

## 12.8 APPLYING LAGRANGIAN DISPERSION ANALYSIS TO THE EXCHANGE OF WATER AND SENSIBLE HEAT WITHIN A CEREALE CROP CANOPY: A SENSITIVITY STUDY AND COMPARISON WITH LEAF LEVEL MEASUREMENTS

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### 1. Introduction

The surface exchange of energy and trace gases at the soil-vegetation-atmosphere interface occurs over a wide range of spatial scales. Various methods to derive the exchange rates between the vegetation and the atmosphere have been developed to overcome the gap between chamber methods and micrometeorological methods at the canopy and ecosystem scale [Katul et al. (2001)]. A promising approach is the inverse Lagrangian dispersion analysis [Raupach (1989b)]. Several successful applications have been presented within the last decade [Denmead and Raupach (1993); Raupach (1989a); Katul et al. (1997); Denmead et al. (2000); Leuning et al. (2000)]. Only a short introduction can be given here. A dispersion matrix  $D$  connects the sources and sinks  $S$  through

$$C_i - C_R = \sum_{j=1}^m D_{ij} S_j \Delta z_j \quad (1)$$

were  $C_i$  and  $C_R$  are measured concentrations at height  $z_{ci}$  and the reference height  $z_R$ ,  $\Delta z_j$  is the thickness of the source layer  $j$ ,  $D_{ij}$  is the dispersion element from  $z_{ci}$  to  $z_j$  and  $S_j$  is the source strength of  $j$ . Eq.(1) is a set of linear equations that can be solved numerically, when the number of unknowns ( $S_j$ ) is less or equal the number of equations (determined by the number of concentration measurements). The solution is called the inverse problem and solved by least square fitting.  $D$  is parameterized by height functions of the standard deviation of vertical wind speed ( $\sigma_w(z)$ ), and the Lagrangian timescale ( $\tau_L(z)$ ).

### 2. Material and Method

A sensitivity analysis was performed to derive an estimate of the uncertainties, that are introduced

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by the input parameters (scalar profile  $C$  and the friction velocity  $u_*$ ). To evaluate the model calculations, net flux of available heat, as the sum of sensible ( $H$ ) and latent heat ( $LE$ ) was compared to the difference between global radiation ( $Rn$ ) and soil heat flux ( $G$ ), which were measured independently.  $G$  is also used to evaluate the source/sink strength for sensible heat above the ground ( $S_{H1}$ ). For the first time to our knowledge, leaf level measurements were used to evaluate the vertical source/sink distributions. For this purpose, enclosure measurements from single leaves were upscaled by their leaf area index (LAI) to the source layers of the Lagrangian model.

#### a. The Inverse Lagrangian Model

For the parameterization of  $D$ , the normalized turbulence profiles  $\sigma_w(z)/u_*$ , and  $\tau_L(z)u_*/h_c$  are used, where  $h_c$  is the mean canopy height. Since no direct measurements of  $\sigma_w$  were available, a power-law fitted function derived for wheat [Raupach et al. (1992); Denmead and Raupach (1993)] has been used for this study:

$$\frac{\sigma_w(z)}{u_*} = \begin{cases} a_1 & z > h_c \\ a_0 + (a_1 - a_0)z/h_c & z \leq h_c \end{cases} \quad (2)$$

with  $a_0 = 0.2$  and  $a_1 = 1.3$ . The Lagrangian timescale can not be measured directly. According to Raupach (1989a), a simple form  $\tau_L u_*/h_c = 0.3$  can be used. For a more detailed discussion see Leuning et al. (2000) and Raupach et al. (1996).

#### b. Site and instrumentation

Measurements were performed in the late growing season from the mid of June to the end of July 1995. The field site (49° 10' N, 8° 16' E) was a 9ha triticale (rye-wheat hybrid) field in southern Germany. Averaged canopy height was 1.35m. Profiles of water vapor and temperature were measured on six different height levels (0.05, 0.3,

