3.6 INVERSE ESTIMATION OF SOIL MOISTURE AND SURFACE ENERGY BUDGET FROM IN-SITU SOIL TEMPERATURE DATA

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Abstract: Because soil thermal properties depend on soil moisture, soil temperature is strongly controlled by soil moisture. This provides a possibility to derive soil moisture from soil temperature measurements. Following this motive, this study develops a system to inversely estimate soil moisture profile from soil temperature profile. The forward model is a single-source land surface model to simulate land surface and subsurface processes. The cost function is a non-dimensional function to describe the discrepancy between measured and model-predicted values of soil temperatures. Besides the soil moisture profile, the estimated parameters also include soil hydraulic and thermal parameters. Applications at one synthetic case and three field cases (two in Tibet, and one in Iowa) show the inverse method can reproduce observed soil moisture when the soil properties can be described by soil hydraulic and thermal function used in this study. In addition, this method can simultaneously produce reasonable surface energy partition.

Key words: Inverse approach, soil moisture estimation, soil vertical heterogeneity, surface energy partition.

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1. INTRODUCTION

At many experimental sites of field projects such as GAME (GEWEX Asian monsoon experiments), CEOP (Coordinated Enhanced Observing Period Project), and SMEX (Soil moisture experiments), soil moisture and temperature profiles were simultaneously measured. Using these data, effective soil thermal and hydraulic properties, and surface energy partition can be derived by inverse methods (Yang et al., 2004c). On the other hand, the soil temperature is strongly controlled by soil moisture, because soil thermal properties depend on soil moisture. This provides a possibility to derive soil moisture from soil temperature. Zhang et al. (2004) presented an inverse method and successfully applied it to two sites within the Oklahoma ARM–CART central facilities. However, the soil thermal diffusivity is not a monotonic function of soil water content, and, particularly, its value is not sensitive to soil moisture when the soil becomes wet. Yang and Koike (2004b) point out that this may lead to multi-solutions if only the thermal diffusion equation is solved. They suggest introducing a heat flux condition in the inverse estimation, because the thermal conductivity is a monotonic function of soil moisture and is sensitive to soil moisture.

This study is an attempt in this aspect. We use a single-source land surface model to predict soil moisture, soil temperature, and surface fluxes, a cost function to calculate the discrepancy between observed and model-predicted values of soil temperature, and an efficient scheme to search the global minimum of the cost function.

The paper is organized as follows: first, we present the inverse approach. It consists of three main steps, comprised of (1) a land surface model (Section 2), (2) a cost function (Section 3), and (3) an efficient minimization scheme (Section 4). Then, the inverse approach is applied to one synthetic dataset and three in situ datasets (Section 5). Finally, we summarize the results (Section 6).

2. A SINGLE-SOURCE LAND SURFACE MODEL

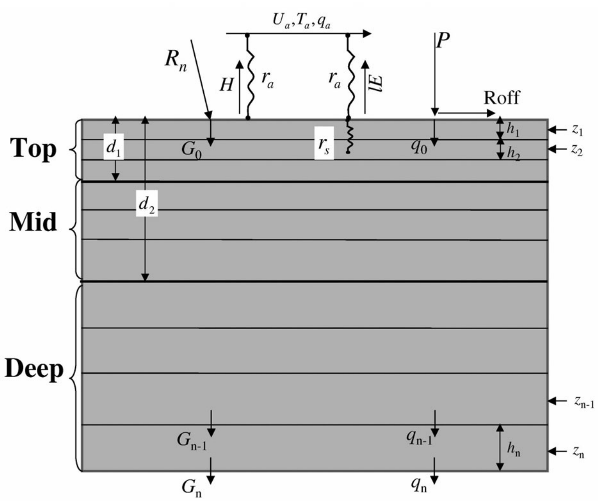

Figure 1 Schematic of the single-source land surface model used in this study. There are three soil domains (Top, Mid, Deep), each of which contains multiple computational layers. All the symbols have their common meaning.

A single-source model does not distinguish the separate contribution to the turbulent fluxes from the vegetation and from the ground, and it usually has fewer parameters to be calibrated than a dual-source model. Yang et al. (2004a) indicates that a single-source model is applicable to bare soil surfaces or sparsely and shortly vegetated surfaces. The model structure used in this study is shown in Figure 1 and has three distinct features.

(1) Single-source flux parameterizations for bare soils and/or shortly vegetated surfaces are improved based on recent experiments in the Tibetan Plateau (Yang et al., 2002; Yang et al., 2003).

(2) Soil subsurface water and heat flows are simulated by a multi-layer scheme. Richards' Law is used to calculate soil water flow, and thermal diffusion equation is used to calculate soil heat flow. The hydraulic functions (hydraulic conductivity and retention curve) are described by Clapp and Hornberger (1978). The thermal conductivity is described by Johansen (1975) and heat capacity by a formula recommended in the Global Soil Data Task (2000).

