Influence of instrument surface heat exchange on CO_2 flux from open-path gas analyzers

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1. Introduction

Open-path infrared gas analyzers are widely used around the world for measuring CO_2 exchange. There have been many comparisons between open-path and closed-path sensors demonstrating substantially similar CO_2 flux measurements. However, there is growing evidence that shows differences between open-path and closed-path measurements, especially in the form of apparent off-season CO_2 uptake when it is physiologically unreasonable to expect it. Measurements made with closed-path analyzers, chambers, and gradient methods have consistently shown small releases of CO_2. To address this issue, a series of laboratory and field experiments were conducted to examine the influence of instrument surface temperature and heat exchange on the open-path CO_2 fluxes.

The following conceptual framework (Burba *et al*. 2005a,b; 2006 a,b) was used: if the instrument surface temperature is different from the ambient temperature (i.e., measured outside the instrument open path), it could cause sensible heat fluxes inside the open-path cell to be different from the ambient, thus affecting CO_2 densities. This phenomenon should be accounted for in Webb-Peraman-Leuning term (WPL, Webb *et al*. 1980). With these issues in mind, this investigation focused on the following specific questions:

i) Is the instrument surface temperature significantly warmer or colder as compared to the ambient air?

ii) Does the resulting instrument surface heat exchange correlate with the vertical wind speed to produce a sensible heat flux inside the path which is different from the ambient sensible heat flux?

iii) Can the effect of this heat exchange be eliminated by enclosing an open-path gas analyzer?

iv) Can a sensible heat flux measured directly inside the path be used in WPL to correct unreasonable open-path fluxes to match closed-path fluxes?

v) Can the instrument surface heat exchange be estimated from co-located meteorological data to correct previously measured open-path fluxes?

vi) What are the consequences of assuming the instrument surface heating effect is negligible?

2. Theoretical Considerations

The impact of instrument surface heating on air density in the optical path of an open-path instrument (Burba *et al*. 2005a, b; 2006a, b) can be described using the Webb-Pearman-Leuning density formulation (WPL, Webb *et al*. 1980), which can be written in the following form for CO_2 flux:

$$F_c = F_0 + \mu \frac{E}{\rho_d} \frac{\rho_c}{1 + \mu \frac{\rho_v}{\rho_d}} + \frac{S}{\rho C_p} \frac{\rho_c}{T_a} \tag{1}$$

and for water vapor flux:

$$E = (1 + \mu \frac{\rho_v}{\rho_d})(E_0 + \frac{S}{\rho C_p} \frac{\rho_v}{T_a}) \tag{2}$$

where F_c is WPL-corrected CO_2 flux (kg m^{-2} s^{-1}); E is WPL-corrected H_2O flux (kg m^{-2} s^{-1}); F_o is initial CO_2 flux, not corrected for WPL (kg m^{-2} s^{-1}); E_o is initial H_2O flux, not corrected for WPL (kg m^{-2} $_s$$^{-1}$); μ is ratio of molar masses of air to water (μ=1.6077); ρ_d is mean dry air density (kg m^{-3}); ρ_v is mean water vapor density (kg m^{-3}); ρ_c is mean ambient CO_2 density (kg m^{-3}); ρ is mean total air mass density (kg m^{-3}); S is sensible heat flux (W m^{-2}); C_p is specific heat of air (J kg^{-1} K^{-1}); T_a is ambient air temperature (K).

Traditionally, S has been measured outside the gas analyzer open path by sonic anemometry, or with the help of a fine-wire thermocouple installed near or in the sonic path. If warm instrument surfaces around the open path heat air in the path, then there may be non-negligible differences between sensible heat flux inside the open path of the gas analyzer and that in ambient air, such that measured or estimated sensible heat flux inside the open path should be used in the WPL term instead of S measured in ambient air (Burba *et al.* 2005a, b; 2006, a, b). T_a is affected in a similar manner as S, but since it is in ^oK, its effect on the WPL term is small (Eqs. 1 and 2).