0.65, 0.95, 1.2, 1.65m) averaged for 30 minutes. Fine wire thermocouples (type E, diameter  $76\mu\text{m}$ ), were used for temperature measurements whereas a closed infra-red gas analyzer (LI-COR 6262) with a manifold valve unit switching between 6 sampling lines was used to measure the water vapor concentration. We assume a standard error of 0.2mb for water vapor and 0.2K for the temperature sensors. Friction velocity was determined by aerodynamic profile method at four heights above the canopy with an error of  $\Delta u_* = \max(0.05\text{m/s}, 0.1u_*)$ . Diurnal courses of water vapor exchange rates of single leaves were measured with a portable leaf chamber (PLC4) and the corresponding analyzer LC4 (both ADC, UK). LAI was determined by a destructive method and independently by using an optical leaf area meter (LAI 2000, LI-COR, USA).  $Rn$  was measured at 2.5m by a net radiometer and  $G$  was derived by heat flux plates placed at  $-0.08\text{m}$  in the soil. On average, there were five subsequent leaves (L1, L2, L3, L4, L5) and the ear (E) on each plant, with L1 as the flag leaf and heights  $z(\text{L1})=1.09\pm 0.11$ ,  $z(\text{L2})=0.78\pm 0.15$ ,  $z(\text{L3})=0.52\pm 0.05$ , and  $z(\text{L4+L5})=0.32\pm 0.03\text{m}$ . Averaged values of LAI from both methods were  $\text{LAI}(\text{L1})=0.9$ ,  $\text{LAI}(\text{L2})=1.5$ ,  $\text{LAI}(\text{L3})=0.8$ ,  $\text{LAI}(\text{L4+L5})=0.5$ . For the application of the inverse Lagrangian model, the canopy was divided into three uniform source layers  $j = 1, 2, 3$  with a thickness of 0.45m. To compare the calculated source/sink distributions with the enclosure measurements, leaves were assigned to the source layers according to their mean height. Transpiration rates of single leaves were multiplied by measured leaf area for that leaf. Since L4+L5 were not active anymore during the selected period, sources and sinks of the lowest layer were assigned to the ground. L3 and L2 were assigned to the middle source layer  $j = 2$ , and the flag leaf was assigned to the upper layer  $j = 3$ .

### 3. Results and Discussion

#### a. Sensitivity study

We compared model results for systematically changed values of  $u_*$  and found that  $\Delta S_j(\Delta u_*)/S_j(\Delta u_*)$ , the relative error in  $S$ , resembles the relative error  $\Delta u_*/u_*$ . Since measurements of  $u_*$  become unreliable at low wind speed, the relative error (given above with a minimum value of 0.05m/s) exceeds 100% for  $u_* \ll 0.5\text{m/s}$ . Fig.1 (left panel) shows the diurnal course of  $\Delta u_*/u_*$  resp.  $\Delta S(\Delta u_*)/S(\Delta u_*)$ . It can be

seen, that especially during night, relative errors become extremely large. By varying the concen-

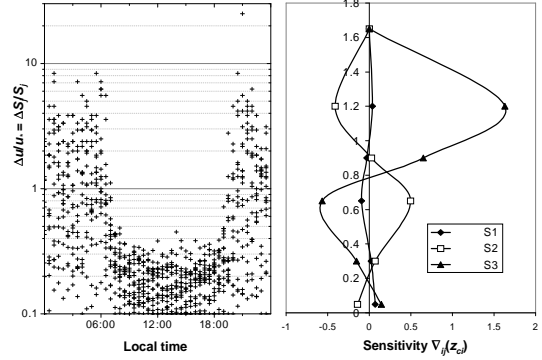


Figure 1: Relative errors in friction velocity and resulting relative errors in the predicted source/sink strength (left). Sensitivity of  $S$  to changes in  $C$  (right)

tration vector, a dimensionless sensitivity matrix  $\nabla$  could be deduced.  $\nabla_{ij}$  expresses the sensitivity of  $S_j$  to a change in  $C$  at  $z_{ci}$ . A comparison of results with systematically and randomly changed normalized concentration profiles showed a uniform sensitivity for a given configuration of input heights and output layers. The derived values for  $\nabla_{ij}$  are plotted against height in Fig.1, resulting in a sensitivity profile  $\nabla_{ij}(z_{ci})$  for each source layer. Weighted by each element  $D_{ij}$ , the least square method to solve Eq.(1) is much more sensitive to errors in the upper heights of  $C_i$ , and most sensitive in the top source layer. In summary, these results led to the formulation

$$\Delta S(\Delta u_*, \Delta c)^2 = \Delta S(\Delta c)^2 + \Delta S(\Delta u_*)^2 \quad (3)$$

$$\Delta S(\Delta c)^2 = u_*^2 \sum_{i=1}^n \frac{1}{n} (\nabla_{j,i} \Delta c_i)^2 \quad (4)$$

$$\Delta S(\Delta u_*)^2 = \frac{S(\Delta S_j)}{u_*} \Delta u_* \quad (5)$$

#### b. Energy budget closure

$Rn$  and  $G$  were used to evaluate the modeled heat flux  $H + LE$ . Fig.2 shows the diurnal course of  $H + LE$  and the residual of the energy budget closure ( $Rn - G - H - LE$ ) for three days. Also shown are the mean errors calculated according to Eq.(3) with a standard error of 0.2mb for water vapor and 0.2K for temperature within the scalar profile. Large deviations from observed values lay mostly within the uncertainty range.

