Inverse Parameter Estimation of the Turbulent Surface Layer from Single-Level Data and Surface Temperature

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ABSTRACT

A simple inverse parameter estimation method is used in a practical diagnostic approach to obtain the surface roughness lengths and surface resistance parameters from a chi-square cost function containing measurements of wind speed and air surface temperature differences in the atmospheric surface layer. The estimated parameters allow the calculation of the turbulent fluxes of momentum and heat and the surface-layer profiles of wind speed temperature and humidity from single-level data of wind speed and variance, air temperature and humidity, surface temperature, and total heat flux (sum of sensible and latent fluxes, estimated as net radiation minus soil heat flux). The procedure, which is potentially applicable when fast response data are not available without the necessity of external parameters (with the exception of the displacement height), is tested over a field dataset in southern Italy.

1. Introduction

The turbulent transfer of energy and momentum between the atmosphere and the earth’s surface determines the structure of the atmospheric boundary layer and the dry and moist convection, while also affecting the hydrological surface budget through evaporation.

Although in recent years several turbulent transfer measurement projects have spread out a good number of fast-response instrumented meteorological towers, a global flux measurement network is far from being implemented for various reasons (cost, management complexity, etc.). On the contrary, a good deal of continuously operating surface weather stations cover several areas of the globe, routinely collecting averaged single-level data of wind speed, temperature, humidity, solar radiation, and precipitation.

However, modeling fluxes from non-fast-response single-level data implies the introduction of site-dependent parameters (surface roughness, soil–canopy resistances, etc.) that must be otherwise estimated (e.g., Van Ulden and Hostlag 1985; Sun et al. 1999). If wind speed and air temperature are available at a single level, the sensible heat and momentum fluxes can be calculated in principle by the Monin–Obukhov (MO) flux-profile relations when the surface temperature is known, but with the introduction of the roughness lengths for momentum and scalars \( z_0 \) and \( z_{0T} \). Then, the latent heat flux can be calculated by applying the energy balance closure if an estimate of the available energy flux (net radiation minus soil/canopy heat flux) is also available. It is also possible to use single-level humidity measurements and the Penman–Monteith equation (e.g., Garratt 1992), but this requires the parameterization of a soil/canopy surface resistance to evaporation.

The necessity of surface parameters can indeed be skipped in retrieving turbulent fluxes using the flux-variance similarity laws (Katul et al. 1995; de Bruin and Hartogensis 2005). De Bruin et al. (1993) also successfully apply the second-moments similarity to the horizontal wind variance of a cup anemometer, which may be used to estimate the friction velocity without sonic anemometer measurements if the MO length or the sensible heat flux are known. However, these methods also need fast-response temperature measurements and do not give direct information on the surface-layer profiles, which depend on the local roughness. These site-dependent quantities can, in principle, be directly estimated from single-level surface meteorological data only if turbulent fluxes are known (Martano 2000); otherwise, the use of models and parameterizations is required.
In this case, a certain degree of uncertainty is generally introduced by the use of mechanistic models for calculating surface parameters over natural landscapes, because of difficulties in properly accounting for the complex random characteristics of the earth surface as well as the scale matching between them and the source area of the fluxes. For example, a possible simple parameterization of \( z_0 \) is proportional to the average effective height of the canopy, but with at least a factor of 2 of uncertainty, which can further increase up to one order of magnitude if the canopy is too “sparse” or too “dense” (Brutsaert 1982; Garratt 1992). More involved parameterizations have been proposed to explicitly take into account the roughness elements’ distribution and shape, but with the introduction of additional parameters such as roughness density and drag coefficient at some characteristic height (Hryama et al. 1996). The use of the momentum roughness instead of the scalar roughness in the temperature profiles, without an appreciable correction of the measured surface brightness temperature (the aerodynamic temperature), is generally found to introduce large errors into the computed fluxes (Sun et al. 1999). The aerodynamic temperature can be directly related to the measured surface temperature, but at the expense of introducing empirical coefficients that must be locally evaluated, although apparently less sensitive to measurements errors than \( z_{0T} \) (Sun 1999).