The concept of using heat flux measured in the optical path was confirmed in a study by Grelle and Burba (2007), where S and T_a were measured inside the instrument open path using a fine-wire thermometer during normal operation, and during a regime in which the instrument was heated by an external heater. In both cases, S measured inside the open path was substantially different from ambient. Also, in both cases, CO_2 fluxes adjusted using a WPL term with S measured inside the open path did not exhibit the unreasonable off-season and nighttime uptakes observed when using ambient S, and they closely matched the reference flux measured with a LI-6262 .

Here we describe, test, and compare several techniques for dealing with S inside the open-path volume, as summarized in Table I. These techniques include: 1) the *traditional approach* (S is measured in the ambient air using sonic anemometry); 2) an *enclosed LI-7500 technique* (S is effectively eliminated by a temperature attenuation in the intake tube of the enclosed analyzer); 3) *a fine-wire* PRT *technique* (*S* is measured directly inside the open path; Grelle and Burba 2007); and 4) *an estimated heating correction technique*, which can be applied to previously collected open-path data (*S* for the WPL term is computed by adding estimated sensible heat fluxes from key instrument surfaces to the ambient sensible heat flux; Burba *et al*. 2006 a, b). In all cases, CO_2 fluxes from closed-path systems (e.g., LI-6262 and LI-7000) are used as references, because high-frequency temperature fluctuations are attenuated in such systems by long intake tubes, thus greatly minimizing or eliminating *S* inside the analyzer cell. Further details on theoretical and experimental approaches can be found in Burba *et. al.* (2008)

3. Results and Discussion

Instrument surface heating and its effect on open-path CO_2 fluxes were tested over four ecosystems: ryegrass, forest clear-cut, maize, and soybean. The surface temperatures of the open-path infrared gas analyzer adjacent to the sampling volume were up to 6^oC warmer than the ambient air during daytime due to heating from the sensor head electronics and solar loading. The heat exchange inside the path was correlated with vertical wind speed. This produced sensible heat fluxes that were on average 14% larger than in the ambient air, at mild air temperatures. This percentage increased further with colder air temperatures and associated increase in sensor head instrument heating by on-board thermoelectric devices.

Figure 1 shows cumulative fluxes measured in four experiments with the closed path LI-6262 and with the open path LI-7500, which was either enclosed or corrected for the heat exchange, using the methods described in Table I. Summary of the integrated CO_2 flux values is provided in Table II. In all experiments, use of solely ambient sensible heat flux in the WPL term (Method 1) causes CO_2 flux integrations to be biased towards the CO_2 uptake as compared to closed-path references. During 4 weeks in winter over dormant ryegrass (Fig 1 A), flux measurements made with the open-path LI-7500 and corrected using Method 1 under-estimated CO_2 release by 12 g C m^{-2} (33%; Table II) as compared to the closed path reference. In contrast, using an enclosed LI-7500 (Method 2) resulted in a nearly perfect match with the reference LI-7000, with an error of 0.3%. When a heating correction was computed from instrument surface temperatures (Method 4) that were estimated from T_a by linear regression, the error was reduced from 12 to 2 g C m^{-2} (from 33% to 5%; Table II). This was not as good as an enclosed LI-7500, but was considerably better than ignoring the instrument surface heat exchange.

In the fine-wire PRT experiment (Figure 1B), use of traditional Method 1 led to a 3 g C m^{-2} (19%) underestimate of CO_2 release during two weeks in October. Meanwhile, the PRT technique (Method 3) and estimated heating correction from T_s computed via linear regression with T_a (Method 4) led to a considerably better match with closed-path references to within 1 g C m^{-2} (Table II). Remaining discrepancies between Methods 3 and 4 may be due to unaccounted heat fluxes caused by nearby structures, since the LI-7500 was mounted close to the base of the sonic anemometer.

