A Variational Method for Estimating Surface Fluxes with Mass Conservation Constraint

SEN LI
College of Meteorology and Oceanography, People's Liberation Army University of Science and Technology, Nanjing, China

ZHONG ZHONG
College of Meteorology and Oceanography, People’s Liberation Army University of Science and Technology, and Institute for Climate and Global Change Research, School of Atmospheric Sciences, Nanjing University, Nanjing, China

WEIDONG GUO
Institute for Climate and Global Change Research, School of Atmospheric Sciences, Nanjing University, Nanjing, China

WEI LU
College of Meteorology and Oceanography, People's Liberation Army University of Science and Technology, Nanjing, China

(Manuscript received 31 March 2013, in final form 23 July 2013)

ABSTRACT

On the basis of the similarity theory of the atmospheric surface layer and the mass conservation principle, a new scheme using a variational method is developed to estimate the surface momentum and sensible and latent heat fluxes. In this scheme, the mass conservation is introduced into the cost function as a weak physical constraint, which leads to an overdetermined system. For the variational method with mass conservation constraint, only the conventional meteorological observational data are taken into account. Data collected in the Yellow River Source Region Climate and Environment Observation and Research Station at Maqu, China, during 11–25 August 2010 are used to test this new scheme. Results indicate that this scheme is more reliable and accurate than both the flux-profile method and the variational method without mass conservation constraint. In addition, the effect of the weights in the cost function is examined. Sensitivity tests show that the fluxes estimated by the proposed scheme are insensitive to the stability functions explored in the cost function and measurement errors.

1. Introduction

The turbulent exchange process plays an important role in land–atmosphere interaction. Accurate representation of the eddy fluxes is essential for understanding the energy transfer in the land–atmosphere system and for successful numerical simulations of the atmosphere processes (Lee 1997). Generally, the momentum and heat fluxes are estimated by the Bowen ratio energy balance (BREB) method (Fritschen and Simpson 1989) and the profile method based on the Monin–Obukhov similarity theory (MOST). It is well known that the BREB, which estimates surface heat fluxes on the basis of measurements of temperature and specific humidity gradients and surface energy budget, becomes computationally unstable and results in spurious large values when the Bowen ratio is in the vicinity of $-1$. Meanwhile, many attempts have been made to develop and improve the profile method. Some flux-profile relationships suitable for various conditions of atmospheric stability have been well documented (Businger et al. 1971, hereinafter B71; Dyer 1974, hereinafter D74; Beljaars and Holtslag 1991, hereinafter BH91; Högström 1996, hereinafter H96; Cheng and Brutsaert 2005; Yang et al. 2008; Song et al. 2010, hereinafter S10). Despite all these efforts, the estimated fluxes are still scattered compared with observations. The disagreements mainly result from the lack of consideration of the energy budget, the limitation of the MOST over a flat
homogeneous surface, and the uncertainties of the input parameters in the flux-profile relationship functions, especially under the stable stratification condition.

To make sufficient use of the observed meteorological information and the similarity law, Xu and Qiu (1997) applied the variational method to compute surface heat fluxes over a flat homogeneous surface. The variational method searches for realistic meteorological variables (e.g., the friction velocity, potential temperature, and specific humidity scale) through constructing a cost function, aiming to minimize the difference between the estimated and observed fluxes. It is found that the variational method is more reliable and useful in practical applications of flux calculations by including different physical constraints in the cost function [i.e., the heat transfer coefficient as a constraint in Ma and Daggupaty (2000), the surface energy budget in Zhang et al. (2004), and temperature variance in Cao and Ma (2005)]. Meanwhile, the applicability of the variational method has been tested over a heterogeneous surface and sea ice surface (Cao and Ma 2005, 2009). Although the results of the variational method with those physical constraints show evident improvements in flux calculations, the observed information such as surface energy flux, radiation measurements, soil temperature, and soil humidity are not included in many observational datasets. This makes it impossible to adopt the physical constraints for use in the variational method. The classical variational method, which is derived from maximum likelihood estimation theory, performs better under overdetermined circumstances (Lorenc 1986), that is, the number of observations in the cost function is greater than the number of unknown parameters. Ma and Daggupaty (2000) also pointed out that the variational method would reduce to the profile method if the number of constraints is equal to that of unknowns. Accordingly, to make use of most of the conventional observational data, it is necessary and important to introduce physical constraints into the cost function in a reasonable way. The mass conservation principle, proposed by Tajchman (1981), is used for determining the zero-plane displacement and roughness length (Molion and Moore 1983; De Bruin and Moore 1985; Lo 1990, 1995; Zhong et al. 2011). It is suggested that the mass conservation principle is a useful concept as a weak constraint for the variational method in most field experiments, where only wind, temperature, and humidity profiles are measured and no additional experimental configurations are available. In this work, on the basis of measurements of wind, temperature, and relative humidity, we intend to verify the application of the variational method with mass conservation constraint to estimate surface fluxes. The results have been compared against those estimated by the variational method without physical constraints and by the conventional flux-profile method. Section 2 introduces the measured dataset used for flux calculations and comparisons. The description of the flux-profile method and the variational method based on the mass conservation principle is given in section 3, the computational results and the sensitivity test are presented and compared with the eddy-correlation-measured fluxes in section 4, and the conclusions are given in section 5.

2. Data

The Yellow River Source Region Climate and Environment Observation and Research Station (hereinafter YRSRORS), which is affiliated with the “ChinaFLUX” program, was established in 2005. The dataset used in the study was collected during 11–25 August 2010 at the Maqu observation site, which is situated at 33°52.77′N, 102°09.27′E, at an altitude of 3423 m. The surrounding area of this site is flat with homogeneously distributed plateau meadows. The aerodynamic roughness length is about 0.035 m and the zero-plane displacement is 0.143 m (Li et al. 2006). A 24-m-high observation tower with five-level sensors for wind (WindSonic, Gill), temperature, and relative humidity (HMP45C, Vaisala) are installed to capture the aerodynamic characteristics and profiles. The observation heights are 2.35, 4.2, 7.17, 10.13, and 18.15 m, respectively, above the ground. The measurement accuracies are ±0.02 m s$^{-1}$ at 12 m s$^{-1}$ for wind speed, ±0.2°C for temperature, and ±2% at 20°C for relative humidity. The absolute limit test and the abrupt change test have been employed to exclude abnormal observations caused by various reasons, for example, the operation problems of the observing system, the thunderstorm weather, and the noise effects. The absolute limit test detects the unrealistic values in the time series by defining the threshold for different observation variables. In the abrupt change test, we specify two thresholds: ±3 times the standard deviations from the mean of the entire observed height record and from the mean of the continuous 2.5-h measurements. When the data at a certain height or time are outside the thresholds, they are excluded from the analysis. Furthermore, the momentum and sensible and latent heat fluxes used to verify the validity of the new scheme are measured by the eddy-correlation technique at a sampling rate of 10 Hz in the dataset. All the data are collected by block averaging over 30 min, so there are 672 time periods of observations. Since the hypothesis of eddy-covariance technique is that the atmospheric turbulence is in steady state and homogeneous, the steady state test and the similarity test of turbulent covariance can be used as the standard for the data quality analysis and control.
(Foken and Wichura 1996). In this study, the flux data are classified into three categories, that is, 0 (good), 1 (average), and 2 (bad), according to the standard from Foken et al. (2004). Only those best samples (category 0) were utilized. After the quality control and classification (Yu et al. 2006; Foken et al. 2004), the number of data samples is reduced to 347. In addition, in an attempt to take anemometer stalling errors into account, the actual wind speed $u$ is also corrected from the measured wind speed $u_m$ by the empirical relationship (Molion and Moore 1983)