Models have been proposed for the parameter (kB\(^{-1}\)) that relates the scalar roughness to the momentum roughness [kB\(^{-1}\) = \( \ln(z_0/z_{0T}) \)]. Classical formulations as functions of the surface Reynolds number have been proposed for smooth surfaces and for bluff roughness elements (Brutsaert 1982) and have been proved to be appropriate for the sea surface (Zilitinkevich et al. 2001). However, there is experimental evidence that the scalar roughness is not related to the momentum roughness over land, especially over nonhomogeneous vegetated surfaces, thus suggesting the benefits of using dual-source models (Blyth and Dolman 1995; Verhoef et al. 1997) and that it also may be dependent on the turbulent surface flow conditions and strictly related to the approach for determining the surface temperature (Sun and Mahrt 1995; Malhi 1996; Verhoef et al. 1997). Su et al. (2001) compare two different dual-source models to estimate kB\(^{-1}\) over the earth’s surfaces as a function of the canopy characteristics (such as fraction cover or leaf area index, canopy height, typical leaf dimension) that appear to perform reasonably well but indeed require a certain amount of local parameters describing the area involved. The use of single-level wind speed, air temperature and humidity, radiation, and surface temperature is also very general in remote sensing estimations of turbulent fluxes, but it requires additional local information. Kustas et al. (1999) use a mixed layer value for wind speed and air temperature and remotely sensed surface temperature to estimate turbulent fluxes by a relatively complex dual-source model in which \( z_0 \), \( z_{0T} \), and the surface resistances are parameterized in term of additional remotely sensed (satellite) surface cover data of the involved region. Boegh et al. (2002, 2004) used remote sensing data in a simpler approach where the surface humidity was estimated as the weighted average between surface saturation and air humidity by a “decoupling coefficient,” which gives good estimates of the turbulent heat fluxes without the parameterization of the surface roughness, but for mainly energy-limited conditions for evaporation.

A different attempt to avoid the need for soil–canopy texture descriptions was made by Caparrini et al. (2004), who used an inverse variational scheme on a prognostic force–restore model for the surface thermal balance to retrieve the evaporative fraction and the thermal bulk transfer coefficient from single-level meteorological data and surface temperature, whenever an effective thermal inertia parameter is known for the land surface. In a very recent application to air pollution problems, Storch et al. (2007) retrieved some relevant boundary layer parameters in the transient advection–diffusion equation from concentration measurements, using the Marquardt–Levenberg method of minimization of the least squares norm.

As noted elsewhere (Martano 2000), in meteorological applications the roughness lengths are defined in terms of the flux-profile relations in the surface layer, so they can be considered to be regression parameters between modeled and measured meteorological variables. In this context a simple turbulent flux model with a minimum number of locally representative parameters (effective roughness lengths and effective surface resistance to evaporation) may be considered reliable if an objective way of tuning the site-dependent parameters is available.

In this work, an attempt is made to skip the modeling of the roughness lengths in terms of additional surface information, in order to retrieve the surface turbulent fluxes from a minimum set of parameters and single-level meteorological data with the addition of the surface temperature. This is achieved by applying a method of inverse parameter estimation to a cost function of the single-level wind speed and air–surface temperature difference measurements, using the energy budget closure as a constraint for the heat fluxes in the form of the Penman–Monteith equation and the horizontal wind variance as a constraint for the momentum flux. The aim is to obtain an objective estimation for
both the fluxes and the surface-layer roughness from single-level measurements and surface temperature, which can also be applied when fast-response measurements are not available.

2. Inverse parameter estimation

If \( \mathbf{X} \) is an \( n \)-valued measurements vector (some properly chosen meteorological data) and \( \mathbf{Y} \) is the \( n \)-valued vector of the model outputs (representing the same \( \mathbf{X} \) data and expressed as a function of the fluxes and of an \( m \)-valued vector \( \mathbf{p} \) of the parameters), then, for a Gaussian distribution of the data uncertainties, the fluxes and parameters determination can be attempted by looking for the minimum of the chi-square cost function \( S^2 \) (e.g., Martin 1971):

\[
S^2 = n^{-1}[\mathbf{Y}(\mathbf{p}) - \mathbf{X}]^T \mathbf{W}[\mathbf{Y}(\mathbf{p}) - \mathbf{X}],
\]

where \( \mathbf{W} \), the weight matrix, is the inverse of the \( n \times n \) covariance matrix of the measurements and the superscript \( T \) indicates the transposed matrix. In the general case in which \( \mathbf{Y}(\mathbf{p}) \) is nonlinear, a simple and effective minimization procedure is the Levemberg–Marquardt minimization method, which can be used to find \( \mathbf{p} \) by iteration as (Beck and Arnold 1977)

\[
\mathbf{p}_{k+1} = \mathbf{p}_k + (\mathbf{J}^T \mathbf{W} \mathbf{J} + \mu \mathbf{D})^{-1}[\mathbf{J}^T \mathbf{W}(\mathbf{X} - \mathbf{Y}(\mathbf{p}_k))],
\]

