A Variational Method for Estimating Near-Surface Soil Moisture and Surface Heat Fluxes*

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ABSTRACT

A variational data assimilation method is proposed to estimate the near-surface soil moisture and surface sensible and latent heat fluxes. The method merges the five parts into a cost function, i.e., the differences of wind, potential temperature, and specific humidity gradient between observations and those computed by the profile method, the difference of latent heat fluxes calculated using the ECMWF land surface evaporation scheme and the profile method, and a weak constraint for surface energy balance. By using an optimal algorithm, the best solutions are found. The method is tested with the data collected at Feixi Station (31.41°N, 117.08°E) supported by the China Heavy Rain Experiment and Study (HeRES) during 7-30 June 2001. The results show that estimated near-surface soil moistures can quickly respond to rainfall, and their temporal variation is consistent with that of measurements of average soil moisture over 15-cm top depth with a maximum error less than 0.03 $m^3\ m^{-3}$. The surface heat fluxes calculated by this method are consistent with those by the Bowen ratio method, but at the same time it can overcome the instability problem occurring in the Bowen ratio method when the latter is about -1. Meanwhile, the variational method is more accurate than the profile method in terms of satisfying the surface energy balance. The sensitivity tests also show that the variational method is the most stable one among the three methods.

Key words: soil moisture, sensible heat flux, latent heat flux, variational method

1. Introduction

Soil moisture is a key variable in the coupled land and atmospheric models. The near-surface soil moisture status has large impact on evaporation for bare soil and land regions with moderate vegetation cover (e.g., short grass) and can control the partition of available energy into sensible and latent heat fluxes. In summer, when the energy partition becomes an important factor for the stability of near-surface atmosphere, soil moisture fields may exert significant influence on the formation of the convective boundary layer (sometimes including moist convection and precipitation) (Castelli et al., 1999; EK and Cuenca, 1994; Ma et al., 2000). Koster et al. (2000) showed that soil moisture dominates over SSTs in controlling summer precipitation over the United States and other large continental region. In addition, soil moisture status can provide some useful information on the prediction of crop yield, infiltration and surface runoff, land use, etc. (Schmugge et al., 1980). Soil moisture can be obtained from point measurements, e. g., the Thermogravimetric Method (AS), the Time Domain Reflectometry (TDR), etc., and from the remote sensing sounding which provides the simultaneous measurements of near-surface soil moisture over large areas but the errors are relatively larger than those from point measurements. Besides direct measurements, soil moisture can be obtained through the indirect methods, such as parameter identification, prediction with the hydrological models, and land data assimilation schemes (Zhang et al., 2004).

Like soil moisture, surface heat flux is also an important variable which characterizes the interaction between land and atmosphere, and its spatial and temporal variations have a large impact on the atmospheric movement over land surface. Regardless of the interaction between atmosphere, ocean, and land, the

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main physical process is the exchange of heat, water, and momentum between earth's surface and lower atmosphere. Therefore, how to accurately calculate the near-surface fluxes is of great importance for weather and climate prediction. Like the soil moisture, the surface heat fluxes can be directly measured and indirectly derived with the aid of other data (Hu and Qi, 1991). The eddy covariance technique provides a relatively direct means of measuring the fluxes without taking an assumption concerning eddy diffusivities. But it should be noted that the eddy covariance sensor is relatively expensive and its maintenance and calibration are also complex. The indirect means include the aerodynamic method (i.e., the profile method), the Bowen ratio energy balance method (i.e., the Bowen ratio method), the combined method, and so on (Hu and Qi, 1991; Thom et al., 1975). Although the influence of the observational errors can be analyzed after the calculation in the indirect method, it is impossible to take the statistic characteristics of errors in measurements as well as aerodynamic formulae into consideration in the process of calculating the fluxes. From the viewpoint of methodology the indirect method is a kind of deterministic method. Because of the errors in measurements (including instrumental error and sampling error), the data always contain some uncertainties; in other words, observation is only a kind of approximation to the true atmosphere and it is almost impossible to perfectly know the true atmospheric states (Du, 2002). To this problem, one of the possible solutions would be to consider observations as random variables and estimate the fluxes by stochastic method. Xu and Qiu (1997) firstly introduced the stochastic view into the estimation of surface heat fluxes by combining the profile method and the Bowen ratio method with a variational technique. In this paper we will extend their method and investigate the estimation of near-surface soil moisture as well as surface heat fluxes over bare soil or vegetated surface with short root.

Castelli et al. (1999) implemented a variational data assimilation procedure for the estimation of surface heat flux and a soil moisture index, in which the ground temperature equation containing surface energy balance is included as part of the data assimilation through an adjoint method. In their method the atmospheric states near the surface are not included. Because evaporation depends not only on the status of soil moisture but also on the stability of near-surface atmosphere, the latter should be considered if we want to correctly estimate those parameters. In this paper we implement a variational scheme for the estimation of surface heat fluxes and near-surface soil moisture by assimilating the observations of air temperature, pressure, humidity, wind, and radiation under the constraints of surface energy balance. In contrast to the indirect method, the proposed variational method makes full use of all information contained in the physical laws and statistical characteristics of observational errors. The scheme is tested with the HeRES data at Feixi Station, showing that it can predict the variation of near-surface soil moisture and overcome the instability in the Bowen ratio method.

