Micrometeorological techniques to measure ecosystem-scale greenhouse gas fluxes for model validation and improvement

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Abstract. Dynamic models are explicit in time and therefore experimental data to validate and improve such models must also be explicit in time. The micrometeorological eddy covariance flux measurement technique is the recommended method for obtaining such data. However, in reality, chemical analyzers for greenhouse gas fluxes such as CH₄ and N₂O are not always fast enough for application with the eddy covariance in a strict sense. Here we show how a combination of the eddy covariance method with the flux-gradient approach could solve the problem, and how current knowledge of the behavior of slow chemical sensors could be used to perform eddy covariance flux measurements even with such sensors. © 2006 Published by Elsevier B.V.

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1. Introduction

To investigate dynamic systems, the knowledge of the system’s state at each point in time, \( X(t) \), and its change over time, \( \frac{dX}{dt} \), needs to be known (e.g., [12]). This is the basis of any prognostic model, be it in weather forecasting, limited-area climate modeling (e.g., [22,24]), atmospheric dispersion modeling of constituents in the air (e.g., [7,21]), or in generalized ecosystem models (e.g., the CENTURY model [20] or the TEM model [18]). Such a dynamic model must predict \( \frac{dX}{dt} \), based on the system’s initial condition \( X(t_0) \), and then for each time step during the model run.

Certainly there are other types of numerical models, such as statistical, empirical, and diagnostic models, to name a few, which all are parameter-based models. The shortcoming
of all these models is that they are not explicit in time, and therefore cannot be considered “prognostic” in a strict sense. Moreover, their validity for predictions is always limited to the range of parameter space for which they were parameterized, since the basic model concepts do not include any theoretical a priori assumptions of model behavior outside the known parameter space.

This is not to say that the latter type of models is not useful. The point to made here is that if one attempts to build and use a prognostic model that bases on the theory of dynamic systems, then one also needs data that fulfill the basic requirement that time must be treated as a special dimension in the system investigated.

First, a short overview is given over dynamic systems modeling concepts that are most widely used in climate modeling, numerical weather forecasting, and atmospheric dispersion modeling, and to an increasing extent also in ecosystem models. Then we will show how eddy covariance flux measurements in the atmosphere can provide the quantitative data for the exchange of trace gases such as methane (CH₄), nitrous oxide (N₂O), carbon dioxide (CO₂), and ammonium (NH₃) that are needed to validate and improve prognostic models. Finally, we discuss how the eddy covariance approach could be extended to applications where instruments are relatively slow.

2. Dynamic systems and prognostic models

A widely used concept in ecosystems research is the one that was introduced by Jenny [14]: a system X under investigation is expressed as a more or less simple function of the environmental variables that determine the observed state of the system, and the time,

\[ X = f(c, o, r, p, t) + z, \]  

(1)

where c is environmental climate, o is organisms (the fauna and flora), r is relief or topography, p is parent material of the soil when pedogenesis started, and t is time expressed as soil age, and z denotes external forcing factors [13]. Huggett [13] refers to this approach as the CLORPT equation or concept. This old concept however does not treat time as a special variable as this is done in the theory of dynamic systems (see [2]). Thus, Huggett [12] introduced the BRASH equation, which is an attempt to take the essentials of the widely established CLORPT concept and modify it to meet the theoretical requirements of a dynamic systems approach. This leads to the two universal equations that are needed for each variable in a dynamic system,

\[ X(t + \Delta t) = X(t) + \frac{dX}{dt}\Delta t + z, \]  

(2)

\[ \frac{dX}{dt} = f(b, r, a, s, h) + z. \]  

(3)

Here, b is the biosphere, r is the troposphere (relief), a is the atmosphere, s is the pedosphere (soils), and h is the hydrosphere. In order to be a fully prognostic system, each variable must be expressed by its current state at an initial time point \( t_0 \), that is \( X(t_0) \), and its first derivative in time at this time point, \( dX/dt(t_0) \).