where \( \mathbf{J} = \partial \mathbf{Y}/\partial \mathbf{p} \) is the \( n \times m \) sensitivity matrix, \( \mathbf{D} \) is a positive definite diagonal matrix (diagonal elements of \( \mathbf{J}^T \mathbf{W} \mathbf{J} \)), and \( \mu \) is the Marquardt parameter. The term \( \mu \mathbf{D} \) is a regularization term that allows the matrix \( (\mathbf{J}^T \mathbf{W} \mathbf{J} + \mu \mathbf{D})^{-1} \) to always be positive definite, ensuring an actual decrease of \( S \) at each step with an appropriate choice of \( \mu \) where necessary. It also generalizes the Gauss–Newton solution (\( \mu = 0 \)) for ill-conditioned \( \mathbf{J}^T \mathbf{W} \mathbf{J} \) (e.g., when the sensitivity of the model to different parameters is very different), retaining the same simplicity of implementation, these being the main reasons for using it in the present context. The use of the diagonal elements of \( \mathbf{J}^T \mathbf{W} \mathbf{J} \) in \( \mathbf{D} \) ensures a comparable order of magnitude for the elements of the two matrices, setting the order of magnitude of \( \mu \) to be increased–decreased with respect to 1. Each iteration starts with a small \( \mu \) that is increased by a multiplicative factor (e.g., 10) until \( S \) decreases. If the diagonal elements of \( \mathbf{W}^{-1} \) are truly representative of the uncertainty (variances) between the model and the measured data, then the approach to the minimum of \( S \) is flagged by too small values of the decrease of \( S \) with respect to 1, so that the procedure can be stopped even before the numerical convergence has been achieved.

In the present work a diagonal form for \( \mathbf{W} \) has been used (assumed independence of the errors of different measurement), in which the diagonal elements are the inverse of the expected variances. Then, the matrix \( \mathbf{W} \) can be formally omitted by Eq. (2) if the elements of \( \mathbf{J} \) have previously been divided by their respective expected standard deviations, simplifying the calculations. A corollary of the procedure is the estimation of the statistical uncertainty of the obtained parameters \( \mathbf{p}_i \) in terms of their variance \( \sigma_i^2 \), as in this case it is easy to show that (e.g., Aster et al. 2005)

\[
\sigma_i^2 = [\mathbf{J}^T \mathbf{J}]^{-1} \sigma_{pi}^2.
\]

3. The cost function

The cost function \( S^2 \) uses a “dual sensor” approach in which two measured quantities, the air–surface temperature difference and the horizontal wind speed, are compared (in the sense of least square differences) with their modeled counterparts. This means that \( \mathbf{X} \) is a vector of both the air–surface temperature difference \( \Delta T = T_a - T_s \) and the wind speed \( U \) measurements, and \( \mathbf{Y} \) is the vector of the correspondingly modeled values \( \Delta T_m \) and \( U_m \).

A prognostic expression for the air–temperature difference has been obtained as function of the total heat flux \( E \) (the sum of the latent and sensible heat fluxes, i.e., net radiation minus soil heat flux for a conservative energy budget), the wind speed \( U \), the air relative humidity \( H_r \), and the air temperature \( T_a \).

Using the Penman–Monteith equation for the evaporation flux, and the MO bulk transfer expression for the sensible heat flux (e.g., Garratt 1992), the modeled surface–air temperature difference \( \Delta T_m \) can be written as

\[
\Delta T_m = [R_a E \gamma (1 + R_s/R_d) - \rho C_p q_s (1 - H_r)] \{\rho C_p dq_s/dT + \gamma (1 + R_s/R_d)\}^{-1}
\]

\[
= \{(k^2 U)^{-1} [(\ln z/z_0) - \psi_m(z/L)][\ln(z/z_{0T}) - \psi_h(z/L)]E \gamma (1 + R_s/R_d) - \rho C_p q_s (1 - H_r)\} \{\rho C_p dq_s/dT + \gamma (1 + R_s/R_d)\}^{-1},
\]

where \( R_a \) is the air resistance for scalars, expressed by its MO equivalent in the second equality; \( R_s \) is the surface resistance to evaporation; \( z \) is the effective measurement height (\( z = Z - d \), where \( Z \) is the height above the ground and \( d \) is the displacement height), \( z_0 \) and \( z_{0T} \) are the roughness lengths for momentum and
the scalars, respectively; \( L \) is the MO length; \( \psi_m \) and \( \psi_h \) are the stability correction functions for momentum and the scalar transfer, respectively; \( q_s \) is the air saturation specific humidity; \( k, \rho, C_p, \) and \( \lambda \) are constants (von Kármán, air density, air specific heat, and evaporation latent heat, respectively), and \( \gamma = C_p/\lambda \).

The parameter \( R_s/R_a \) is expected to be determined, in general, by the state of the soil (e.g., soil moisture and temperature) and the vegetation (e.g., leaf area index, stomatal resistance). However, it should be expressed solely in terms of the measured variables to obtain a closed model parameterization; an attempt to express the resistance ratio by its expected close correlation with the evaporative fraction in the context of the inverse estimation is presented in section 5.