(3) Soil vertical heterogeneity is parameterized. Soil structures are not only horizontally heterogeneous but also often vertically heterogeneous. The top layer of a soil can have different soil textures and amounts of organic matters from the deep layer. A typical example is the prairie in the Central and Eastern Tibetan Plateau, where the surface is covered by short vegetation. The vegetation develops very plentiful roots in the top 10 to 20 centimeters to adapt the harsh climate in the plateau. Yang et al. (2004c) pointed out that existence of dense vegetation roots in topsoils may significantly reduce thermal conductivity, increase soil water potential, and enhance surface evaporation. Numerical experiments (Koudelova, 2003; Gao et al., 2004) have shown the difficulties in producing observed soil moisture, ground temperature, and surface energy partition at several plateau sites. Therefore, the vertically heterogeneous soil column is approximated by two uniform domains – a near-surface soil domain and a bottom soil domain, and a transitional domain between the two.

To accurately simulate soil heat flow and water flow, each domain consists of a number of layers, thinner in the top domain (~1 cm) and thicker in the bottom domain (~10 cm). The number of computational layers is adjustable. In our case studies (Section 5), there are 30 or 40 computational layers, and the total soil depth is 1.6 m. The LSM is integrated over 2~3 months with a time step of several minutes. More details are presented in the case studies (Section 5). The process parameterizations have been described in Yang et al. (2004c), and will not be duplicated here.

3. INVERSE MODEL

3.1 Input data

Input data of the inverse model include forcing data to drive the LSM, soil temperature for model calibration, soil moisture and/or heat fluxes for validations. The forcing data are routinely measured at an automatic weather station (AWS). Soil moisture and temperature are measured by a soil moisture and temperature measuring system (SMTMS). The SMTMS consists of multiple temperature sensors (accuracy ~ 0.1 K) and TDR (time domain reflectometry) moisture sensors (accuracy ~ 0.03), and the sampling frequency can be 30 ~ 60 minutes or finer. Additional details about the case studies are presented in Section 5.

3.2 Optimized parameters

There are many parameters in the LSM. Surface albedo can be derived from measured downward and upward short-wave radiations, or estimated by empirical formulas (Pleim and Xiu, 1995). Aerodynamic roughness length can be derived from wind profiles (Kohsiek et al., 1993; Yang et al., 2003). The surface emissivity is specified as 0.97 since it does not significantly affect simulated results. Soil hydraulic parameters are estimated by empirical formula (Cosby et al., 1984):

$$K_s = 7.0556 \times 10^{-6.884+1.53 sand} \ \mathrm{m\,s^{-1}}, \quad (1)$$

$$\psi_s = -0.01 \times 10^{1.88-1.31 sand} \ \mathrm{m}, \quad (2)$$

$$b = 2.91 + 15.9 clay, \quad (3)$$

where $sand$ and $clay$ denote percentage of sand and clay in a dry soil.

The optimized parameters are listed in Table 1. They are: the soil porosity θ_s, the soil bulk density ρ_d, the maximum soil thermal conductivity λ_m, the boundary depths of transitional domain (d_1, d_2), and $sand$ and $clay$. The initial profile of soil water content is nonlinearly interpolated by soil water content at the surface θ_{01} and at the surface and the bottom θ_{0n}. Both θ_{01} and θ_{0n} are optimized.

3.3 Objective function

$$F = RMSE_T, \quad (4)$$

where $RMSE_T$ represents the root mean square errors of soil temperature over all measuring depths during the optimizing period.

Table 1 Optimized parameters of the land surface model.

Symbol	Unit	Lower bound	Upper bound
θ_s	$\mathrm{m^3\,m^{-3}}$	0.25	0.7
ρ_d	kg m^{-3}	$1900(1-\theta_s)$	$2650(1-\theta_s)$
$sand$	—	5	95
$clay$	—	3	60
λ_m	$\mathrm{W\,m^{-1}\,K^{-1}}$	0.5	3
d_1	m	0	0.3
d_2	m	$d_1 + 0.02\,\mathrm{m}$	1.6
θ_{01}.	$\mathrm{m^3\,m^{-3}}$	θ_{rsd}	θ_s
θ_{0n}	$\mathrm{m^3\,m^{-3}}$	θ_{rsd}	θ_s

4. OPTIMIZATION ALGORITHM

Optimizing parameters is a tough task in inverse problems of soil parameters because cost functions usually have multi-parameters and are highly nonlinear, non-derivable and even discontinuous. The parameter space usually contains multiple minima. To find the global minimum, the Levenberg-Marquardt method (Marquardt, 1963) is widely used in inverse models (e.g., Parkin *et al*., 1995; Simunek and van Genuchten, 1996; Hopmans *et al*., 2002), but the inverse solution is sensitive to initial parameter guesses. To overcome this problem and to find globally optimal parameters, several effective methods has been developed in past twenty years, such as the simulated annealing [Kirkpatrick et al., 1983], the annealing-simplex method (Pan and Wu, 1998), genetic algorithms (Goldberg, 1989), the sequential uncertainty fitting inverse (Abbaspour, et al., 1997). This study adopts the Shuffled Complex Evolution method developed at The University of Arizona (SCE-UA) (Duan *et al*., 1992; Duan *et al*., 1993). This method is based on a synthesis of four concepts: (1) combination of deterministic and probabilistic approaches; (2) systematic evolution of a 'complex' of points spanning the parameter space, in the direction of global improvement; (3) competitive evolution; (4) complex shuffling. The synthesis of these elements makes the SCE-UA method effective and robust, and also flexible and efficient. It has been widely used in parameter calibration of various models.

