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1. INTRODUCTION

Turbulence and convection act to transport and mix near-surface heat and moisture within a region of the lower troposphere known as the planetary boundary layer (PBL). The daytime (or convective) PBL is variable and is directly affected by interactions at the land surface, in effect serving as a "short-term memory" of land surface processes on diurnal time scales (Stull, 1988). As a result, the time evolution of atmospheric temperature and humidity profiles in the PBL, and of turbulent fluxes and temperature and moisture conditions at the land surface, are dependent upon and feed back on one another.

One problem yet to be resolved in studies of these interactions is how conditions at the land surface can be diagnosed using observations of the PBL and its diurnal evolution. The need for this type of approach has become evident in light of the many challenges involved in modeling land surface interactions via soil-vegetationatmosphere-transfer (SVAT) schemes and the inability to directly measure or estimate these interactions outside of short-term field experiments. Further. atmospheric forecast models at regional to global scales require accurate representation of surface energy and water budgets, and estimating these processes at the scales applicable to such models using discontinuous point-scale observations is a major challenge. A key hypothesis of this work is that by using PBL information it may be possible to estimate regional scale landsurface fluxes without the need for specification of soil and vegetation properties, upscaling procedures, or insitu flux measurement.

Within this framework, the objectives of this paper are to improve understanding and develop methods of estimating conditions and processes at the landatmosphere interface, focusing on how land surface properties and energy budgets influence PBL height and structure. The emphasis will be on *daily* variability in these properties, using the PBL as an integrator of surface conditions on *regional* scales.

2. BACKGROUND AND METHODOLOGY

Previous attempts to exploit PBL-land surface relationships have focused on closure of the heat budget in the PBL and similarity theory, but there has been little application of conservation equations to individual days, little consensus on the treatment of some of the components involved such as entrainment and advection, and available methods require many parameterizations, assumptions, and in-situ measurements of PBL properties. These issues need to be addressed in order for daily surface fluxes and properties such as soil water content and surface temperature to be diagnosed operationally. The conservation of heat in the PBL, including all sources and sinks, is represented by

$$\frac{\partial \overline{\theta}}{\partial t} + \frac{\overline{U_j}}{\partial x_j} \frac{\partial \overline{\theta}}{\partial x_j^2} = \frac{v_{\theta} \partial^2 \theta}{\partial x_j^2} - \frac{1}{\overline{\rho} C_p} \left[L_{\nu} E - \frac{\partial \overline{R_{nj}}}{\partial x_j} \right] - \frac{\partial (\overline{u_j} \overline{\theta})}{\partial x_j} \quad (1)$$

where Θ is the potential temperature, *t* is the time, U_j is the mean wind speed in the jth direction, v_{θ} is the molecular thermal diffusivity, C_p is the specific heat of moist air, ρ is the air density, R_{nj} is net radiation in the jth direction, and u_j' and θ' are the turbulent wind and temperature components (Stull 1988).

i. Storage: The first term $(d\theta/dt)$ is the time rate of change of potential temperature in the PBL, and can be measured using successive radiosonde soundings. The remaining terms of Eq. (1) represent the components of this heat input. The main sources of error in this term are uncertainties in the PBL height and inter-radiosonde calibration between soundings (Betts and Barr, 1996).

The PBL height is identified by a sharp and consistent change in the lapse rates of potential temperature $(d\theta/dz)$ and specific humidity (dq/dt). It can be detected visually from the θ and q profiles, but to eliminate subjectivity, an algorithm was implemented which assigned PBL height to the level where the gradients of θ and q exceed a prescribed threshold $(0.02 \text{ Km}^{-1}, -.025 \text{ g kg}^{-1} \text{ m}^{-1})$.

ii. Advection: Although the main processes affecting PBL development are heat fluxes at the lower and upper boundaries, horizontal advection of heat and moisture $(U_j d\theta/dx)$ must also be accounted for. Numerous methods to estimate this term have been developed including: (1) using a synoptic network of radiosonde data; (2) using a regional atmospheric model; (3) computing advection as the residual term of the conservation equation; (4) assuming it to be zero for multi-day composites; and (5) assuming it to be negligible based on selected case studies.