2. HeRES location and data

The observational data used in this study were collected by the surface Bowen ratio energy balance system (SERBS) supported by the HeRES Program during 7-30 June 2001 at Feixi Experimental Station in the Huaihe River Basin. The surface around the station was flat and covered with short sparse grasses. The soil type is clay. The SERBS included the following measurements: three-level horizontal wind speeds, temperatures, and water vapor pressures, respectively, at heights of 1, 4, and 10 m, precipitation, net radiation flux (near the surface), soil heat flux, and soil temperatures at depths of 0, 10, 20, and 40 cm. The averaged soil moistures at 2 layers (0-15 and 15-30 cm below the surface) were also measured. All observational instruments were calibrated at the gauging center of the China Meteorological Administration before the field observation.

3. Profile relations and the variational method

Based on the Monin-Obukhov similarity theory, the vertical profiles of wind, temperature, and specific humidity for turbulent flows in the surface layer can be described by the following equations:

$$u(z)=\frac{u_*}{k}\Big[\ln(\frac{z}{z_{0\mathrm{m}}})-\psi_\mathrm{m}(\frac{z}{L})+\psi_\mathrm{m}(\frac{z_{0\mathrm{m}}}{L})\Big], \tag{1}$$

$$\theta(z)=\theta_\mathrm{s}+\frac{\theta_*}{k}\Big[\ln(\frac{z}{z_{0\mathrm{h}}})-\psi_\mathrm{h}(\frac{z}{L})+\psi_\mathrm{h}(\frac{z_{0\mathrm{h}}}{L})\Big], \tag{2}$$

$$q(z)=q_\mathrm{s}+\frac{q_*}{k}\Big[\ln(\frac{z}{z_{0\mathrm{q}}})-\psi_\mathrm{q}(\frac{z}{L})+\psi_\mathrm{q}(\frac{z_{0\mathrm{q}}}{L})\Big], \tag{3}$$

where u_* is the frictional velocity defined by $u_*=\tau/\rho$ in association with wind stress τ and air density ρ; θ_* and q_* are flux temperature and humidity scales, respectively; $z_{0\mathrm{m}}$, $z_{0\mathrm{h}}$, and $z_{0\mathrm{q}}$ are roughness lengths for momentum, heat, and humidity, respectively; $L=u_*^2\theta/kg\theta_*$ is the Obukhov length; $k\approx0.4$ is the Von K*á*m*á*n constant; ψ_m, ψ_h, and ψ_q are the stability functions. For an unstable case ($\theta_*<0$ or $L<0$), the stability functions ψ_m and ψ_h are taken as (Paulson, 1970; Xu and Qiu, 1997)

$$\psi_\mathrm{m}=2\ln\frac{1+x}{2}+\ln\frac{1+x^2}{2}-2\mathrm{arctg}x+\frac{\pi}{2}, \tag{4}$$

$$\psi_{\mathrm{h,q}}=2\ln\frac{1+x^2}{2}, \tag{5}$$

where $x=(1-16z/L)^{1/4}$. For a stable case ($\theta_*>0$, or $L>0$), the stability function ψ_m and ψ_h are given by (Beljaars and Holtslag, 1991)

$$-\psi_\mathrm{m}=a\frac{z}{L}+b(\frac{z}{L}-\frac{c}{d})\exp(-d\frac{z}{L})+\frac{bc}{d}, \tag{6}$$

$$-\psi_{\mathrm{h,q}}=(1+\frac{2az}{3L})^{3/2}+b(\frac{z}{L}-\frac{c}{d})\cdot\exp(-d\frac{z}{L})+\frac{bc}{d}-1, \tag{7}$$

where a=1, b=0.667, c=5, d=0.35, and the stability function ψ_q=ψ_h is assumed. Sensible and latent heat fluxes are computed, respectively, by

$$H=-\rho c_p u_*\theta_*, \tag{8}$$

$$\lambda E=-\rho\lambda u_* q_*, \tag{9}$$

where c_p is the specific heat at constant pressure and λ is the latent heat of evaporation.

Various formulations of evaporation over the land surface have been proposed (Stull, 1991; Manfouf and Noihan, 1991), but we will not compare them since our main focus is to test the proposed variational method in this paper. For facility estimation of the near-surface soil moisture, we use the evaporation formulation adopted by the European Centre for Medium-Range Weather Forecasts (ECMWF) (Viterbo and Beljaars, 1995), and the impact of soil type is considered. In this scheme, evaporation comes from three parts, i.e., the interception reservoir, vegetation transpiration, and bare soil. It is relatively difficult to accurately calculate the interception reservoir coming from precipitation and dew, hence the evaporation from the interception reservoir is not included in our data assimilation scheme but we will try to reduce its impact on the estimation by implementing other methods (see Section 4.2 for further explanation). For bare soil, the evaporation is calculated as

$$E_\mathrm{g}=\frac{\rho}{r_\mathrm{a}}\Big[\alpha q_\mathrm{sat}(T_\mathrm{sk},p_\mathrm{s})-q_\mathrm{L}\Big], \tag{10}$$

where q_L is the specific humidity near the surface; p_s is the surface pressure; T_sk is the skin temperature which can be derived from the surface potential temperature θ_s; and α is the soil moisture index which depends on the soil moisture w of the top model layer with the following relationship:

$$\alpha=\begin{cases}0.5\Big[1-\cos(\dfrac{\pi w}{1.6w_\mathrm{cap}})\Big] & w<w_\mathrm{cap},\\ 1 & w\geqslant w_\mathrm{cap.}\end{cases} \tag{11}$$

Here, w_cap is the soil moisture at field capacity.