$$u(z) = u_m(z)/\{1 - \exp[-8.03u_m(z)]\}. \quad (1)$$

### 3. Descriptions of methods

#### a. Flux-profile method

On the basis of the similarity hypothesis of Monin and Obukhov, the profiles of wind, potential temperature, and specific humidity for turbulent flows in a horizontally homogeneous surface layer are expressed as follows (BH91):

$$u(z) = \frac{\kappa}{u_*} \left[ \ln \left( \frac{z - d}{z_{0m}} \right) - \psi_m \left( \frac{z - d}{L} \right) + \psi_m \left( \frac{z_{0m}}{L} \right) \right], \quad (2)$$

$$\Delta \theta = [\theta(z) - \theta(z_{0h})] = \frac{\theta_0}{\kappa} \left[ \ln \left( \frac{z - d}{z_{0h}} \right) - \psi_h \left( \frac{z - d}{L} \right) + \psi_h \left( \frac{z_{0h}}{L} \right) \right], \quad (3)$$

and

$$\Delta q = [q(z) - q(z_{0q})] = \frac{q_0}{\kappa} \left[ \ln \left( \frac{z - d}{z_{0q}} \right) - \psi_q \left( \frac{z - d}{L} \right) + \psi_q \left( \frac{z_{0q}}{L} \right) \right], \quad (4)$$

where $u_*$ is the friction velocity; $\theta_0$ and $q_0$ are the potential temperature and humidity scale, respectively; $z_{0m}$, $z_{0h}$, and $z_{0q}$ are the roughness lengths for momentum, heat, and humidity, respectively ($z_{0h} = 0.1z_{0m}$ and $z_{0q} = z_{0h}$; see Lo 1996); $\kappa = 0.4$ is the von Kármán constant; $d$ is the zero-plane displacement associated with the upward displacement in the mean airflow trajectory; $P_0$ is the turbulent Prandtl number; $\psi_m$, $\psi_h$, and $\psi_q$ are the stability functions determined experimentally in various fields; and $L$ is the Monin–Obukhov length given by $L = \overline{u^2}/\kappa g \theta_*$, where $g$ is gravitational acceleration. The momentum flux, namely, the wind stress, is related to the friction velocity by

$$\tau = \rho u_*^2, \quad (5)$$

where $\rho$ is the air density. The sensible heat flux is associated with the temperature scale by

$$H = -c_p \rho u_* \theta_*, \quad (6)$$

where $c_p$ is the specific heat of air at constant pressure. The latent heat flux is given by

$$\lambda E = -\lambda \rho u_* q_*, \quad (7)$$

where $\lambda$ is the latent heat of evaporation. The negative in Eqs. (6) and (7) represents the upward flux.

Various analytical expressions for stability functions have been given in previous works. No consensus, however, has been reached so far on the values of the experimentally determined constants or functions. Guilloteau (1998) suggested that under unstable stratification condition, the schemes of H96 give good approximations to the measurements. H96 is proportional to powers of $z/L$ and can be expressed as

$$\psi_m \left( \frac{z}{L} \right) = 2 \ln \left( \frac{1 + x}{2} \right) + \ln \left( \frac{1 + x^2}{2} \right) - 2 \tan^{-1}(x) + \frac{\pi}{2}, \quad (8)$$

and

$$\psi_h \left( \frac{z}{L} \right) = \psi_q \left( \frac{z}{L} \right) = 2 \ln \left( \frac{1 + y^2}{2} \right), \quad (9)$$

where $x = [1 - 19(z - d)/L]^{1/4}$ and $y = [1 - 11.6(z - d)/L]^{1/4}$. For the stable condition, the universal functions of BH91 are reliable across a wider range of stable stratification. The functions of BH91 are expressed as

$$-\psi_m \left( \frac{z}{L} \right) = a \left( \frac{z}{L} \right) + b \left( \frac{z}{L} - \frac{c}{d} \right) \exp \left( -\frac{d \cdot z}{L} \right) + \frac{bc}{d} \quad (10)$$

and

$$-\psi_h \left( \frac{z}{L} \right) = -\psi_q \left( \frac{z}{L} \right) = \left( 1 + \frac{2az}{3L} \right)^{3/2} + b \left( \frac{z}{L} - \frac{c}{d} \right) \exp \left( -\frac{d \cdot z}{L} \right) + \frac{bc}{d} - 1, \quad (11)$$

where $a = 1$, $b = 0.667$, $c = 5$, and $d = 0.35$.

Since the wind speed, temperature, and specific humidity gradients are measured directly, the Monin–Obukhov
length can be computed by an iterative procedure through substituting Eqs. (7)–(11) into Eqs. (2)–(4). The three unknowns, that is, the friction velocity, temperature, and humidity scale, can be obtained to calculate momentum and sensible and latent heat fluxes simultaneously by Eqs. (5)–(7). While only the vertical profiles are needed in the flux-profile method, it is evident that the disagreement between the estimated and observed fluxes can be attributed to the uncertainty of universal stability functions and the inadequacy of observational data.

b. Variational method with mass conservation constraint

The variational method makes full use of the observed meteorological data through a searching procedure for $u_g$, $\theta_g$, and $q_g$ to minimize the cost function $J$, which is defined as the summation of differences in wind speed, potential temperature, and specific humidity between the computed and observed values. In the study, the mass conservation hypothesis is included in the cost function to serve as a weak physical constraint. In previous papers (Molion and Moore 1983; De Bruin and Moore 1985), it is assumed that the mass flow is given by

$$m(z) = \int_0^z \rho u(z) \, dz,$$

where $m$ is the mass flow, $z$ is the height, and $\rho$ is air density.