5. CASE STUDIES

The inverse approach described above is used to calibrate the land surface model to two types of data sets. The first is a numerically generated data set (hereafter identical twin). The second is field-collected data set at a GAME-Tibet site (Anduo), a CEOP-Tibet site (Naqu), and a SMEX02 site (WC33). The following introduce the results of these case studies.

5.1 Identical twin

5.1.1 Data set. The experiment design is very similar to that of the GAME-Tibet observations (see section 5.2.1). We assume that the total soil depth is 1.6 m and that this total depth is represented by three soil layers with thickness values of 0.10, 0.15, 1.35 meters (in other words, $d_1 = 0.1\,\mathrm{m}$, $d_2 = 0.25\,\mathrm{m}$). We also assume that the topsoil is a typical clay loam with a higher porosity and water potential and the bottom soil is a typical sandy loam with a lower porosity and water potential. The ground is a bare soil surface, which is wetted by two-day continuous precipitation every 10 days in the first month, and dried in other days. A diurnally varying wind speed, temperature, radiations, and a constant specific humidity are used to drive the model.

Table 2 Parameter values of the identical twin study in the forward run.

Parameter	Top domain (Clay loam)	Bottom domain (Sandy loam)
θ_s ($m^3\,m^{-3}$)	0.476	0.416
ρ_d (kg m-3)	1309	1460
θ_r ($m^3\,m^{-3}$)	0.141	0.043
K_s ($m\,s^{-1}$)	1.31×10^{-6}	7.11×10^{-6}
n	1.35	1.41
α (cm^{-1})	0.00435	0.0230
λ_m ($W\,m^{-1}\,K^{-1}$)	1.59	2.16
Soil depth (m)	0~0.1	0.25~1.6

To examine the sensitivity of the inverse estimation, we deliberately introduce "measurement" errors and model errors. "Measurements" errors are introduced by using a coarse spatial resolution (30 layers) and temporal resolution (400 s) in the forward run, while using a fine resolution (40 layers, 200 s) in the inverse estimation. Model errors are introduced by using different soil thermal and hydraulic functions in the forward run and the inverse runs.

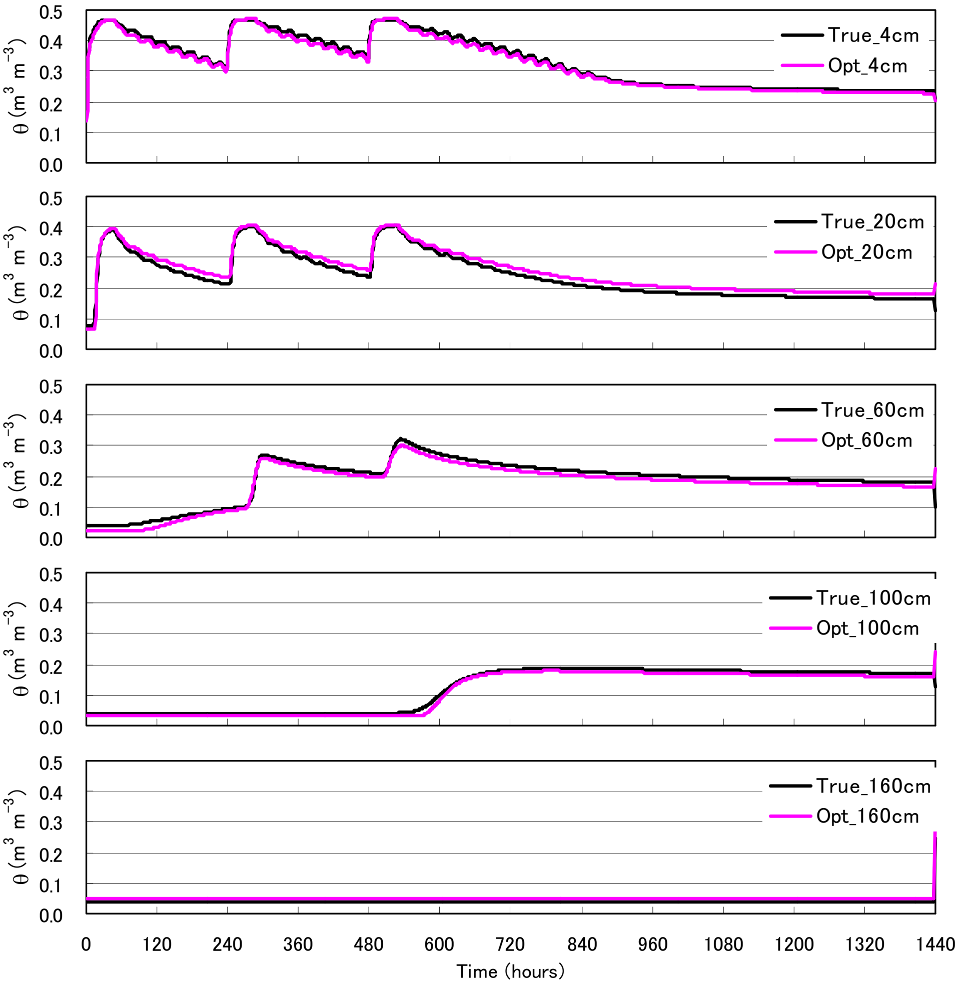

Figure 2 Comparison of soil moisture between the truth run (from the forward run) and the optimized values (from the inverse calibration) for the synthetic dataset.