The dry vegetation transpires at the rate

$$E_\mathrm{v}=\frac{\rho}{r_\mathrm{a}+r_\mathrm{c}}\Big[q_\mathrm{sat}(T_\mathrm{sk},p_\mathrm{s})-q_\mathrm{L}\Big], \tag{12}$$

where r_a is the aerodynamic resistance and r_c is the canopy resistance which can be expressed as

$$r_\mathrm{a}=\frac{1}{ku_*}\Big[\ln(\frac{z}{z_{0\mathrm{h}}})-\psi_\mathrm{h}(\frac{z}{L})+\psi_\mathrm{h}(\frac{z_{0\mathrm{h}}}{L})\Big], \tag{13}$$

$$r_\mathrm{c}=\frac{r_\mathrm{smin}}{L_\mathrm{f}}f_1(P_\mathrm{AR})f_2(\overline{w}). \tag{14}$$

Here, r_smin is the minimum stomatal resistance of a single leaf; L_f is the leaf area index; P_AR is the photosynthetically active radiation (P_AR=0.55R_s, and R_s is the net radiative flux near the surface); and $\overline{w}$ is the mean soil moisture in the root zone. Since the vegetation roots are short at Feixi Station, we assume that

$\overline{w}$ is equal to the near-surface soil moisture. f_1 and f_2 are stress functions defined as

$$\frac{1}{f_1(P_{\rm AR})} = 1 - a_1 \log\frac{a_2 + P_{\rm AR}}{a_3 + P_{\rm AR}}, \tag{15}$$

$$\frac{1}{f_2(\overline{w})} = \begin{cases} 0 & \overline{w} < w_{\rm pwp} \\ \dfrac{\overline{w} - w_{\rm pwp}}{w_{\rm cap} - w_{\rm pwp}} & w_{\rm pwp} \leqslant \overline{w} < w_{\rm cap}, \\ 1 & \overline{w} \geqslant w_{\rm cap} \end{cases} \tag{16}$$

where a_1=0.19, a_2 = 1128 W m^{-2}, a_3=30.8 W m^{-2}, and $w_{\rm pwp}$ is the soil moisture at permanent wilting point. In Feixi Station, $w_{\rm pwp}$=0.123 and $w_{\rm cap}$=0.311 are specified (Pielke, 1990; Peng, 1999). If vegetation fraction $c_{\rm v}$ (0.5 in Feixi Station) is known, the sum of latent heat fluxes from the above two parts is calculated as

$$\lambda E_{\rm evp} = c_{\rm v}\lambda E_{\rm v} + (1 - c_{\rm v})\lambda E_{\rm g}. \tag{17}$$

As we know that the semi-empirical profile formulations, the evaporation parameterization and observations all contain errors. On the other hand, to improve the accuracy of results, all observations should be used if we are not sure at which level the observations are relatively accurate. Owing to overdeterminacy, it is difficult for the deterministic method to implement all observations (nine observations in Feixi Station) to find the solution to five unknown variables (i.e., u_*, θ_*, q_*, $\theta_{\rm s}$, and w), while the maximum likelihood theory may be a good choice because it can consider all observations as well as error statistics at the same time (Lorenc, 1986). If the probability distribution functions (PDFs) for the formulations and observations are multidimensional Gaussian functions and the observational errors and model errors are mutually uncorrelated, the maximum likelihood estimation changes into the variational technique with L_2 norms (Lorenc, 1986; Sasaki, 1970). Based on the above considerations and observations, we adopt the variational approach to estimate the five parameters by minimizing the following cost function

$$J = \frac{1}{2}\Bigg\{W_u \sum_{i=1}^{3}\Big[u(z_i) - u_i^{\rm ob}\Big]^2 + W_\theta \sum_{i=1}^{3}\Big[\theta(z_i) - \theta_i^{\rm ob}\Big]^2 + W_q \sum_{i=2}^{3}\Big[q(z_i) - q(z_1) - (q_i^{\rm ob} - q_1^{\rm ob})\Big]^2 + W_E(\lambda E_{\rm evp} - \lambda E)^2 + W_{\rm eq}(R^{\rm ob} - G^{\rm ob} - H - \lambda E)^2\Bigg\}, \tag{18}$$