The hypothesis of Marunich (1971) (referenced in Tajchman 1981) assumes that the rate of mass flow between ground level and level $z_1$ over the smooth surface is equal to the rate of mass flow between ground level and level $z_2$ above the rough surface. This is considered to be the “mass conservation hypothesis” and is expressed as

$$\int_0^{z_1} u_1(z) \, dz = \int_0^{z_2} u_2(z) \, dz.$$

Marunich further hypothesized that if levels $z_1$ and $z_2$ are high enough, then the velocities at $z_1$ and $z_2$ are nearly constant and equal. On the basis of this hypothesis, he suggested the distance between $z_1$ and $z_2$ is the zero-plane displacement. De Bruin and Moore (1985) extended the Marunich’s approach without the need of a hypothetical smooth surface, taking into account the existence of the transition layer above the surface. They assumed the condition of mass conservation could be imposed on the logarithmic wind profiles, such that the logarithmic wind profile, extrapolated to $z = z_{0m} + d$, transports the same amount of mass flow as the actual wind profile. Although the method to impose a condition of conservation of mass flow on the logarithmic wind profile is primarily developed for practical reasons, theoretically, it also bears a physical meaning when parameters $z_{0m}$ and $d$ are linked to mass flow. This condition can be written as

$$\int_{d + z_{0m}}^z \rho u \, dz = \int_0^z \rho u_m(z) \, dz,$$

where $u$ is calculated by Eq. (2) according to different stability cases and $u_m$ is the measured velocity. In this study, we assume that the airflow in the surface layer is incompressible and that air density is constant with height; hence, the density is negligible. The left-hand side of Eq. (14) represents the estimated mass flow, and the right-hand side of Eq. (14) represents the mass flow transported by the measured velocity profile, which can be regarded as the area enclosed by the measured wind profile. For simplicity, we employ the trapezoidal rule to compute it directly, and the calculation can be expressed as

$$\int_0^z u_m(z) \, dz = \frac{1}{2} U_1 Z_1 + \sum_{i=1}^{N-1} \frac{1}{2} (U_i + U_{i+1})(Z_{i+1} - Z_i),$$

where $U_i$ means the measured wind speed at $i$th level of $Z_i$ and $N = 5$ in the dataset.

On the basis of the study of De Bruin and Moore (1985), the mass conservation assumption could be used as a reasonable working hypothesis in neutral condition. Lo (1990, 1995) applied the mass conservation hypothesis to determine zero-plane displacement height and roughness length. In their study, the general forms of the logarithmic wind and temperature profiles, including diabatic influence functions, are introduced. Zhong et al. (2011) have extended the hypothesis to non-neutral conditions to estimate the effective roughness length. Figure 1 shows the comparison between the measured and estimated mass flow during 11–25 August 2010, where the estimations are computed by Eqs. (2) and (14) using the measured $u_g$ and the measurements are obtained by Eq. (15) through measured wind profiles. It can be seen in Fig. 1a that within the entire range of $-6 \leq z/L \leq 2$, the estimations are consistent with the measurements, especially under near-neutral and stable conditions. The estimations are somewhat larger than the measurements in unstable stratifications. Further analysis reveals that the discrepancy can be attributed to the uncertainties in idealistic flux-profile functions and the inaccuracy in measured $z_{0m}$ and $d$, as well as large samples under unstable conditions. Nevertheless, the difference between them is not significant, with the absolute error closing to zero and the relative error less than about 10% (Figs. 1b,c). In general, the mass conservation hypothesis
in this study can be applied for non-neutral conditions, agreeing with the studies of Lo (1990, 1995) and Zhong et al. (2011).

The cost function can be written as

\[
J = \frac{1}{2} \left[ \sum_{i=1}^{5} C_u (u_i - u_{i,\text{obs}})^2 \right] + \frac{1}{2} \left[ \sum_{j=1}^{4} C_i (\Delta \theta_j - \Delta \theta_{j,\text{obs}})^2 \right] + C_q (\Delta q_j - \Delta q_{j,\text{obs}})^2 + \frac{1}{2} C_m \delta_{\text{mass}},
\]

where \( u_i \), \( \Delta \theta_i \), and \( \Delta q_i \) are derived from Eqs. (2)-(4); the subscript letters obs stand for observations; and \( i \) and \( j \) denote the number of observation levels for wind speed and temperature, respectively. Note that the surface temperature and humidity are not included in the dataset, \( \Delta \theta_j \) and \( \Delta q_j \) in the cost function represent the differences between the above four levels, and the lowest level instead of the height \( z_{0h} \).

The residual error in the mass conservation is given by

\[
\delta_{\text{mass}} = \int_{d + z_{0m}}^{z} \frac{u_s}{\kappa} \left[ \ln \left( \frac{z - d}{z_{0m}} \right) - \psi_m \left( \frac{z - d}{L} \right) + \psi_m \left( \frac{z_{0m}}{L} \right) \right] dz - \frac{1}{2} U_i Z_i - \sum_{i=1}^{N-1} \frac{1}{2} (U_i + U_{i+1})(Z_{i+1} - Z_i).
\]
The variables $C_u$, $C_r$, $C_q$, and $C_m$ are dimensional weights, which can be specified empirically to be inversely proportional to the respective observation error. In this study, the weights are set to be $C_u = 50 \text{ m}^2 \text{s}^{-2}$, $C_r = 25 \text{ K}^{-2}$, $C_q = 5.4 \times 10^6$, and $C_m = 20$. Weight determination is examined in detail in the following section.

To obtain optimal estimates of $u_*$, $\theta_*$, and $q_*$, it is necessary to minimize $J$. Namely, the three gradients of $J$ relative to the unknowns should be zero:

$$\frac{\partial J}{\partial u_*} = \frac{\partial J}{\partial \theta_*} = \frac{\partial J}{\partial q_*} = 0.$$  \hspace{1cm} (18)

The analytical expressions of the gradient components are given in the appendix. The “non parameter” problem arises as a result of the confusion of unknowns when the unknowns in the study are related to each other (Schaudt, 1998), for example, the Monin–Obukhov length $L = \theta_0 g / (k g \theta_*)$ in the cost function. To avoid this problem, a scanning procedure instead of a searching one is applied to find the optimal solution. The scanning scales are set up approximately: a maximum of $1 \text{ m} \text{s}^{-1}$ for the friction velocity, from $-1.5$ to $1 \text{ K}$ for the potential temperature scale, and from $-1.5 \times 10^{-5}$ to $1.0 \times 10^{-5}$ for the specific humidity scale. Thus, an extension of the limited-memory, quasi-Newton Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm (L-BFGS) for unconstrained optimization, which we call the L-BFGS-B method, is employed instead of the L-BFGS (Liu and Nocedal 1989) used in Xu and Qiu (1997). The main improvement is that L-BFGS-B is able to deal with large nonlinear optimization problems subject to simple constraints.

