)		
vegetation fraction	*Kustas et al.* [1994a]	(0.42)		
albedo, wet vegetation	*Dickinson et al.* [1993]	(0.2)		
albedo, dry vegetation	*Dickinson et al.* [1993]	(0.25)		
albedo, bare soil	*Dickinson et al.* [1993]	(0.33)		
root activity factor	*Famiglietti* [1992]	10,000		(348025)
root density, m m^{-3}	*Famiglietti* [1992]	1		(86.5)
root resistivity, s m^{-1}	*Famiglietti* [1992]	1e9		(4.8e11)
critical leaf water potential, m	*Famiglietti* [1992]	-210		(-500)
Soil parameters				
surface zone depth, m	Based on PBMR sensitivity depth	(0.1)		
initial surface soil moisture, %	*Schmugge et al.* [1994]	(10.0)		
root depth, m	*Schmugge et al.* [1994]	1.5	(0.8)	
initial root zone soil moisture, %	*Schmugge et al.* [1994]	(17.0)		
maximum rate of capillary rise, m s^{-1}	*Famiglietti* [1992]	(0.1)		
initial transmission zone soil moisture, %	*Schmugge et al.* [1994]	(17.0)		
percent sand, %	*Kustas and Goodrich* [1994]	70.9	63.1	(14.4)
percent clay, %	*Kustas and Goodrich* [1994]	8.5	22.1	(8.1)
bulk density, g cm^{-3}	*Kustas and Goodrich* [1994]	(1.6)		
residual soil moisture, %	*Rawls et al.* [1993]	1	5.1	(2.2)
saturated soil moisture, %	*Kustas and Goodrich* [1994]	38.0	33.6	(30)
saturated hydraulic conductivity, m s^{-1}	*Rawls et al.*, [1993]	6.9e-5	4.7 e-6	(8.7e-6)
bare soil roughness length, m	assumption	(0.001)		
bare soil zero plane displacement, m	assumption	(0.0)		
Water table parameters				
average topographic index	calculation from $A(\tan(B))$ image	(8.314)		
K$_s$ exponential decay parameter	*Famiglietti* [1992]	(7.0)		
initial water table depth, m	*Gilbert* [1996]	(100.0)		
Energy balance parameters				
soil moisture for calculation of PET, %	Sellers *et al.* [1986]	28		(47)
diurnal heat penetration, m	from observations [*Houser*, 1996]	0.5		(0.33)
temperature of deep soil layer, °K	from observations [*Houser*, 1996]	297.0		(287.6)

[a] Values in parentheses produce the "best" Monsoon '90 simulation. Read 1e9 as 10^{-9}.

4.2. Spatially Variable Parameters

Spatial distributions of the soil and vegetation parameters were estimated using GIS maps of Walnut Gulch vegetation and soils. The potential rooting depths for each soil series were taken from a recent Walnut Gulch soil survey (D. J. Breckenfeld, unpublished document, 1993). Values of the effective porosity, ϕ_e, residual soil moisture, θ_r, and the saturated hydraulic conductivity, K_s, were determined by *Mayeux* [1995] using values suggested by *Rawls et al.* [1993] and *Bouwer* [1966]. J. Berglund, unpublished report, (1995) calculated saturated soil moisture, θ_e, for each soil class as follows:

$$\theta_e = \phi_e + \theta_r . \qquad (1)$$

Percent sand and clay were calculated by J. Berglund (1995) from values of percent material passing through certain sieves

for each soil series in the soil survey. Bulk density, *B*, was estimated using an empirical formula [*Rawls et al.*, 1993]:

$$B = 1.51 + 0.0025(S) - 0.0013(S)(O) - 0.0006(C)(O)$$
$$- 0.0048(C)(E) . \qquad (2)$$