where $z_i, u_i^{\rm ob}, \theta_i^{\rm ob}$, and $q_i^{\rm ob}$ are observed heights, wind speeds, potential temperatures, and specific humidity, respectively; the first three terms on the right side of Eq.(18) measure the fits to the observed wind speeds, temperatures, and specific humidity gradients; the fourth term measures the mismatch between computed latent heat fluxes with the evaporation scheme and the profile method; the last term measures the fit to the surface energy balance with $R^{\rm ob}$ and $G^{\rm ob}$ being observed net radiative flux and soil heat flux. According to the maximum likelihood theory, weights W_u, W_θ, W_q, W_E, and $W_{\rm eq}$ should be inversely proportional to variances of the corresponding term in Eq.(18) which depend on the error statistics of the profile formulations, evaporation schemes, and observations, but it is very difficult to exactly know those characteristics. Alternatively, the weights are calculated only according to possible observational errors by the accuracy of sensors: $W_u = 0.5^{-2} = 4$(s^{2}m^{-2}) (note that the impact of wind speed is considered), W_θ=0.2^{-2}=25(K^{-2}), W_q=(2.2×10^{-4})$^{-2}$=2.066×10^7, $W_{\rm eq} = W_E = 15^{-2} = 4.4 \times 10^{-3}$(m^4 W^{-2}) (Xu and Qiu, 1997). Although above weights cannot be accurate, computations are found not to be sensitive to the weights in the vicinity (within the same orders of magnitudes) of these values. The quasi-Newton algorithm is used to find the optimal solutions to five variables ($u_*, \theta_*, q_*, \theta_{\rm s}$, and w), and then the sensible and latent heat fluxes are calculated according to Eqs.(8) and (9). In the quasi-Newton algorithm five gradient components of the cost function J are needed at each iterative step and can be derived from Eqs.(1)-(18). For simplicity, the analytical expressions of the gradient components are not presented in this paper. With a specified convergence criterion, for example, $|\nabla J| \leqslant 10^{-4}$, the minimization procedure is found to converge within no more than 20 iterative steps.

4. Results and analyses

4.1 The surface roughness length

In this paper, we use the method from Xu and Qiu (1997) to calculate the surface roughness length.

Assume that $z_{0\mathrm{m}}$ remains unchanged during the selected observational periods (24 days). For a selected $z_{0\mathrm{m}}$, sensible and latent heat fluxes can be estimated by the profile method. With the estimated sensible and latent heat fluxes and the observed R^{ob} and G^{ob}, the residual $\delta E = R^{\mathrm{ob}} - G^{\mathrm{ob}} - H - \lambda E$ is calculated. For total N time-level observations, the RMS value of δE is computed by

$$\varepsilon = (N^{-1}\sum_{n=1}^{N}\delta E_n^2)^{1/2}. \tag{19}$$

It has been found that ε reaches the minimum when $z_{0\mathrm{m}}$ is about 3 cm, which suggests that 3 cm should be used as the surface roughness length in order to closely satisfy surface energy budget. It is assumed that the roughness length $z_{0\mathrm{h}}$ is approximately equal to $0.1z_{0\mathrm{m}}$ for non smooth surface (Thom, 1972; Brutsaert, 1982).

4.2 The estimated near-surface soil moisture

Irrigation and rainfall make soil quickly become wet, and evaporation and infiltration make soil gradually become dry. Except irrigation and rainfall, the soil moisture changes slowly during one day so that only daily averaged soil moisture is estimated. To investigate whether our method can make a quick response to the soil wetting after rainfall, a comparison between the observed precipitation and estimates of near-surface soil moisture is plotted in Fig.1, showing that the increase of estimates of near-surface moisture is temporally consistent with the precipitation.

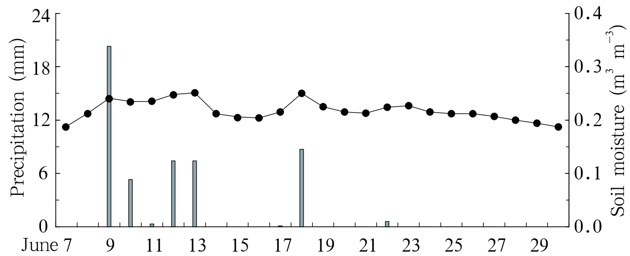

Fig.1. Comparison between the daily precipitation observations (solid columns) and daily averaged soil moistures retrieved (line with solid circles).

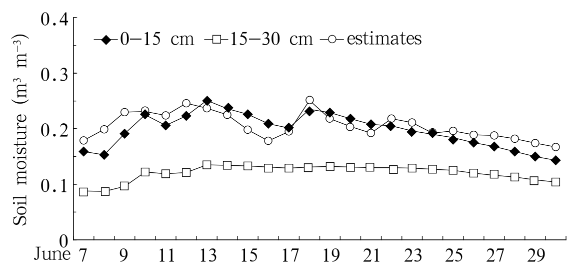

Fig.2. Comparison of the soil moisture observations at 2 layers: one layer between 0 and 15 cm (diamonds) and the other between 15 and 30 cm (squares) with daily averaged soil moistures retrieved (line with circles).

In Fig.2 the estimated soil moistures are compared with the daily averaged observations of soil moisture at two layers, showing that changes of estimated near-surface soil moisture with time are consistent with those of observations at the first layer in depths of 0-15 cm, and their differences are within $\pm 0.03\ \mathrm{m^3\ m^{-3}}$; however, almost no correlation is found in the estimates and the observed soil moistures at the second layer in depths of 15-30 cm. The vegetation around Feixi Station is grass with short root, and thus the contribution of soil moisture at deep layer to evaporation through root extraction is obviously very small. On the other hand, during the observational period the soil moisture at the second layer is very dry and almost near the permanent wilting point, and thus it is either impossible to make contribution to evaporation. Inversely, because of the above two reasons it is difficult to retrieve the soil moisture at deep layer just based on evaporation within a short time.