Figures 1C and 1D show cumulative yearly CO_2 fluxes determined in the Mead, NE experiment from maize and soybean, respectively. During the off-season period (October-May) traditionally corrected open-path fluxes were 39 to 66 g C m^{-2} (75-81%) lower than the closed-path flux because of the systematic underestimation of CO_2 loss due to instrument surface heating (Table II). Consistent underestimation of CO_2 flux by the traditional technique has resulted in a considerable overestimation of the yearly CO_2 uptake at both sites by 92-100 g C m^{-2} (14-16%) as compared to closed-path fluxes. In contrast, cumulative fluxes from an open-path sensor corrected using Method 4 from T_s estimated via both linear and multiple regressions were consistently similar to closed-path fluxes throughout the entire year (Figures 1 C,D). On an integrated basis over the off-season, the multiple regression technique resulted in a larger error in

Maize (-10% vs. -4% for linear regression with T_a), but was better in Soybean (4% vs. 7% for linear regression with T_a). On a yearly basis both regressions gave good results, with the LI-7500 CO_2 flux matching the closed-path reference within 1%.

Overall, on a seasonal basis, any technique accounting for instrument surface heating (Methods 2-4) resulted in a significant improvement in CO_2 flux estimates compared with the traditional approach, which uses only ambient sensible heat flux in WPL term (Method 1). The most significant improvements were observed when the effect of instrument surface heat exchange was eliminated by enclosing the LI-7500 (CO_2 flux error of 0.3%), followed by measuring sensible heat flux in the open path using the fine-wire PRT technique (CO_2 flux error of -4%; Grelle and Burba 2007). Estimating the instrument surface heat exchange (Burba *et al*. 2006b) using measured T_s reduced the CO_2 flux error to -6%, while estimating T_s by linear regression with T_a reduced the error to -6 to 7%; estimating T_s by multiple regression with weather variables reduced CO_2 flux error to -10% to 4%. By contrast, in the ecosystems studied, neglecting the instrument surface heat exchange and using only ambient sensible heat flux in the WPL term (Method 1), produced underestimates of CO_2 release ranging from 14 to 81% (Table II).

4. Conclusions

Among the tested techniques the best performance was yielded by an enclosed LI-7500 (Method 2), followed by the fine-wire PRT technique (Method 3), and by the estimated heating correction technique which utilizes measured T_s, and T_s evaluated by linear regression with T_a, or by a multiple regression with weather variables (Method 4). The least successful performance was yielded by a traditional approach (Method 1) that uses solely ambient sensible heat flux in WPL term, resulting in a significant underestimate of long-term CO_2 release in all conducted experiments. Further details on results from this study, as well as on conceptual and methodological considerations, can be found in Burba *et. al.* (2008).

These results may have important implications for global carbon cycle research and climate modeling. Systematic underestimation of the CO_2 release during off-season periods by open-path sensors would likely be biased towards cold-climate ecosystems. As a result, longer and colder off-season periods would have greater underestimates of CO_2 release. Yearly estimates of net ecosystem exchange then may be significantly biased toward CO_2 uptake in such cold-climate ecosystems, and may need to be revised in some cases. Warm-climate ecosystems are less likely to be strongly affected, especially when air temperatures do not drop below freezing and when CO_2 fluxes stay large throughout the year. Open-path CO_2 fluxes calculated with the traditionally computed WPL term were not corrected for this previously unknown instrument surface heat exchange effect, so it is likely that biases already exist in data from colder ecosystems, and have affected a number of studies, their conclusions, and resulting models. Additional research is required to evaluate the potential impact of such bias, and to develop a strategy to correct the large volume of previously collected open-path data, including further investigation and validation of the proposed techniques for correction of instrument surface heat exchange in a wide range of ecosystems and experimental settings.