The iterative procedure is run to compute the cost function and its gradients until the convergence criterion is satisfied. The procedure consists of the following steps.

1) Suppose the initial guessed values of the unknowns are $u_0 = 0.01 \text{ m} \text{s}^{-1}$, $\theta_0 = -0.01 \text{ K}$, and $q_0 = 0$; $L$ can be computed.

2) Calculate $u$, $\Delta \theta$, and $\Delta q$ from Eqs. (2)–(4) and $\delta_{\text{mass}}$ from Eq. (17) based on the estimated $L$.

3) Calculate the cost function $J$ in Eq. (16) and its gradients with respect to the three unknowns. If the convergence criterion is reached, the expected estimates $(u_*, \theta_*, q_*)$ are obtained; otherwise, the scanning direction and the step size can be determined in terms of the gradients and the scanning direction of the previous iteration.

4) Along the scanning direction, a line search is performed within predetermined bounds to find the minimum $J$, and new estimates are obtained at each iteration.

5) Repeat steps 2–4 until the procedure converges.

The variational method explores all conventional observed data of wind speed, temperature, and relative humidity. It is suitable for the variational approach whereby an overdetermined system including three unknowns and four constraints is formed when additional information of mass conservation is introduced.

4. Results and discussion

4.1. Estimations of the momentum, sensible, and latent heat fluxes

To evaluate the performance of the variational method with mass conservation (hereinafter VWM) in this study, we compare the fluxes computed by the new scheme and by the conventional flux-profile method with those measured by eddy correlation. In addition, the variational method without the mass conservation constraint (hereinafter VOM) is designed following the same approach of Xu and Qiu (1997), which simply inputs multiple-level observed data into the cost function and constructs the overdetermined system. The results estimated by VOM are also examined. Note that for the flux-profile method, the schemes of H96 for unstable cases and BH91 for stable cases are used and are denoted as BHH. The results are plotted as points in their respective correlation diagrams (Fig. 2). In the stable stratification (Figs. 2a–c), the correlation diagram contains 101 points corresponding to the 101 samples of observations during the selected period. For unstable stratification, there are 246 samples (Figs. 2d–f). It is seen in Fig. 2a that the correlation points of the three methods are distributed near the diagonal line in most cases. Note that they are above the diagonal line when the momentum fluxes $\tau$ are small. This means that an underprediction appears for strongly stable conditions because of the uncertainty of stability functions. Still, the measured and the computed results using the three methods agree well and their correlation coefficients are similar, as shown in Fig. 2a. In contrast, under the unstable conditions, obvious discrepancies in $\tau$ estimated from the three methods are found in Fig. 2d. Many points of the VOM results are scattered below the diagonal line, indicating significant underestimations. On the contrary, most points of the BHH results are
distributed above the diagonal line, suggesting distinct overestimations. The above results clearly show that neither VOM nor BHH can provide satisfactory flux calculation. The points of the VWM results, however, are distributed along the diagonal line and correspond to the highest correlation coefficient. This result suggests that among the three methods discussed above, VWM is the most effective one to calculate momentum fluxes, although several underestimations cannot be neglected.

Sensible heat fluxes $H_s$ and latent heat fluxes $\lambda E$ computed by the three methods are compared with observations under different stratifications in Figs. 2b–f. The points representing the BHH results are sparsely distributed, showing large vertical deviations from the diagonal line, particularly when the sensible heat flux is largely negative. Similar patterns are found in latent flux calculations under stable conditions by VOM. The results demonstrate evident underestimations. Note that the BHH overestimates latent heat flux in all cases, and some of these average errors are quite significant. For example, the average $\lambda E$ from YRSRORS observations is 19.7 W m$^{-2}$ for stable cases and 209.9 W m$^{-2}$ for unstable cases, whereas from BHH results it is 39.6 W m$^{-2}$ and 284.8 W m$^{-2}$, representing a nearly twofold increase in magnitude under stable conditions. In comparison with results of the other methods, sensible and latent heat fluxes estimated by VWM show relatively weaker fluctuation and agree better with observations. Meanwhile, the correlation coefficients between VWM results and measurements are the highest among all three methods. It is recognized that the validity of the mass conservation approach can be established in all stability classes. On the basis of its definition, the mass conservation constraint is used to adjust the wind profile, mainly manifesting in the friction velocity, so as to make the rate of mass flow within the logarithmic wind profile equal to that within the actual wind profile. From Eq. (5), the momentum flux is only affected by the friction velocity; therefore, the difference of results under stable and unstable condition is insignificant. The correlation coefficients between VWM results and measurements reach 87% under both conditions. Estimation of the heat fluxes, however, is determined not only by the friction velocity, but also by the potential temperature and humidity scale. As shown in Figs. 2b, 2c, 2e, and 2f, the calculated results by VWM show better agreement with the measurements under unstable condition than that under stable condition, which is consistent with results from the other two methods. This behavior may possibly be related to the stability functions. In unstable

![Fig. 2](image_url)

**Fig. 2.** For (top) stable and (bottom) unstable conditions, the (a),(c) momentum fluxes, (b),(d) sensible heat fluxes, and (c),(e) latent heat fluxes of the observed vs the values computed by the flux-profile method (dots), the variational method without mass conservation constraint (circles), and the VWM constraint (plus signs).
Table 1. RMSE (W m⁻²) between the observed momentum fluxes (τ), sensible heat fluxes (Hₜ), and latent heat fluxes (λE) and those computed by the three methods BHH, VWM, and VOM. The terms Uns, Sta, and Ent stand for unstable stratification, stable stratification, and entire stratification, respectively.

