

Chapter 7

CONCERNING THE MEASUREMENT OF ATMOSPHERIC TRACE GAS FLUXES WITH OPEN- AND CLOSED-PATH EDDY COVARIANCE SYSTEMS: THE DENSITY TERMS AND SPECTRAL ATTENUATION

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Abstract

Atmospheric trace gas fluxes measured with an eddy covariance sensor that detects a constituent's density fluctuations within the *in situ* air need to include terms resulting from concurrent heat and moisture fluxes, the so called 'density' or 'WPL corrections' (Webb et al. 1980). The theory behind these additional terms is well established. But, virtually no studies to date have examined the constraints imposed on the theory by different instrumentation technologies and by limitations inherent to eddy covariance systems. This study extends the original WPL theory by examining how eddy covariance instrumentation, particularly spectral attenuation and an instrument's basic technology, influences the application of this theory to flux measurement. Specific issues discussed here include the importance of static pressure fluctuations to the WPL theory, the possible systematic overestimation of the WPL vapor term, and the transfer functions associated with signal processing and volume averaging effects of a fast-response closed-path CO₂/H₂O sensor. This different perspective on the WPL theory suggests that current methods of applying the WPL theory, particularly with closed-path systems, can yield significant biases in the annual carbon balance derived from eddy covariance technology and can cause the surface energy imbalance to increase with increasing wind speed. Furthermore, it is suggested that spectral corrections should be made before applying the WPL theory to estimate fluxes and that high frequency point-by-point conversions from mass density to mixing ratio is not the preferred method for estimating fluxes by eddy covariance.

1. Introduction

Webb et al. (1980), henceforth WPL80, showed that eddy covariance trace gas fluxes measured with a sensor that detects a constituent's density fluctuations within the *in situ* air need to include terms resulting from concurrent heat and moisture fluxes. These additional terms arise as a consequence of the density fluctuations of the ambient air sampled by an instrument that measures trace gas density rather than the constituent's molar mixing ratio (WPL80; Paw U et al. 2000; Fuehrer and Friehe 2002; Massman and Lee 2002). Unfortunately, so far no technology has been developed that allows a single instrument to directly sense a constituent's mixing ratio. So measured mass fluxes will continue to require additional instrumentation for heat and moisture fluxes.

Since WPL80 this theory has been validated for an open-path eddy covariance system (e. g., Leuning et al. 1982), developed and compared for open- and closed-path systems (Leuning and Moncrieff 1990; Leuning and King 1992; Suyker and Verma 1993; Lee et al. 1994; Leuning and Judd 1996), extended to include other terms, most notably the fluctuating pressure term, (e. g., Fuehrer and Friehe 2002; Massman and Lee 2002), and redeveloped in three dimensions (Paw U et al. 2000; Massman and Lee 2002), and further refined by Leuning (2003).

In general there is little doubt about the validity or appropriateness of this theory. However, much of the discussion and development of this theory to date has centered on applying it to different types of eddy covariance instruments, i. e., to open- and closed-path systems. This study takes a different approach by examining how the instrumentation, particularly spectral attenuation and an instrument's basic technology, influences the application of the WPL80 theory to the measurement of eddy covariance fluxes. Central to this issue are the questions of whether spectral corrections should be made before or after applying the WPL80 theory to estimate fluxes and whether making high frequency point-by-point conversions from mass density to mixing ratio is useful for estimating fluxes. Some of these issues have been (at least partially) addressed in previous work and some have not.

To accomplish this goal three fundamentals need to be presented. First, in this study the terms flux and covariance are not used synonymously. Here flux refers to mass transfer rates in the atmosphere. Covariance, on the other hand, refers to the covariance between signals, or truncated data streams, obtained by two different instruments. Thus covariances are associated with instruments. Furthermore, it is assumed here that no eddy covariance instrument is necessarily free of high frequency attenuation and that the amount of attenuation can be unique to

any given instrument or eddy covariance system. In most cases it is generally assumed that correcting the covariances for spectral attenuation yields an estimate of the flux. However, as discussed later, this is not necessarily the case for a closed-path system. Therefore, a distinction is also made between corrected and uncorrected covariances.

Second, the WPL80 terms are not a consequence of inadequate sensor performance, and in that sense they are not instrument related corrections. Any properly functioning CO₂ instrument that employs infrared gas analysis technology detects the number of absorbing CO₂ molecules within the path of its infrared light beam. Assuming that an instrument detection volume is constant, then a CO₂ instrument indirectly measures the density (or number density) of the CO₂ molecules in a sample. Consequently, the WPL80 temperature, pressure, and vapor terms are not required to ‘correct’ the measured trace gas density—Fuehrer and Friehe (2002) make the same point. Rather they are required to compensate for the concurrent density fluctuations in the air sampled with this type of instrument. In essence the WPL80 terms are required to distinguish between the true surface exchange (or biologically relevant) flux and the atmospheric flux measured with a sensor that detects mass density rather than mixing ratio. As a result this study will not refer to the WPL80 terms as corrections.

Third, in principle the WPL80 terms apply to (or characterize) the ambient environment in which the trace gas density is measured. For example, the ambient environment at the place of measurement in a closed-path system is not characterized by a fluctuating temperature field because the intake tube attenuates the temperature fluctuations so strongly that they can be ignored (Frost 1981; Leuning and Moncrieff 1992; Rannik et al. 1997). In effect, therefore, the intake tube alters the sample used to measure the atmospheric trace gas density. This ability to alter the measurement sample is a crucial difference between open- and closed-path sensors. Both open- and closed-path sensors are similar in that they include an infrared gas analyzer that responds to the attenuation (by absorption) of an infrared light beam. However, they are fundamentally different in their sampling strategy because the open-path system is a passive system (i. e., it does not fundamentally alter the measurement sample), whereas the closed-path system is an active system because it does alter the sample. When estimating fluxes this distinction is critical to the application of spectral corrections to the covariances and the WPL80 terms.

The intent of this study is to systematically examine open- and closed-path systems by applying the above three fundamentals to each in turn. Consequently, this study also examines the transfer functions appropri-

ate to the signal processing software and volume averaging effects of a closed-path instrument, as well as, possible influences that the pressure fluctuations can have on fluxes measured with a closed-path system. The next section formulates the relationship between the flux, the WPL80 (temperature, pressure, and vapor) terms, and spectral attenuation. After that sections 3 and 4 discuss open- and closed-path systems, with section 4 presenting some new aspects of closed-path systems. The final section of this study summarizes the conclusions.