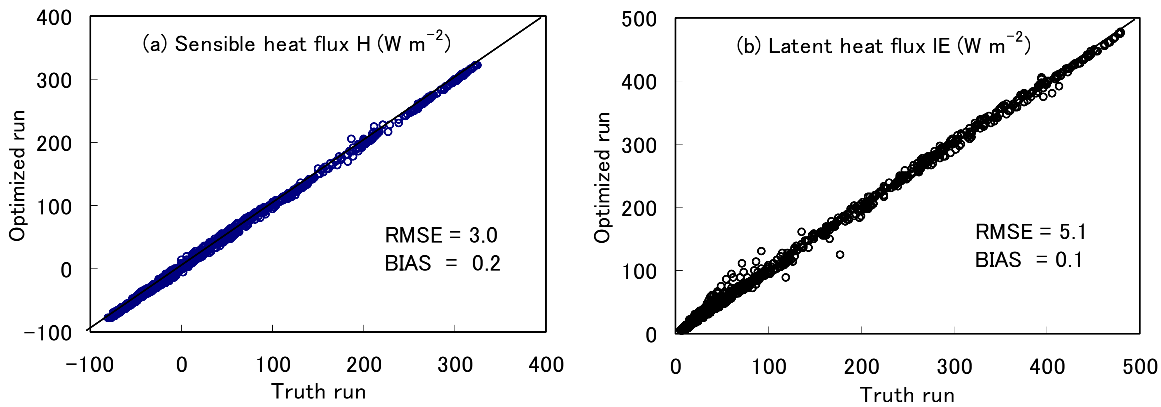

Figure 3 Comparison of sensible heat flux and latent heat flux between the truth run (from forward run) and the optimized values (from the inverse calibration) for the synthetic dataset.

The "true" values of soil parameters used in the forward run are shown in Table 2. Soil moisture is initialized by the residual values θ_r , and soil temperatures are initialized with a constant temperature of 298 K. The model is then integrated 60 days (hereafter forward run). Soil moistures at five depths (0.04, 0.2, 0.6, 1.0, 1.6 m), and soil temperatures at nine depths (0.0, 0.04, 0.2, 0.4, 0.6, 0.8, 1.0, 1.3, 1.6 m) are recorded hourly, analogous to measurements at the GAME-Tibet experiments. These data are used as input data in the inverse estimation.

5.1.2 Estimated soil moisture and surface energy budget. Figure 2 shows a good agreement between estimated soil moisture and "measured" one at five depths. Figure 3 present the comparisons of energy partition between the "truth" run and the optimized run. The derived sensible heat fluxes and latent heat fluxes are close to the true values.

5.2 GAME-Tibet Anduo site

5.2.1 Description of site and data set. The GAME-Tibet Anduo site (Lat. 32.241° N, Lon. 91.635° E, Alt. 4700m) locates at the central Tibetan Plateau. This site is covered by sparse and short grasses in the summer, but vegetation. roots share a large volume of the surface soil layer in all seasons and the bulk density of the soil is therefore much lower than the deeper soil. This discontinuity of the soil structure is also found at other GAME-Tibet sites. Observations show soil water content is high near the surface, decreases in the transitional soil, and increases again in the deep soil. By a sensitivity study using a dual-source land surface model, Yang et al. (2004a) show that the vegetation can change the energy partition between the vegetation and the ground surface, but the surface energy partition between the sensible heat and the latent heat is insensitive to the leaf area index and the vegetation coverage for the plateau sparse and short prairie, and thus a single-source model is applicable to this site.

Table 3 Measurement items and levels at the GAME-Tibet Anduo site, 1998.

Items	Height or depth (m)
Planetary Boundary Layer (PBL) station (30 min. average):	
Wind speed and direction	1.90, 6.00, 14.10
Air Temperature	1.55, 5.65, 13.75
Humidity	1.55, 5.65, 13.75
Pressure	Surface
Precipitation	Surface
Radiation	14.0
Turbulent fluxes	2.85
Soil temperature	0.0, 0.05, 0.1, 0.2
SMTMS (60 min. average):	
Soil moisture	0.05, 0.2, 0.6, 1.0, 1.6, 2.58
Soil temperature	0.05, 0.2, 0.4, 0.6, 0.8, 1.0, 1.3, 1.6

To understand the land-atmosphere interactions on the plateau, intensive observations were carried out at Anduo during May-Sepetember 1998. Table 3 lists the field-collected data concerning the inverse estimation, including 30-minute-recorded forcing data for driving the LSM, hourly-recorded soil temperature and moisture profiles for the inverse estimation. Moreover, there are two sets of observed energy partitions for verifying model output: in one set, the sensible heat fluxes were measured by the eddy-correlation technique, and the latent heat fluxes were derived from the surface energy budget equation (Note: the latent heat fluxes were actually measured by the eddy-correlation, but the measurements are not trustable due to a sensor problem, see Yang et al. (2004a) for more details); the other set was calculated from the observed air temperature and humidity profile by the Bowen ratio method.