where *S* is percent sand, *C* is percent clay, *O* is percent organic matter, and *E* is the cation exchange capacity of clay normalized by percent clay. Measurements at the eight Monsoon '90 Metflux sites [*Daughtry et al.*, 1991] and parameter ranges given by *Jones* [1983] were used in conjunction with the Walnut Gulch vegetation GIS coverage to estimate the spatial distribution of leaf area index (LAI) and minimum stomatal resistance. The topographic index was calculated from digital elevation models (DEMs) derived from 23 1:5000 stereo aerial photos [*Matthews*, 1992]. DEM
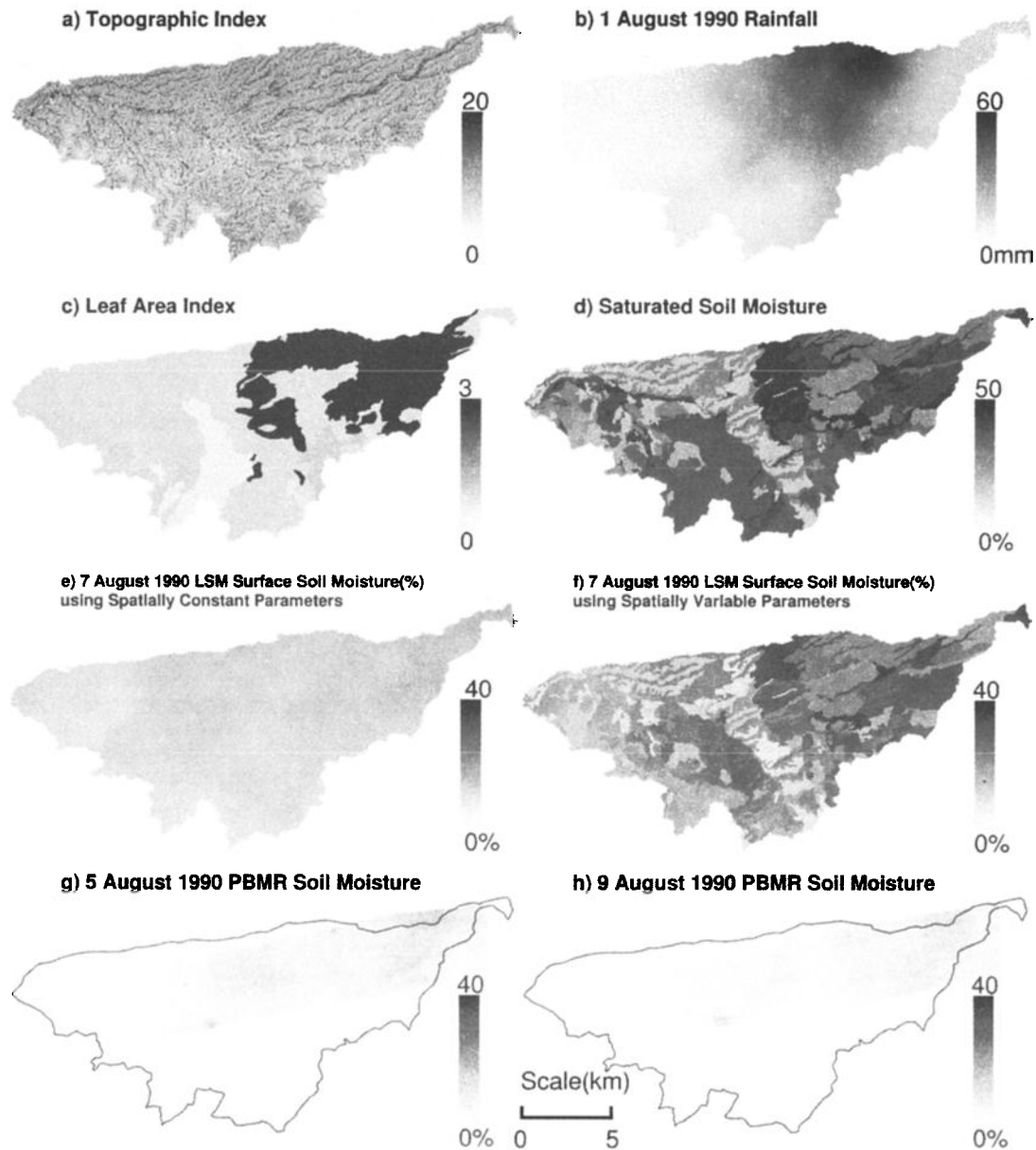
Figure 1. Spatially distributed Walnut Gulch Experimental Watershed: (a) topography, (b) precipitation, (c) vegetation, and (d) soils. LSM spatial predictions of surface soil moisture at 1200 LT on August 7 (DOY 219) using (e) spatially constant and (f) spatially variable soils and vegetation parameters (all simulations using spatially variable topography and precipitation). Push broom microwave radiometer (PBMR) derived soil moisture for (g) August 5, 1990 (DOY 217) and (h) August 9, 1990 (DOY 221) [Houser et al., 1998]. The addition of spatially variable soils and vegetation produces unrealistic polygon artifacts in the simulation.

overlaps were averaged, then a smoothing algorithm was applied to reduce noise, and isolated runoff sinks were filled. The watershed was delineated and the topographic index was derived using the standard methodology detailed by *Beven* [1995]. A selection of representative spatially variable Walnut Gulch parameters is shown in Figure 1a-1d, and the watershed averages of these parameters are reported in Table 1.

4.3. Results and Discussion

The simulated spatial patterns of surface soil moisture for August 7, 1990 (DOY 219), using both the spatially constant and the spatially variable parameters, are shown in Figures

1e-1f. It is evident that the spatially variable parameters have a large impact on the spatial patterns of the simulation. Further, the soil moisture patterns derived using the spatially variable parameters appear to be unrealistic and do not compare well with observed push broom microwave radiometer (PBMR) surface soil moisture (Figures 1g-1h).

A series of simulations, where only one spatially variable parameter set was used at a time (the other parameters were set to their estimated catchment-averaged values), were performed to determine which subset of spatial parameters contribute most to these patterns (the topographic index and the precipitation fields were spatially variable in all these simulations). The simulations with spatially variable

vegetation parameters perform similarly to the control run, indicating that spatial variation in these parameters has little effect on predictions. All of the simulations using spatially variable soil parameters show distinct polygon patterns. The parameter specifying saturated soil moisture has the most influence on simulated spatial patterns, while those which specify the percentages of sand and clay, the saturated hydraulic conductivity, and the residual soil moisture have a more moderate influence. The soil characteristics are extremely important, and the vegetation characteristics are less important in regulating soil moisture variability and other surface water and energy components in this watershed. The results of this sensitivity also show that the spatially variable topographic index has very little influence on the simulations; this result is a consequence of the large depth to the water table at Walnut Gulch.

The pattern of enhanced spatial soil and vegetation polygons apparent in the simulations is an artifact of both assigning lumped values of the parameters to discretely partitioned areas as well as the misspecification of parameter values. A more appropriate specification of spatial parameters would reflect their continuous variability in space, as obtained with remote sensing. It is also clear that the specification of the spatial parameter values using scattered observations, table lookup, and physical relationships (as described in section 4.2) result in inadequate parameter specification. These results indicate that the available WGEW parameter observations simply have insufficient accuracy and spatial frequency to realistically constrain the LSM. Because the simulations using spatially constant vegetation and soil parameters compare well to the PBMR patterns, the subsequent parameter calibration studies reported in section 5 assume spatially constant soil and vegetation parameters across the catchment, leaving only topographic index and precipitation as spatially varying entities.

The use of catchment-averaged parameters in this study is supported by *White et al.* [1997], who found that the difference between the calculated area-averaged surface energy fluxes given for the WGEW by a single point land surface model with aggregate parameters and that given by a distributed array of land surface models was small. This conclusion was tested here; although there was more variability than reported by *White et al.* [1997] because of the finer spatial resolution, there was overall agreement. The relevance of this finding to the present study is that it supports the use of catchment-averaged parameters and forcing for the WGEW if catchment-averaged surface fluxes are required. This conclusion is only valid when catchment-averaged fluxes are of interest; for cases where downslope flows or water availability in valley bottoms is of interest, then spatially variable parameters and forcing are required. In this study, the spatially distributed LSM is required to allow prediction of spatial patterns of soil moisture at the resolution of the available remotely sensed observations.