2. The WPL80 terms and spectral attenuation

The turbulent atmospheric mass flux of a trace gas measured with an instrument that measures the mass mixing ratio of the gas (ω_g) rather than its density (ρ_g) is expressed as $\overline{\rho_d w' \omega'_g}$; where the overbar is the time averaging or covariance operator, $\overline{\rho_d}$ is the time-averaged (mean) dry air density, w' is the fluctuating vertical velocity, and ω'_g is the fluctuation of the trace gas mass mixing ratio (ω_g), where ω_g is defined as the ratio of the trace gas density to the dry air density: $\omega_g = \rho_g / \rho_d$. WPL80 developed the following relationship between $\overline{\rho_d w' \omega'_g}$ and the heat, pressure, and mass fluxes measured with instruments that detect changes in density rather than mixing ratio:

$$\overline{\rho_d w' \omega'_g} = \overline{w' \rho'_g} + \overline{\rho_g} (1 + \overline{\chi_v}) \left[\frac{\overline{w' T'_a}}{\overline{T_a}} - \frac{\overline{w' p'_a}}{\overline{p_a}} \right] + \mu_v \overline{\omega_g w' \rho'_v} \quad (7.1)$$

where ρ'_g is the trace gas density fluctuation, $\overline{\chi_v}$ is the mean volume mixing ratio for water vapor (which is the ratio of mean vapor pressure, $\overline{p_v}$, to the mean partial pressure of the dry air, $\overline{p_d}$; $\overline{\chi_v} = \overline{p_v} / \overline{p_d}$), $\overline{T_a}$ is the mean ambient temperature, T'_a is the fluctuation in ambient temperature, $\overline{p_a}$ is the mean ambient pressure, p'_a is the fluctuation in ambient pressure, μ_v is the ratio of the molecular mass of dry air, m_d , to the molecular mass of water vapor, m_v , (i.e., $\mu_v = m_d / m_v$), and ρ'_v is the fluctuation in the ambient water vapor density. The first term on the right hand side (RHS) of Equation 7.1, $\overline{w' \rho'_g}$, is the density covariance. The second term includes the temperature covariance, $\overline{\rho_g} (1 + \overline{\chi_v}) [\overline{w' T'_a} / \overline{T_a}]$, and the pressure covariance, $\overline{\rho_g} (1 + \overline{\chi_v}) [-\overline{w' p'_a} / \overline{p_a}]$. The $\mu_v \overline{\omega_g w' \rho'_v}$ term is the water vapor covariance.

Although Equation 7.1 is fairly standard there are several associated issues that should be mentioned. First, of the four covariances comprising the RHS of Equation 7.1 only the last three are WPL80 terms and only they are associated with fluctuations in the ambient environment at the point of the measurement of the trace gas density, ρ_g . Second, strictly speaking, WPL80 did not include the pressure flux term in their

development although they were aware of it. This term is included here because it has been shown to be important for open-path systems for some atmospheric conditions (Massman and Lee 2002) and because it is needed in order to assess its importance to closed-path systems. Third, the subscript ‘*g*’ is used in Equation 7.1 and throughout this study to denote any general trace gas. Carbon dioxide is specified with a ‘*c*’ subscript and water vapor is specified by a ‘*v*’ subscript.

Equation 7.1 basically assumes that all instruments make perfect measurements (no high frequency attenuation, immediate response, high signal to noise ratios), that such instruments are co-located at a point in space and make simultaneous measurements (no spatial separation or time lag effects), and that the data archiving system is perfect (no digitization noise, no external electronic contamination of the signal, perfect signal processing). In this case the three WPL80 covariance terms are true atmospheric fluxes, the density covariance term, $\overline{w'\rho'_g}$, is the true atmospheric mass flux measured with an instrument that detects fluctuations in mass density rather than mixing ratio, and $\overline{\rho_d w'\omega'_g}$ is the true surface exchange flux. Of course no such system exists and all quantities and covariances measured in Equation 7.1 are compromised somewhat. Thus the measured (or more properly the uncorrected) surface flux, $(\overline{\rho_d w'\omega'_g})_m$ is better represented by

$$(\overline{\rho_d w'\omega'_g})_m = (A_{wg}^d \overline{w'\rho'_g}) + \overline{\rho_g}(1 + \overline{\chi_v}) \left[\frac{(A_{wT} \overline{w'T'_a})}{\overline{T_a}} - \frac{(A_{wp} \overline{w'p'_a})}{\overline{p_a}} \right] + \mu_v \overline{\omega_g} (A_{wv} \overline{w'\rho'_v}) \quad (7.2)$$

where the subscripted *A* is an attenuation factor that represents the aggregated instrument and system related effects that tend to reduce the true covariance (i. e., $0 \leq A \leq 1$). For this study each of the four terms on the RHS of Equation 7.2 represents an uncorrected covariance between the vertical velocity and another instrument and the subscript attached to each attenuation factor identifies a particular covariance. The ‘*d*’ superscript on the first term is to distinguish between the attenuation factor for the density term and those associated with the WPL80 terms. This last distinction is important for closed-path systems.

Correcting these covariances for spectral attenuation has been the subject of many recent studies (see the following papers and their references for a summary: Massman 2000, 2001; Rannik 2001; Chapter 4). This study is similar to these previous studies in that it also develops some new transfer functions appropriate to (at least some) closed-path eddy covariances systems. These transfer functions are based on filters implemented as part of the signal processing software and the volume av-

eraging effects of the sampling chamber. But this study also extends the previous studies of spectral corrections by placing them in the context of the WPL80 terms as they relate to open- and closed-path systems. In essence the next two sections address the steps required to derive a corrected flux estimate, $\overline{\rho_d w' \omega'_g}$, from an uncorrected flux estimate, $(\overline{\rho_d w' \omega'_g})_m$ for open- and closed-path systems.

3. Open-path systems

Both open- and closed-path systems produce attenuated signals. However, attenuation of CO₂ or H₂O density fluctuations in an open-path sensor results from the sensor's inability to resolve data on scales smaller than the detection volume. This is an instrument design issue and is not related to physically altering the sample's temperature, pressure, water vapor, or CO₂ content. In the case of a closed-path sensor the intake tube physically attenuates the temperature fluctuations and the CO₂ and H₂O density fluctuations by mechanical mixing, molecular diffusion, and interaction with the tube walls. It can also both enhance and attenuate the pressure fluctuations (Iberall 1950; Holman 2001). Beyond these tube effects the instrument itself (e. g., a Licor 6262 or other closed-path instrument) also attenuates the signal. Some of this attenuation is flow-related and is similar to the tube effects. Some of it is related to volume averaging and signal processing, which like the open-path sensor do not physically alter the sample. Only the flow path actively (although possibly inadvertently) acts to alter the sample by changing its temperature, damping its moisture and CO₂ variations, and altering its pressure fluctuations.

Strictly speaking there are several (albeit relatively minor) reasons why an open-path sensor is not a truly passive sensor. For example, the energy of the infrared signal absorbed by the CO₂ molecules increases their vibrational and rotational energy (a quantum physical effect). In addition, the sensor can actually remove mass from the sample when condensation occurs on the lenses, which generally causes an easily diagnosed problem by rendering the data useless. There are also the possibilities that the sensor may distort the flow and that there are boundary-layer effects associated with flow near the flat surfaces that enclose the optical path. Further, open-path sensors are a heat source to the atmosphere because of their infrared signal generator and because (and maybe more importantly) the sensor body radiates absorbed solar radiation as heat. Conceivably, these last two effects could alter the temperature of the sample before or during its passage through the

instrument's optical path. However, these issues and all the previous effects can be ignored for the present discussion.