Because the observations (vertical profiles of wind, temperature, humidity, and radiation) represent the averaged states around the station, the estimates can only represent the spatially averaged soil moisture. However, the soil moisture observations are measured only at one point, which may be one reason for the difference between the estimates and measurements. On the other hand, the estimate is the average soil moisture over a 7-cm depth while the measurement is an averaged value over a 15-cm depth (Viterbo and Beljaars, 1995), which may be another reason for the difference between the estimates and observations. Finally, it should be noted that evaporation from the interception reservoir is not included in Eq.(17) but its impact can be reduced to some extent by the weak constraint of energy balance in the cost function. If the vegetation roots are not short, it is unreasonable to assume that the average soil moisture over the root area is equal to the near-surface soil moisture; however, if we know the empirical relationship between near-surface soil moisture and root zone soil moisture (Montaldo and Albertson, 2003), our method may be applicable to this case. For the bare soil, our method can be easily used because the above assumption is not needed.

4.3 The estimated latent and sensible heat fluxes

In addition to the estimates of soil moisture, our method can provide more reasonable estimates of surface heat fluxes by only using the conventional observations compared with the profile method and the Bowen ratio method. Of course, the three methods should be compared with the eddy covariance method. Because there was no eddy covariance sensor in Feixi Station, comparisons could only be carried out in terms of the surface energy balance and stability. As we know that the profile method is based on the Monin-Obukhov similarity law and has good computational stability, but the calculated heat fluxes sometimes deviate largely from the surface energy balance (Hu and Qi, 1991; Thom et al., 1975); on the contrary, the Bowen ratio method is based on the surface energy balance, but becomes computationally instable and results in spurious large values in the computed fluxes when the Bowen ratio is about -1 (Xu and Qiu, 1997). In the combined method, the two methods are merged to overcome the problem of surface energy unbalance, but it still needs the profile-gradient observations of high quality (Hu and Qi, 1991; Thom et al., 1975). From the viewpoint of methodology, the combined method belongs to deterministic methods and is difficult to take into consideration the stochastic errors in the observations and samples. Our method is based on the theory of optimal estimation; it can take all errors into consideration and use all observations which may be larger than the number of the variables to be estimated in order to increase the accuracy of estimation.

Firstly, comparison is made between the heat fluxes (averages over 30 min) calculated with the variational method and profile method (Fig.3). The two sensible heat fluxes almost have the same daily variation, but the fluxes from the profile method are almost smaller than those from the veriational method around the midday, especially the clear-sky midday (Fig.3a). The similar results can be found in their correlation plot (Fig.4a). For the latent heat flux, the daily variation trends of the fluxes from two methods are almost similar, but the fluxes from the profile are no longer smaller, sometimes even larger than those from the variational method around the midday (Fig.3b) so that their correlation is poor (Fig.4b). If all heat fluxes calculated by two methods are substituted into the equation for surface energy balance, the RMS deviation from the surface energy balance will be 86 W m^{-2} for the profile method while only 14 W m^{-2} for the variational method. Based on data from Huaihe River Basin experiment (HUBEX) intensive observation period (IOP), Zhu et al. (2003) found that the heat fluxes calculated with the eddy covariance technique did not deviate from the surface energy balance in this area. Therefore, we can infer that the fluxes calculated with the profile method have large errors; in other words, the heat fluxes estimated by the variational method are more reliable than those by the profile method from the viewpoint of the surface energy balance.

Comparison of fluxes between the Bowen ratio method and the variational method is plotted in Fig.5. In contrast to the Bowen radio method, the variational method can effectively eliminate the spurious spikes in the heat fluxes when the Bowen ratio is close to -1. If the spurious spikes are deleted, the fluxes computed by the two methods are in better agreement than those by the profile method and variational method (Fig.6). Smith et al. (1992) compared the fluxes obtained by the Bowen radio method with those by the eddy covariance technique and found no serious problem for the consistency of heat fluxes obtained by the two methods (except when Bowen ratio is about -1). Zhu et al. (2003) also found that there was no large discrepancy between the Bowen ratio method and eddy covariance method in the Huaihe River Basin. In general, the above results indirectly show that our method is reliable, and moreover it can give the estimates of heat fluxes when the Bowen ratio is about −1.