5. Multiobjective Calibration of Nonobserved Model Parameters

The purpose of this study was to obtain estimates of the nonobserved model parameters that would result in improved simulations of the overall behavioral responses of the watershed. In particular, the desire was to select values for the parameters that minimized the error in predicted soil moisture and sensible, latent, and ground heat fluxes. As discussed by

Gupta et al. [1999], this situation involves the problem of finding parameter estimates which can simultaneously minimize several noncommensurable criteria. This section examines the hypothesis that a multiobjective parameter calibration method can be used to improve the estimates of the nonobserved model parameters of the LSM model.

5.1. Data Available for Calibration

The primary observations used to calibrate the LSM parameters in this study were hourly time series of catchment-averaged, water balance corrected, latent heat flux during unstable atmospheric conditions, soil heat flux, and gravimetric calibrated near-surface soil moisture measured with resistance sensors (Table 1). During the Monsoon `90 study period, three replicate gravimetric surface soil moisture samples were collected each day at the eight Metflux sites [*Schmugge et al.*, 1994]. Resistance sensors collected continuous time series of soil moisture at 2.5 cm and 5 cm below the surface at all eight Metflux sites [*Amer et al.*, 1994]. Because such sensors are generally difficult to calibrate and tend to drift, they were recalibrated each day against gravimetric measurements for the purpose of this study. The energy balance was determined from measurements of net radiation, soil heat flux, and estimates of sensible and latent heat flux by either eddy covariance or temperature variance methods [*Kustas et al.*, 1994a]. A detailed water balance study showed that during Monsoon `90 the sensible heat flux was underestimated because of eddy correlation propeller stalls, source area mismatch, or horizontal flux divergence in hilly terrain [*Houser et al.*, 1997; *Williams*, 1996; *Keefer et al.*, 1997]. Therefore, for this study the observed latent and sensible heat fluxes were adjusted to be consistent with the water balance, and unreliable observations during stable

Table 2: Calibration Parameter Ranges and Objective Functions[a]

Calibration Parameter	Possible Range
Root activity factor	1 to 1e6
Root density, m m^{-3}	1 to 100
Root resistivity, s m^{-1}	1e6 to 1e12
Critical leaf water potential , m	-1 to -1000
Potential evaporation soil moisture, %	10 to 50
Penetration of diurnal heating, m	0.1 *to* 0.7
Temperature of deep soil layer, K	285 to 310
Minimum stomatal resistance, s m^{-1}	0 to 700
Percent sand, %	1 to 100
Percent clay, %	1 to 100
Residual soil moisture, %	1 to 20
Saturated soil moisture, %	20 to 50
Surface saturated hydraulic conductivity, m s^{-1}	5e-5 to 5e-7

Objective Function
sensible heat flux (eight sites, water balance corrected, daytime average from temperature variance)
latent heat flux (eight sites, water balance corrected, daytime average from temperature variance)
soil heat flux (eight sites average from soil heat flux plates)
surface soil moisture (eight sites, gravimetric corrected average from resistance sensors)

[a] The sensible heat flux objective function was included as a diagnostic; it was not used in the determination of the Pareto set. Read 1e6 as 10^{-6}.

atmospheric conditions were excluded from objective function calculations.

5.2. Parameters Calibrated

The 13 parameters listed in Table 2 were identified for calibration. Table 2 also lists the typical range of their values; these ranges were specified larger than might normally be expected in order to allow the calibration procedure some leeway in accounting for model and data error. Moreover, because some of the parameters are nonphysical, the specification of their ranges is somewhat arbitrary. Note that the soil heat flux parameters (temperature of the deep soil layer and penetration of diurnal heating) were included in this list even though they were measured with confidence. This is because the soil heat flux was poorly simulated by the LSM owing to the simplicity of its soil heat flux submodel; this suggests that nonphysical values for these parameters may be necessary for the model to perform adequately. Note also that the five soil water retention parameters, which can be estimated from observations, were also included in the calibration, because this greatly improved the simulation of soil moisture and yielded insight into the use of observed soil parameters.

5.3. Theoretical Background to the Multiobjective Calibration Approach

A theoretical and practical basis for the calibration of models with multiple and noncommensurable output fluxes has been presented by *Gupta et al.* [1998, 1999], *Bastidas et al.* [1999], and *Meixner et al.* [1999]. Because of errors in the model (structure) and in the data it is impossible to find a single "best" parameter set that simultaneously minimizes the errors in matching all of the observable model outputs. This leads to a multiobjective optimization problem for which the "solution" is a region of the parameter space that reflects different trade-offs in the matching of the outputs. An acceptable solution can be selected by the user from this region of trade-off solutions using subjective judgment.

To clarify, a simple one-parameter example is presented in Figure 2; we assume that data are available for two model output fluxes that must be matched, and we let $f_1(\theta)$ and $f_2(\theta)$ represent the mean square error (MSE) in matching these fluxes for selected values of a specific model parameter θ.

Figure 2a illustrates how each of the mean square error functions $f_1(\theta)$ and $f_2(\theta)$ might vary with θ. Note that the parameter value $\theta = \theta_1$ minimizes the function f_1 but has a relatively poor value for f_2, while a different value $\theta = \theta_2$ minimizes the function f_2 but has a relatively poor value for f_1. In other words, the individual solution $\theta = \theta_1$ that gives the best match to the first model flux might give rather poor performance in terms of matching the second model flux and vice versa. However, in general, we wish to have a model solution that simultaneously gives acceptable "good" matching of both fluxes.