An open-path sensor is intended to be used in the open atmosphere. It is in that sense an *in situ* sensor. Therefore, it samples the ambient environmental conditions and all the WPL80 terms are associated with the ambient environment. Consequently all the covariances in Equation 7.2 are related to atmospheric fluxes. Furthermore, all uncorrected covariances measured with an open-path system must be spectrally corrected before summing them to produce an estimate of $\overline{\rho_d w' \omega'_g}$. A simple thought experiment should help to clarify this issue. Consider two cases for measuring the surface CO₂ flux. The first case is for the perfect instrument or system, for which no spectral corrections apply; i. e., all instruments are co-located and perfectly measure data at a point so that $A_{wc}^d = A_{wT} = A_{wp} = A_{wv} = 1$ and $(\overline{\rho_d w' \omega'_c})_m = \overline{\rho_d w' \omega'_c}$. In this case the WPL80 terms are simply added to the density covariance term, $\overline{w' \rho'_c}$, to yield the true CO₂ surface mass flux, $\overline{\rho_d w' \omega'_c}$.

The second case differs from the first only in that the CO₂ measurement is attenuated by 25% (i. e., $A_{wc}^d = 0.75$ and $A_{wT} = A_{wp} = A_{wv} = 1$). For this example the only way to recover the true surface flux, $\overline{\rho_d w' \omega'_c}$, from the uncorrected surface flux, $(\overline{\rho_d w' \omega'_c})_m$ is to correct the attenuated density covariance, $A_{wc}^d \overline{w' \rho'_c}$, then add all the WPL80 terms to it. Applying the spectral corrections after including the WPL80 terms would be equivalent to correcting $(\overline{\rho_d w' \omega'_c})_m$ directly, which in turn would also multiply (or over-correct) the three WPL80 terms by a correction factor that applies only to the CO₂ instrument. This could yield a significantly biased estimate of the true surface flux because for most environments the WPL80 temperature covariance term is often the dominant term. This example can be extended to include any combination of imperfect (spectrally attenuated) covariance measurements and in general one must conclude that for open-path sensors spectral corrections must be applied to the uncorrected covariances before including the WPL80 terms in the final estimate of the trace gas surface flux. The only exceptions to this are the very unlikely situations where either all covariance attenuation factors are identical or all WPL80 terms are negligibly small compared with the density covariance term. In general it must be assumed that spectral (or cospectral) corrections are specific to the instruments involved and that they are not necessarily transferable from one covariance measurement to another. In other words, individual instruments are often based on fundamentally different technologies, which can impose different physical designs and separation distances, different time constants, and different noise reducing filters. All of these define instrument specific response functions.

This basic principle of instrumentation and the other fundamentals, discussed previously, are also relevant to closed-path systems and to the estimation of surface fluxes by converting high frequency CO₂ mass density measurements (ρ'_c) to high frequency CO₂ dry-air mass mixing ratio (ω'_c).

4. Closed-path systems

A closed-path system is a combination of both active and passive sampling. Attenuation of the temperature fluctuations in a closed-path system qualifies as active because it results from a combination of molecular and turbulent diffusion within the intake tube and the associated heat exchange with the tube walls. In essence the tube acts as a heat exchanger and brings the sample to a uniform temperature before it is drawn into the detection chamber of the infrared gas analyzer.

Attenuation of fluctuations in trace gas mass density result from a combination of diffusional smoothing of density variations inside the flow path (defined by the tube and the detection chamber), possible interaction with the walls of the flow path, design (line or volume averaging) aspects of the infrared gas analyzer's detection chamber, and any signal processing or electronic filtering inherent to the instrument's electronic circuitry. Of these only the tube and chamber flow effects qualify as active, all others are passive.

Usually, however, these active and passive effects are lumped together into a single time constant, which is then used to describe the closed-path system. But, including the WPL80 terms in a manner appropriate to a closed-path system requires careful consideration of the nature of the sampling and its associated spectral correction. In general the spectral corrections made to the WPL80 covariance terms should *not* include any active (or flow path) attenuation effects. Rather, they should include only passive attenuation effects associated with the other parts of the system. This may seem surprising at first, but it follows directly from the fact that the WPL80 covariance terms refer to the environment in which the trace gas density is measured. Therefore, the appropriate measure of p'_a in the WPL80 pressure covariance term, $\bar{\rho}_g(1 + \bar{\chi}_v)[-w'p'_a/\bar{p}_a]$, and of ρ'_v in the WPL80 vapor covariance term, $\mu_v\bar{\omega}_g\overline{w'\rho'_v}$, are those occurring within the detection chamber of the closed-path system. This result follows from the same logic (or physical manipulation of the sample) that eliminates T'_a and the temperature covariance term from the environment of the detection chamber. It's just that in the case of T'_a the attenuation can be considered 100% effective, but for p'_a and ρ'_v the physical attenuation of the signals is not as complete. [Note that the

attenuation of p'_a by the flow path is made more precise later in this study.]

This result, which applies to both CO₂ and water vapor because they are often measured with the same closed-path system, has some surprising implications for physical interpretation of the WPL80 terms and for estimating and correcting the attenuation factors included in Equation 7.2. For CO₂ the spectral correction factor ($1/A_{wc}^d$) for the density covariance, $A_{wc}^d \overline{w'\rho'_c}$, must exceed the correction factor ($1/A_{wv}$) for the vapor covariance, $A_{wv} \overline{w'\rho'_v}$, because both CO₂ and water vapor covariances share exactly the same set of passive attenuation factors, but only the CO₂ density term includes the active (flow path) attenuation effects as well (i.e., $A_{wc}^d < A_{wv}$). If the active portion of all the attenuation factors is included when spectrally correcting the WPL80 vapor covariance, then the surface CO₂ flux, $\overline{\rho_d w' \omega'_g}$, will be overestimated as a result. The same applies for water vapor as well, therefore (and even more surprisingly) $A_{wv}^d < A_{wv}$. In other words, when measuring the water vapor covariance $\overline{w'\rho'_v}$ with a closed-path system the attenuation (or correction) factor that applies to the density covariance is different than the one that applies to the WPL80 term even though they are the same measured quantity.

The reason for this surprising difference is that the density covariance should be interpreted in terms of an atmospheric- or surface-related flux (which is external to the environment in which the measurements are made in a closed-path sensor), whereas the WPL80 terms refer to conditions internal to the instrument. Thus the WPL80 terms lose their interpretations as surface exchange fluxes. Rather they are simply covariances between the sonic anemometer and measurements made inside the chamber of a closed-path system. This is very different than the open-path case for which the WPL80 terms retain their interpretation as surface-related fluxes. But because the closed-path system actively alters the sample the WPL80 terms lose their immediate association with surface fluxes.

Given this distinction between the density covariance and the WPL80 covariance terms and its importance to spectral corrections and the estimation of surface fluxes, the next section develops the transfer functions for the detection chamber of a closed-path system.

4.1 Detection chamber transfer functions

There are two aspects of the closed-path detection chamber that compromise its ability to produce a precise estimate of ρ'_c and ρ'_v within the chamber: the signal processing software and the volume averaging ef-

fects of the chamber. Both of these issues are appropriate to open-path instruments as well. But, for open-path instruments the signal processing software effects are usually minimal and can typically be ignored and the volume effects (and related line averaging) have been discussed (Gurvich 1962; Silverman 1968; Andreas 1981; Moore 1986; Massman 2000).

For this study the Licor 6262 is used as an example of how to address these concerns. However, the general approach for developing these transfer functions (if not the specific transfer functions themselves) applies to any closed-path sensor. The next three subsections provide a detailed discussion.