In summary, there is no consensus on how to treat advection, and it typically represents the largest uncertainty in PBL budget analyses. However, a variety of studies have shown that using the change in potential temperature in the free atmosphere (just above the mixed layer) between successive soundings provides a better estimate of large-scale advection relative to more complex treatments (Hipps et al. 1994; Diak and Whipple 1993; Swiatek 1992). This method estimates advection as being maximum at the top of the PBL, decreasing to 30 percent of the maximum at the

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land surface, with linear variation between these two heights. In all, the dataset includes 55 warm (+1.39 K average) and 22 cold (-1.55 K average) advection days, and contributions to the heat budget range between \pm 100 W m⁻².

iii. Molecular Diffusion and Latent Heating: The third and fourth terms are the molecular diffusion of potential temperature and body sources of heat in the PBL. These quantities are orders of magnitude smaller than the other terms in Eq. (1) (Stull 1988) and are neglected.

iv. Radiative Flux Divergence: Radiative flux divergence (RFD; (dR_{nj}/dx_j)) is often ignored in heat budget analyses and is generally assumed to be negligible during the daytime (Arya 2001). However, Glazier et al. (1976), Kustas and Brutsaert (1987), Peters-Lidard and Davis (2000), and Freedman et al. (2001) all emphasize the possible significance of RFD in the conservation equation, which may comprise up to 40 percent of the total heat budget under certain conditions.

For this work, a radiative transfer model was used to estimate RFD and assess the significance of this term in the overall heat budget. STREAMER (Key et al. 1998) is a robust radiative transfer model that uses at minimum a 2-stream approximation of the full radiative transfer equation. STREAMER was run for four times daily to examine the daytime evolution and the response of radiative fluxes to different surface and initial profile conditions.

v. Surface Sensible Heat Flux: The sensible heat flux into the PBL is estimated using $d(u_j\theta)/dx$, which is composed of surface sensible heat flux (H_s) and entrainment of heat into the top of the PBL (H_i). H_s is typically only measured routinely during short-term field experiments which commonly have uncertainties of at least 10 percent due to instrument and sampling error. Further, point measurements of surface fluxes are not necessarily representative of areas larger than the local field in which they are collected, and instrumentation to measure such fluxes are expensive and labor intensive. These difficulties are the main reason why alternative methods to estimating surface fluxes have been a popular topic of study in recent years.

vi. Entrainment: The upper-air flux of heat (H_i) into the PBL is difficult to estimate directly. It can be estimated using gradients of temperature and moisture at or near the PBL height, but such methods require numerous assumptions. The 'slab' model developed by Tennekes (1973) is a simplification of the conservation equation that ignores advection, subsidence, and RFD, but can be problematic because of its sensitivity to small errors in PBL height (on the order of 60 m) and uncertainty in inversion-level temperature, humidity, and vertical velocity, measurements (Cleugh and Grimmond 2001).

Therefore, a great deal of work has been done to develop an entrainment parameter such that

$$-H_i = A_R \cdot H_s \tag{2}$$

where A_R provides the magnitude of entrainment relative to surface sensible heat flux. For long term averages

typical values of A_R in the literature vary from 0.2 (Stull 1988) to 0.39 (Peters-Lidard and Davis 2000; Dolman et al. 1997; Barr and Strong 1996; Barr and Betts 1997; Betts and Ball 1994; Betts and Barr 1996), while hourly values range from –0.2 to greater than 2.0 (Kustas and Brutsaert 1987; Peters-Lidard and Davis 2000; Cleugh and Grimmond 2003). An accurate estimate of this parameter would enable entrainment to be specified without the need for detailed measurements of the PBL at the inversion height, but agreement on values for daily average and diurnal time scales has proven problematic. Because H_S is available, the entrainment fluxes were estimated as a residual from the conservation equation.