The expression for the modeled wind speed \( U_m \) is simply the MO similarity form, but writing the friction velocity as \( u_* = \sigma_u \varphi \), where \( \sigma_u \) is the standard deviation of the horizontal wind speed and \( \varphi \) is a function of the stability. This results in

\[
U_m = (u_*/k)[\ln(z/z_0) - \psi_m(z/L)]
\]

\[
= (1/k)\sigma_u \varphi[\ln(z/z_0) - \psi_m(z/L)].
\]

The function \( \varphi \) as used here is defined in Eq. (7) in the next section. It fits the dataset well (see next section) and has also been used with cup anemometer data (de Bruin et al. 1993).

The alternative forms proposed by Wilson (2001) for the stability correction functions of momentum and heat \( \psi_m(z/L) \) and \( \psi_h(z/L) \) in the unstable surface layer are preferred here to the generally used Businger–Dyer expressions (Businger et al. 1971). The Wilson expressions are intended to be analytically simpler and allow an easier estimate of the sensitivity matrix \( \mathbf{J} \) in terms of derivatives of the model expression with respect to the parameters. Indeed, the derivatives have been represented using the chain rule as analytical recursive expressions, instead of as numerical increment ratios to avoid roundoff problems, and the whole Marquardt–Levemberg algorithm has been implemented on a programmable pocket calculator.

Last, the form of the cost function \( S \) is

\[
S^2 = n^{-1} \sum [(\Delta T_m - \Delta T)^2/\epsilon_{\Delta T}^2 + (U_m - U)^2/\epsilon_U^2],
\]

where the sum \( \Sigma \) is over the available measurements and \( \epsilon_{\Delta T} \) and \( \epsilon_U \) are the expected standard deviations for \( \Delta T \) and \( U \), respectively.

If the MO bulk transfer relations are used to express \( z/L \) in Eqs. (4) and (5) as recursive functions of \( U, T_a, T_0, z_0, \) and \( z_{0T} \), the unknown (nondimensional) parameters remaining in Eq. (6) are \( \ln(z/z_0), \ln(z/z_{0T}) \), and \( R_s/R_a \).

Any attempt to further simplify the cost function, retaining only the temperature difference terms, just depending on \( \ln(z/z_0), \ln(z/z_{0T}) \), and \( R_s/R_a \) by themselves (“single sensor” approach), caused the algorithm to fail in finding proper values for \( z_0 \) and \( z_{0T} \), with large bias in the determination of the fluxes. The structure of the logarithmic MO expressions for the wind–temperature profiles, which implies circular relationships between the roughness and turbulent scale parameters when no information about turbulent scales/fluxes is available (Sun and Mahrt 1995), caused the results to be partially undetermined. The additional information from the horizontal wind variance \( \sigma_u \) fixes the magnitude of the turbulence velocity scale \( u_0 \) and is the solution adopted here to obtain good estimates of \( u_0 \) and \( z_0 \). The turbulence temperature scale \( T_0 \) remains constrained by the sensible heat flux through the energy conservation condition (total heat flux \( E \)) included in Eq. (4).

4. The dataset

The dataset of measurements used to test the inversion model was collected at the university campus in Lecce (southeastern Italy) between May and June 2005, in a Mediterranean landscape field covered with shrubs and partially surrounded by trees, as described elsewhere (Martano 2000). Here, a 16-m-high mast is equipped with standard meteorological instruments and routinely collects half-hour averages of the above-mentioned meteorological variables, including surface brightness temperature (as measured by a surface Everest 4004 GL thermodiometer), soil heat flux (measured by a Hukseflux HFP01-SC heat plate at 0.02 m under bare soil surface), and net radiation (measured by a Rebs Q*7.1 net radiometer). A fast-response eddy correlation system (Solent–Gill ultrasonic anemometer, and Campbell Krypton hygrometer Kh20) outputs half-hour-averaged turbulent fluxes and variances in streamline coordinates, as described by Martano (2000) as well as the averaged horizontal wind speed.

The relevant displacement height \( d = 8 \) m in the described site, found in previous studies (Martano 2000), has been taken into account to correct the measurement height \( Z \) in the MO similarity profiles as \( z = Z - d \). A global quality test of the fast-response measurements has then been performed to assess the degree to which the dataset fits MO similarity. Figure 1 shows the ratios between the measured turbulent variances \( \sigma_u/u_0 \) and \( \sigma_T/T_0 \) and their similarity expressions, the right-hand sides of Eqs. (7)–(9), versus the stability parameter \( z/L \).
The relation between \( u^* \) and the horizontal wind variance \( u^*/H_{9268} \) is very controversial in the literature. Classically (Panofsky and Dutton 1984), it is not a local MO similarity function of \( z/L \) but rather depends on \( z_i/L \), where \( z_i \) is the boundary layer height (inversion base height in daytime). However, experimental data are controversial and the dependence on \( z_i/L \) often appears to be very weak.

