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Agricultural and Forest Meteorology 136 (2006) 108–113
AGRICULTURAL AND FOREST METEOROLOGY
www.elsevier.com/locate/agrformet

The storage term in eddy flux calculations

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Received 20 April 2004; received in revised form 9 December 2004; accepted 11 December 2004

Abstract

Formal derivation of the storage term in eddy flux estimates of surface exchange shows that it is just the difference between instantaneous concentration profiles at the tower measured at the beginning and end of the averaging period, T, divided by T. As such, the storage term is likely to be a poorer estimate of the true concentration change in a representative volume around the tower than the time-averaged eddy flux is of exchange from the surface patch. This is because instantaneous profiles are easily biased by a single gust. To avoid this, many workers compute the storage from time-averaged concentration profiles centered on the beginning and the end of the averaging period. Here we show that this procedure underestimates the storage by at least 50% in most conditions with larger errors occurring when the integral time scale of the turbulence is much smaller than the averaging time T. Reducing the averaging time to the minimum required to smooth out the influence of individual gusts does not improve things significantly.

Keywords: Eddy flux; Canopy flow; Turbulent exchange; Flux measurement

1. Introduction

Calculation of surface-atmosphere scalar exchange by the aerodynamic or 'eddy flux' approach used in the FLUXNET (Baldocchi et al., 2001) involves the estimation of two kinds of term. The first includes the aerodynamic fluxes, both advective and turbulent and the second is the storage term. They reflect the conceptual basis of the method which is to erect a notional control volume V over a representative patch of surface, to measure all the fluxes across the aerial faces of the volume and any change of concentration within it and then to infer the exchange across the surface patch by difference.

Usually, only measurements from a single tower are available and the mass balance in V is approximated by assuming horizontal homogeneity and integrating the point valued mass balance equation from the ground to height h, the location of a sonic anemometer measuring the eddy flux $\overline{w'c'}$, and then averaging over a period T. Defining the time average operator by,

$$\overline{\phi} = \frac{1}{T}\int_{-T/2}^{T/2} \phi(t)\,\mathrm{d}t \tag{1}$$

we obtain,

$$\int_0^h \frac{\overline{\partial c}}{\partial t}\mathrm{d}z + \int_0^h \frac{\partial\overline{w'c'}}{\partial z}\,\mathrm{d}z = \int_0^h \frac{\overline{\partial c}}{\partial t}\mathrm{d}z + \overline{w'c'}(h) = \bar{S} \tag{2}$$

In Eq. (2), z is the vertical coordinate, w' and c' the turbulent fluctuations in vertical velocity and scalar concentration, respectively, and S is the surface exchange rate in flux density units. In the airspace, molecular diffusion has been ignored relative to turbulent fluxes, however, at the soil surface ($z = 0$) or at solid surfaces through the canopy, molecular diffusion is the

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0168-1923/$ – see front matter © 2005 Published by Elsevier B.V.
doi:10.1016/j.agrformet.2004.12.010

initial means of transport of scalars into the airspace. This process is absorbed in the definition of $\overline{S}$. For a more considered derivation of this equation, see Finnigan et al. (2003).

We see from Eqs. (1) and (2) that the storage term can be written as,

$$\int_0^h \overline{\frac{\partial c}{\partial t}} \mathrm{d}z = \int_0^h \left[\frac{1}{T}\int_{-T/2}^{T/2} \frac{\partial c}{\partial t}\,\mathrm{d}t\right]\mathrm{d}z = \int_0^h \frac{1}{T}\left[c\left(z, \frac{T}{2}\right) - c\left(z, -\frac{T}{2}\right)\right]\mathrm{d}z \tag{3}$$

Hence, the storage term is the difference in the *instantaneous* profiles of $c(z, t)$ at the beginning and end of the averaging period, divided by T. In practical cases, the difference between two instantaneous $c(z, t)$ profiles can be very noisy and many workers adopt the strategy of replacing $c(z, \frac{T}{2}) - c(z, -\frac{T}{2})$ in Eq. (3) by $\bar{c}(z, \frac{T}{2}) - \bar{c}(z, -\frac{T}{2})$, the difference between time-averaged vertical profiles centered on the beginning and the end of the flux-averaging period. While removing the problem of a noisy storage term, this procedure is not supported by formal manipulation of the mass balance equation.