To this end we note that there exists a region of values $\Theta_p = \{\theta_1 < \theta < \theta_2\}$ consisting of those parameter values for which it is possible to obtain improvement in $f_2(\theta)$ (by varying θ) while simultaneously allowing some deterioration in $f_2(\theta)$; this region is called the "Pareto," "non-inferior," or "trade-off" solution. Similarly, all values of $\theta \notin \Theta_p$ are called "inferior" solutions. Figure 2b shows the problem plotted in the function space with $f_1(\theta)$ and $f_2(\theta)$ on the axes, and the curve represents the trajectory obtained by varying θ over its feasible range. Clearly, the objective is to find θ such that we come as close to the origin $\{f_1, f_2\} = \{0,0\}$ as possible. Note that the segment of the curve between B and C represents the trade-off region, while other portions of the curve represent inferior solutions. Any one of the trade-off solutions can be selected by the user as "best," depending on which trade-off in matching of model performance is considered most acceptable by the user.

5.4. Objective Function

Three objective functions were used to calibrate the model parameters: the hourly mean square error in matching of latent heat flux during unstable atmospheric conditions, soil heat flux, and gravimetric calibrated near-surface soil moisture. In each case the mean square error objective function, F, was computed using the normalized sum of the squared difference between the catchment-averaged, water balance corrected observations, O_i, and the predictions, P_i, whenever the observation was available; thus

$$F = \frac{1}{n}\sum_{i=1}^{n}(O_i - P_i),\qquad(3)$$

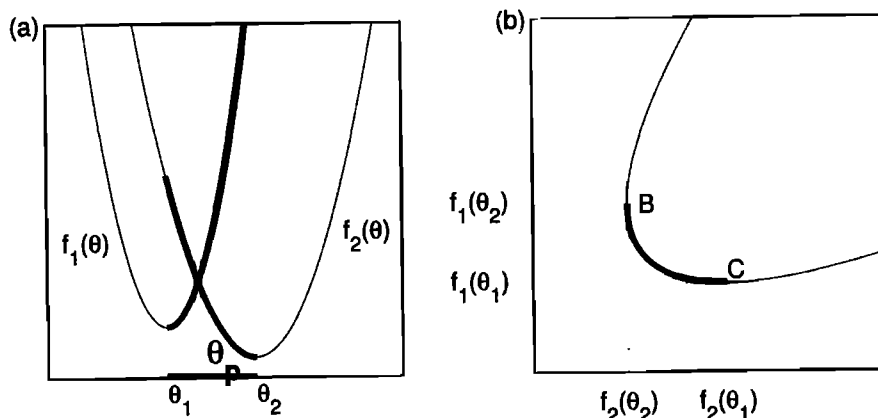where i is the time step and n is the number of observations.

Figure 2. A simple one-parameter, two-objective model calibration example: (a) how each of the mean square error functions, $f_1(\theta)$ and $f_2(\theta)$, might vary with model parameter θ, and (b) problem plotted in the function space with the curve representing the trajectory obtained by varying θ over its feasible range.

5.5. Multiobjective Calibration Methodology

The procedure adopted for the multiobjective calibration of the LSM parameters at Walnut Gulch was to conduct a Monte-Carlo search of the feasible parameter space indicated in Table 2. A total of 200,000 parameter set realizations were randomly generated, and the three objective function values were computed at each parameter set. From these, the "noninferior" trade-off parameter region was estimated by finding those points for which there did not exist at least one other member of the original 200,000 realizations for which all three objective function values were better. Only 125 parameter set realizations were found to belong to this estimated noninferior region, indicating a rather substantial reduction in overall parameter uncertainty. In addition, at each noninferior point, the mean square error in matching of hourly sensible heat flux was also computed for diagnostic purposes.

The estimated noninferior region is displayed in Figure 3 using the formats introduced by *Sorooshian et al.* [1993] and *Gupta et al.* [1998, 1999]. Figure 3 (left) shows the trade-off among the objectives, while Figure 3 (right) shows the corresponding trade-off among the parameters. Note that the objective function values have been normalized onto a zero-to-one scale, where zero corresponds to the smallest error and one corresponds to the largest error in the feasible region. Similarly, the parameter sets are also normalized onto a zero-to-one scale, with zero corresponding to the minimum value of the parameter and one corresponding to the maximum value in their defined ranges. These plots enable ease in identifying which parameters are poorly or well identified and also how various parameter values affect prediction errors. The estimated noninferior solution region shows relatively low values for most of the objectives, with the largest spread being in the matching of soil moisture. Some of the calibrated (noninferior) parameters ranges are quite tight (e.g., deep soil temperature and percent clay), showing that these parameters are identified well. The noninferior parameter values also are generally confined to moderate ranges of the parameter space. However, quite a lot of parameter interaction is observed, with two clusters of parameters evident (i.e., see minimum stomatal resistance, potential evaporation soil moisture, diurnal heating penetration, residual soil moisture, etc.).

Despite the relatively low objective function values produced by the noninferior parameter range the corresponding total range of LSM flux prediction remains high. The eight Metflux site average ranges of prediction obtained from the Pareto parameter sets are shown in Figure 5. There is still a large amount of prediction variability even within the Pareto set, and hence the final parameter set must be chosen carefully.

All of the noninferior parameter sets are good but with different compromises as to which objective is more fully minimized. To select a single "best" parameter set from the 125 noninferior solutions, a necessarily subjective procedure was followed. For each of the three objectives, the five noninferior parameter sets giving the best value of that objective function were selected (a total of 15 solutions); in addition, the five members of the noninferior region giving the best value of hourly mean square error in matching of sensible heat flux also were selected as shown in Figure 4. Note that the sensible heat flux objective function was not used in the estimation of the noninferior region. Each row of plots corresponds to a different optimized objective function, while Figure 4b shows the trade-off among objectives and Figure 4a

shows the corresponding trade-off among the parameters. Inspection of these results shows that the five solutions giving best matching to soil moisture also give relatively good matching of the other four fluxes. In addition, it was decided that the soil moisture objective was most important for the purposes of this study. Therefore the parameter set that produced the lowest soil moisture objective was chosen (bolded line in Figure 4). The selected parameter values are shown in Table 1.