De Bruin et al. (1993) show that MO similarity can reasonably relate \( u^* \) to the horizontal wind variances measured by cup anemometers as

\[
\sigma_u/u^* = 1/\phi = 2.2(1-3z/L)^{1/3},
\]

and this relation for the horizontal wind variance is tested here and will be used in the context of Eq. (5). For the vertical velocity and the temperature variances, the test functions are respectively (Panofsky and Dutton 1984; Liu et al. 1998)

\[
\sigma_w/u^* = 1.25(1-3z/L)^{1/3} \quad \text{and} \quad \sigma_T/T^* = 2.0(1-8z/L)^{-1/3}.
\]

It appears in Fig. 1 that the wind variances fit the MO similarity very well, but some scatter is present for the temperature variances, mainly when approaching neutral conditions.

The MO flux-profile relations have been solved for the parameters \( p_1 = \ln(z/z_0) \) and \( p_2 = \ln(z/z_{0T}) \) [using the Wilson (2001) stability functions and the measured fluxes], and the result is shown in Fig. 2 versus \( z/L \). It appears that the parameter \( p_1 \) is very well defined over the whole dataset while the parameter \( p_2 \) shows a higher degree of scatter that increases when approaching neutral conditions. This is probably related to the effects of vanishing \( T^* \) and the related increased uncertainty in the surface temperature measurements at sunrise-sunset, but is also possibly affected by the influence of the high roughness sublayer in the turbulence measurements taken at a level that is only about 2 times the displacement height, which may cause larger discrepancies with respect to the similarity laws approaching the neutral regime (Garratt 1978). Moreover, in Fig. 2 a possible actual increase in \( p_2 \) with the wind speed cannot to be excluded (Malhi 1996), although \( z_{0T} \), like \( z_0 \), is treated as a constant in this context. The averages and standard deviations for \( p_1 \) and \( p_2 \) over an 18-day dataset (only daytime conditions) are found to be \( p_1 = \ln(z/z_0) = 2.7 \pm 0.8 \), which means that \( z_0 = 0.56 \) m, in good agreement with Martano (2000), and \( p_2 = \ln(z/z_{0T}) = 15 \pm 4.6 \), which means an average value of \( z_{0T} = 2.5 \times 10^{-6} \) m.

5. Expressions for the resistance ratio

Considering \( R_s \) as representative of the effective evaporative response of the (nonhomogeneous) sur-
face, the nondimensional ratio $R_s/R_a$ in Eq. (4) should be expressed in terms of the model variables, that is, based only on information coming from the surface temperature along with air temperature humidity and wind speed, and total heat flux.

A similar approach to flux estimation can be found in Boegh et al. (2002), from which a possible simple closed expression for $R_s/R_a$ could be directly obtained from the flux-gradient similarity. The expression of the total heat flux (the sum of the sensible and latent heat fluxes) can be written in terms of air–surface temperature and humidity differences and air resistance through the bulk transfer relations, and the soil surface resistance can be defined in terms of surface saturation humidity $q_s(T_0)$ and actual surface humidity $q_0$ (e.g., Garratt 1992). This standard set of two equations can be closed, expressing the unknown surface humidity $q_0$ in terms of its limiting values, the air humidity $q_a$, and the saturation humidity at soil temperature $q_s(T_0)$:

$$d q_a = \beta d q_s(T_0) + (1 - \Omega) q_a,$$

with the weighting factor

$$\Omega = \frac{q_s(T_0) / q_a + 1 + R_s/R_a}{q_s(T_0) / q_a + 1},$$

as a function of the external parameter $\beta$ ($0 < \beta < 1$) that limits ad hoc the effective evaporation (Boegh et al. 2002). Boegh et al. (2004) obtain good results in estimating surface heat fluxes in a Danish landscape with $\beta = 0.9$, which allows the surface humidity to get close to its saturation value at the surface temperature, but noting that “one significant drawback of the method is that when the temperature of the evaporating front is not represented by the measured surface temperature . . . it is necessary to adjust the parameter [\beta].” In the case of the present paper (mainly far from saturation conditions), the unknown parameter $\beta$ may be retrieved by the inverse method, because it is possible to obtain an analytical expression for $R_s/R_a$ as a function of $\beta$ from the above-mentioned set of four equations [numerically solved in Boegh et al. (2002, section 2)]. Unfortunately, the obtained expression contains singularities coming from vanishing values of $q_0 - q_a = \Omega[\beta q_s(T_0) - q_a]$ as $\beta$ decreases that make it of impractical and uncertain use in an inverse estimation of the $\beta$ parameter and generally tends to limit the validity of the approach to close-to-saturation conditions. Thus, a different solution has been attempted here.