5.2.2 Estimated soil moisture and surface energy budget. Figure 4 shows the comparison between estimated soil moisture and "measured" one at five depths; Figure 5 presents the scatter-plots showing the comparisons of energy partition between the simulation and the observation by eddy-correlation technique (or by Bowen ratio method). Both retrieved soil moisture and surface energy partition are comparable to the observed ones. Particularly, the optimized sensible heat fluxes ranges between the two sets of observations (by the eddy-correlation and by the Bowen ratio), i.e., larger than the observation by the eddy correlation while smaller than the observation by the Bowen ratio method. However, SiB2 cannot produce observed soil moisture, surface temperature, and energy partition, as demonstrated by Koudelova (2003). These comparisons in surface energy budget suggest that the inverse approach considering soil vertical heterogeneity successfully provides a reasonable estimate to the turbulent fluxes, while fails to do when the vertical heterogeneity is ignored. The dense vegetation roots in the topsoil lead to high latent heat fluxes while low sensible heat fluxes. This, in turn, suggests the importance of soil vertical heterogeneity in controlling surface soil state and thus surface energy partition.

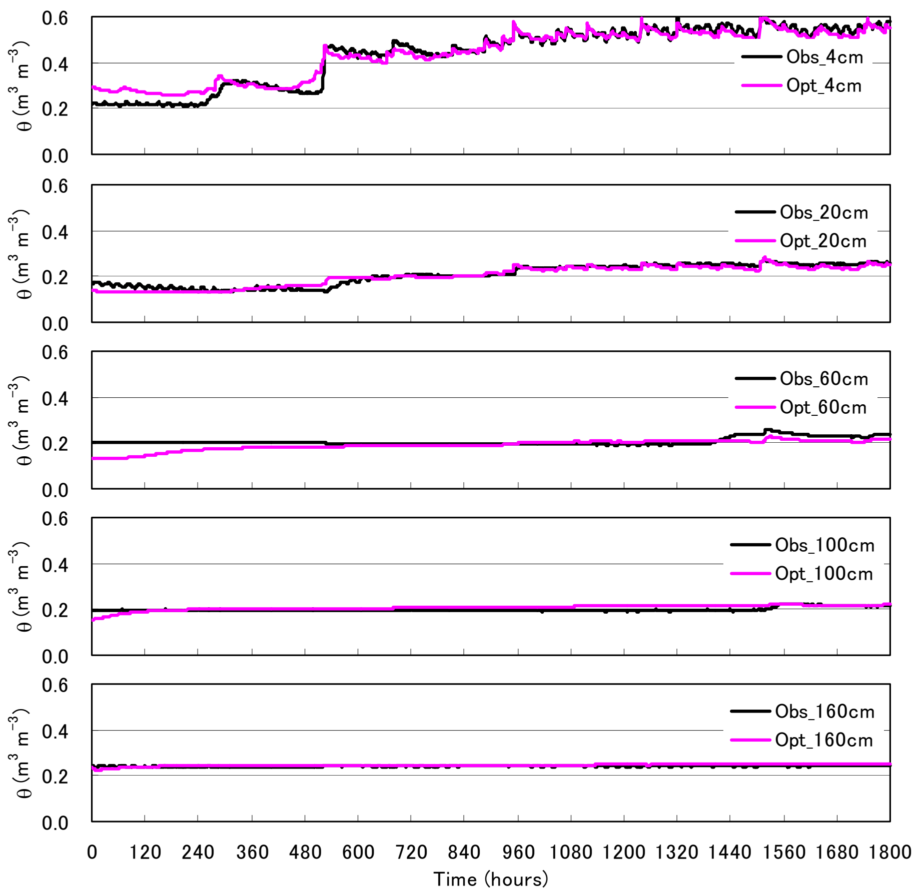

Figure 4 Comparison of soil moisture between observation (Obs) and the retrieved one from soil temperature (Opt) for the GAME-Tibet Anduo site, 1998.