Shortly, the basic theoretical background is that time is a special dimension or variable in a dynamic system. It only progresses forward and it cannot be randomly varied. All other variables adhere much more to the simplified concepts of ensemble statistics that are the basis of most analyses we perform whenever we neglect time.
In reality it is difficult to establish a model that is fully prognostic in all its parts. Although the concept of dynamic systems has been introduced in meteorology and atmospheric sciences long ago, it is still the case that numerical weather forecasting systems and global climate models only have a framework of a prognostic system, while many components driving this model core are statistical, empirical, and diagnostic algorithms which are not explicit in time. Without going into the details, it can be said that the wind vector and thus turbulence are quickly varying entities of the atmosphere such as temperature, atmospheric moisture, and trace gas contents. In a dynamic model they are treated as fully prognostic variables, while other entities such as soil moisture, radiation fluxes (e.g., solar radiation input from the sun) and many others are not prognostic.

The critical issue in prognostic systems is that although there is a solid theoretical basis of the model, one needs to find a way to close the system of equations that describe the model. As an example: if one constructs a fully prognostic model with 3 variables, then a set of equations with 3, 6, and 10 unknowns is needed for the zero, first, and second order closure, respectively [25]. The dilemma is that the number of unknowns increases with the level of complexity of the model, although our common sense would expect the reverse, namely that a system of equations is more easily to close as we increase the resolution (level of closure) of our system. Thus, an approximation is always needed to tackle such a model system, no matter how complex it is.

A useful approximation that is widely used is a second-order closure. This means, that all second-order terms in the equation system are resolved, but third-order terms of interactions are neglected, either by setting them zero if there is a reason to do so, or to parameterize them. With this assumption, it becomes clear that all interaction terms at the fourth and higher levels become zero by definition and can be neglected as well.

The eddy covariance technique is an experimental method (Fig. 1) to measure the higher order terms of a dynamic system. Although there is a wealth of publications that also consider the measurements of terms higher than the second order (which is of course useful to test the validity of the approach to parameterize or neglect third and higher order

Fig. 1. Eddy covariance instrumentation for flux measurements of CO₂ and water vapor at ETH research stations Chamau (left; 393 m a.s.l.) and Früebüel (right; 1024 m a.s.l.). The instrument in the center is a 3-dimensional sonic anemometer measuring the wind vector, and the inclined instrument next to it is an open-path infrared gas analyzer (Licor 7500, Logan UT, U.S.A.) for CO₂ and H₂O concentration measurement at 20 Hz temporal resolution. The slanted mounting reduces the time after rain events until the optical path is dry again, and the orientation of the sensor minimizes interferences with direct sunlight.
terms in a prognostic model), we restrict ourselves to the standard eddy covariance flux measurements done with one set of instruments at one site, which allows to measure the turbulent exchange of trace gases in the atmosphere with the local surface.

3. The eddy covariance method combined with the flux-gradient approach

3.1. The eddy covariance method

The basic equation for the eddy covariance flux measurement method is

\[ F_c = \text{cov}(w'c') \]  

(4)

with \( F_c \) the vertical net flux of entity \( c \) (e.g. CO\(_2\), H\(_2\)O, CH\(_4\), N\(_2\)O, temperature), \( w \) is the wind speed perpendicular to the surface, and \( \text{cov}(\cdot) \) and primes denote a temporal average of the covariance function (typically 30 min, Fig. 2) and the short-term deviation from it, respectively. Depending on instrumentation, additional conversion factors are needed in Eq. (4) to yield the net flux in the desired units (e.g., specific heat capacity in the case of sensible heat flux if \( c \) is temperature). Moreover, corrections such as the density flux correction [26] and the high frequency and damping loss correction [8] need to be applied. Although the theoretical basis is relatively simple, in practice there are a whole variety of details that need to be carefully considered to yield defensible flux estimates. The reader is referred to the Handbook of Micrometeorology [16] for such details.