It is interesting to note that the calibrated parameter values are reasonably close to the default values, with the exception of the root parameters, and are in general more realistic. A root density of 86 m m⁻³ is much more realistic than 1 m m⁻³, for instance, while the high minimum stomatal resistance is realistic for water-conserving semiarid plants. The default percent sand and clay parameters that were derived from a number of soil analyses (J. Berglund, unpublished report, 1995) were likely too high because the large coarse fraction (D. J. Breckenfeld, unpublished document, 1993) was removed prior to analysis. Basically, if the sand, silt, and clay percentages (which in the published soil analysis add up to 100%) are adjusted so that they add up to 100% minus the coarse fraction, then they get very close to the parameters found using calibration. These insights lead to the inclusion of a coarse fraction correction in the model physics [*Houser*, 1996]. The large differences in soil heat flux parameters are probably an artifact of the LSM having a simplified soil heat flux submodel. Finally, the high values of critical leaf water potential and soil moisture for the calculation of potential evapotranspiration (PET) reflect the fact that the plants do not wilt and that the environment rarely experiences potential evaporation.

There is a clear compromise in the calibration between latent heat flux prediction and soil moisture prediction (Figure 5). The range of prediction shows that latent heat flux can be calculated well by the LSM but at the expense of soil moisture. By choosing to predict soil moisture most accurately, rather than latent heat flux, we obtain "flat tops" or "hats" in the simulated latent heat flux time series. According to *Carlson* [1991, p. 353], "there is considerable observational evidence of [such] behavior in the field." This LSM prediction of latent heat flux may not be entirely incorrect, but it is certainly not supported by the Monsoon '90 observations. It is difficult to draw any definitive conclusions here because the accuracy of these latent heat flux observations has been questioned [*Williams*, 1996; *Keefer et al.*, 1997; *Houser et al.*, 1997].

6. Conclusions

High-quality land surface water and energy balance simulations are essential for the prediction of drought, floods, agricultural production, land surface inputs to the atmosphere, and the response of land surfaces to climate change. However, the land surface water and energy balance models that make these predictions generally utilize large numbers of parameters, many of which are not regularly measured and some of which describe abstract land surface characteristics that cannot be measured. The inherent heterogeneity of land surfaces requires spatially distributed LSM predictions, which complicates the optimum selection of parameters. Further, LSMs are expected to predict multiple land surface states and fluxes reasonably well, which requires the use of a multiobjective calibration procedure to achieve optimal
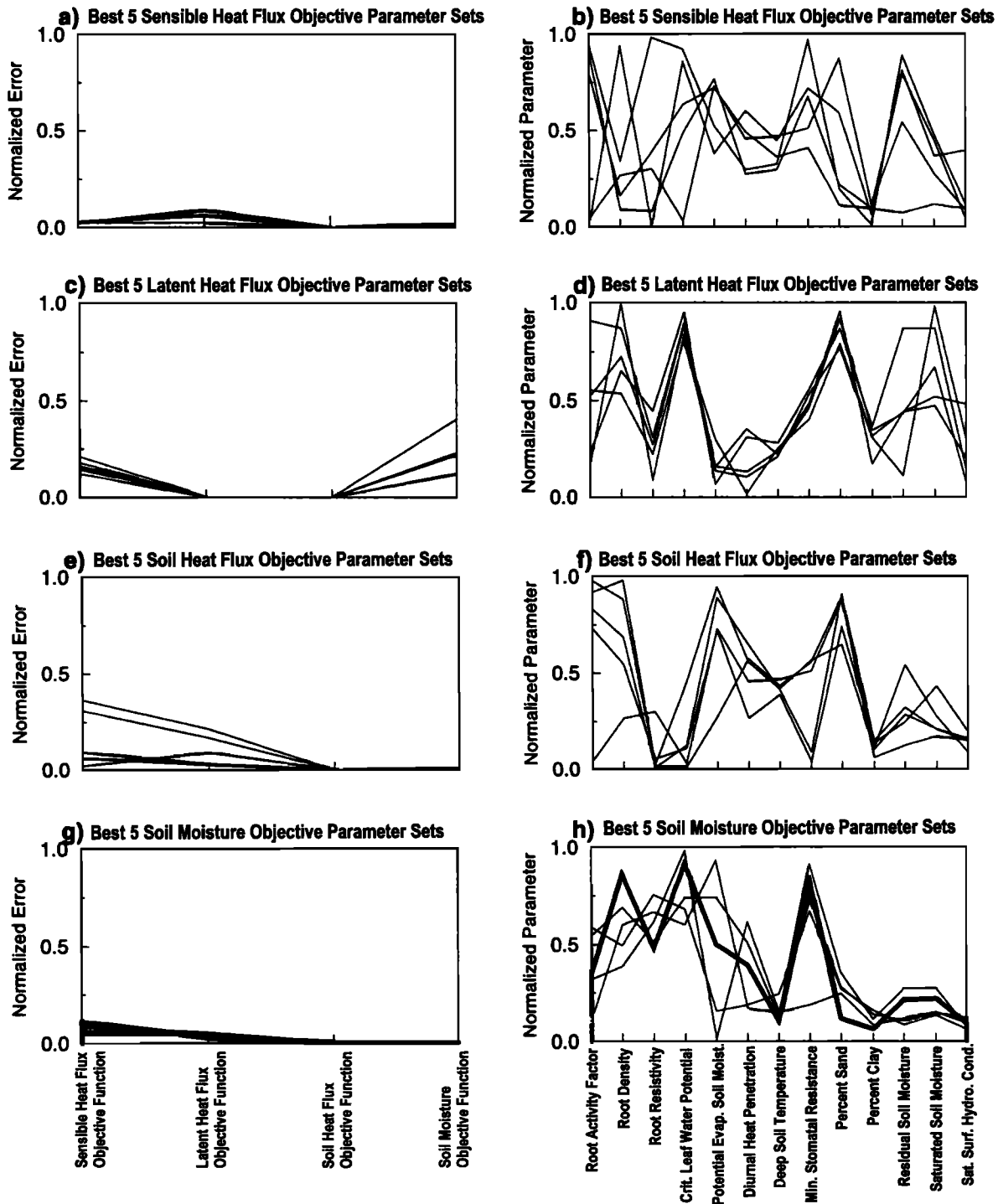
Figure 3. Pareto set normalized objective function and parameter values for the 13-parameter, three objective function Monte-Carlo calibration. The best five parameter sets and objective function values for each objective function are shown, with the subjectively chosen "best" parameter set shown in bold. Parameter and objective function definitions are shown in Table 2.

performance. Therefore, this study has explored the feasibility of using spatially distributed soils and vegetation information and a multiobjective parameter calibration method to improve the predictive ability of a spatially distributed LSM at the WGEW.