As noted by Salvucci (1997), the transition between moisture-limited (far from saturation) and energy-limited (close to saturation) evaporation is often characterized by an abrupt change in $T_0 - T_a$, which suggests the use of this quantity as the main variable for a simple ad hoc parameterization of the nondimensional variable $R_s/R_a$. Indeed, over a generic surface, the temperature difference controls the sensible heat flux through the air resistance (function of the roughness lengths), and then, together with the total available heat flux (incoming net radiation minus soil flux), the flux partition, that is, either the Bowen ratio or the evaporative fraction (latent heat flux divided by total heat flux).

The candidate expression to parameterize $R_s/R_a$ should then depend on $T_0 - T_a$ in a nondimensional form, but also normalized to the total heat flux, because it should control the evaporative fraction more than the absolute evaporation flux (depending on the total heat flux). An expression of this kind could be simply the outgoing longwave radiation normalized to $E$: $\sigma T_0^4 - \sigma T_a^4)/E$, which has a first-order dependence on $T_0 - T_a$ ($\sigma$ is the Stefan–Boltzmann constant). However, if $R_s/R_a$ is the main parameter governing the evaporative fraction in the Penman–Monteith equation, the “corrected” complement of the evaporative fraction, $(Q_s - Q_{sat})/E = \rho C_p(T_0 - T_a)(R_s/E) - Bo_s(1 + Bo_s)^{-1}$, where $Q_s$ is the sensible heat flux and $Q_{sat}$ is the saturation sensible heat flux at the saturation Bowen ratio $Bo_s = 0.79(q_s/dT) - 1(q_s/dT + \gamma) - 1$ (e.g., Garratt 1992), is expected to be a function of the resistance ratio. Indeed, this nondimensional group should be strongly correlated with $R_s/R_a$ as it must directly increase with decreasing evaporative fraction (increasing $R_s$), it depends on $R_a^{-1}$, and it vanishes in saturated conditions (vanishing $R_s$). Obviously, other groups or a combination of the two groups are possible in principle, and the data test is necessary to make a proper choice. With known (measured) fluxes, temperature, and humidity, the Penman–Monteith equation can be inverted to calculate the ratio $R_s/R_a$ from the experimental data. Figure 3 shows the experimentally retrieved values of $R_s/R_a$ versus the measured $(Q_s - Q_{sat})/E$ (squares) and the product $[(Q_s - Q_{sat})/E] [(\sigma T_0^4 - \sigma T_a^4)/E]$ (circles). The proposed nondimensional expressions seem to be very consistent with the Penman–Monteith equation in representing the resistance ratio for the present dataset, but further investigations for different datasets may be useful to test their general applicability. The first scatterplot is very well represented by a two-parameter exponential law, as shown by the continuous line, while in the second case the plot is somehow linearized, although at the expense of a larger amount of scatter, with the advantage of suggesting a simpler one-parameter proportionality law. Both resulting formulations have been tested in the inverse model as

$$R_s/R_a = R_1 \exp[R_2(Q_s - Q_{sat})/E]$$

$$= R_1 \exp[R_2(\rho C_p(T_0 - T_a) (R_s(z_0,z_{0T}))E]$$

$$- Bo_s(1 + Bo_s)^{-1}),\text{ (10)}$$

for the four-parameter model in section 6 and
within the expected errors, to their experimental values $\Delta T$ and $U$;
2) the Penman–Monteith equation with $R$ (or $R_1$ and $R_2$) updated at each iteration, which also includes the energy budget closure with the measured $E$ for the estimated fluxes; and
3) the logarithmic (MO) flux-profile relations, with fluxes and roughness lengths updated at each iteration.

Equation (6) has been minimized iteratively over a 1-h-averaged dataset of 18 days in daytime conditions (say, $n \sim 150–200$), using Eq. (2) for the above-mentioned $p$ parameter vectors. To avoid large errors that are due to the uncertainty of the data and the applicability of the similarity relations, only wind speed larger than 1 m s$^{-1}$ and total heat fluxes larger than 50 W m$^{-2}$ have been selected in these calculations.

From previous experience with measurements at the same site, constant standard deviations of 2 K and 0.5 m s$^{-1}$ were used in all computations, which are considered to be representative of the uncertainties $e_{\Delta T}$ and $e_U$ in Eq. (6). Although affected by the ability of the model to reproduce the measured data, the uncertainty depends on the measurement errors and the statistical variance, for the average wind speed, while for the temperature difference it is expected to be due mainly to the measurement error and the ability of the small measurement area of the surface temperature (about 1 m$^2$) to represent the whole source area of the fluxes. In this case, a comparison with some available satellite surface temperature data of 1-km$^2$ resolution (land surface temperature maps derived from the National Oceanic and Atmospheric Administration Advanced Very High Resolution Radiometer) confirmed a reasonable reliability of the surface temperature measurements within about 2 K of the standard deviation. Anyway, the obtained values for the minimum of $S$ of order 1 (between 0.7 and 1.1 in all cases) confirmed this choice to be reasonable, and this test can always be used for a correction of the weights $e_{\Delta T}^2$ and $e_U^2$ of Eq. (6) after a first “trial” run of the algorithm. The algorithm numerically converges within about 20 iterations typically (from initial values of the parameters: $z_0 = 10^{-1}$ m, $z_{0T} = 10^{-3}$ m, $R = R_1 = R_2 = 1$), but a stopping condition has been used to halt the program when $S$ is close to 1 and the iteration decrement $dS$ is much less than the expected standard deviation of the chi-square distribution of $S^2$ (e.g., $S < 1 + 4n^{-1/2}$ and $dS < 0.1n^{-1/2}$), thus reducing the number of iterations to 10–15. Both the three-parameter model of Eq. (11) and the four-parameter model of Eq. (10) have been tested in two different cases:

6. Results

The inversion procedure looks for the vector parameter $p$ [either $p = [\ln(z/z_0), \ln(z/z_{0T})]$, $R_1$, $R_2$] or $p = [\ln(z/z_0), \ln(z/z_{0T})]$, $R$] according to either Eq. (10) or Eq. (11) for $R/R_a$. and the turbulent fluxes that best satisfy the following conditions:

1) the optimization of the modeled $\Delta T_m$ and $U_m$ to be as close as possible (in the least chi-square sense),

$$
\frac{R}{R_a} = \frac{R[(Q_s - Q_{sat})/E]}{[(\sigma T_0^4 - \sigma T_0^3)/E]}
= \frac{R[pC_p(T_0 - T_a)/[ER_a(z_0, z_{0T})]}
- Bo_s(1 + Bo_s)^{-1}[(\sigma T_0^4 - \sigma T_0^3)/E],

$$ (11)

for the three-parameter model in that section.

Here, $R$, $R_1$, and $R_2$ are the nondimensional parameters to be determined, and the air side resistance $R_a(z_0, z_{0T})$ in the right-hand side is expressed by MO bulk transfer relations as being a function of $z_0$ and $z_{0T}$ and the measured variables. Note that the second expression for $R/R_a$ in Eqs. (10) and (11) is applied in the inversion model (parameterized form: fluxes to be estimated) while the regression lines in Fig. 3 refer to the first equality in Eqs. (10) and (11) (with measured fluxes), and in this case the regression parameters are found to be (18-day dataset, daytime conditions) $R = 65$, $R_1 = 0.15$, and $R_2 = 5.9$. 

![Figure 3. Retrieved $R/R_a$ from the Penman–Monteith equation vs $(Q_s - Q_{sat})/E$ (squares) and $(Q_s - Q_{sat})/E \times (\sigma T_0^4 - \sigma T_0^3)/E$ (circles). The continuous lines represent exponential and linear
](image-url)}
FIG. 4. Calculated vs measured friction velocity in case 2 for the four-parameter (circles) and three-parameter models (squares). The crosses represent case 1 for the four-parameter model.

FIG. 5. As in Fig. 4, but for sensible heat flux.

1) \( E = R_n - G \), where \( R_n \) and \( G \) are respectively the measured net radiation and ground heat flux, and

2) \( E = Q_s + Q_e \), where \( Q_s \) and \( Q_e \) are the true measured sensible and latent heat fluxes, to get rid of errors from imperfect energy balance closure such as, for example, uncertainty in soil heat flux measurements (Cava et al. 2008).

The obtained results for the parameters are (roughness lengths in meters)

1) \( p_1 = \ln(z/z_0) = 2.71 \pm 0.04 (z_0 = 0.53), p_2 = \ln(z/z_{0T}) = 15.5 \pm 1.1 (z_{0T} = 1.4 \times 10^{-6}), p_3 = R = 53 \pm 14 \) and \( p_1 = \ln(z/z_0) = 2.7 \pm 0.04 (z_0 = 0.54), p_2 = \ln(z/z_{0T}) = 14.1 \pm 0.7 (z_{0T} = 6.0 \times 10^{-6}), p_3 = R_1 = 0.37 \pm 0.09, \) and \( p_4 = R_2 = 5.5 \pm 0.7, \) and

2) \( p_1 = \ln(z/z_0) = 2.73 \pm 0.04 (z_0 = 0.52), p_2 = \ln(z/z_{0T}) = 14.1 \pm 0.9 (z_{0T} = 6.0 \times 10^{-6}), p_3 = R = 80 \pm 14 \) and \( p_1 = \ln(z/z_0) = 2.71 \pm 0.04 (z_0 = 0.53), p_2 = \ln(z/z_{0T}) = 14.2 \pm 0.9 (z_{0T} = 5.0 \times 10^{-6}), p_3 = R_1 = 0.56 \pm 0.15, \) and \( p_4 = R_2 = 4.9 \pm 0.7. \)

These results compare well to those from section 4 and also with those from Martano (2000) for \( z_0 \); the differences in the resistance parameters are somehow expected as they are evaluated by complex expressions (Penman–Monteith and \( R/R_{s} \) as functions of the measured fluxes in section 5 (see Fig. 3) and by the parameterized forms of (10) and (11) in the present section (see end of section 5). The roughness parameters appear to be insensitive to both the resistance closure scheme and to the energy balance errors, as they essentially depend on the logarithmic flux-profile relations.