Fig. 2. Example of a 16-day time series measured with the eddy covariance method at the Oensingen cropland site of ETH (47°17’N, 7°44’E, 450 m a.s.l.). Data recorded at 20 Hz were averaged over 30-min intervals. Raw fluxes are covariances before damping loss [8] and density flux [26] corrections were applied. Note how the optical dirtiness housekeeping variable of the Licor 7500 CO\(_2\) and H\(_2\)O analyzer, which indicates poor data quality during rain events and foggy conditions, influence the respective fluxes. Experience shows that data up to 70–80% dirtiness are still useable (the typical value for clean optics is around 50%).
The eddy covariance flux measurement technique delivers information on the ecosystem scale, i.e., from tens of m$^2$ to several ha of the surface area upwind from the tower. The area influencing the flux measurements is referred to as footprint area [15,23]. In contrast to flux measurements with sharply delimited chambers, the boundary of the footprint of eddy covariance flux measurements are gradual. Moreover, the size of the footprint depends on atmospheric conditions, namely stability of the atmosphere, horizontal wind speed, and surface roughness, and measurement height. Generally, the footprint area is much smaller during daytime with unstable atmospheric stratification than during nighttime. Therefore, it is always recommended to measure over a surface that is horizontally homogeneous and large enough to provide similar surface characteristics in the footprint area irrespective of its size. This is not always possible and it should therefore be recalled that the eddy covariance method by itself delivers a point information and thus works also in complex landscapes (see e.g. [27]). However, the relationship between the point information and its footprint area is not as straight forward as if the criterion of horizontal homogeneity of the surface is met.

While eddy covariance flux measurements are well established in the literature for CO$_2$, H$_2$O, sensible heat and momentum flux, some further details on how it is possible to carry out nitrous oxide and methane flux. There are a few instruments for fast measurements of N$_2$O and CH$_4$ concentrations for eddy covariance flux measurements on the marked, mostly based on the tunable diode laser technique. The high price and the manpower needed to maintain such an instrument during field deployments, however, are still prohibitive in many cases. Therefore, we shall spend some thoughts on how one could perform eddy covariance flux measurements with slow sensors. With most available slow gas analysers we expect a considerable time-dependent damping of the signal at high frequencies. In Eugster and Senn [8], we developed the basis for the correction of such measurements which we have been successfully using in the past more than 10 years for NO$_2$, O$_3$, CO$_2$, H$_2$O, and liquid fogwater flux measurements. Section 4 provides the basic information to be considered when an attempt to measure eddy covariance fluxes with slow instruments is planned.

3.2. The modified eddy covariance and gradient method (mECG)

This method is also known in the literature as the “modified Bowen-ratio method” (e.g. [4]), although it does not require the knowledge of the Bowen ratio (the ratio between sensible and latent heat flux [3]). This method combines the advantage of direct eddy covariance flux measurements with the need for slower sampling times of, say, N$_2$O and CH$_4$. To determine the vertical flux of the latter components, one measures the vertical gradient close to the canopy and at some distance above, and then yield the flux

$$F_c = K \Delta c / \Delta z,$$

where $K$ is the turbulent diffusion coefficient and $\Delta c / \Delta z$ is the measured finite-differences gradient of concentration $c$ in the vertical direction $z$. A very variable and therefore difficult to obtain entity is $K$. If we are capable to measure another flux, say, the CO$_2$ flux with the eddy covariance method and at the same time measure its concentration gradient, then it is possible to determine $K$ using Eq. (5). Now, for the N$_2$O and CH$_4$ fluxes we only must assume that the $K$ value is the same as that for CO$_2$, which allows us to determine the
N₂O and CH₄ fluxes. As an example, Griffith et al. [9] showed very good agreement between fluxes measured directly by eddy covariance, and those measured indirectly via the modified eddy covariance and gradient method.

At our research sites we measure the eddy covariance fluxes of H₂O and CO₂ using a Lico(r) (Logan, UT, USA) open path infrared gas analyzer, model 7500 (Fig. 1). The gradients of H₂O, CO₂, CH₄, N₂O, and NH₃ are measured using an INNOVA (Ballerup, DK) model 1312-5 photoacoustic analyser.

Although we expect to be able to detect peak fluxes with the mECG whenever the magnitude of the flux is relevant for longer-term budgets, the resolution will most likely not be sufficient to also resolve small fluxes. Therefore, we lay out new concepts on how to improve flux measurements with slow sensors in the following section.