Taken over a day, the storage term for most scalars of biological interest becomes negligible compared to the eddy flux term but when we aim to resolve the diurnal cycle over periods like an hour, storage can be significant, particularly around sunrise and sunset. When stratification is strong and turbulence levels are low, particularly at night, the storage term assumes greater importance, often being the dominant term in the mass balance calculation. In this short paper, therefore, we aim to clarify the 'correct' form of this term by formal manipulation of the mass balance equation and to discuss the most appropriate form to use in practice.

2. Analysis

We would like to average the concentration over the volume V, which for convenience we take to be a rectangular box of height h and plan area L^2. With data from a single tower, we can only perform this spatial average in height z. So for quasi-stationary flows, where the turbulent integral time scales are much smaller than the time scale of background variation in concentration, we assume that a time average over period T is equivalent to first performing a spatial average over a plane L^2 at height z and then taking the time average of this spatial average.

Generalizing the time averaging operator in Eq. (1) to a moving average filter, we define,

$$\overline{\phi(t)}^P = \frac{1}{2P}\int_{t-P}^{t+P} \phi(t')\,\mathrm{d}t' \tag{4}$$

where it is convenient to write $T = 2P$. With only a single tower, we cannot average the primitive conservation equation over the control volume V. Instead, we assume that the moving average filter in Eq. (4) can serve as a surrogate for volume averaging and use it rather than the simple time average in Eq. (1). Eq. (2) then becomes,

$$\int_0^h \overline{\frac{\partial c(t)}{\partial t}}^P \mathrm{d}z + \overline{w'c'}^P(h, t) = \bar{S}^P(t) \tag{5}$$

Comparing Eqs. (4) and (1), it is clear that $\bar{c} = \bar{c}^P(0)$ and it is straightforward to show that,[1]

$$\frac{\partial \bar{c}^P}{\partial t} = \overline{\frac{\partial c}{\partial t}}^P; \quad \left.\frac{\partial \bar{c}^P}{\partial t}\right|_{t=0} = \left.\overline{\frac{\partial c}{\partial t}}^P\right|_{t=0} = \overline{\frac{\partial c}{\partial t}} = \frac{1}{T}\left[c\left(\frac{T}{2}\right) - c\left(-\frac{T}{2}\right)\right] \tag{6}$$

Since we can always, without loss of generality, select the origin of the time coordinate $t = 0$ in the centre of our averaging period T, it is clear that we can write the storage term in three precisely equivalent ways, viz,

$$\int_0^h \frac{\partial\left(\overline{c(z,t)}^P\right)}{\partial t}\mathrm{d}z\bigg|_{t=0} = \int_0^h \overline{\frac{\partial c(z,t)}{\partial t}}^P \mathrm{d}z\bigg|_{t=0} = \int_0^h \overline{\frac{\partial c(z,t)}{\partial t}}\mathrm{d}z = \int_0^h \frac{1}{T}\left[c\left(z, \frac{T}{2}\right) - c\left(z, -\frac{T}{2}\right)\right]\mathrm{d}z \tag{7}$$

and that each of these forms reduces to the difference between instantaneous profiles of $c(t)$ measured at the beginning and end of the averaging period.

The form represented by the first term on the LHS of Eqs. (6) or (7) is the time derivative of the moving-average filtered concentration taken at $t = 0$ or more generally, in the middle of the averaging period. Approximating this derivative by a first order central difference, we have,

[1] A direct way to do this is to calculate the several terms in Eq. (6) using Eq. (10), the Fourier Integral representation of $c(t)$.