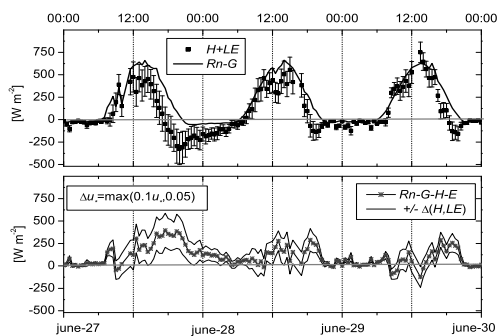


Figure 2: Closure and residual of energy budget

### c. Vertical source/sink distributions

For the upscaling of leaf level transpiration rates to latent heat source in the two upper layers we used measurements during a sunny, cloudless day (27th of June). Fig.3 shows good agreement between upscaled measured rates and inferred source strengths. High values of the upscaled enclosure measurements during early morning and late evening hours are probably effected by high relative humidity inside the chamber and not real. Relative small uncertainties were found compared to available heat flux Fig.(2), where sensible heat is included.

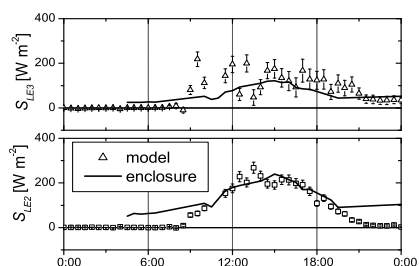


Figure 3: Comparison of modeled source/sink distribution for latent heat with upscaled enclosure measurements in the upper two canopy layers for 27th of June 1995

### d. Nighttime mixing

During calm nights, a free convection regime occurred near the ground due to radiative cooling of the upper canopy, a phenomena that has been observed in dense canopies [Jacobs et al. (1994); Bosveld et al. (1999)]. Under free convective con-

ditions, mixing in the lower canopy does not scale well with the friction velocity but with the free convective velocity  $w_*$ . Neglecting the role of free convection in the parameterization of  $\sigma_w$  leads to an underestimation of vertical mixing and to an underestimation of  $|S_j|$  by the Lagrangian model. Therefore we performed a combined scaling of  $\sigma_w$  that incorporates a convective part. Garrat (1992) gives a first guess with  $\sigma_w/w_* \approx 0.6$  under free convective conditions. As proposed by Jacobs et al. (1994), we used the standard deviation of temperature (at 0.3m height) to approximate  $w_*$ . A linear profile of  $\sigma_w(z, w_*)$ , decreasing with height was added to Eq.(2) for calm nighttime conditions with  $u_* < w_*$ . In Fig.4, modeled

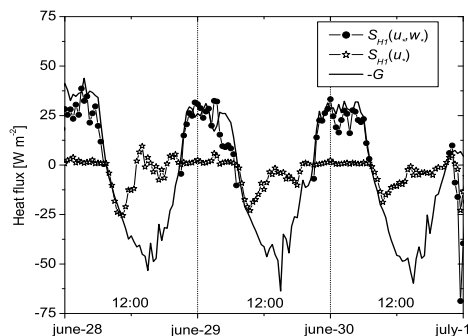


Figure 4: Sensible heat source of the ground layer and measured soil heat flux. The sensible heat source does not include the heat fraction from direct beam radiation during the day

heat flux of the lowest layer is shown with the common scaling procedure ( $S_{H1}(u_*)$ ) and with the modified one ( $S_{H1}(u_*, w_*)$ ). The measured soil heat flux ( $G$ ), also shown in Fig.4, includes a non-turbulent heat fraction from direct beam radiation, which is not included in the modeled values of  $S_{H1}$ . From the early morning to midday,  $S_{H1}(u_*)$  follows  $G$ . With increasing inclination angle of the sun, the beam fraction of  $G$  increases and leads to the deviations of  $S_{H1}(u_*)$  from  $G$  later in the day. During the night, exchange with the air above is underestimated using the scaling based on  $u_*$ . Consequently the sensible heat loss by the soil is also underestimated. By incorporating the convective transport into the dispersion model, the nighttime heat flux above the ground could be simulated quite well using  $S_{H1}(u_*, w_*)$ .