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Table I. Techniques for correcting open-path fluxes for the effect of instrument surface heat exchange (Burba *et.al*, 2008)

General Equations

General equation for the gas flux (F_c) over a homogenous horizontal plain for steady state conditions including WPL term (Webb et al, 1980)	$F_c = F_0 + \mu \frac{E}{\rho_d} \frac{\rho_c}{1+\mu \frac{\rho_v}{\rho_d}} + \frac{S}{\rho C_p} \frac{\rho_c}{T_a}$
General equation for the water vapor flux (E) over a homogenous horizontal plain for steady state conditions including WPL term (Webb et al, 1980)	$E = (1+\mu \frac{\rho_v}{\rho_d})(E_0 + \frac{S}{\rho C_p} \frac{\rho_v}{T_a})$

Sensible Heat Flux, S, for General Equations

Traditional WPL correction technique. Sensible heat flux is computed in the ambient air from sonic temperature or from a fine-wire thermocouple in the open air (Baldocchi *et al.*, 1988)	$S = \rho C_p \overline{w' T_a'}$	*Method 1*
Enclosed LI-7500 technique. Sensible heat flux has been eliminated by attenuating temperature fluctuations in the long intake tube. Same principle is used in the reference closed-path measurements (LI-6262 or LI-7000)	$S = 0$	*Method 2*
Fine-wire PRT technique. Sensible heat flux inside the open path is measured directly by fine-wire PRT and used instead of ambient sensible heat flux measured in the open air (Grelle and Burba, 2007)	$S = \rho C_p \overline{w' T_{PRT}'}$	*Method 3*
Estimated heating correction technique. Total sensible heat flux for WPL term is computed by adding estimated sensible heat fluxes from key instrument surfaces (bottom window, top window and spar) around the open-path to the ambient sensible heat flux (Burba, 2006b).	$S = \rho C_p \overline{w' T_a'} + S^{bot} + S^{top} + 0.15 S^{spar}$	*Method 4*

Surface Sensible Heat Fluxes for Nobel Formulation used in Method 4

Nobel (1983) formulation for S^{bot}, S^{top} and S^{spar}. T_s can be measured, or estimated via linear regression with Ta (Table III) or via multiple regression with key weather variables (Table II).	$S^{bot} = k^{air} \frac{(T_s^{bot} - T_a)}{\delta^{bot}}$ $S^{top} = k^{air} \frac{(r^{top} + \delta^{top})(T_s^{top} - T_a)}{r^{top}\delta^{top}}$ $S^{spar} = k^{air} \frac{(T_s^{spar} - T_a)}{r^{spar} \ln(\frac{r^{spar} + \delta^{spar}}{r^{spar}})}$ $\delta^{bot} = 0.004 \sqrt{\frac{l^{bot}}{U}} + 0.004$ $\delta^{top} = 0.0028 \sqrt{\frac{l^{top}}{U}} + 0.00025 / U + 0.0045$ $\delta^{spar} = 0.0058 \sqrt{\frac{l^{spar}}{U}}$

w is vertical wind speed (m s^{-1}); T_a is ambient air temperature (°K); T_{PRT} is temperature measured inside the open path with fine-wire PRT (°K); S^{bot}, S^{top}, S^{spar} - sensible heat fluxes from key instrument surfaces of bottom window, top window and spar, respectively (W m^{-2}); T_s is the mean surface temperature of the bottom window (T_s^{bot}), top window (T_s^{top}) and spar (T_s^{spar}) (°K); δ is average thickness of the boundary layer above the bottom window, top window, and spar (m); r^{top} is the radius of the sphere (0.0225 m); r^{spar} is the radius of the cylinder (0.0025 m); l^{bot} is diameter of the source housing treated as a plane (0.065 m), 0.004 m is added to compensate for the 20° angle of the shoulders in relation to the horizontal bottom window; l^{top} is the diameter of the detector housing treated as a sphere (0.045 m), , 0.0045 m is added to compensate for the non-spherical surface of the top window; l^{spar} is the diameter of the spars treated as cylinders (0.005 m); k^{air} is the thermal conductivity coefficient of air (W m^{-1} °K^{-1}); U is mean horizontal wind speed (m s^{-1}). Other terms are defined in the text.