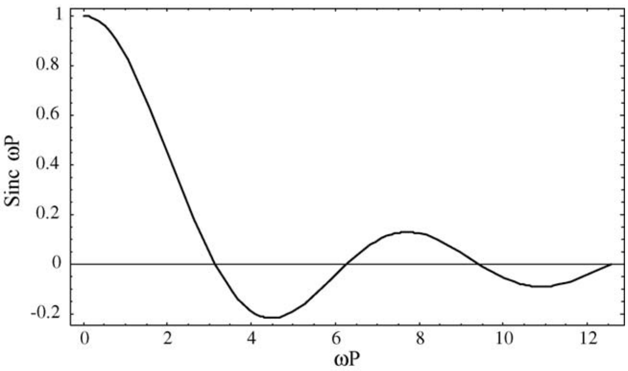

Fig. 1. The transfer function of the moving average window, sinc(ωP). As sinc(x) is even in x, only positive frequencies are shown.

$$\left.\frac{\partial \overline{c}^P}{\partial t}\right| t=0 \simeq \frac{\overline{c}^P(P)-\overline{c}^P(-P)}{2P} \tag{8}$$

but we see from Eq. (4) that this is just the difference between time averages of $c(t)$ centered on the beginning and the end of the averaging period, then divided by $T = 2P$. In other words, the strategy adopted at some flux sites to smooth out noise in the storage term amounts to taking a first order central difference approximation to the exact form of the storage term.

We can make the effect of this procedure more quantitative in the following way: define the Fourier transform of $c(t)$ as,

$$\hat{c}(\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty} c(t)\exp(\mathrm{i}\omega t)\,\mathrm{d}t \tag{9}$$

where we assume that $c(t)$ has a mean of zero over a time scale much larger than T so that the integral in Eq. (9) converges and $\hat{c}(\omega)$ exists (Lenschow et al., 1994). Then,

$$c(t)=\int_{-\infty}^{\infty}\hat{c}(\omega)\exp(-\mathrm{i}\omega t)\,\mathrm{d}\omega \tag{10}$$

and it follows directly by applying Eq. (4) to Eq. (10) that,

$$\left.\frac{\partial \overline{c}^P}{\partial t}\right| t=0 = -\int_{-\infty}^{\infty}\mathrm{i}\omega\,\hat{c}(\omega)\,\frac{\sin\omega P}{\omega P}\,\mathrm{d}\omega \tag{11}$$

while,

$$\frac{\overline{c}^P(P)-\overline{c}^P(-P)}{2P} = -\int_{-\infty}^{\infty}\mathrm{i}\omega\,\hat{c}(\omega)\left[\frac{\sin\omega P}{\omega P}\right]^2\mathrm{d}\omega \tag{12}$$

The function sinc(ωP) = sin(ωP)/(ωP) is the Fourier transform of the moving average window defined by Eq. (4) and so, when a function of time $c(t)$ is filtered by Eq. (4), its Fourier transform is multiplied by the transfer function sinc(ωP). The form of sinc(ωP) is illustrated in Fig. 1. The zero crossings of sinc(ωP) are at $\pm n\pi|$ so the width of the central lobe is $2\pi/P$.

Comparing Eqs. (11) and (12), we see that approximating the exact form of the storage term $\frac{\partial \overline{c}^P}{\partial t}$ by the central difference formula in Eq. (8), is equivalent to low-pass filtering the exact storage term by the moving average window. As we see from Fig. 1, this attenuates the high frequency content of the exact term but not with a sharp filter cut-off. Some high frequency content 'leaks' into the filtered storage term through the positive and negative lobes of sinc(ωP).

3. Discussion

Ideally we would like to compute the storage term as $\overline{\partial\langle c\rangle/\partial t}$, the time average of the rate of change of the concentration, averaged over the volume V. Similarly, we would like to compute the eddy flux term as $\overline{\langle\langle wc\rangle\rangle}(h)$, the time average of the covariance averaged over the plane $4L^2$ at height h.[2] We have seen that instead we are forced to approximate both of these terms using measurements at a single tower, whereupon the storage term becomes simply the difference between instantaneous profiles at the beginning and end of the averaging period and the eddy flux the time average at one level on the tower. It is likely that the time-averaged eddy flux is a better approximation to $\overline{\langle\langle wc\rangle\rangle}(h)$, the true flux through the plane capping the volume V, than the difference between two instantaneous profiles is to

[2] Here, $\langle\,\rangle$ denotes the volume and $\langle\langle\,\rangle\rangle$ the planar averaging operator.