#### 4. Conclusions

The evaluation of available heat fluxes as the sum of latent and sensible heat inferred by Lagrangian dispersion analysis showed a good agreement with independent measurements. Modeled source distributions of latent heat and transpiration rates upscaled from leaf level measurements agreed also well. This offers the applicability of the inverse Lagrangian approach, to estimate canopy conductance in multiple vertical layers within the canopy. These estimates are essential to force and calibrate multilayer models describing the exchange between the vegetation and the atmosphere. By a detailed sensitivity study, error propagation due to  $u_*$  and the input scalar profiles has been analyzed. The proposed error estimation can help to evaluate the modeled source/sink distributions and to distinguish uncertainties caused by inaccurate measurements on one hand and theoretical problems on the other. An important improvement of the inverse Lagrangian analysis would be the incorporation of stability effects into the dispersion model as already proposed by Leuning (2000). Additionally, the role of near-ground free convection during calm nights could be demonstrated in this study since the combined scaling scheme for  $\sigma_w$  using  $u_*$  as well as  $w_*$  showed a significant improvement of the model. For a general use of the modified scaling scheme, intensive investigations of the thermal processes leading to these turbulence characteristics are desired.

#### References

- Bosveld, F., A. Holtslag, and B. Van den Hurk, 1999: Nighttime convection in the interior of a dense douglas forest. *Bound.-Layer Meteorol.*, **93**, 171–195.
- Denmead, O. and M. Raupach, 1993: Methods for measuring atmospheric gas transport in agricultural and forest systems. *ASA Special Publication*, **55**, 19–43.
- Denmead, O. T., L. A. Harper, and R. R. Sharpe, 2000: Identifying sources and sinks of scalars in a corn canopy with inverse lagrangian dispersion analysis i. heat. *Agric. Forest Meteorol.*, **104**, 67–73.
- Garrat, J., 1992: *The atmospheric boundary-layer*. Cambridge atmospheric and space science series, Cambridge University Press, Cambridge.
- Jacobs, A., J. Van Boxel, and R. El-Kilani, 1994: Nighttime free convection characteristics within a plant canopy. *Bound.-Layer Meteorol.*, **71**, 375–391.
- Katul, G., C.-T. Lai, M. Siqueira, K. Schäfer, J. Albertsson, K. Wesson, D. Ellsworth, and R. Oren, 2001: Inferring scalar sources and sinks within canopies using forward and inverse methods. *Observations and modeling of land-surface fluxes within hydrological systems*, V. L. Albertson and J.D., eds., American Geophysical Union, Washington D.C., 31–45.
- Katul, G., R. Oren, D. Ellsworth, C. Hsieh, N. Phillipps, and K. Lewin, 1997: A langrangian dispersion model for predicting co2 sources and sinks, and fluxes in a uniform loblolly pine (pinus taeda l.) stand. *J. Geophys. Res.*, **102**, 9309–9321.
- Leuning, R., 2000: Estimation of scalar source/sink distributions in plant canopies using lagrangian dispersion analysis: Corrections for atmospheric stability and comparison with a multilayer canopy model. *Bound.-Layer Meteorol.*, **96**, 293–314.
- Leuning, R., O. Denmead, A. Miyatat, and J. Kim, 2000: Source/sink distribution of heat, water vapor, carbon dioxide and methane in a rice canopy estimated using lagrangian dispersion analysis. *Agric. Forest Meteorol.*, **104**, 233–249.
- Raupach, M., 1989a: Applying langrangian fluid mechanics to infer scalar source distributions from concentration. *Agric. Forest Meteorol.*, **47**, 85–108.
- , 1989b: A practical langrangian method for relating scalar concentrations to source distributions in vegetation canopies. *Q.J.R. Meteorol. Soc.*, **115**, 609–632.
- Raupach, M., O. Denmead, and F. Dunin, 1992: Challenges in linking atmospheric co2 concentrations to fluxes at local and regional scales. *Aust. J. Bot.*, **40**, 697–716.
- Raupach, M., J. Finnigan, and Y. Brunet, 1996: Coherent eddies and turbulence in vegetation canopies - the mixing-layer analogy. *Bound.-Layer Meteorol.*, **78**, 351–382.