In the present form, the method calculates the parameters \( p_1 = \ln(z/z_0) \) and \( p_2 = \ln(z/z_{0T}) \), and needs in principle the displacement height \( d \) as input. However, Martano (2000) showed that \( d \) can be estimated from single-level data satisfying the MO similarity, if the fluxes are also known. In this context, an extension of the procedure to the simultaneous estimation of \( d \) is not to be excluded; however, it is expected to be more sensitive to possible deviations from the MO similarity in the dataset, because it should be based solely on the optimization of the correction terms, \( \psi([(Z - d)L]) \), in the flux-profile relations (Martano 2000).

Scatterplots of the calculated fluxes are presented in Figs. 4–6 for \( u_s, Q_s, \) and \( Q_e \) (calculated as \( Q_e = E - Q_s \)), respectively. They show that the different forms of the resistance parameterizations in Eqs. (10) and (11) have little effect on the calculated fluxes, as is also suggested by the good regressions in Fig. 3, while the errors in the energy balance closure affect the heat fluxes but not the friction velocity. A thorough discussion of the causes and corrections of the energy imbalance, although apparently important in the practical application of the method, is outside of the scope of the present paper but has been extensively presented elsewhere for the same measurement site (Cava et al. 2008).

Figures 7–10 show the time evolution of the relative error (relative differences between calculated and mea-
measured variables) of $\Delta T_m$, $U_m$, and $Q_s$ for a subset of 10 consecutive days of measurements (from 27 May to 5 June 2005), in daytime conditions, for the three- and four-parameter models in cases 1 and 2 above. Overall, the figures show a reasonable result with a relative uncertainty generally within 20% for $\Delta T_m$ and $U_m$ and 40% for $Q_s$. A slightly positive diurnal trend tends to appear in the estimated sensible heat flux, together with a negative trend in the surface temperature. The figures confirm the insensitivity of the calculated wind speed to both resistance parameterization and energy balance closure, as expected, and also confirm the sensitivity of the heat fluxes to the energy balance closure. They also show that the uncertainty in the calculated temperature difference $\Delta T_m$ is clearly reduced in the four-parameter model, which is apparently connected with the best parameterization of the resistance ratio $R_s/R_a$, as shown in Fig. 3.

7. Comments and conclusions

The approach proposed in this paper is intended to be a practical evaluation of the surface turbulent fluxes together with the correspondent roughness lengths and is applicable to a minimum set of single-level micrometeorological data (horizontal wind speed and standard deviation, air temperature and humidity, total heat flux, and surface temperature) without the introduction of site-dependent parameters. To be generally applied in the present form with surface single-level data, the algorithm needs an estimate of the total heat flux (sum of the latent and sensible heat fluxes), and an estimate of the horizontal wind variance. If the former can be obtained from the net radiation and the soil heat flux, and the latter is obtained by either cup anemometers (de
Bruin et al. (1993) or by the more recent 2D sonic anemometers for weather stations, the procedure is independent of both eddy correlation measurements and external site-dependent parameters (at present, with the exception of the displacement height). The roughness parameters and the surface resistance are optimized over the measurement dataset via an inverse estimation procedure. The simultaneous estimation of heat and momentum fluxes and the related roughness lengths allows a complete description of the vertical structure of the surface layer in terms of flux-profile (MO) relations. As based on diagnostic expressions, the procedure can also be easily used over discontinuous datasets. The proposed algorithm shows stable results in terms of the computed (average values of) roughness lengths, while the estimated heat fluxes are mainly sensitive to a possible energy flux imbalance, in the context of the proposed simple expressions for the air–surface resistance ratio. However, it is possible that more detailed expressions for the surface resistance (in terms of more physical/physiological variables) and/or for the scalar roughness length (in terms of the surface fluxes) could reduce the scatter in the calculated fluxes, although it would probably require sensible changes in the model formulation (e.g., the use of the Penman–Monteith approximation), as well as an increased number of unknown parameters to be found. In the proposed version, with a very reduced number of parameters, and for the considered dataset, the proposed simple formulations of the resistance ratio appear to be consistent with the use of the Penman–Monteith equation and the calculated average values of the roughness lengths are consistent with those obtained from the MO profiles, which are the two basic modeling ingredients. Eventually, testing the present model over different datasets could be of interest in assessing its general applicability, and further developments of the inversion approach may be possible in terms of surface resistance and roughness parameterizations, basic model equations, and the simultaneous estimation of the displacement height.

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