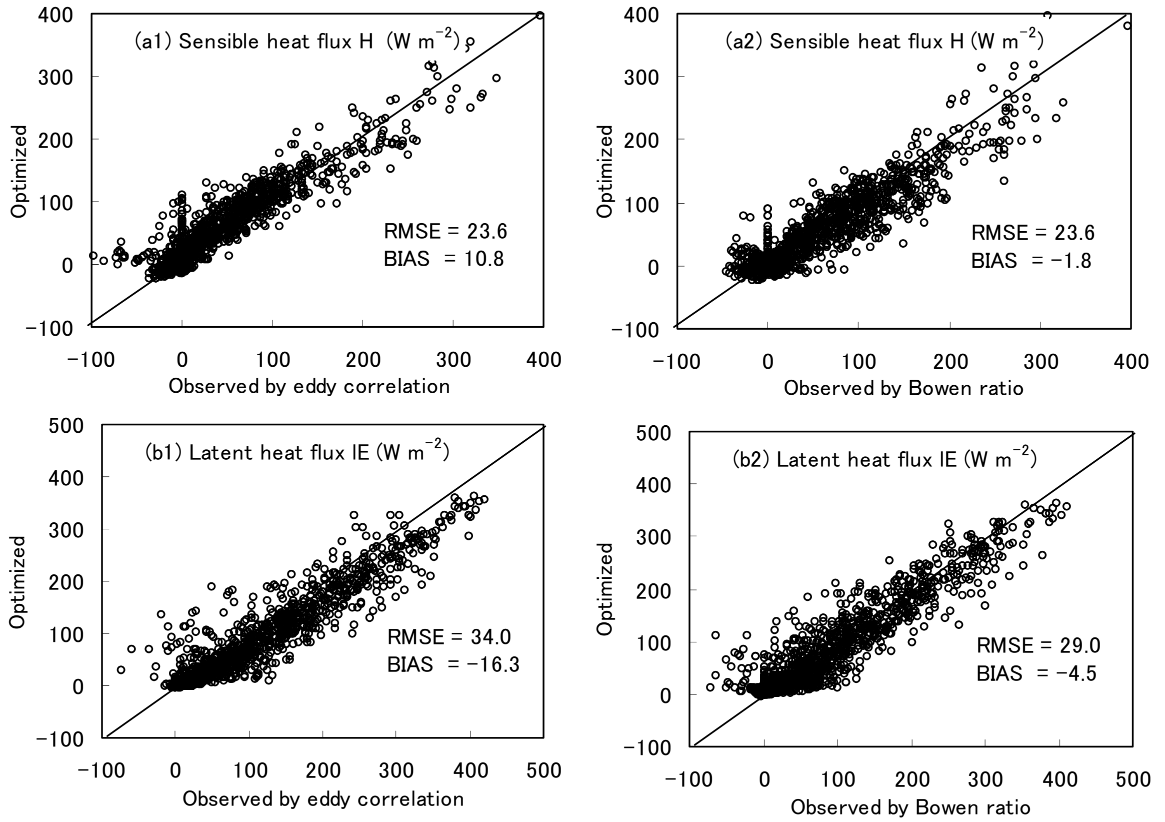

Figure 5 Comparison of sensible heat flux and latent heat flux between the observations and the optimized values (from the inverse calibration) for the GAME-Tibet Anduo site during 16 June ~ 30 August, 1998.

5.3 CEOP-Tibet Naqu site

5.3.1 Description of site and data set. The CEOP-Tibet Naqu site (Lat. 31.379°N, Lon. 91.900°E, Alt. 4580 m) locates at the central Tibetan Plateau. This site is covered by sparse and short grasses in the summer, but vegetation roots are not as dense as at Anduo site. A distinct feature is that below the root layer, gravels share a big volume, which makes difficulties in measuring soil moisture and also describing soil thermal and hydraulic behaviors.

Data collection at this site was implemented from September 2000 to August 2002, but failed occasionally in wintertime. Table 4 lists the field-collected data concerning the inverse estimation. Turbulent fluxes can be derived from Bowen ratio method by temperature and specific humidity profiles.

Table 4 Measurement items and levels at the CEOP-Tibet Naqu site, 2001.

Items	Level (m)
AWS (average of 50:05～60:00 of each hour):	
Wind speed and Direction	0.5, 2.0, 10.0
Air Temperature	0.5, 2.0
Humidity	0.5, 2.0
Pressure	Surface
Precipitation	Surface
Radiation	
Soil temperature	0.0, 0.04, 0.1, 0.2, 0.4
SMTMS (60 min. average):	
Soil moisture	0.05, 0.2, 0.6, 1.0, 1.6, 2.10
Soil temperature	0.05, 0.2, 0.4, 0.6, 0.8, 1.0, 1.3, 1.6