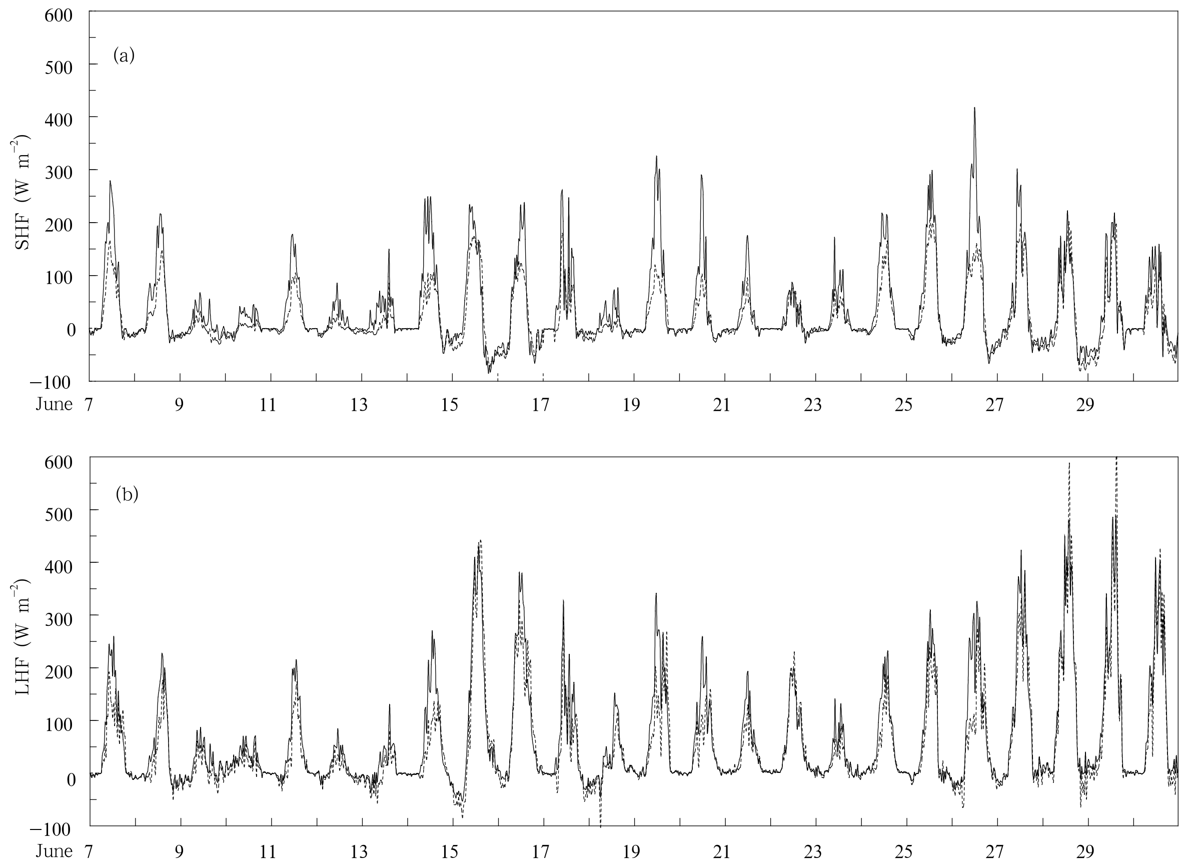

Fig.3. Comparisons between fluxes estimated by the variational method (solid line) and those computed by the profile method (dashed line) for (a) sensible heat flux (SHF) and (b) latent heat flux (LHF).

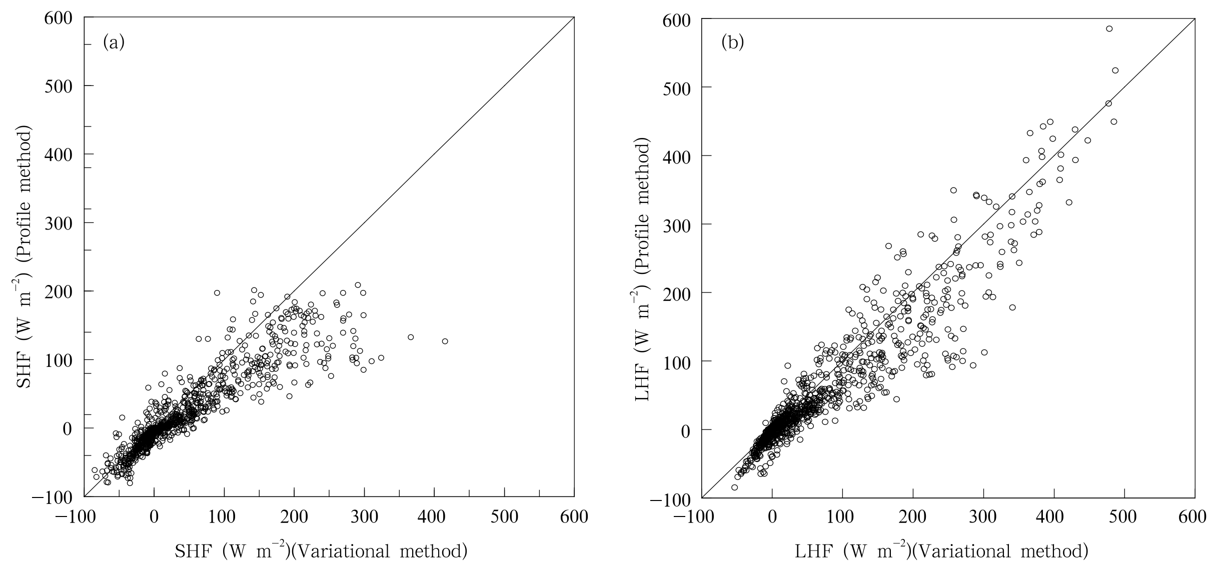

Fig.4. Correlation plots of fluxes estimated by the variational method and those computed by the profile method for (a) SHF and (b) LHF.