4.1.1 The signal processing algorithm. To provide a good signal to noise ratio the Licor 6262 uses a third-order Bessel filter as an antialiasing filter. Its associated (complex) transfer function, $h_{3B}(\omega)$, is given as follows:

$$h_{3B}(\omega) = \frac{15}{(15 - 6\Omega^2) - j(15\Omega - \Omega^3)} \quad (7.3)$$

where $j = \sqrt{-1}$, $\Omega = \omega\tau_{3B}\sqrt{3.0824}/(2\pi)$, τ_{3B} [s] is the time constant of the third order Bessel filter, $\omega = 2\pi f$ [radians s⁻¹] and f [Hz] is frequency. Because this filter is complex there is both a real part, the gain function or $H_{3B}(\omega)$, and an imaginary part or phase function, $H_{3B}^\phi(\omega)$. The gain function is expressed as

$$H_{3B}(\omega) = \frac{15}{\sqrt{\Omega^6 + 6\Omega^4 + 45\Omega^2 + 225}} \quad (7.4)$$

The importance of the phase function (to first order instruments) was pointed out by Hicks (1972) and Horst (1997) and further developed to include the effects of any longitudinal displacement between the sonic and the mouth of the intake tube and any possible (unresolved) tube lag times by Massman (2000). Following Massman (2000), the phase function for the third-order Bessel filter appropriate to the present example is

$$H_{3B}^\phi(\omega) = \frac{(15 - 6\Omega^2) \cos[\phi(\omega)] - (15\Omega - \Omega^3) \sin[\phi(\omega)]}{\sqrt{\Omega^6 + 6\Omega^4 + 45\Omega^2 + 225}} \quad (7.5)$$

where $\phi(\omega) = \omega(l_{lon}/u + L_t/U_t)$ and l_{lon} is the longitudinal displacement, u is the mean horizontal atmospheric wind speed, L_t is the tube length, and U_t is the tube flow velocity. In most applications the phase effects associated with the tube lag time, L_t/U_t , are eliminated from Equation 7.5 by digitally shifting sonic time series so that it will be

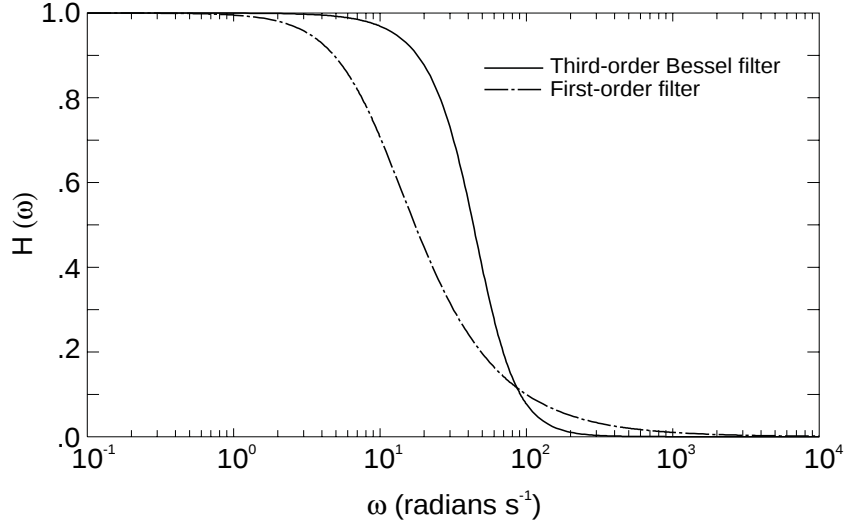


Figure 7.1. Gain functions, $H(\omega)$, for a first order filter with a time constant $\tau_1 = 0.1$ s and third-order Bessel filter with a time constant $\tau_{3B} = 0.2$ s. Equation 7.6 is the first order filter's gain function and Equation 7.4 is for the third-order Bessel filter.

synchronized with the closed-path sensor. However, depending on the sampling frequency and the exact value of the lag time, some unresolved lag time may still remain as part of the phase. Here L_t/U_t is included for completeness and will be understood as any possible unresolved tube lag time.

It is possible to compare each of these last two transfer functions with their first order counterparts, $H_1(\omega)$ and $H_1^\phi(\omega)$, which is done by the next two equations and Figures 7.1 and 7.2.

$$H_1(\omega) = \frac{1}{\sqrt{1 + \omega^2 \tau_1^2}} \quad (7.6)$$

$$H_1^\phi(\omega) = \frac{\cos[\phi(\omega)] - \omega \tau_1 \sin[\phi(\omega)]}{\sqrt{1 + \omega^2 \tau_1^2}} \quad (7.7)$$

where τ_1 is the time constant of the first order instrument. [Note that these last two equations are expressed differently by Massman (2000), but that their multiplicative effect for spectral correction factors is the same regardless.]

For the purposes of comparisons only, Figures 7.1 and 7.2 assume that $\tau_1 = 0.1$ s and that $l_{on}/u + L_t/U_t = 0.001$ s. For the Licor 6262 $\tau_{3B} = 0.2$ s with 0.1 s being its recommended nominal first order equivalent time

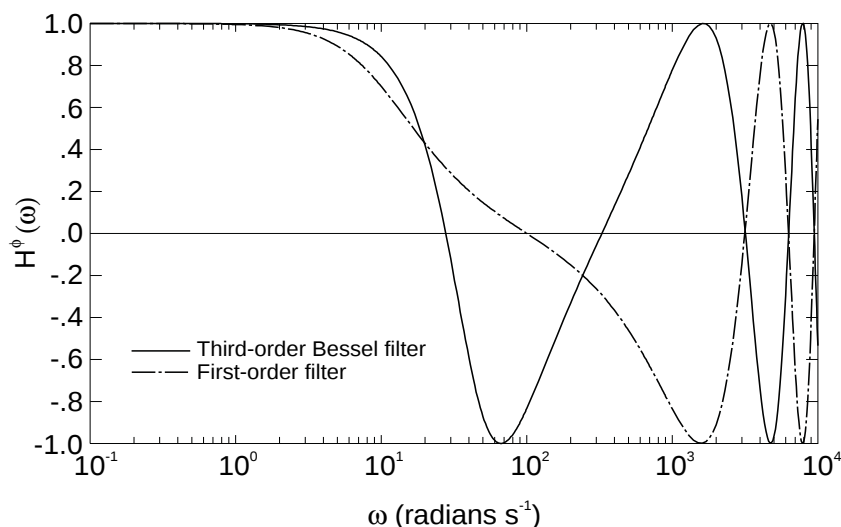


Figure 7.2. Phase functions, $H^\phi(\omega)$, for a first order filter with a time constant $\tau_1 = 0.1$ s and third-order Bessel filter with a time constant $\tau_{3B} = 0.2$ s. Equation 7.7 is the phase function for first order filter and Equation 7.5 is for the third-order Bessel filter. The phase $\phi(\omega) = 0.001\omega$ for both filters.

constant. As indicated in both Figures 7.1 and 7.2 the third-order Bessel filter (with $\tau_{3B} = 0.2$ s) produces less filtering than (or out performs) the first order filter (with $\tau_1 = 0.1$ s). In the case of the phase functions Figure 7.2 indicates that each filter has a different effect on the phase at high frequencies ($\omega \geq 20$ radians s^{-1} or $f \geq 4$ Hz). However, the phase-shifting portions of these filters occur in the cospectral region with very little power so that this behavior is not particularly significant to spectral correction factors or observed cospectra.