Although it seems reasonable that the inclusion of spatially variable soil and vegetation information in a spatially distributed LSM should improve local predictions, this study shows that the polygon nature of these data sets results in unrealistic simulations which were inconsistent with observations. A parameter sensitivity study revealed that spatial variations in vegetation parameters have little effect on predictions, but that soil parameters have a large effect. This problem is both an artifact of discretely assigning a single set
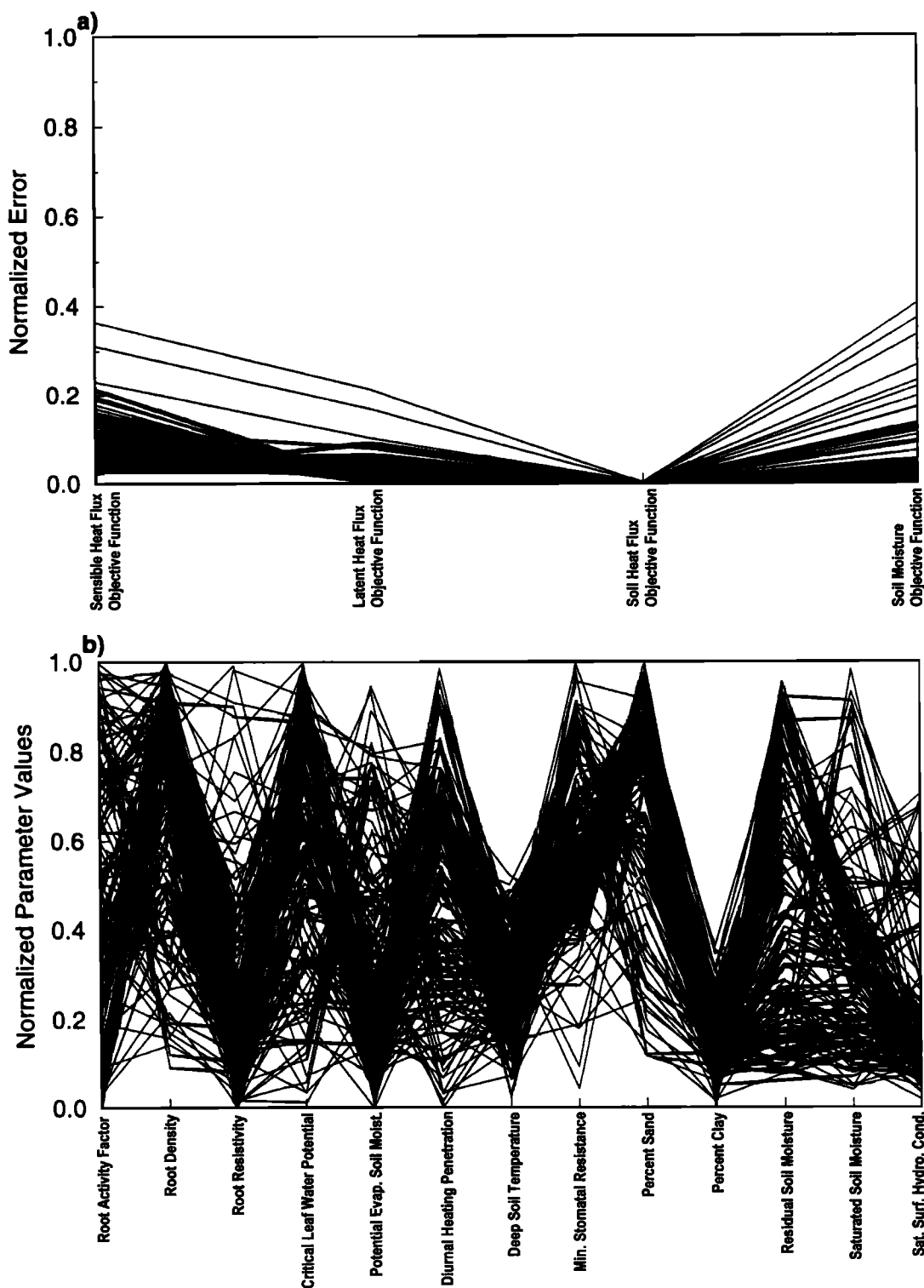
Figure 4. Pareto set normalized (a) objective function and (b) parameter values for the 13-parameter, three objective function calibration. Parameter and objective function definitions are shown in Table 2.

of parameters to large areas of the catchment and a misspecification of spatial parameter fields due to inadequate measurement of the required parameters.

˙ It is also recognized that the choice of spatially constant soil moisture initialization on July 22, 1990 and the short model spinup influences the spatially distributed predictions and influences thus the calibration of the distributed model.