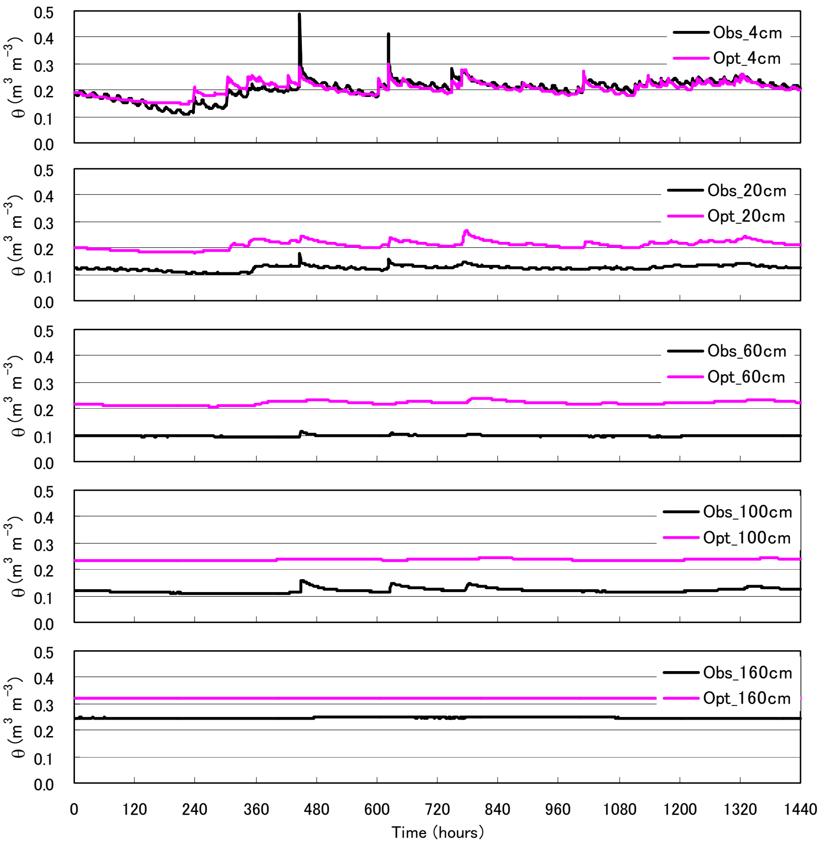

Figure 6 Same as Figure 4, but for CEOP-Tibet Naqu site, 2001.

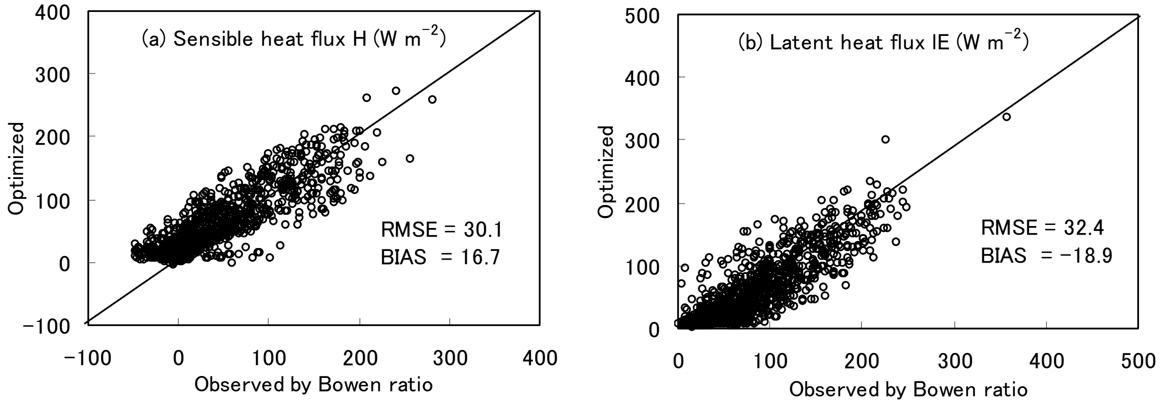

Figure 7 Comparison of sensible heat flux and latent heat flux between the values derived from Bowen ratio and the optimized values (from the inverse calibration) for the CEOP-Tibet Naqu site during 1 July ~ 30 August, 1998. The root mean square error and bias are indicated for each variable.

5.3.2 Estimated soil moisture and surface energy budget. Figure 6 shows the comparison between estimated soil moisture and "measured" one at five depths; Figure 7 presents the scatter-plots showing the comparisons of energy partition between the simulation and the observation by Bowen ratio method. We can see the surface soil moisture is well reproduced by the inversion, but observed soil moisture in deep layers is obviously less than the retrieved one. We suspect that the normal soil hydraulic and thermal functions used in this model are not suitable for the mixture of sandy particles and gravels at this site. Since the surface state (soil moisture and temperature) are well reproduced, the surface energy partition looks comparable to the fluxes derived from Bowen ratio method.

5.4 SMEX02-WC33 site

5.4.1 Description of site and data set. The SMEX02 was conducted during the summer (middle June – middle July). At SMEX02 WC33 site (Lat. 41.978°N, Lon. 38.642°E, Alt. 318m), the University of Tokyo collected ground data and microwave brightness temperatures for developing algorithm to derive soil moisture from satellite data. Although this site was covered by soybean and corn during the experimental period, vegetation on a small area is cleared, where soil moisture and temperature were measured. The measurements are shown in Table 5, including soil moistures were measured at six depths, and soil temperatures were measured at 10 depths. Flux data was not available.

Table 5 Measurement items and levels at the SMEX02 WC33 site, 2002.

Items	Level (m)
AWS (10 min. average):	
Wind speed and Direction	2.0
Air Temperature	2.0
Humidity	2.0
Pressure	Surface
Precipitation	Surface
Radiation	
SMTMS (10 min. average):	
Soil moisture	0.015, 0.04, 0.08, 0.15, 0.25, 0.50
Soil temperature	0.0, 0.015, 0.04, 0.06, 0.08, 0.10, 0.15, 0.25, 0.50

5.4.2 Estimated soil moisture. Figure 8 shows a good consistence between the measured and the estimated soil moisture at all depths except at 4 cm. The moisture at 4cm is lower than the moisture in the shallower layer (at 1.5cm) and the deeper layer (8cm). This observed complex moisture profile cannot be reproduced by our simple sandwich-soil structure.