4.1.2 Spatial averaging of the detection chamber. The Licor 6262 detection chamber is approximately 0.15 m long, 0.0063 m high, and 0.0126 m wide. The volume flow through the detection chamber and the infrared signal path are parallel and down the length of chamber. The light beam tapers somewhat between one end of the sample chamber and the other, but this will be neglected for the present discussion. Also neglected here is any flow path (active) attenuation of mass fluctuations associated with the detection chamber itself. This is justifiable because the tube length is usually much greater than the length of the detection chamber.

The rectangular geometry of the detection chamber suggests the use of Cartesian coordinates for modeling the volume averaging effects of

the sample chamber. It is possible to show, but will not be done here, that this approach is formally or mathematically the same as those used to express the effects of line averaging by open-path sensors on the measured spectra (Gurvich 1962; Silverman 1968). However, there is one important difference. The flow velocity within the detection chamber can be very different than the wind speed of the ambient atmosphere near the tube mouth, so that the transfer functions need to be expressed in terms of the volume flushing time constant of the detection chamber, τ_{vol} , rather than averaging lengths. Therefore, for an instrument with a flow path that is parallel to the infrared light beam the spectral transfer function associated with volume averaging, $H_{vol}(\omega)$, is

$$H_{vol}(\omega) = \frac{\sin^2(\omega\tau_{vol}/2)}{(\omega\tau_{vol}/2)^2} \quad (7.8)$$

Given the maximum flow rate of the Licor 6262 is 10 L min^{-1} and that the volume of the detection chamber is 0.0119 L , then the minimum value that τ_{vol} that can be expected is about 0.07 s (i.e., $\tau_{vol} \geq 0.07 \text{ s}$).

Although it is reasonable to assume that the infrared light beam is parallel to the flow path, it is possible that they could deviate slightly from one another. But, it is also possible to account for these deviations. For example, Gurvich (1962) developed the appropriate transfer function for the perpendicular case and Silverman (1968) generalized the Gurvich function to any angle less than 90 degrees. However, these deviations are expected to be small for the 6262 and they will not be investigated here.

4.1.3 Is a closed-path sensor a first order instrument?.

The nominal (first order) time constant for the Licor 6262 sensor is often taken to be 0.1 s . This presumption is now tested with a simple example by calculating the spectral correction factors for a first order sensor and a sensor that combines the effects of the third-order Bessel filter with volume averaging. These calculations are performed using the integration approach summarized by Equation 3 of Massman (2000) or Equation 1 of Chapter 4. Here the focus is on the correction factor rather than the transfer functions because, first, the results and conclusions are the same regardless and, second, a practical example using correction factors is more insightful for this comparison. All further closed-path scenarios assume the following: (i) the height of the covariance measurement is 5 m above the zero plane displacement, (ii) the sampling rate is 10 Hz and the sampling period is 30 minutes , (iii) the atmosphere is neutrally stable, (iv) the sonic path length is 0.15 m , (v) the mouth of the intake tube is displaced both laterally and longitudinally by 0.15 m from the center

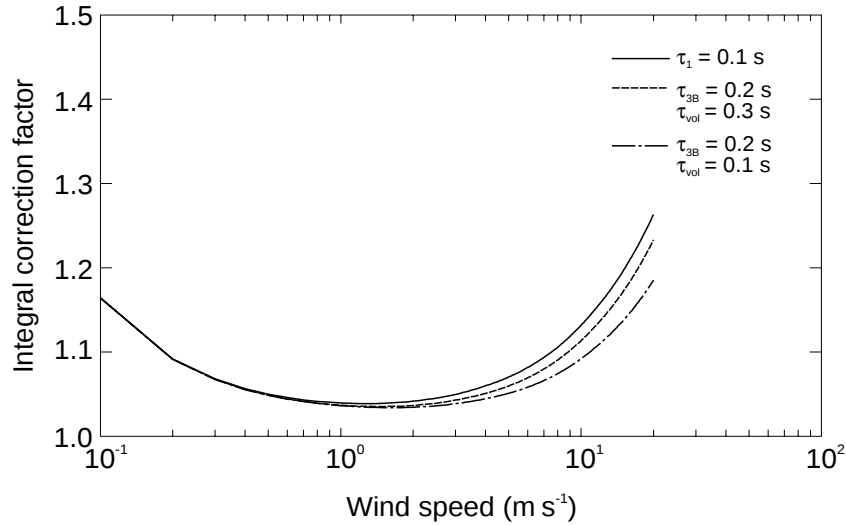


Figure 7.3. Comparison of integral correction factors for three different Licor 6262 scenarios. The first two scenarios combine the effects of the third-order Bessel filter, which is part of the instrument's signal processing software, with the volume averaging effects of the detection chamber. Two different values for the volume flushing time constant, τ_{vol} , are shown. The third scenario assumes that the Licor 6262 is a first order instrument with a response time, τ_1 , of 0.1 s. Neutral atmospheric stability is assumed.

of the sonic, (vi) flow in the tube is turbulent and the corresponding Reynolds number is about 20,000, (vii) the ratio (including Massman's (1991) tube attenuation factor, Λ) of the tube radius to its length is 0.03 and the total tube lag time (not the unresolved portion) is 2.0 s, and (viii) the maximum nondimensional frequency of the frequency-weighted cospectrum, η_x (Massman 2000), is 0.085 after the flat terrain cospectrum of Kaimal et al. (1972), (ix) the high pass block averaging filter is included in the calculations of the spectral correction factor, and (x) the shape of the cospectrum is taken from Chapter 4.

The results, shown in Figure 7.3, indicate (a) that describing the Licor 6262 as a first order instrument with a time constant of 0.1 s overpredicts the true attenuation somewhat at wind speeds greater than about 3 m s⁻¹ and therefore, overpredicts the spectral correction factor for these wind speeds and (b) that the volume averaging effects of the Licor 6262 detection chamber, although relatively small, can contribute to spectral attenuation. Regarding (a), some trial and error comparisons suggested that the Licor 6262 was better described as a first order instrument with a time constant of 0.06 to 0.08 s, depending on τ_{vol} . Result (b) is, of

course, somewhat dependent upon the exact values of τ_{vol} and η_x . Larger values for either of these parameters will increase the spectral correction factor.

Part of the reason for (b) is that the appropriate transfer function is actually $\sqrt{H_{vol}(\omega)}$ (e. g., Moore 1986), rather than $H_{vol}(\omega)$ itself, which applies to spectra rather than ρ'_c or ρ'_v . This will tend to reduce the attenuation that would have otherwise have been predicted by $H_{vol}(\omega)$. But, this also highlights an important aspect of making spectral corrections, which is that the assumptions made when deriving a transfer function also determine how it is applied. For example, if the transfer function is developed on the basis of spectra, then taking the square root is appropriate to describe the attenuation of fluctuations. This is usually the case for line averaging or volume averaging effects (e. g., Andreas 1981). However, if the transfer function is derived directly on the basis of mass density fluctuations then taking the square root is not appropriate. A good example of this last case is the transfer function describing tube attenuation effects (e. g., Massman 1991).