However, the unrealistic very strong surface soil spatial patterns predicted on August 7 (Figure 1) would likely be enhanced given a spatially variable soil moisture initialization or longer term model spinup. It is possible that the spatially distributed initial conditions could be manipulated to produce a better spatially distributed prediction. However, we had no spatially distributed observations on July 22, for validating
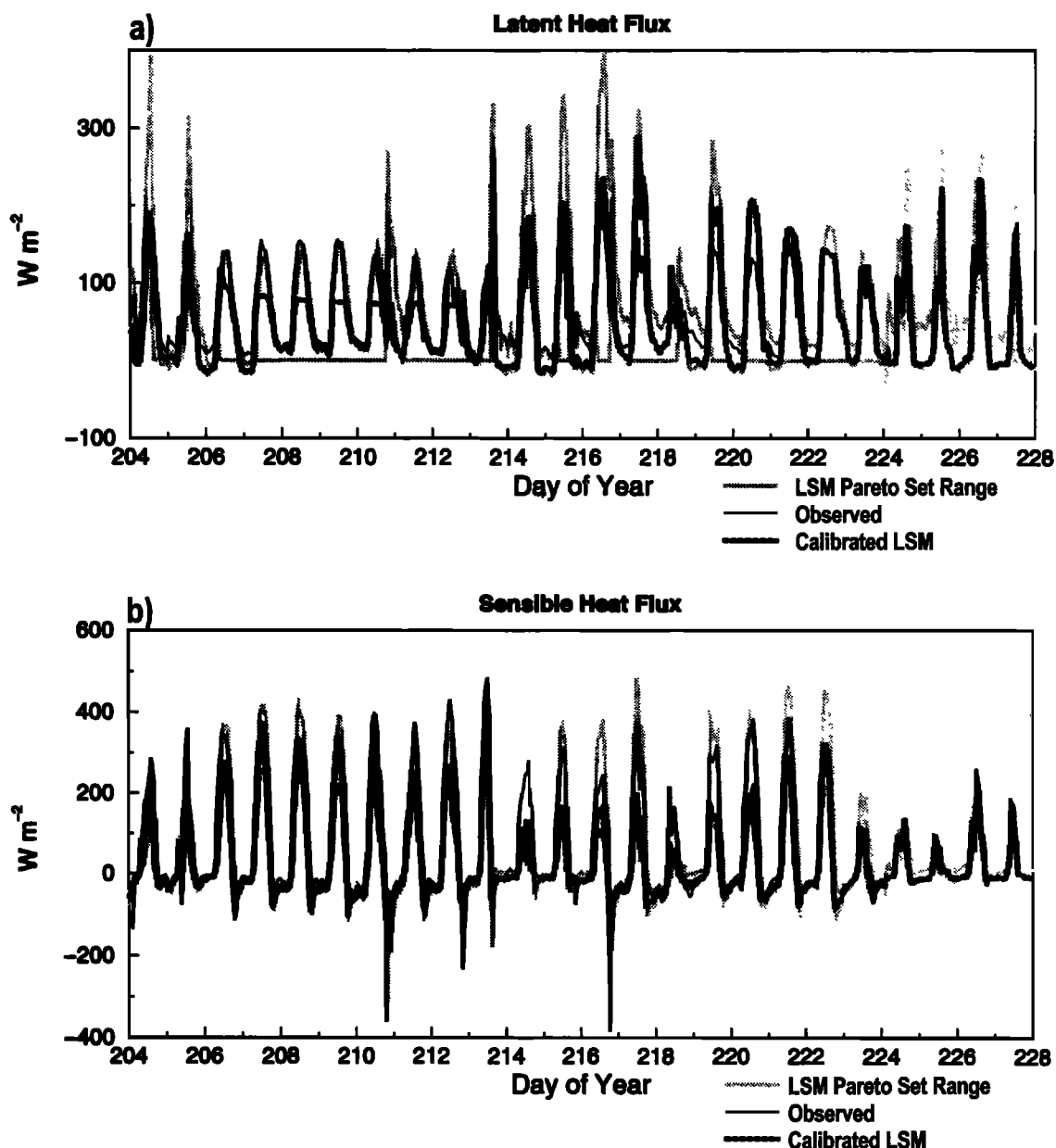
Figure 5. Catchment-averaged time series of (a) latent, (b) sensible, (c) soil heat flux, and (d) near-surface soil moisture and their associated prediction ranges for the 13-parameter, three objective function Pareto set. The subjectively chosen calibrated parameter set prediction and area-averaged observations are also indicated.

such manipulations, and we seriously doubt that such manipulation would change our conclusions given the very strong spatial patterns observed in the subsequent predictions.

There is doubt that the process of deriving the spatially variable parameter fields from a few scattered observations using established physical relationships and table lookup is sufficient for realistically constraining a complex distributed land surface model. The spatially variable parameter fields were derived from a variety of sources, which leads to inconsistencies in the resulting parameter set and degraded LSM performance. Ideally, the model should be calibrated for each point in the domain to produce consistent parameter sets that account for the spatial variability of surface characteristics. For the WGEW this is a poorly posed problem, being that there are 90,000 model grid points and

only eight surface flux observation points. Given that the available spatial information is insufficient to accurately specify the LSM spatial parameter distributions, we chose to calibrate the catchment average parameters to provide the best possible simulation. Because precipitation is the dominant driver of spatial variability in soil moisture at the WGEW, this approach results in reasonable LSM spatial predictions.