$\overline{\partial\langle c\rangle/\partial t}$, the rate of change of $c(t)$ averaged over V. An errant gust can dominate an instantaneous profile of $c(z, t)$, whereas a long-period time average of $w'c'(t)$ will smooth over many eddies. This seeming paradox arises because implicit in the replacement of the volume average by a time average is the assumption that the time rate of change at any point in the plane is representative of the whole plane.

We want to know how large an error we will generate by using either Eq. (7) or Eq. (8) to compute the storage term. In the first case, using Eq. (7), we will be liable to large random errors from under-sampling $c(t)$ in V, whereas by using Eq. (8) we will lose high frequency content in the storage term that might be needed to balance the eddy flux term and as a result might bias our deduced value for $\bar{S}$.

There are two sources of variation of $c(z, t)$ in V. The first is systematic variation in the x–z plane caused by heterogeneity in the biome in which the tower is placed. The second is the time variation in $c(z, t)$, caused primarily by the intermittent penetration of large turbulent eddies into the canopy (e.g. Gao et al., 1989). If we average for a period long enough to capture a representative number of these eddies, we can avoid the problem of single eddies biasing the profiles of $c(z, t)$ in Eq. (7). At the same time, since these large eddies are accompanied by significant azimuthal variation in the instantaneous wind vector, averaging over a few of them will mean that a volume of the canopy around the tower is effectively sampled. There is little more we can do through time averaging to redress serious problems of biome heterogeneity and tower siting.

For arguments sake, let us suppose that we want to sample for long enough to record the passage of at least 10 such eddies at the tower. It is reasonable to take τ, the integral time scale of the turbulent time series $w(z,t)$ and $c(z, t)$ or of their eddy covariance $w'c'(t)$, as a measure of the time between these eddies. We would want to sample for at least 10τ to form a reasonable surrogate for $\langle c\rangle(t)$ to use as the basis of the storage term calculation. Most Fluxnet sites are in the surface layer or in the roughness sublayer of tall canopies so that typical values for τ under stationary conditions in near-neutral flow are some tens of seconds, so we require an averaging time of $200\ \mathrm{s} \geq 10\tau \geq 100\ \mathrm{s}$. This is much shorter than the averaging time T used at flux tower sites, where typically $3600\ \mathrm{s} \geq T \geq 1800\ \mathrm{s}$. However, we expect that it will be in non-stationary conditions that the storage term is most important so in the next section we want to calculate the difference between the 'exact' value of the storage term given by Eq. (7) with the assumption that the profile on the tower is representative of the whole volume V, and approximate values given by the central difference approximation in Eq. (8) with two different averaging times. First we construct Eq. (8) with $2P = T$, the full average time and then we see if the central difference approximation can be improved by using a shorter averaging time equal to $2P = 10\tau$ in Eq. (8).

To do this, we want to know the effect of using these two choices for averaging period on Eq. (12) for some realistic choice for $\hat{c}(\omega)$. We generally do not have the Fourier transform of $c(z, t)$ available. More usually we have the power spectrum of $c(z, t)$, which is the Fourier transform of the autocovariance function, $R(t - t')$. We define,

$$R(t-t') = \overline{c'(t)\,c'(t+t')} \tag{13}$$

and assume after Lenschow et al. (1994),

$$R(t-t') = \sigma_c^2 \exp\left[-\frac{|t-t'|}{\tau}\right]; \quad \text{with } \sigma_c^2 = \overline{c'^2(t)} \tag{14}$$