4.2 Pressure fluctuations within the detection chamber

For most atmospheric conditions the variations in ambient density due to the pressure covariance term, $\bar{\rho}_g(1 + \bar{\chi}_v)[-w'p'_a/\bar{p}_a]$, can be ignored. However, for windy, turbulent conditions and open-path sensors this may not be true (Massman and Lee 2002). It is, therefore, worthwhile to explore the possible nature of the pressure fluctuations inside the detection chamber of a closed-path instrument. This involves two related issues. First, how does the flow within the tube affect pressure fluctuations between the mouth of the tube and the detection chamber and second, does the presence of the eddy covariance equipment or the creation of a local external flow field caused by pulling the sample into the tube affect or distort the unperturbed ambient atmospheric pressure fluctuations? Each of these questions is examined in turn.

4.2.1 Pressure fluctuations and tube flow. For eddy covariance applications ($f \leq 20$ Hz) the tube acts as a first order filter when the flow is uniform and laminar or nonturbulent (Iberall 1950; Holman 2001). The corresponding complex transfer function, $h_{p'}(\omega)$, and associated first order time constant, $\tau_{p'}$, for the attenuation of pressure fluctuations by uniform laminar tube flow are

$$h_{p'}(\omega) = \frac{1}{1 - j\omega\tau_{p'}} \quad (7.9)$$

$$\tau_{p'} = \frac{8\mu L_t}{\pi a^4} \frac{V}{\gamma \bar{p}_a} \quad (7.10)$$

where $\mu [\approx 0.18(10^{-4}) \text{ Pa s}]$ is the dynamic viscosity of air, a is the tube radius, V is the volume of the detection chamber, and $\gamma = 1.4$ is the ratio of C_p to C_v for air. (Here C_p and C_v are the specific heats of air at constant pressure and volume.)

The time constant, $\tau_{p'}$, of a system defined by a Licor 6262 with internal pressure, $\bar{p}_a$, of about 96 kPa attached to a tube of length 10 m and inside diameter of 6.35 mm is approximately 0.0004 s, which suggests that for most eddy covariance applications the pressure fluctuations are negligibly attenuated by uniform laminar tube flow. But turbulent tube flow tends to increase $\tau_{p'}$ and the resulting attenuation (Rohmann et al. 1957, Brown et al. 1969). As the flow Reynolds number increases $\tau_{p'}$ increases from a few percent (Rohmann et al. 1957) to maybe an order of magnitude or slightly more (Brown et al. 1969). Even so $\tau_{p'}$ should be quite short and pressure attenuation should be fairly small for many closed-path eddy covariance applications.

On the other hand, for some frequencies the total volume of the tube and detection chamber can act as a resonance cavity (Aydin 1998; Holman 2001) with a resonance frequency $f_n = n\sqrt{3\pi a^2 C_s^2 / (4L_t V)} / (2\pi)$; where C_s is the speed of sound and $n = 1, 2, 3, \dots$, specifies the harmonic frequency. For the present example $f_1 \approx 24.5 \text{ Hz}$ suggesting that these higher frequency pressure fluctuations would be amplified in the detection chamber. Another possible source of high frequency pressure fluctuations is the pump, which for closed-path eddy covariance systems should be downstream of the detection chamber. These pumps typically are diaphragm pumps which operate at 50 or 60 Hz, which, if some design precautions in the tubing connecting the pump and the detection chamber are not taken, could contaminate the detection chamber with 50 or 60 Hz pressure fluctuations. However, these two high frequency effects can be ignored for the present study because the spectral power is too small in this range to be of any concern.

Overall therefore it seems that tube flow is likely to have very little impact on the transmission of pressure fluctuations, so that p'_a inside the detection chamber is nearly the same as p'_a just outside the mouth of the intake tube. Therefore, as with the open-path system the WPL80 pressure covariance term may also be important to estimates of surface fluxes for closed-path systems during windy, turbulent conditions.

4.2.2 Possible influence of the instrumentation on ambient pressure fluctuations at the tube mouth.

The sonic, the instrumentation mounting structure, the mouth of the tube, and the flow

field created by the intake system can interact with the local ambient flow field to create dynamic pressure fluctuations near the mouth of the intake tube. For example, eddies can be shed from the equipment or the mounting boom when the Strouhal number is about 0.2. Assuming a characteristic length scale of 0.05 to 0.25 m for the eddy covariance equipment and a typical wind speed between 2 to 8 m s⁻¹, then the characteristic eddy shedding frequency could be anywhere between about 2 and 30 Hz. Conceivably, the associated dynamically-induced pressure fluctuations could suppress or enhance any ambient atmospheric static pressure fluctuations that may be present naturally. There are also internal and external tube boundary layers that are created by the ambient flow that will depend on the wind direction and speed (e. g., Kim et al. 2001). However, these effects are likely to be relatively small scale and confined to high frequencies. But, there may also be larger quasi-static pressure fields that are formed by the interaction of the instruments and the wind, which would likewise be a function of wind speed and direction. A full discussion of this issue is beyond the intention of the present study, but it is important that this possibility be mentioned as a research need for closed-path systems. But, in general, the discussions just presented suggest that p'_a within the chamber may or may not reflect the true atmospheric static p'_a , so that estimating $\overline{w'p'_a}$ from ambient measurements, which is exemplified in the next section, may or may not provide an accurate estimate of the covariance between w' and p'_a inside the detection chamber.

4.3 Synthesis: Possible consequences for flux estimates

The traditional application of the WPL80 theory to closed-path systems assumes that the temperature covariance term has been eliminated because $T'_a = 0$ within the detection chamber, that the pressure covariance term never contributes because $p'_a/\overline{p_a}$ is negligible, and that any spectral correction to the vapor covariance term includes the tube attenuation effects. This approach basically uses the mass density and water vapor measurements to form covariances and then combines the results to estimate the surface mass flux, $\overline{\rho_d w' \omega'_g}$. An alternative to this approach is to convert the measured mass density to mass mixing ratio at the high frequency data rate and then to estimate the surface mass flux by decomposing ω_g into its mean and fluctuating parts and calculating $\overline{w' \omega'_g}$ directly. This section applies the insights developed earlier to these two approaches. For the first approach a numerical example is