<table>
<thead>
<tr>
<th>Methods</th>
<th>BHH</th>
<th>VOM</th>
<th>VWM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stratification</td>
<td>Uns</td>
<td>Sta</td>
<td>Ent</td>
</tr>
<tr>
<td>RMSE_τ</td>
<td>0.042</td>
<td>0.021</td>
<td>0.038</td>
</tr>
<tr>
<td>RMSE_λE</td>
<td>85.926</td>
<td>28.755</td>
<td>81.606</td>
</tr>
</tbody>
</table>

Stratification, stability functions are reliable and supposed to be more important because of the larger turbulent fluxes under that condition. The stability functions and turbulence under stably stratified conditions, however, have remained less understood and controversial (Cheng and Brutsaert 2005). The strongly stable boundary layer is characterized by large temperature gradients, weak momentum fluxes, light wind, and small mass flow. Therefore, the constraint derived from mass conservation becomes weak. As a result, the VWM generates more realistic estimation of heat fluxes under unstable conditions than in stable conditions. We further calculate the root-mean-square error (RMSE) to quantitatively evaluate the performance of the three methods. As demonstrated in Table 1, in all cases the BHH has an RMSE of 0.038 for τ, of 27.190 for Hₜ, and of 81.606 for λE, whereas the RMSEs for the same quantities are 0.036, 19.584, and 66.245 for the VOM method and 0.02, 13.443, and 40.654 for the VWM method. These results suggest that the VWM method gives the most realistic estimation of momentum and heat fluxes and performs best among the three methods.

Figure 3 shows the time evolution of the relative errors (relative differences between measured and calculated variables) of u₀, Hₜ, and λE during a period of 10 consecutive days (from 11 to 21 August 2008). The weather condition during the period was relatively fair, with mean winds blowing mostly from the south or the southwest. There were no recorded rainfalls and the soil experienced gradual drying. After the quality control procedure, 253 wind, temperature, and humidity profiles, of which 179 are for unstable stratification and 74 are for stable stratification, are selected. Simultaneous flux measurements are obtained also. Figure 3c shows that VWM can give a reasonable result, with relative uncertainty generally within 40% for Hₜ and λE, and 50% for u₀. Results of the other two methods, however, have much larger biases than that of VWM. Overestimation of sensible and latent heat fluxes by BHH is evident (Fig. 3a) with relative error up to about 170%. The overestimation is less severe in results of the VOM, but the relative error of friction velocity can reach about 100%. Figure 3d shows the variation of mean relative difference of Hₜ and λE for the consecutive days. A slightly negative diurnal cycle tends to appear, especially in the first, fourth, and tenth days. During the daytime, the mean relative error becomes smaller but increases in magnitude during the nighttime. Although the diurnal cycle looks weak, it provides evidence to support our previous results that the VWM performs best under unstable stratification conditions (i.e., daytime). Table 2 lists the mean relative difference between the observed and computed heat fluxes by the VWM during the daytime (0800–1800 LST) and the nighttime (2000–0600 LST), respectively. The biases in the daytime are significantly less than that in the nighttime, indicating that the estimated results for the daytime are more consistent with observations. This can be attributed to the sufficient number of samples and reliable stability functions under unstable and convective conditions. In general, the VWM shows substantial improvements in the flux calculations relative to the VOM and the flux-profile method.

b. Sensitivity tests

Since there is no clear way to select the weights in the cost function J, it can be related to the observational errors empirically and even arbitrarily (Daley 1996; Cao et al. 2006). Moreover, although the mass conservation is derived from the vertical wind profile, this does not mean that the weight of the mass conservation term depends solely on the accuracy of wind speed measurements. Thus, to search for Cₘ and examine the sensitivity of the estimated fluxes to the weights, we compute the RMSE of sensible heat fluxes between the observed and estimated values and those estimated by VWM with different weight groups. First, suppose Cₙ is proportional to the measurement resolution in specific humidity of a constant 5.4 × 10⁶, Cₘ is determined within the range of 0–100, and Cₙ and Cₗ are changing from 1 to 100; thus, there are 100 × 100 × 101 experiments in all. Next, the sensitivity of the estimated heat fluxes to Cₙ is tested. As shown in Fig. 4, when Cₘ is assumed to be 0 (i.e., the VOM), the RMSE ranges from 13.7 to 32, with different combinations of Cₙ and Cₗ. It is clear that with
FIG. 3. Time series of relative differences between observed and computed friction velocity (circles), sensible heat flux (dots), and latent heat flux (plus signs) obtained by the (a) BHH, (b) VOM, and (c) VWM methods. (d) The variation of mean relative difference of estimated heat fluxes by the VWM method or continuous days. Time starts at 0000 LST 11 Aug 2010.
larger values of $C_t$, the variation of RMSEs is significant. On the contrary, when the mass conservation constraints are constructed in the cost function, it can be seen from Fig. 5 that with different weight groups RMSEs vary from 12.65 to 13.85, which is not distinct at all. This result further proves the advantage of VWM and indicates its weaker sensitivity to weights compared to the VOM. Figure 5 also shows that the RMSEs are barely dependent on $C_u$ when $C_m$ and $C_t$ are fixed. It should be mentioned, however, that as the assumed $C_m$ increases, the relatively small value strip in RMSE (shaded with slanted lines in each panel) shifts to the larger $C_t$. It seems that there probably exists a comprehensible relationship between $C_m$ and the averaged $C_t$ denoted by the dashed line over the shaded area, which may provide a basis for setting $C_m$. To ascertain whether the relationship exists, we choose the weight combinations with which the RMSEs of estimated sensible heat fluxes are within the range of $(1 + 1.005) \text{RMSE}_{\text{min, all}}$, and compute the respective correlation coefficients of selected $C_m$ values with $C_u$ and $C_t$. The $\text{RMSE}_{\text{min, all}}$ represents the minimum RMSE regarding all weights experiments. On the basis of the calculation, the correlation coefficient of $C_m$ with $C_t$ is equal to 0.9153 ($p = 0.01$) at the statistically significant level of 99.9%. This indicates a reasonable linear relationship between them. Meanwhile, the correlation coefficient of $C_m$ with $C_u$ is 0.1453, suggesting a poor linear relationship between them. As a result, $C_m$ can be determined through regression by minimizing the RMSE. The linear regression

### Table 2: The mean relative difference between the observed and computed heat fluxes by the VWM with constraint during the daytime (0800–1800 LST) and nighttime (2000–0600 LST).