The measurements inevitably contain observational and sampling errors, which definitely have negative impact on the accuracy of estimates. Although it is impossible to completely reduce their influences, the estimates are relatively reliable if one method is not very sensitive to these errors; on the contrary,

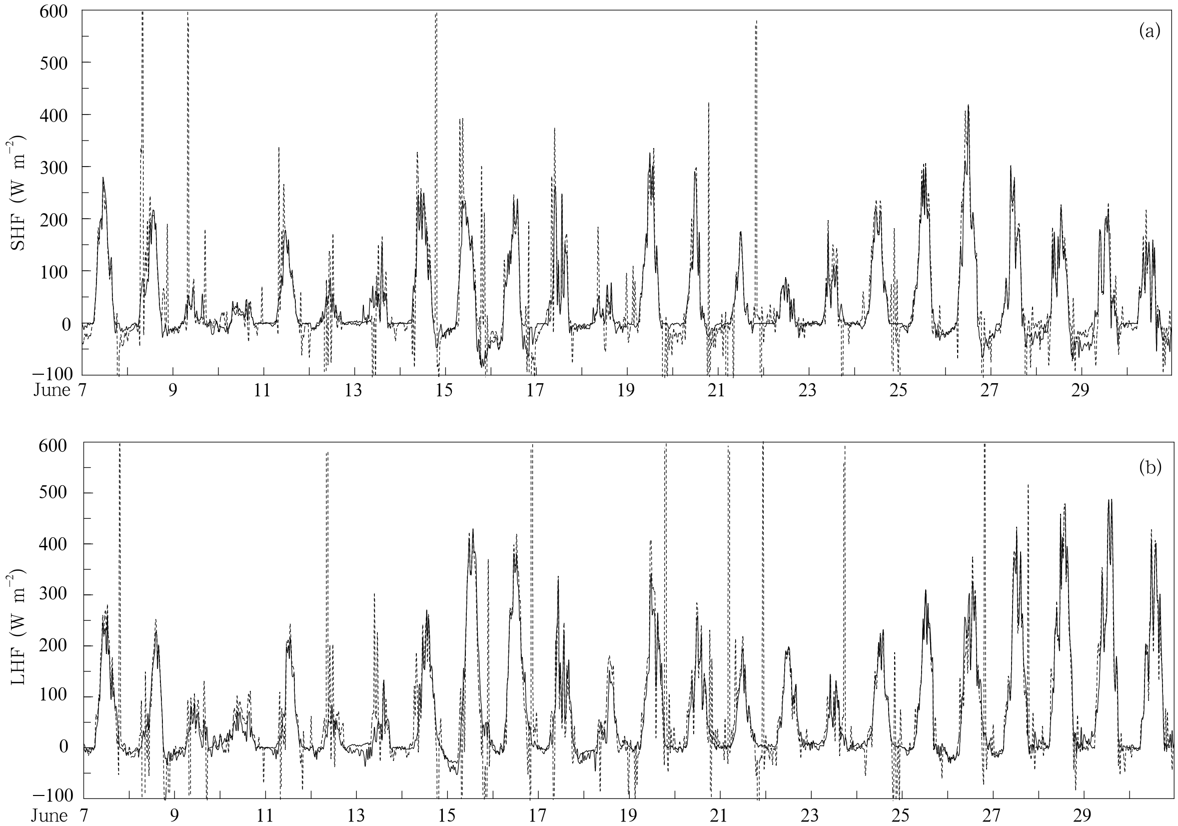

Fig.5. Comparisons between fluxes estimated by the variational method (solid line) and those computed by the Bowen ratio method (dashed line) for (a) SHF and (b) LHF.

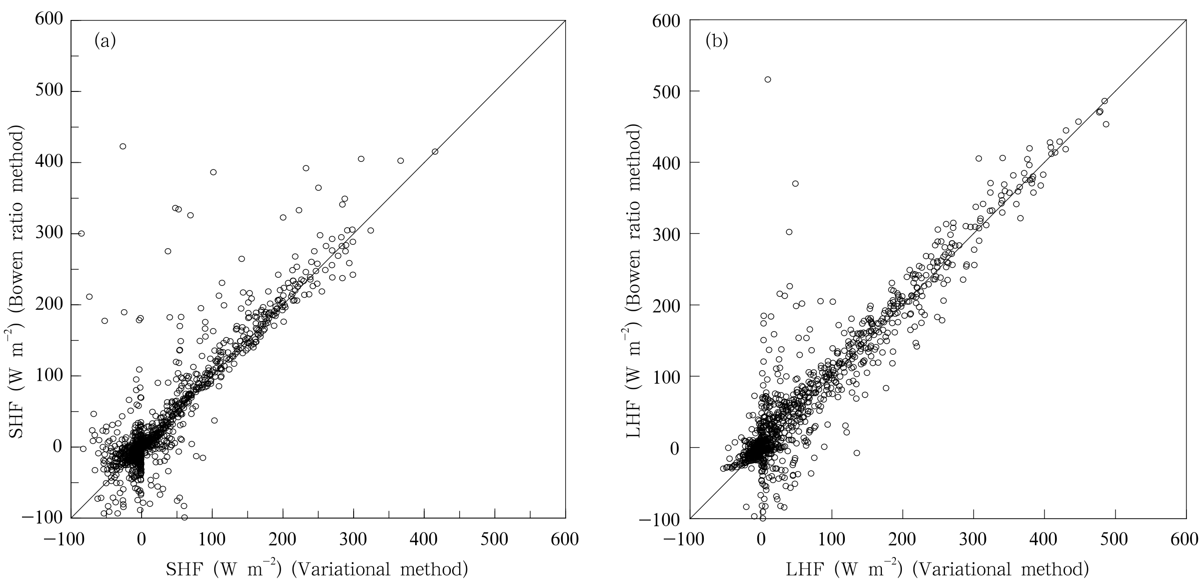

Fig.6. Correlation plots of fluxes estimated by the variational method and those computed by the Bowen ratio method for (a) SHF and (b) LHF.