Table II. Comparison of the integrated CO_2 release measured in three different field experiments with four different techniques for computing WPL term. All tables and plots include only hours with complete data, i.e. when actual readings from the LI-6200/7000, LI-7500, and other instruments used in the proposed corrections were available. Non-stationary conditions, rain, snow, instrument malfunctions and other filled-in periods were excluded to assure proper comparison between LI-7500 F_c and LI-6262/7000 F_c. The error in F_c calculated by these techniques is computed using closed-path LI-6262 or LI-7000 as reference such that % error=100*(F_{7500}-$F_{6262/7000}$)/$F_{6262/7000}$. Off-season periods are considered to be periods without green foliage area. In all three experiments, use traditionally computed WPL term with open-path LI-7500 (Method 1) leads to significant underestimates of CO_2 release or overestimates of CO_2 uptake, while LI-7500 flux corrected for surface heating by either of three proposed alternative methods is close to reference closed-path LI-6262/7000 flux which is not affected by heating problem (Burba *et.al*, 2008)

	Technique	**Units**	**Experiments**						**Essence of Technique**
			Enclosed LI-7500	**Fine-Wire PRT**	**Study at Mead**				
			Nebraska Dec-Jan Ryegrass	Sweden October Forest clear-cut	Nebraska Off-season Maize fallow	Off-season Soy fallow	Year Maize	Year Soybean	
Reference	Closed-path Fc: LI- 6262 or LI-7000 (used as reference)	g C	36	14	88	48	-630	-643	Heat exchange effect is minimized by attenuation of high frequency temperature fluctuations in intake tube. Only latent heat flux portion is used in the WPL term
Method 1	Fc from open-path LI-7500 with traditionally computed WPL (Webb et al., 1980)	g C	24	11	22	9	-730	-735	Ambient sensible heat flux measured outside the open path is used in the WPL term
		% error	**-33**	**-19**	**-75**	**-81**	**16**	**14**	
Method 2	Fc from an enclosed LI-7500	g C	36	-	-	-	-	-	Heat exchange effect is minimized by high frequency temperature attenuation in intake tube. Only latent heat flux portion is used in the WPL term
		% error	0.3	-	-	-	-	-	
Method 3	Fc from open-path LI-7500 with fine-wire PRT correction (Grelle and Burba, 2007)	g C	-	13	-	-	-	-	Sensible heat flux measured using fine-wire PRT in the open path is used instead of the ambient sensible heat flux in the WPL term
		% error	-	-4	-	-	-	-	
Method 4	Fc from open-path LI-7500 with estimated heating correction (Burba et. al., 2006b): Ts is measured	g C	34	-	-	-	-	-	Additional sensible heat flux in the open path is computed from instrument surface temperature, T_s, using the formulation by Nobel (1983), and then added to ambient sensible heat flux in the WPL term. Ts can be measured directly near top and bottom windows and on spars, or estimated from air temperature, or multiple regression with key weather variables.
		% error	-5	-	-	-	-	-	
	Fc from open-path LI-7500 with estimated heating correction (Burba et. al., 2006b): Ts is estimated from linear regression with Ta	g C	34	15	85	51	-626	-646	
		% error	-5	6	-4	7	-1	0.5	
	Fc from open-path LI-7500 with estimated heating correction (Burba et. al., 2006b): Ts is estimated from multiple regression from Table II	g C	-	-	79	50	-639	-651	
		% error	-	-	-10	4	1	1	