<table>
<thead>
<tr>
<th></th>
<th>Sensible heat flux</th>
<th>Latent heat flux</th>
</tr>
</thead>
<tbody>
<tr>
<td>Daytime</td>
<td>0.1662</td>
<td>0.1251</td>
</tr>
<tr>
<td>Nighttime</td>
<td>0.2189</td>
<td>0.1842</td>
</tr>
</tbody>
</table>

![Figure 4](attachment:image.png)  
**Fig. 4.** The RMSEs of sensible heat fluxes between the measured values and values estimated by the VOM method, namely, the weight of the mass conservation term ($C_m$) in the cost function is equal to zero. The $x$ axis and the $y$ axis represent the weight of differences in the potential temperature term ($C_t$) and that of differences in the wind speed term ($C_u$), ranging from 1 to 100, respectively.
shown in Fig. 6 is valid for sufficiently large samples and the optimally fitted function for $C_m$ relative to $C_t$ is given by

$$C_m = 0.6763C_t - 0.0877. \tag{19}$$

This helps to improve the choice of weights in the cost function. After $C_m$ is obtained, the sensitivity of the estimated heat fluxes to $C_q$ is examined. We assume that $C_u = 50$, $C_i = 25$, and $C_m = 18$, derived from Eq. (19), and eight different values for $C_q$ are listed in Table 3. Note that the magnitude of the selected $C_q$ is presumably the inverse square of the observational error in specific humidity. The RMSEs between the computed heat fluxes and the measurements are also listed in Table 3 for each $C_q$ value. In general, the variation of RMSEs for sensible heat fluxes is smaller than that for latent heat fluxes in eight tests. As shown, the RMSEs of sensible heat fluxes vary from 12.8 to 13.1 and RMSEs of the latent heat fluxes vary from 41.5 to 42.3, indicating that the computed heat fluxes do not correspond clearly to the change in $C_q$, which is mainly caused by the small difference in specific humidity.

As mentioned above, in this study the cost function $J$ is based on the stability functions derived from BHH. These stability functions are supposed to be reliable. On the basis of different in situ experiments, however, various empirical coefficients and functions have been developed, leading to large differences in flux calculations, especially in the stable stratification condition. To verify the impact of empirical functions on results of the VWM, four empirical functions resulting from B71, D74, S10, and BHH are employed and are incorporated into the cost function. The sensible heat fluxes estimated by profile methods and VWM with different flux-profile functions are shown in Fig. 7. It is clear that, for all kinds of stratification (unstable, neutral, and stable) and all flux variables, the biases estimated by VWM using different functions are pretty small (Fig. 7a), corresponding to the similar tendency. For profile methods, as seen in Fig. 7b, the discrepancies between results with different empirical functions are not evident and are similar to those of the VWM under unstable conditions. This is ascribed to the analogous $-1/2$ law, which is adopted as the empirical functions with different coefficients in various experiments. In
contrast, results with profile methods under stable stratification remain largely scattered because of the uncertainties of the applicable stability interval and various forms of flux-profile functions. The mean absolute error (MAE) and correlation coefficients ($R$) between the empirical functions are listed in Table 4. The MAE can be evaluated by

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^{n} |F_{i,x} - F_{i,y}|,$$

(20)

where $F_{i,x}$ and $F_{i,y}$ are the $i$th (the number of samples) results computed by the different empirical functions. As shown in Table 4, for the unstable stratification there is insignificant difference between the two methods. For the stable cases, however, the MAE between results of VWM using different functions is only about half of that generated by the profile methods. This indicates that the VWM places weak dependence on the empirical equations.

To investigate the sensitivities of the estimated fluxes to the observational errors in wind, temperature, and specific humidity, eight sensitivity experiments were conducted. Errors of $\pm 0.5$ m s$^{-1}$, $\pm 0.2$ K, and $4 \times 10^{-4}$ (about 2% relative humidity) are added to the wind at 4.2 m, temperature and specific humidity at 7.17 m, respectively, for the $n = 318$ time levels. Eight combinations of errors and the MAE of fluxes estimated by each method with and without the errors are listed in Table 5.

Because the mass flow is defined by the wind profile

![Fig. 6. The scatterplot of selected values of $C_m$ vs $C_t$ with which the RMSEs of sensible heat fluxes estimated by VWM method are less than 1.005 times the minimum RMSE relevant to all weights experiments. The solid line represents the mean $C_m$ relative to $C_t$, where the linear regression relationship is shown by a dashed line.](image)

**Table 3.** List of experiments, parameters of assumed $C_q$, and the RMSEs (W m$^{-2}$) in sensible and latent heat fluxes between the observations and those estimated by experiments for different $C_q$ values.

<table>
<thead>
<tr>
<th>Expts</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_q$</td>
<td>$2 \times 10^6$</td>
<td>$3 \times 10^6$</td>
<td>$4 \times 10^6$</td>
<td>$5 \times 10^6$</td>
<td>$6 \times 10^6$</td>
<td>$7 \times 10^6$</td>
<td>$8 \times 10^6$</td>
<td>$1 \times 10^7$</td>
</tr>
<tr>
<td>RMSE$_{\lambda E}$</td>
<td>41.728</td>
<td>41.526</td>
<td>40.988</td>
<td>41.248</td>
<td>41.487</td>
<td>41.845</td>
<td>42.026</td>
<td>42.231</td>
</tr>
</tbody>
</table>
Eq. (12)], the mass conservation constraint is certainly affected by the wind error. This explains why the MAE generated by VWM is slightly larger than that by the VOM (see the fourth and fifth rows in Table 5) when wind error is imposed. The VWM method, however, exhibits the lowest sensitivities to temperature and specific humidity errors since it uses the observational information and extra physical constraint based on wind speed. For the flux-profile method, the estimated latent heat fluxes are most sensitive to specific humidity error and moderately sensitive to temperature error. The estimated sensible heat fluxes are highly sensitive to temperature error. Note that the specific humidity is not used in sensible heat flux calculations by the profile method, so error of specific humidity exerts no influence on the results. Relative to the flux-profile method, the VOM method is much less sensitive to errors of wind and specific humidity. But the VOM is sensitive to temperature errors, as discussed by Zhang et al. (2004). The above results clearly show that among all three methods used in this study, the VWM is the least sensitive to observation errors, except for speed error, and the profile method is the most sensitive.

5. Conclusions

In this study, the mass conservation principle, which is based on wind profiles and has clear physical meanings,
is chosen as a weak constraint in the cost function in the variational method for turbulent flux calculations. With the mass conservation constraint, the number of observations in the cost function is greater than the number of unknown parameters, namely, the overdetermined situation, and only the conventional meteorological data are taken into consideration. By using the limited memory quasi-Newton algorithm for large-scale bound-constrained optimization (L-BFGS-B), the optical friction velocity, potential temperature, and specific humidity scales are scanned within predefined scales for estimation of momentum and sensible and latent heat fluxes.