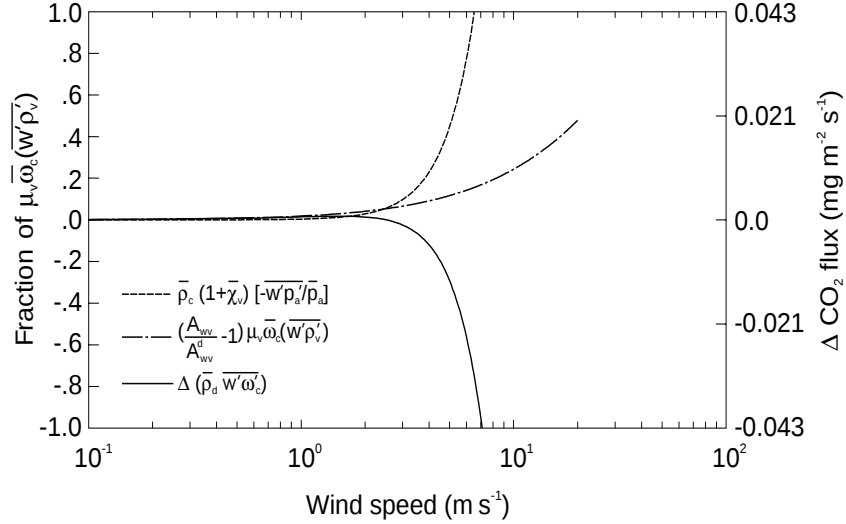


Figure 7.4. Equivalent CO₂ flux magnitudes and wind speed dependencies for the various terms of Equation 7.11, showing the consequences of ignoring the WPL80 pressure covariance term and of overcorrecting the vapor covariance term. The combined effect (solid line) indicates that the surface flux for CO₂, $\bar{\rho}_d \overline{w' \omega'_g}$, is underestimated (negative quantities). For the purposes of comparison note that $0.02 \text{ mg CO}_2 \text{ m}^{-2} \text{ s}^{-1} = 1.72 \text{ tC ha}^{-1} \text{ yr}^{-1}$.

provided. In the second, the discussion outlines possible discrepancies with the first approach.

4.3.1 Influence of spectral corrections and pressure fluctuations.

This subsection estimates the errors in estimates of the surface flux associated with ignoring the WPL80 pressure covariance and overcorrecting the water vapor covariance. Including the tube attenuation as part of the spectral correction to $\mu_v \bar{\omega}_g \overline{w' \rho'_v}$ overcorrects the spectral attenuation by an amount $A_{wv}/A_{wv}^d - 1$. Combining this overestimate with the pressure covariance term yields the following expression for the error, $\Delta(\bar{\rho}_d \overline{w' \omega'_g})$, in the estimate of $\bar{\rho}_d \overline{w' \omega'_g}$ resulting from a misapplication of the WPL80 theory:

$$\Delta(\bar{\rho}_d \overline{w' \omega'_g}) = \frac{A_{wv}}{A_{wv}^d} \mu_v \bar{\omega}_g \overline{w' \rho'_v} - \left\{ \mu_v \bar{\omega}_g \overline{w' \rho'_v} + \bar{\rho}_g (1 + \bar{\chi}_v) \left[-\frac{\overline{w' p'_a}}{\bar{p}_a} \right] \right\} \quad (7.11)$$

This error and its components are evaluated numerically using the same scenario and assumptions listed in section 4.1.3 for Figure 7.3.

However, it is more convenient to express the pressure covariance in terms of the wind speed, u . This is done first by noting that $-\overline{w'p'_a} = C\overline{\rho_a}u_*^3$, where $C \approx 2$ for neutral atmospheric conditions (Wilczak et al. 1999; Massman and Lee 2002), and second by assuming that $u_* = Bu$, where $B \approx 0.2$ for forested canopies and $B \approx 0.1$ is more appropriate for agricultural crops. Note that this relationship between u and u_* does not necessarily apply universally. It is useful here for numerical purposes only and should not be taken as indicative of any particular site, where it will depend upon the measurement height, the atmospheric stability, the canopy roughness length, etc. For estimating $-\overline{w'p'_a}$ at any given eddy covariance site the relationship $-\overline{w'p'_a} = C\overline{\rho_a}u_*^3$ should use u_* values measured with the sonic anemometer rather than estimating u_* from the wind speed. However, the multiplier C increases as the atmosphere becomes more unstable (Wilczak et al. 1999).

The numerical evaluation of Equation 7.11 is performed for both CO_2 and water vapor and assumes: $\mu_v = 0.622$, $\overline{\omega}_c = 0.57 \text{ mg g}^{-1}$, $\overline{w'\rho'_v} = 0.12 \text{ g m}^{-2} \text{ s}^{-1} \approx 300 \text{ W m}^{-2}$, $\overline{\rho}_c = 730 \text{ mg m}^{-3}$, $\overline{\chi}_v = 0.02$, $\overline{\rho}_a = 1.28 \text{ kg m}^{-3}$, $\overline{p}_a = 100 \text{ kPa}$, and $\overline{\rho}_v = 15 \text{ g m}^{-3}$. The ratio A_{wv}/A_{wv}^d is computed following the integral approach for estimating correction factors (see Equation 3 of Massman 2000). For A_{wv}^d is it assumed that the first order response time of the closed-path system (tube + Licor 6262) was determined empirically to be 0.3 s. Thus the equivalent response time includes the tube attenuation as well as the 6262's signal processing software and its volume averaging effects. For A_{wv} only the third order Bessel filter and the volume averaging effects, both discussed earlier, are used.

The results for CO_2 are shown in Figures 7.4 and 7.5 shows the water vapor results. Each figure includes $\Delta(\overline{\rho}_d \overline{w'\omega'_g})$, $[\frac{A_{wv}}{A_{wv}^d} - 1]\mu_v \overline{\omega}_g \overline{w'\rho'_v}$, and the pressure covariance term, $\overline{\rho}_g(1 + \overline{\chi}_v)[-\overline{w'p'_a}/\overline{p}_a]$. Each expression is evaluated as a fraction of $\mu_v \overline{\omega}_g \overline{w'\rho'_v}$ (left axis) and an absolute amount (right axis) for the case $B = 0.2$.

To aid in the interpretation of Figure 7.4 it should be noted that $0.02 \text{ mg CO}_2 \text{ m}^{-2} \text{ s}^{-1} = 1.72 \text{ tC ha}^{-1} \text{ yr}^{-1}$. Consequently, even small biases resulting from these discrepancies can lead to significant biases in the annual carbon budget estimated by eddy covariance. In general, these CO_2 results suggest that ignoring the pressure covariance term introduces a larger bias into the estimate of the surface CO_2 flux, $\overline{\rho}_d \overline{w'\omega'_g}$, than overcorrecting the water vapor covariance term. But, the overcorrected water vapor covariance does partially compensate for the lack of the pressure covariance term. Figure 7.5 suggests that the consequences to the surface water vapor flux are similar, but less significant than for

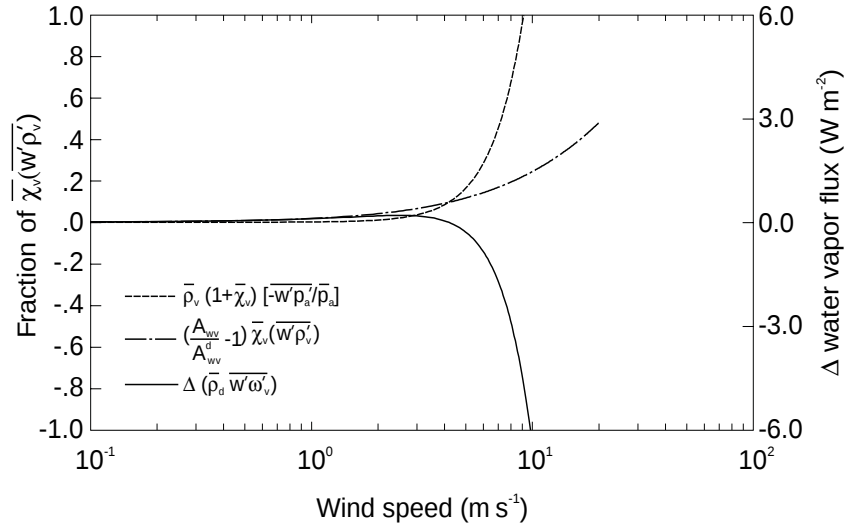


Figure 7.5. Equivalent water vapor flux magnitudes and wind speed dependencies for various terms of Equation 7.11, showing the consequences of ignoring the WPL80 pressure covariance term and of overcorrecting the vapor covariance term. The combined effect (solid line) is that the true surface flux for water vapor, $\bar{\rho}_d \overline{w' \omega'_v}$, is underestimated (negative quantities). For this example the water vapor flux is assumed to be about 300 W m^{-2} .

the CO_2 surface flux. Figure 7.5 also indicates that ignoring the pressure covariance term can cause the lack of closure (underestimation) of the surface energy balance to worsen as wind speed increases.