Then the power spectrum of $c(z, t)$ is,

$$\hat{S}_C(\omega) = \sigma_c^2 \frac{\tau}{\pi(1+\omega^2\tau^2)} \tag{15}$$

and from Eq. (11) it follows directly that the power spectrum of $\partial\bar{c}^P/\partial t$ is given by,[3]

$$\hat{S}_{\partial\bar{c}^P/\partial t}(\omega) = \omega^2 S_C(\omega)\left[\frac{\sin\omega P}{\omega P}\right]^2 \tag{16}$$

whence the variance of the 'exact' value of the storage term is given by,

$$\overline{\left(\frac{\partial\bar{c}^P}{\partial t}\right)^2} = \overline{\left(\frac{\partial\bar{c}^P}{\partial t}\right)^2} = \int_{-\infty}^{\infty} \hat{S}_{\partial\bar{c}^P/\partial t}(\omega)\,\mathrm{d}\omega$$
$$= \int_{-\infty}^{\infty} \omega^2 S_C(\omega)\left[\frac{\sin\omega P}{\omega P}\right]^2 \mathrm{d}\omega \tag{17}$$

and a measure of the magnitude of the storage term is provided by the square root of Eq. (17).

[3] Note that $\omega^2\hat{S}_C(\omega)$, the power spectrum of $\partial c/\partial t$ does not approach zero as $\omega \to \infty$ but approaches $\sigma_c^2/\pi\tau$ asymptotically. In a real power spectrum of $\partial c/\partial t$, molecular conductivity would ensure an approach to zero at high frequencies. The filtered power spectrum $\hat{S}_{\partial\bar{c}^P/\partial t}(\omega)$, in Eq. (16), does converge to zero however as $\omega \to \infty$.

$$\mathrm{ST}_E = \sqrt{\int_{-\infty}^{\infty} \omega^2 S_C(\omega) \left[\frac{\sin\omega P}{\omega P}\right]^2 \mathrm{d}\omega} \tag{18}$$

Because we derived ST_E starting from the power spectrum $\hat{S}_C(\omega)$, where each spectral component is the squared magnitude of the corresponding component in $\hat{c}(\omega)$, ST_E can only be interpreted as an upper bound on the true value of the storage term in Eq. (11).

We now define a comparable upper bound estimate of the central difference approximation, Eq. (12). Following the same steps as in Eqs. (15–18) we define,

$$\mathrm{SCD}_T = \sqrt{\int_{-\infty}^{\infty} \omega^2 S_C(\omega) \left[\frac{\sin\omega P}{\omega P}\right]^4 \mathrm{d}\omega} \tag{19}$$

where SCD_T is the upper bound on the central difference approximation to the storage term formed from averages of length $2P = T$ centered on the beginning and the end of the averaging period, T. Finally, we form a similar measure, SCD_τ for the central difference approximation but where we use time averages of length $2P = 10\tau$ centered on the beginning and the end of the averaging period, T. From Eqs. (11) and (12) it follows that

$$\mathrm{SCD}_\tau = \sqrt{\int_{-\infty}^{\infty} \omega^2 S_C(\omega) \left[\frac{\sin\omega P}{\omega P}\right]^2 \left[\frac{\sin 5\omega\tau}{5\omega\tau}\right]^2 \mathrm{d}\omega} \tag{20}$$

We can calculate the relative magnitudes of these three upper-bound estimates assuming the form given in Eq. (15) for $\hat{S}_C(\omega)$ and choosing values for $2P = T$ and τ. At most flux sites, default values for T are 3600 s > T > 1800 s while, as we have already noted, in stationary near-neutral conditions, a typical lower bound for τ at tower height is 10 s. In such conditions, however, the storage term will be small and recent re-analysis of flux tower data (Sakai et al., 2001; Finnigan et al., 2003) has shown that low frequency eddies in the boundary layer play a much more significant role in scalar transport near the surface than hitherto realized. Such non-stationary conditions can be represented by increasing the integral time scale in Eq. (15). For example, if we set $\tau = 200$ s then 21% of the variance in $c(t)$ occurs at periods longer than 3600 s. In Table 1, we have compared the ratios $\mathrm{SCD}_T/\mathrm{ST}_E$ and $\mathrm{SCD}_\tau/\mathrm{ST}_E$ for various choices of $2P = T$ and τ.[4]

Several things are obvious from this table:

(1) From the last column, we see that applying the central difference approximation with an averaging time of 10τ, the best we can do is to retrieve around 45% of the true storage term. Hence, the minimum feasible averaging time that will avoid the tower profiles being biased by single gusts returns less than half the exact storage term.
(2) Using the central difference approximation with the full averaging period T gives the poorest result when T/τ is largest with only around 10% of the true storage term being recovered when the integral time scale is 10 s and ~20% when $\tau = 50$ s.
(3) As 10τ, the 'shorter' averaging period in the central difference approximation, approaches T, then the two different forms of the central difference approximation converge.