Data collected by YRSRORS during 11–25 August 2010 at the Maqu observation site are used to test the variational method with mass conservation constraint (VWM). Briefly, the computational results of momentum and sensible and latent heat fluxes are consistent with the eddy-correlation measurements. In addition, it is shown that the VWM results are highly correlated with the measured fluxes. Biases of fluxes calculated by the VWM method are much smaller than that by the VOM method and by the conventional flux-profile method. Note that the heat fluxes estimated by the VWM agree better with the measurements under unstable conditions because of the sufficiently large number of samples and reliable stability functions.

Sensitivity tests of the weights in the cost function have been carried out for the VWM method. The results show that compared to the VOM, the effect of changing weights is insignificant in estimation of sensible heat flux. Although the estimated fluxes varied in a limited range, an evident linear relationship is found between the weight of the mass conservation term and that of the temperature difference term, resulting in smaller RMSEs. Moreover, the computed heat fluxes by the VWM have similar values when the weight of the specific humidity difference term is changed within certain scales. Relative to the VOM and the flux-profile method, the VWM method shows less sensitivity to errors in meteorological data. The sensible heat fluxes’ sensitivity to errors in temperature and the latent heat fluxes’ sensitivity to errors in specific humidity are greatly reduced in VWM than in VOM and BHH, whereas the heat fluxes’ sensitivity to wind speed errors is intermediate. In addition, since no consensus has been reached on the stability functions experimentally, in the paper the sensible heat fluxes estimated by the VWM using different empirical functions are examined. The results show good agreement, especially for the stable cases, and the mean absolute errors of computed fluxes using different functions are only about half of those by the profile methods. This suggests that the stability function has no substantial impact on the VWM results. Hence, introducing the mass conservation into the cost function is a reliable and simple way to carry out flux calculations. It makes full use of the existing conventional observational information in an effective approach. It is noteworthy that the VWM can be applied for flux estimations over a heterogeneous underlying surface because the mass conservation applies to significantly heterogeneous terrain complexity (Andre and Blondin 1986).

Acknowledgments. This work was supported by National Key Basic Research and Development Project of China under Grants 2010CB428505 and 2011CB952002 and by the R&D Special Fund for Public Welfare Industry (Meteorology) under Grant GYHY201306025.

APPENDIX

Analytical Expressions of the Gradient Components

The detailed analytical expressions of the gradient components of the cost function, defined in Eq. (16) relative to \((u_0, \theta_0, q_0)\), are derived as follows:

<table>
<thead>
<tr>
<th>Error combinations</th>
<th>Mean absolute error (W m(^{-2}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(u (m s^{-1}))</td>
<td>Sensible heat flux</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>q (10(^{-2}))</td>
</tr>
<tr>
<td>0.5</td>
<td>0</td>
</tr>
<tr>
<td>−0.5</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>0.2</td>
</tr>
<tr>
<td>0</td>
<td>−0.2</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0.5</td>
<td>0.2</td>
</tr>
<tr>
<td>−0.5</td>
<td>−0.2</td>
</tr>
</tbody>
</table>
\[
\frac{\partial J}{\partial u_0} = \sum_{i=1}^{5} \left[ C_a(u_i - u_{i0}) \frac{\partial u}{\partial u_0} \right] + \frac{4}{\sum_{j=1}^{5} \left[ C_d(\Delta \theta_j - \Delta \theta_{j0}) \frac{\partial \Delta \theta}{\partial \theta_0} \right] + C_m(\Delta q_j - \Delta q_{j0}) \frac{\partial \Delta q}{\partial \theta_0} \right] + C_m \delta_{\text{mass}} \frac{\partial \delta_{\text{mass}}}{\partial \theta_0},
\]

\[
\frac{\partial \delta_{\text{mass}}}{\partial \theta_0} = \frac{\partial \delta_{\text{mass}}}{\partial q_0}, \quad \frac{\partial \delta_{\text{mass}}}{\partial q_0} = 0.
\]

The stability functions \(\psi_m, \psi_h,\) and \(\psi_q\) are given by Eqs. (8) and (9) for unstable condition and Eqs. (10) and (11) for stable condition. Accordingly, the gradient components of stability functions are given, for unstable conditions, by

\[
\frac{\partial \psi_m}{\partial x} = 2 \left( 1 + x + \frac{1}{1 + x^2} \right),
\]

\[
\frac{\partial \psi_h}{\partial y} = \frac{4y}{1 + y^2},
\]

and the gradient components of mass conservation are given by

\[
\frac{\partial \delta_{\text{mass}}}{\partial u_0} = \frac{1}{u_0} \int_{d+z_{0m}}^{z} u dz + \frac{4L}{19g} \left( \frac{1}{2} f_1^2 - f_2 \right)
\]

\[
+ \frac{u_0}{19g} \left( \Delta f_1 + \frac{1}{2} \frac{\partial f_2}{\partial u_0} - \frac{\partial f_3}{\partial u_0} \right) - 2u_0 \frac{\partial f_4}{\partial u_0},
\]
\[
\frac{\partial \delta_{\text{mass}}}{\partial \theta_*} = -\frac{2u_*L}{19\kappa} \left( f_1 + \frac{1}{2} f_2 - f_3 \right) + \frac{u_* 2L}{\kappa} \left( \frac{\partial f_1}{\partial \theta_*} + \frac{1}{2} \frac{\partial f_2}{\partial \theta_*} - \frac{\partial f_3}{\partial \theta_*} \right) - \frac{2u_* \partial f_4}{\kappa}.
\]

(A19)

\[
\frac{\partial \delta_{\text{mass}}}{\partial q_*} = 0,
\]

(A20)

where \( \int_{d+z_{0m}}^{\infty} u \, dz \) represents the mass flow estimated by logarithmic wind profile, which is defined in the left term of Eq. (14) and can be expressed by

\[
\int_{d+z_{0m}}^{\infty} u \, dz = \frac{u_*}{\kappa} \left[ \int_{d+z_{0m}}^{\infty} \ln \left( \frac{z-d}{z_{0m}} \right) \, dz + \frac{2L}{19} \left( f_1 + \frac{1}{2} f_2 - f_3 \right) - 2f_4 \right];
\]

(A21)

\[
f_1 = (x^4 - 1) \ln \frac{1 + x}{1 + x_0} \frac{(x^4 - 4)}{4} + \frac{(x^3 - x_0)}{3} - \frac{(x^2 - x_0^2)}{2};
\]

(A22)

\[
f_2 = (x^4 - 1) \ln \frac{1 + x^2}{1 + x_0} + \frac{1}{2} (x^4 - 2x^2 + \frac{1}{2}(x_0^2 - 1)^2;
\]