3. STUDY SITE AND DATA

The Atmospheric Radiation Measurement Cloud and Radiation Test Bed in the Southern Great Plains (ARM-SGP) provides surface flux, meteorological, and hydrological observations along with atmospheric profiling for a network of sites in and near the winter wheat belts of Oklahoma and Kansas. Radiosondes were launched up to 4 times daily from the SGP central facility (Lamont, OK) during intensive field campaigns. Soundings at 1130 Z and 2030 Z are representative of the onset of surface heating (sunrise) and maximum PBL height, and serve as ideal endpoints for daily measurements of PBL growth. ARM-SGP employs Bowen ratio (EBBR) flux instruments that provide 30minute average fluxes of net radiation, sensible, latent, and soil heat, along with co-located surface radiant temperature, soil water content (averaged 0-5 cm over 5 locations), 2-m air temperature, mixing ratio, and wind data measurements from micrometeorological instrumentation.

Fluxes were averaged from three sites closest to and possessing similar land cover characteristics as the central facility where the radiosondes were launched. Spatial averaging helps to smooth out localized anomalies in flux data and is more representative of the 10-100 km fetch over which the PBL tends to interact with the land surface (Ek and Holstag 2003; Cleugh and Grimmond 2003; Dolman et al. 1997; Oke 1987).

Data for the summer months (JJA) of 1997, 1999, and 2001 were examined, characterized by high available energy at the land surface and a wide range of boundary layer growth. Overall, 132 dates were used in the analyses.

4. RESULTS

4.1 RFD

RFD in the PBL (as simulated by STREAMER) is characterized by strong diurnal variation with negative values of RFD at night and in the early morning, maximum values just after noon, and positive RFD through the afternoon. Daily means of RFD range from 0 to +20 W m⁻², but are much larger at any single time of day (\pm 80 W m⁻²). These diurnal patterns reflect variability in solar radiation and humidity in the lower 1-2 km of the atmosphere. The net effect is that humidity moderates the diurnal near-surface temperature cycle, and in effect lowers the gradient of net radiation from the surface to the top of the PBL. To incorporate RFD into conservation analyses, a linear model was employed predicting daily RFD across the range of specific humidities present in the dataset.

4.2 Conservation Analyses

Contributions to total heat storage for each term of the conservation equation range from 1.5-7.8 percent for advection, 2.9-4.3 percent for RFD, 62.3-65.8 percent for H_s , and 23.3-32.8 percent for H_i . The relative unimportance of advection and RFD on daily time scales is apparent as together they contribute less than 10 percent of the heat added to the PBL throughout the day.

The mean value of the entrainment parameter, A_R , for all 132 days is 0.48, which is over two times the conventional estimate of 0.20. Based on wind measurements from ARM-SGP, the mean friction velocity (u^* ; the scaling parameter for mechanical turbulence) was 0.828 ms⁻¹ for the dates considered, indicating that a significant amount of wind shear is likely the cause of some of the high entrainment fluxes (Pino et al. 2003; Betts and Barr 1996, 1997; Kustas and Brutsaert 1987).

By using this estimate of A_R in combination with the conservation equation, we can solve for H_s . There is little skill in predicting surface sensible heat flux in this manner ($R^2 = 0.146$), which lends credence to the hypothesis that large day-to-day variability is present in the proportion of heat added to the PBL from the surface versus entrainment. This result also illustrates the inability of *average* budget parameters to capture PBL variability using heat conservation principles.

4.3 Controls on PBL/Land-Surface Relationships

The results presented above suggest that conservation analyses are confounded by fundamental properties such as PBL height, atmospheric stability, soil water content, near-surface temperature and moisture, and wind speed. In fact, there are direct and causal relationships between such basic properties and conservation terms, as well as among the properties themselves.

Heat storage is essentially a function of and bounded by PBL height, stability, and near-surface temperature, and as a consequence should be directly related to all three. Our results show that stability, soil water content (SWC), 2m-potential temperature change (DELT), and 2m-specific humidity change (DELQ) exhibit well-defined covariance with PBL height (Fig. 1). DELT by itself explains more than 48 percent of the variance in PBL height, and stronger relationships exist when DELT versus PBL height is stratified by stability and SWC.

Statistical models indicate that stability in the layer of mixed-layer growth is the variable most strongly correlated with PBL height. This differs from the free atmosphere stability typically employed in PBL growth models. Also interesting to note are the non-linearities that are evident in the relationships in Figure 2. For example, when stability drops below 0.0048 K m⁻¹, PBL height increases rapidly. A similar threshold is observed when SWC drops below 10 percent, in which case Bowen ratio (not shown) and PBL height increase sharply. These effects are not captured by slab or conservation-based approaches because these variables are not included.