For the case $B = 0.1$ the results (not shown) were similar to those shown in these last two figures, except that the pressure covariance term, although still significant to the surface flux estimates, was reduced relative to the $B = 0.2$ scenario. Finally, it is important to reiterate that all results presented in this section are intended as plausible examples only. They are useful for indicating general features and general consequences. But the specific numerical results do not necessarily apply universally, because each eddy covariance site is likely to have different sensor deployment, potentially different sensor time constants, different measurement heights, and different data processing algorithms. The same caveat is true for the next section.

4.3.2 High frequency conversion of mass density to mixing ratio.

This section examines the consequences of estimating the surface flux by converting the high frequency data, point-by-point to $\omega_g = \rho_g/\rho_d$, then decomposing it to $\bar{\omega}_g + \omega'_g$, and finally using ω'_g

to form $\overline{\rho_d w' \omega'_g}$. For this case the WPL80 theory still applies so that $\omega'_g = \rho'_g + \overline{\rho_g}(1 + \overline{\chi_v})[-p'_a/\overline{p_a}] + \mu_v \overline{\omega_g} \rho'_v$. But no single instrument measures ω_g directly, rather it can only be determined by combining data (or data streams) from more than one instrument. Consequently, it is $\rho'_g + \overline{\rho_g}(1 + \overline{\chi_v})[-p'_a/\overline{p_a}] + \mu_v \overline{\omega_g} \rho'_v$ that is being measured, not ω'_g . Therefore, when forming the covariances it is still appropriate to be concerned with how and with what instruments are the quantities ρ_g , ρ_d , ρ'_g , p'_a , and ρ'_v being measured or calculated. This issue must be addressed if spectral corrections are to be applied appropriately and if the pressure fluctuations need to be included. In general, Equation 7.2 still applies when estimating $\rho_d \overline{w' \omega'_g}$.

Consider the following, and final, example. Assume that mean pressure inside the tube is known, but measured with a relatively slow response sensor so that p'_a cannot be measured and the pressure covariance term is thereby implicitly ignored. Further assume that all other conditions and parameter values are the same as those already provided in the previous example except that the response time of the CO₂ sampling system has been found empirically to be 0.3 s and for water vapor the response time was found to be 0.5 s. In this case applying the correction factor associated with $\overline{w' \rho'_c}$ to $(\overline{\rho_d w' \omega'_c})_m$ would yield the same result as shown in Figure 7.4. This approach would properly correct the measured CO₂ density covariance, $A_{wc}^d \overline{w' \rho'_c}$, but would again overestimate the vapor covariance term exactly as shown in Figure 7.4. For water vapor the results are similar to those shown in Figure 7.5, except that the overestimation factor, A_{wv}/A_{wv}^d , is now about 50% greater, a consequence of using a response time of 0.5 s rather than 0.3 s.

These last two examples indicate that the application of WPL80 terms and spectral corrections to closed-path eddy covariance systems do not commute and that the preferred approach must be first to apply appropriate spectral corrections to each of the terms in Equation 7.2, then add them together to form the surface flux. If this is not done the use of an active trace gas sampling system will virtually guarantee that any estimate of the surface flux will be biased because the amount of attenuation of the density covariance term, A_{wg}^d , is likely to exceed the amount of attenuation of the WPL80 vapor covariance term, A_{wv} . In other words, it is very important to estimates of surface flux not to confuse combining data streams from different instruments, which is a mathematical operation, with making a direct measurement of ω_g with a single instrument.

5. Summary and conclusions

Open- and closed-path CO₂ and water vapor eddy covariance systems are similar in their use of infrared gas analyzers to measure trace gas fluctuations. But, they are different in their handling of the air being sampled. These differences are crucial when applying spectral corrections and the WPL80 terms for flux estimation. Open-path systems are purely passive, i. e., they do not physically alter the sample. Whereas closed-path systems combine aspects of both active and passive sampling with the intake tube acting as the active portion. It is the active portion of the system that physically alters the sample by eliminating the temperature fluctuations and attenuating the water vapor and CO₂ fluctuations through a combination of diffusional smoothing and interaction with the tube walls.

The spectral corrections associated with passive sampling describe instrument or data processing compromises and they apply to all covariances (including the WPL80 terms) and to either an open- or closed-path system. However, these corrections are specific to a particular instrument and data processing system and they are not necessarily the same for any of the covariances: $\overline{w'T'_a}$, $\overline{w'p'_a}$, $\overline{w'\rho'_c}$, or $\overline{w'\rho'_v}$. Spectral corrections associated with active sampling describe sample-handling compromises and they apply only to the density covariance term, $\overline{w'\rho'_g}$, not to the (closed-path-associated) WPL80 vapor or pressure covariance terms. This is a consequence of the fact that the WPL80 terms characterize the environment in which the trace gas measurements are made. In the case of the open-path the WPL80 covariance terms can be interpreted as fluxes (after spectral correction). In the case of the closed-path the WPL80 covariance terms lose their interpretation as fluxes, because fluctuations in temperature, pressure, and water vapor of the air being sampled by the detection chamber have been physically altered by the tube and the tube flow.

This study has attempted to provide a template for the application of spectral corrections to the WPL80 terms and the estimation of fluxes by reexamining the original WPL80 theory from the perspective of the instrumentation and its supporting technology. The major conclusions are that (i) with current technology the application of spectral corrections and the WPL80 terms do not commute and spectral corrections should be made to all covariances first before summing the WPL80 terms to estimate surface fluxes, (ii) high frequency point-by-point conversions from mass density to mixing ratio is not the preferred method for estimating fluxes by eddy covariance, (iii) for closed-path systems the spectral corrections for the WPL80 covariance terms and the density

covariance term, $\overline{w'\rho'_g}$, are not the same, (iv) for some atmospheric conditions the WPL80 pressure covariance term, which is usually ignored, can be significant for closed-path estimates of both the CO₂ flux and the surface energy balance, in part because pressure fluctuations are not likely to suffer significant attenuation with turbulent tube flow, and (v) using the same spectral corrections for the density covariance term, $\overline{w'\rho'_g}$, and the WPL80 water vapor covariance term can introduce significant biases into the annual estimates of the carbon balance, as can ignoring the WPL80 pressure covariance term.

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