(A23)

\[
f_3 = (x^4 - 1) \tan^{-1}(x) - (x_0^3 - 1) \tan^{-1}(x_0) - \frac{1}{3} (x^3 - x_0^3) + x - x_0;
\]

(A24)

\[
f_4 = (z - d - z_{0m}) \tan^{-1}(x_0);
\]

(A25)

\[
\frac{\partial f_1}{\partial x} = 4x^3 \ln \frac{1 + x}{1 + x_0} + \frac{(x^4 - 1)}{1 + x} - x^3 + x^2 - x;
\]

(A26)

\[
\frac{\partial f_1}{\partial x_0} = -\frac{x^4 - 1}{(1 + x)(1 + x_0)} + x^3 - x_0^2 + x_0;
\]

(A27)

\[
\frac{\partial f_2}{\partial x} = 4x^3 \ln \frac{1 + x^2}{1 + x_0^3} + \frac{2(x^4 - 1)}{1 + x^2} - 2x^3 + 2x;
\]

(A28)

\[
\frac{\partial f_2}{\partial x_0} = -\frac{2x_0(x^2 - 1)}{(1 + x_0^3)} + 2x^2 - 2x_0;
\]

(A29)

\[
\frac{\partial f_3}{\partial x} = 4x^3 \tan^{-1}(x), \quad \frac{\partial f_3}{\partial x_0} = -4x_0^3 \tan^{-1}(x_0);
\]

(A30)

\[
\frac{\partial f_4}{\partial u_*} = \frac{z - z_{0m} - d \partial x_0}{1 + x_0^2} \quad \frac{\partial f_4}{\partial \theta_*} = \frac{z - z_{0m} - d \partial x_0}{1 + x_0^2}.
\]

(A31)

\[
\frac{\partial x}{\partial u_*} = 8(z - d)\kappa \theta_*\frac{T u_*^{4}}{x^3}, \quad \frac{\partial x}{\partial \theta_*} = -\frac{4(z - d)\kappa \theta_*^{2}}{x^3};
\]

(A32)

\[
\frac{\partial x_0}{\partial u_*} = \frac{8z_{0m} \kappa \theta_*}{T u_*^{4}}x^{-3}, \quad \frac{\partial x_0}{\partial \theta_*} = -\frac{4z_{0m} \kappa \theta_*}{T u_*^{4}}x^{-3};
\]

(A33)

\[
\frac{\partial y}{\partial u_*} = \frac{8(z - d)\kappa \theta_*}{x^3}, \quad \frac{\partial y}{\partial \theta_*} = -\frac{4(z - d)\kappa \theta_*}{x^3},
\]

(A34)

where \( x = [1 - 19(z - d)/L]^{1/4}, \quad x_0 = (1 - 19z_{0m}/L)^{1/4}, \quad y = [1 - 11.6(z - d)/L]^{1/4}, \) and \( L = Tu_0^2/(\kappa \theta_*). \) For stable conditions, the gradient components of stability functions are given by

\[
\frac{\partial \psi_m}{\partial x} = -a - b \exp(-dx) + db \left( x - \frac{c}{d} \right) \exp(-dx);
\]

(A35)

\[
\frac{\partial \psi_h}{\partial x} = \frac{\partial \psi_m}{\partial x};
\]

\[
= -a \left( 1 + \frac{2}{3} \frac{x}{d} \right)^{1/2} - b \exp(-dx) + db \left( x - \frac{c}{d} \right) \exp(-dx);
\]

(A36)

the gradient components of mass conservation are given by

\[
\frac{\partial \delta_{\text{mass}}}{\partial u_*} = \frac{1}{u_*} \int_{d+z_{0m}}^{\infty} u \, dz + \frac{u_*}{\kappa} \left[ \frac{\partial f(z-d)}{\partial u_*} - \frac{\partial f(z_{0m})}{\partial u_*} + (z - d - z_{0m}) \frac{\partial \psi_m}{\partial u_*} \right];
\]

(A37)

\[
\frac{\partial \delta_{\text{mass}}}{\partial \theta_*} = \frac{u_*}{\kappa} \left[ \frac{\partial f(z-d)}{\partial \theta_*} - \frac{\partial f(z_{0m})}{\partial \theta_*} + (z - d - z_{0m}) \frac{\partial \psi_m}{\partial \theta_*} \right];
\]

(A38)

\[
\frac{\partial \delta_{\text{mass}}}{\partial q_*} = 0,
\]

(A39)
\[
\int_{\zeta}^{\zeta_{om}} u \, dz = \frac{u_0}{k} \left[ f(z - d) - f(z\zeta_{om}) \right] + (z - d) \zeta_{om} \theta_{s} \left( \frac{z_{om}}{L} \right); \tag{A40}
\]

\[
f(y) = \frac{y}{\ln \frac{z}{z_{om}}} - y + \frac{a}{2} \frac{y^2}{L^2} 
- \left( \frac{b}{d} + \frac{L}{d^2} \right) \exp \left( -\frac{d}{L} y \right) + \frac{bc}{d} y; \tag{A41}
\]

\[
\frac{\partial f(y)}{\partial L} = -\frac{a}{2} \frac{y^2}{L^2} \left( \frac{b}{d} + \frac{L}{d^2} \right) \exp \left( -\frac{d}{L} y \right) 
- \frac{dy}{L^2} \left( \frac{b}{d} + \frac{L}{d^2} \right) \exp \left( -\frac{d}{L} y \right); \tag{A42}
\]

\[
\frac{\partial L}{\partial u_0} = \frac{2u_0}{k \theta_s}, \quad \frac{\partial L}{\partial \theta_s} = -\frac{Tu_0^2}{k \theta_s^2}; \tag{A43}
\]

\[
\frac{\partial x}{\partial u_0} = \frac{-2(z - d)k \theta_s}{Tu_0^2}, \quad \frac{\partial x}{\partial \theta_s} = \frac{(z - d)k g}{Tu_0^2}, \tag{A44}
\]

where \( x = (z - d)/L = (z - d)k \theta_s/Tu_0^2, a = 1, b = 0.667, c = 5, \) and \( d = 0.35, \) as in Eqs. (10) and (11).

REFERENCES


Cao, Z., and J. Ma, 2005: An application of the variational method to computation of sensible heat flux over a deciduous forest. \textit{J. Appl. Meteor.}, \textbf{44}, 144–152.


Ma, J., and S. M. Daggupaty, 2000: Using all observed information in a variational approach to measuring \( z_{om} \) and \( z_{ao} \). \textit{J. Appl. Meteor.}, \textbf{39}, 1391–1401.