Table 1
Comparison of the ratios of the central difference approximations to the storage term with two averaging periods, T and 10τ, to the 'exact' value of the storage term

τ (s)	21% of $c(t)$ variance is above this period (s)	$2P = T$ (s)	$\mathrm{SCD}_T/\mathrm{ST}_E$	$\mathrm{SCD}_\tau/\mathrm{ST}_E$
10	180	1800	0.10	0.44
50	900	1800	0.22	0.40
100	1800	1800	0.31	0.41
200	3600	1800	0.42	0.39
10	180	3600	0.08	0.47
50	900	3600	0.17	0.41
100	1800	3600	0.24	0.44
200	3600	3600	0.34	0.45

The ratios are calculated for turbulent time series with different long term-trends associated with different integral scales.

4. Summary and conclusions

A formal derivation of the storage term $\int_0^h \overline{\partial c/\partial t}\,\mathrm{d}z$ at a single tower shows that it is simply the difference between the vertical profiles of $c(z, t)$ at the beginning and end of the averaging period T, divided by T. Either of these profiles is easily biased away from its average over the representative volume V by concentration differences carried by a single gust. As a result, many workers replace the instantaneous profiles by time-averaged profiles centered on the beginning and the end

[4] Convergence of the integrals in Eqs. (18–20) is slow. They were integrated numerically to a frequency of $50\pi/T$. Increasing the integration limit above this frequency changed the final value of the integrand less than 0.01%.

of the averaging period, T. The time constant for these time-averaged profiles is usually also taken as T for convenience.

We have shown that this central difference approximation to the exact storage term is equivalent to a further filtering of the 'exact' storage term by a rectangular window of width T. Typical values of T used at tower sites are much longer than the averaging time necessary to smooth out profile anomalies caused by eddies in well mixed, stationary and fully turbulent flows. We identify this necessary smoothing time as $\sim 10\tau$, where τ is the integral time scale of the turbulence and in such conditions, $\tau \sim 10$ s. In non-stationary flows, when the storage term is likely to make a significant contribution to the mass balance, however, the effective value of τ is much larger, as long as 200 s in many cases.

We have formed measures of the upper bound on the storage term by assuming that the power spectrum of the $c(z, t)$ fluctuations follows the classic Cauchy form, Eq. (15), and also equivalent measures for the central difference approximations with the window width of the additional filtering operation being both the conventional T and the (usually) shorter value 10τ. A comparison of these measures in Table 1 shows that the true storage term can be underestimated by as much as 90% when the integral timescale is short ($\tau \sim 10$ s) and the averaging time used in the central difference approximation is long, $3600\text{ s} > T > 1800$ s. Using the central difference approximation with a shorter averaging time of 10τ improves matters somewhat when $\tau \ll T$ with only $\sim$60% of the exact term lost but as $10\tau \to T$ there is no obvious advantage in using a different averaging period for the central difference approximation to that used in forming the standard tower averages, T. In both cases, about 50% of the true storage term is lost.

In practical operations, many other factors will determine the actual averaging times and procedures used to estimate the storage term. Time delays involved in multiplexing tower concentration profiles through a single gas analyzer may be the prime determinant of the central difference averaging time. Similarly, we must re-emphasize that the measures of comparison of the different approximations, being based on power spectra, are upper bounds and actual values of the storage term may be smaller than indicated here. The largest losses, that we identify with central differencing with T and a short integral time scale, correspond also to quasi-stationary times when the storage term is likely to be negligible compared to the eddy flux term. At other times, when storage may be significant, these calculations indicate that it will be generally underestimated by at least 50% whatever averaging procedure is used. Hence, there is an irreducible error associated in calculating the storage from a single tower, where the worker must choose between the random error associated with using instantaneous profiles and a certain loss of high frequency information if the storage term is calculated from time-averaged vertical profiles.

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