It is acknowledged that the simulation should improve if there were sufficient information to truly calibrate the LSM spatially. It may have been possible to use the spatially distributed PBMR soil moisture remote-sensing estimates to calibrate the spatially distributed parameters. However, this was not done because our intention in this study was to perform a multiobjective calibration that would improve the prediction of a number of quantities. If the LSM had been
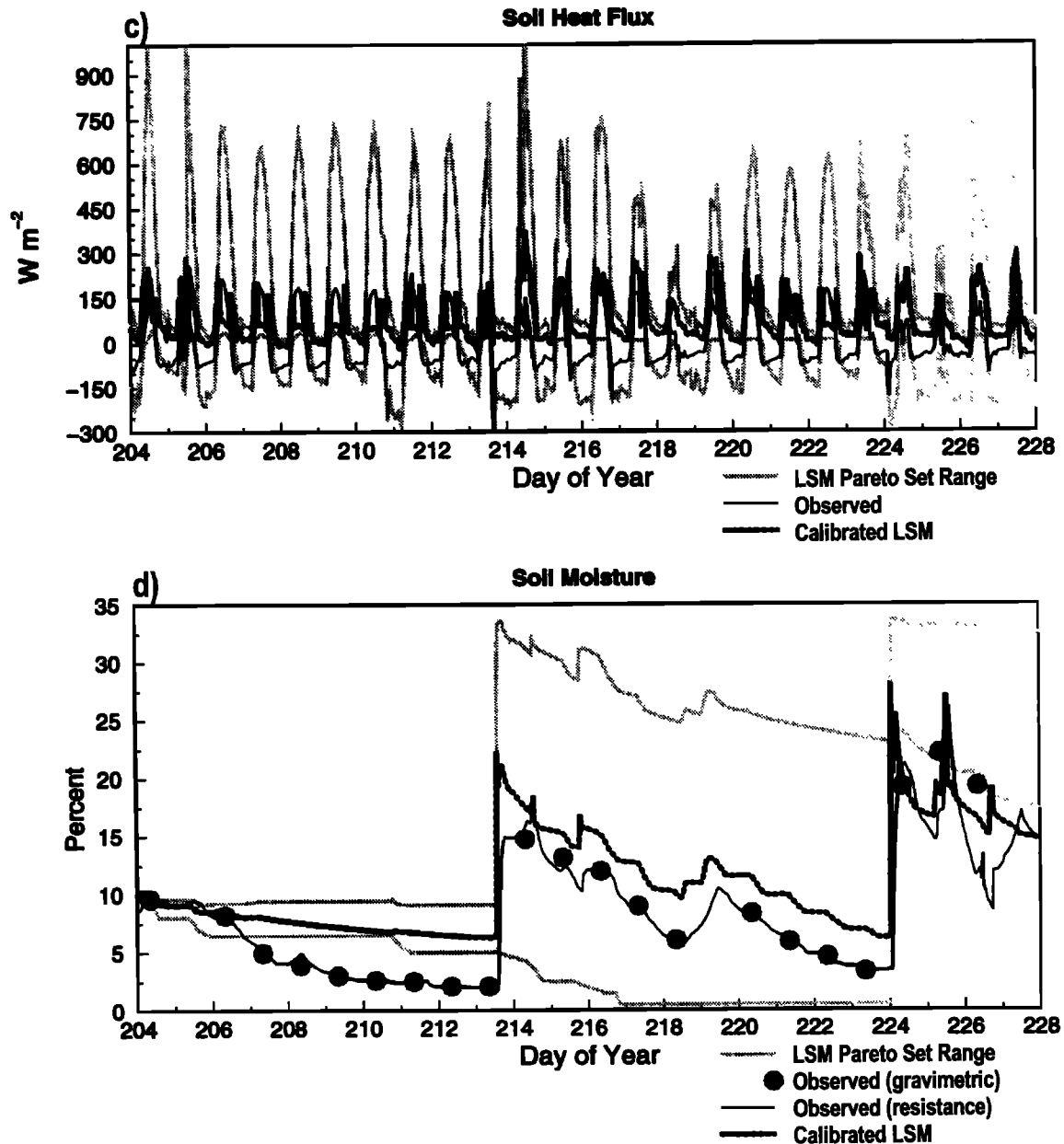
Figure 5. (continued)

calibrated spatially using only remotely sensed soil moisture, then the surface energy flux prediction skill may have degraded.

The use of catchment-averaged parameters in this study is also supported by the small difference between the calculated surface energy fluxes given by a single LSM with aggregate parameters and that given by a distributed array of LSMs. This finding also suggests that a spatially distributed LSM applied at the WGEW with the resolution used in this study is probably not needed if catchment-averaged surface fluxes are required. However, a spatially distributed LSM is required for prediction of spatial patterns of soil moisture at the resolution of the available observations.

LSMs have many parameters which must be carefully specified for their optimal implementation. Several parameters were directly observable at Walnut Gulch, and their values could be readily specified, but others were nonphysical and

were derived by optimization. A multiobjective LSM calibration technique was used to calibrate these parameters by estimating the noninferior parameter region based on a large number of Monte-Carlo parameter set realizations, then selecting the "best" parameter set in a semisubjective way. The chosen parameter set contained physically reasonable values which, in the case of the soil water retention parameters, were superior to measured values (because of the removal of the coarse fraction prior to measurement).

Several additional insights into multiobjective calibration were gained as a result of additional experiments not reported in this paper and for which additional investigation is required. These include the following: (1) Some parameters tend to have similar values for minimum objectives from several sites, indicating that watershed average parameters may be acceptable. However, the spatial patterns present in the PBMR data suggest that improved distributed representations may be

possible, and therefore a lumped representation may not be acceptable for all the parameters. (2) Pareto optimal parameter sets often produce objective functions with large error indicating that some model components may require improvement (the soil heat flux component for example). (3) Some objectives that are linked through model physics, such as sensible and latent heat fluxes, contain similar information. To make the multiobjective calibration more identifiable, only objective functions with significantly different model performance information should be used in the calibration process. (4) The inclusion of soil parameters in the calibration results in significantly better LSM performance because measurements of these parameters were likely biased owing to the removal of the coarse fraction (i.e., rocks and gravel), the presence of macropores, etc. (5) A large number of objective functions leads to a large Pareto set size, making identification of a preferred parameter set impossible. Therefore, when implementing a multiobjective calibration, it is critical to select a minimum number of most relevant objectives. (6) Because multiple parameter sets can be Pareto, multiobjective calibration problems are inherently subjective. Procedures for finding the Pareto parameter sets are relatively automatic and will help to identify parameter sets that minimize all the objectives to some extent. However, to choose a single parameter set from those that are Pareto, a set of rules about which objective (or trade-off among objectives) is most critical to minimize must be adopted. Alternatively, in this context, the concept of a preferred parameter set may not be meaningful. It might be better to understand the range of model behaviors given by the Pareto set. The range and character of the Pareto set may be an indication of model physical deficiencies, as when the observations lie outside the pareto set range. However, a large Pareto set parameter range may also result from a poorly posed parameter estimation problem.

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