if the method is very sensitive to the error, the results will be questionable. Based on the above consideration, we devise a set of tests to investigate the sensitivities of three methods to the errors in the observations: 0.5 m s^{-1} is added into the observed wind speed at the height of 10 m, 0.2°C is added into the observed temperature at 1-m height, 2.2×10^{-4} (about 1 % relative humidity at 28°C) is added into the specific humidity at 1-m height, and 15 W m^{-2} is added into the observed available energy ($R-G$). Fluxes computed from original data and error-contaminated data are respectively denoted by F and F'. The RMS error ($E_{\rm rms}$) for the estimated heat fluxes during 24 days can be evaluated by

$$E_{\rm rms}=\left[N^{-1}\sum(F'-F)^2\right]^{1/2}, \tag{20}$$

where N=3456 (Table 1). Among the three methods, the Bowen ratio method is the most sensitive to the observational errors except for errors in wind speed (since the Bowen ratio method does not need the wind observation). For the profile method, the estimated latent heat fluxes are very sensitive to the errors in air humidity and moderately sensitive to the errors in wind speed (see the sixth column in Table 1), while sensible heat fluxes are very sensitive to the errors in temperature (see the third column in Table 1). The errors in radiation have no influence on the results because the profile method does not use them. The heat fluxes estimated by the variational technique are not very sensitive to all observational errors, therefore they are more stable and reliable. One possible reason is that our method combines the advantages of the profile and the Bowen ratio methods, and another reason is the use of the optimal estimation for the improving performance of the variational technique (Daley, 1991; Zhang et al., 2004).

Table 1. Sensitivity of the SHF and LHF estimated by profile, Bowen ratio, and variational methods to the observational errors

Variables	Data errors	RMS errors for SHF (W m^{-2})			RMS errors for LHF (W m^{-2})		
		Profile	Bowen	Variational	Profile	Bowen	Variational
T	+0.2°C	24.5	259.0	14.5	13.8	259.3	14.0
	−0.2°C	22.2	399.1	13.8	12.4	399.0	13.5
u	+0.5 m s^{-1}	5.7	0.0	3.8	13.8	0.0	3.7
	−0.5 m s^{-1}	5.3	0.0	3.6	12.5	0.0	3.6
q	$+2.2\times10^{-4}$	4.5	843.0	9.0	50.4	843.4	10.1
	-2.2×10^{-4}	3.0	1011.2	8.1	49.5	1011.8	9.5
$R-G$	+15 W m^{-2}	0.0	137.8	4.4	0.0	137.7	6.8
	−15 W m^{-2}	0.0	137.4	4.5	0.0	137.8	3.7

5. Conclusions and further discussion

To correctly estimate the near-surface soil moisture and surface sensible and latent heat fluxes, the variational method is proposed which merges the information from the profile method, the Bowen ratio method, observations and their error statistics using the theory of maximum likelihood estimation. The input data are observations of wind, temperature, and humidity at different heights and the available surface energy; the number of estimates is five so that the minimum observations should be the same number. Besides necessary observations of two-level humidity and the available surface energy, the rest observations are two-level temperature and one-level wind or two-level wind and one-level temperature. If we could not make sure at which level the observation is more accurate, using more observations may help reduce the impact of uncertainties in observations and samples on the accuracy of estimates. The variational method just has the ability of merging more observations than the number of estimates, e.g., nine observations in Feixi Station but only five estimates.

The method is tested with the observational data, showing that it can quickly respond to the soil wetting due to precipitation and makes a good estimate of near-surface soil moisture with an absolute error less than 0.03 m^3 m^{-3}. The possible reason for the difference is that the estimated soil moisture represents the near-surface soil moisture (an averaged value over a 7-cm depth), while the observation is an averaged soil moisture over a 15-cm depth.

The estimated heat fluxes have a good correlation with those by the Bowen ratio method, but it can overcome the instability in the Bowen ratio method and provide the flux estimates when the Bowen ratio is around -1. The fluxes calculated by the profile method generally are smaller than those by the variational method, especially at the clear-sky midday. The possible reason for the discrepancies of fluxes is that the profile method does not take the surface energy balance into consideration and the forms of stability functions adopted in our tests may not be appropriate for Feixi Station. It is possible to make the calculated heat fluxes by the profile method satisfy the surface energy balance by choosing the more realistic semi-empirical forms. At the same time, more appropriate functions will also help improve the accuracy of estimation with the variational method, since they are very important integrants of the variational method. However, if the correct semi-empirical functions could not be sought out, our results demonstrate that the variational method can effectively reduce large deviation from the surface energy balance. The sensitivity tests show that the variational method is the least sensitive to the errors; this characteristic is very important to the accurate estimation, because all data cannot avoid the observational, sampling, and representative errors.

For the bare soil, the variational method can directly be used to estimate the near-surface soil moisture and surface heat fluxes because of no need of calculation of dry vegetation evaporation. For the land with deep-root vegetation cover, our method may be extended to estimate the average soil moisture over the root zone, but cannot provide the near-surface soil moisture information unless the empirical relationship between soil moistures at different depths is known. If the third term in Eq.(18) is discarded, the new cost function can be used to estimate the heat fluxes only.

Although the semi-empirical stability functions adopted in this study have been widely applied and the constraints in the cost function also reduce their impact on the estimates, different functions will certainly have some influences on the results which may need quantitative investigation in the future. Also the method needs further validating by using the data at different experimental locations with different soil types and weather conditions.

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