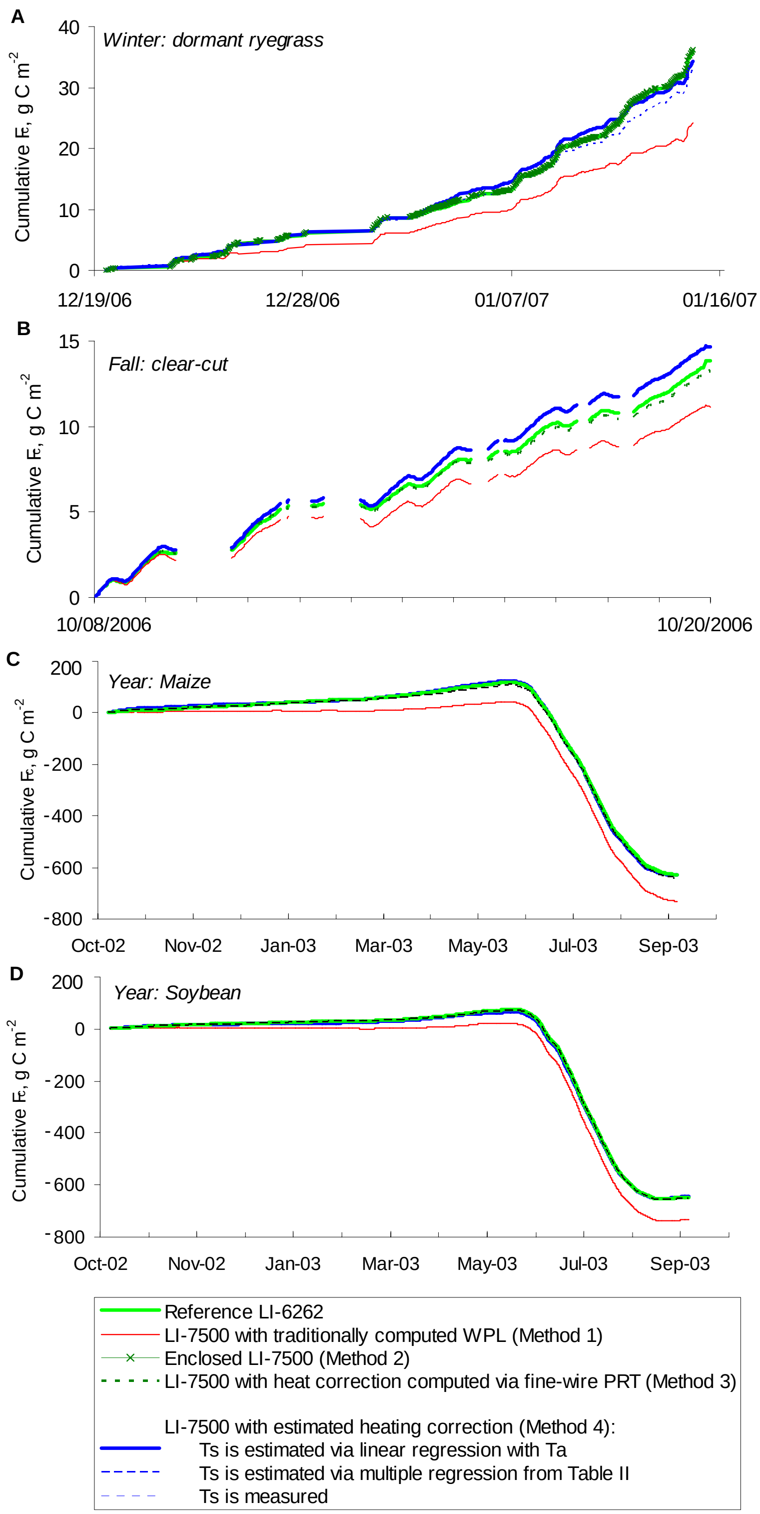

Figure 1. Cumulative plot of hourly Fc values (in g C m^{-2}) in four ecosystems. (A) enclosed LI-7500 experiment over dormant ryegrass; (B) fine-wire PRT experiment; and study and Mead, NE: (C) maize, and (B) soybean. In all cases data were used only when actual readings from the LI-6200/7000, LI-7500, and other instruments used in the proposed corrections were available. Non-stationary conditions, rain, snow, instrument malfunctions, and other filled-in periods, were excluded to assure proper comparison between LI-7500 and LI-6262/7000. In all experiments, use of traditionally computed WPL term (Method 1) with the open-path LI-7500 leads to underestimates of CO_2 release, and overestimates of CO_2 uptake, while LI-7500 flux corrected for surface heating by any of the proposed methods is quite similar to the reference closed-path LI-6262/7000 flux (Burba *et.al*, 2008)