4.4 Stability and Soil Water Content as Controls

Based on these results, the two most influential and fundamental properties controlling PBL variability are *stability* and *soil water content*, and the two following functional relationships were examined:

PBL Height = f(soil water content, stability) DELT = f(soil water content, stability)

Soil moisture controls partitioning of available energy at the land surface, which in turn fuels the growth of the convective PBL and determines the nearsurface temperature equilibrium. Stability restricts the growth of the mixed layer and entrainment, and as a consequence controls the structure of the PBL that is reflected in the 2m-temperature change over the course of the day.

To investigate these relationships, we employed a procedure similar to one described by Diak and Stewart (1989), Diak (1990), and Diak and Whipple (1993), but without the need for modeling or simplifications. This method estimates three-dimensional surfaces that predict PBL height and DELT as separate functions of soil water content and stability, and enables any one of these variables to be predicted from observations of the other three.

Figure 2 shows PBL height predicted across the full range of stability and soil water content present in the data set. This surface explains 63 percent of the variance in PBL height when tested against the full dataset. Further, a linear model using DELT is able to explain 6 percent of the residual variance not explained by the PBL height surface (i.e., together, stability, soil water content, and DELT explain 69 percent of the variance in PBL height). A second surface (not shown) predicts DELT across the same range of stability and soil water content, and explains 51 percent of the variance in DELT, with PBL height adding an additional 7 percent.

When the two surfaces are overlain, two of the four variables can be solved for simultaneously from observations of the remaining two. With stability and DELT as predictors, this overlaying method explains 76 percent of the variance in PBL height. This accuracy is better than any simple or multiple regression model predicting PBL height from this dataset.

Estimating soil moisture is not as straightforward because: a) stability is not predictive of soil water content, and b) soil water content is not evenly dispersed against the other three variables and a large portion of the predicted surface is data-sparse. Also, because trend surfaces capture the *general variability* of PBL height and DELT, the observed ranges of PBL height and DELT are greater than those predicted. As a result, using observations of PBL height or DELT that are outside of the contoured range to predict soil moisture results in unreasonable estimates of soil water content.

To account for these limitations, we inverted the expressions for the PBL height and DELT surfaces to enable soil moisture to be predicted from the remaining three variables. Further, we assumed values for the saturation and wilting points for soil moisture and used these bounds to constrain and re-scale predicted soil moisture. Resultant predictions explain 66 percent of the variance in soil water content (92 percent when grouped by 5 percent volumetric soil moisture), and all values are within reasonable bounds of observed soil moisture.

5. DISCUSSION AND SUMMARY

By examining a large sample of daily PBL and land surface data, we have transformed noisy and complex observations of such variables into robust methods to estimate and explain daily PBL development and structure. The results from conservation analyses show that estimation of daily surface fluxes is not possible using traditional or mean approximations for budget Further, entrainment and advection are not terms. observable on the scales necessary to obtain accurate budgets. Given these limitations, additional influential and confounding variables were examined and alternative methods of describing these relationships were developed to better describe the day-day variability in PBL-LSEB relationships. More importantly, these methods are based on easily observable variables (namely stability, soil moisture, PBL height, and 2mpotential temperature change) relative to those necessary for conservation approaches.

A natural and useful extension of the methods described in this paper is that soil water content can be estimated inversely from the same variables. Daily observations of surface moisture availability are extremely difficult to obtain directly, and this method does a good job of estimating soil moisture from routinely measured variables. Further, because of the close relationship between soil moisture and Bowen ratio, these estimates also provide information on LSEB. Because the PBL serves as an integrator of surface conditions and fluxes, this approach provides a particularly attractive strategy for estimating regional scale land surface fluxes. These results will also be useful from a remote sensing perspective, as highresolution observations of PBL structure are now available from sensors onboard satellite platforms such as Terra and Aqua.

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Figure 1: Observations of PBL and land surface properties plotted against one another for all 132 days of the study.

Trend Surface of PBL Height



Figure 2: PBL height as a function of stability and soil water content for all 132 days of the study. The highest heights are found under conditions of low soil water content and low stability.