6. CONCLUSIONS

This work develops an inverse system to derive soil moisture and surface energy budget from soil temperature. It consists of a single-source land surface model to predict soil moisture and temperature profiles and surface fluxes, a cost function to calculate the discrepancy between observed and model-predicted values of soil temperature, and an efficient scheme SCE-UA to search the global minimum of the cost function. We parameterize vertically heterogeneous soils by a sandwich-like model structure (two uniform domains and a transitional domain). Unlike early studies that solves the thermal diffusion equation, we introduce surface heat flux as the upper boundary condition from surface energy balance, which can lead to more reliable soil moisture estimation.

We apply this system to a numerical synthetic data set and three field sites. The results suggest that the inverse method can reproduce observed soil moisture when the soil properties can be described by normal soil hydraulic and thermal functions. In particular, surface soil moisture, which is our most concerning, can be derived quite reliably. The method also simultaneously produces reasonable surface energy partition. The results may serve to simplify field experiment design in the future.

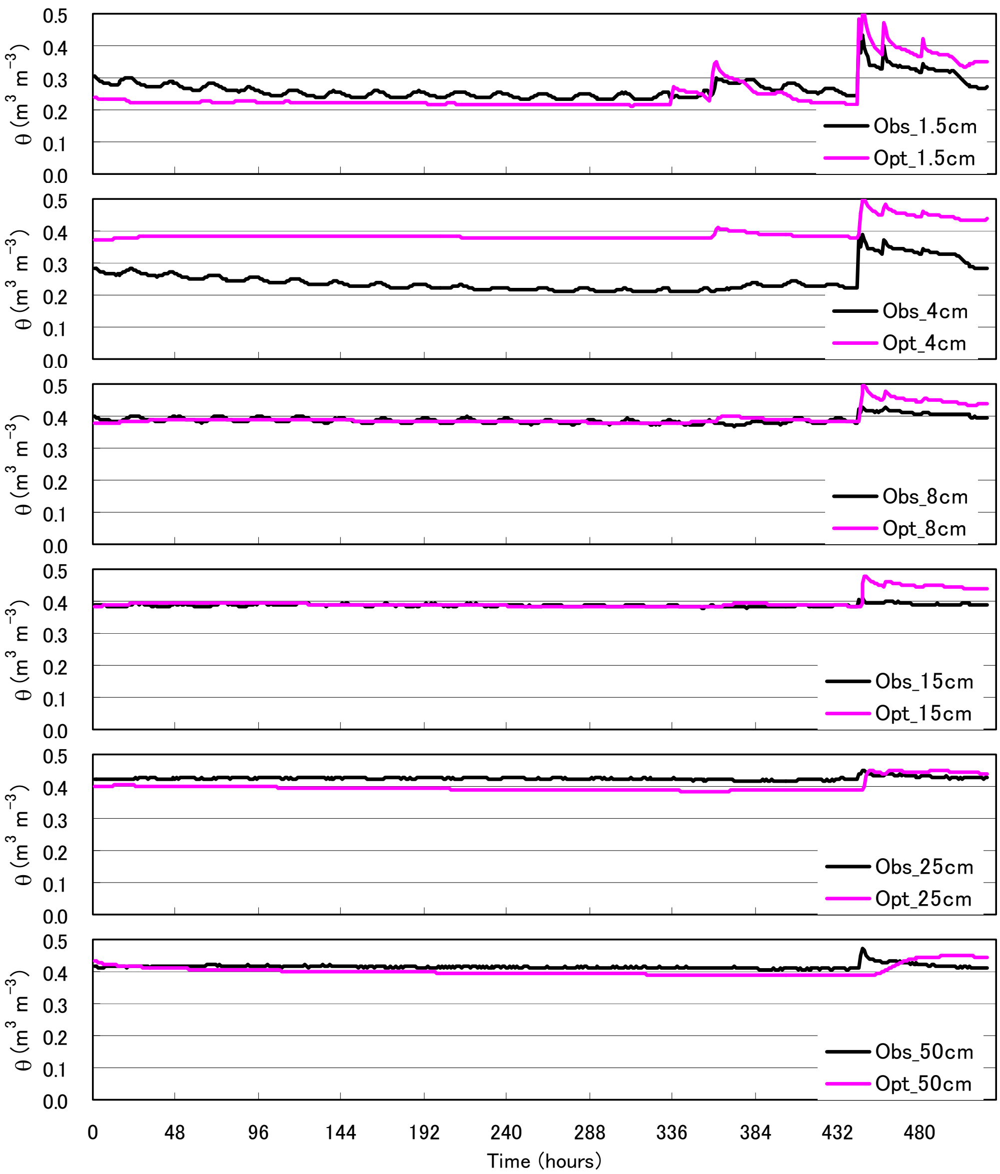

Figure 8 Same as Figure 4, but for SMEX02 WC33 site, 2002.

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