4. Eddy covariance flux measurements with slow instruments

So far the emphasis in research has always been on finding and producing very fast analyzers that can achieve a 10 Hz temporal resolution or better. If instruments were slow and needed several minutes to analyse a single sample, the relaxed eddy accumulation method [6,5,1] was used, for example for measurement of fluxes of volatile organic compounds [10]. However, now there are many instruments available on the market that have a time resolution that lies somewhere in-between the range of very expensive ideal fast instruments and more affordable very slow ones, which could open a new field of application if they were used for eddy covariance flux measurements.

Here we will summarize the two most important aspects that need to be considered when trying to perform direct flux measurements with such instruments: (a) the problem of the cut-off frequency; and (b) the problem of damping. Since both aspects are quite well understood in theory and also in practice, the question is not so much whether the method can produce meaningful results, but rather whether the additional assumptions to be made and the corresponding uncertainties in flux estimates are acceptable for a certain application or not. As with any indirect flux measurement (e.g. with the relaxed eddy accumulation, an enclosure measurement, or a dispersion model based approach) such assumptions are often made implicitly.

4.1. The influence of the cut-off frequency

Even a fast instrument has a natural upper limit of frequencies that it can resolve. For example, a modern open-path infrared gas analyzer measures CO₂ and H₂O concentrations 20 times per second. Based on the Nyquist frequency theorem which states that there are at least to samples needed to resolve a regularly oscillating structure, the highest frequency that can be resolved is thus the cut-off frequency $f_{\text{cutoff}} = 10$ Hz. Fig. 3 shows how this cutoff frequency influences the flux measurements.

The bold line represents the universal normalized cospectrum of turbulent flux measurements in the atmosphere under neutral and unstable atmospheric stratification (which in general represents daytime conditions [8]). The statistical behavior of turbulence becomes quite universal if natural frequency $f$ is normalized by multiplying $f$ with $z/u$, which is the ratio between measurement height $z$ above local ground (in meters; in case of
dense vegetation the reference height is not ground level but roughly 2/3 of canopy height), and \( u \) is the mean horizontal wind speed (in m/s). In Fig. 3 \( n \) is this normalized frequency. Since \( f_{\text{cutoff}} \) is a constant value for a given instrument, but \( u \) varies under natural conditions while \( z \) is normally kept constant, the fraction of resolved flux depends on environmental conditions. Fig. 4 shows how cutoff frequency and the choice of \( z/u \) relate to Fig. 3. Since \( u \) varies naturally, only \( z \) can be controlled by appropriate experimental

![Fig. 3. Influence of various examples of cut-off frequencies on flux measurement. Each vertical line drawn at a specific cut-off frequency separates the resolved share of the true flux on the left side from the unresolved fraction to the right. The numbers correspond to the numbers in Fig. 2 and are equal to the sampling frequency if \( z/u = 1 \).](image3)

![Fig. 4. Isolines with equal share of resolved turbulent flux by a system with a given combination of \( z \), \( u \), and \( f_{\text{cutoff}} \). The line numbers correspond to the numbers given in Fig. 3. All lines show that if \( z/u \) is large, then a slow instrument has the same quality for flux measurements as a fast instrument deployed at a location where \( z/u \) is small. As an example, two points with equal performance are drawn at a sampling rate of 4 Hz with \( z/u = 0.5 \) and at 0.25 Hz with \( z/u = 8 \).](image4)
design. For a given location, the value of $z/u$ increases curvilinearly in the near-surface atmosphere (typically the lowest 50 to 100 m depending on atmospheric conditions) as $z$ is increased. Thus, with a slow instrument, it is suggested to measure higher up in the air than with a really fast one.

4.2. The influence of damping

In addition to what was discussed in Section 4.1 most instruments are subject to damping effects, where slow variations are perfectly resolved, but the higher the frequency of the variations the greater the problem of the instrument to resolve such fluctuations. This is called damping [8]. This is particularly important for closed-path instruments (effect of volume averaging) and instruments measuring over a longer distance (effect of line averaging), while a perfect eddy covariance instrumentation is normally expected to provide a point measurement. Fig. 5 starts with the same idealized cospectrum as in Fig. 4 and the effect of damping on the resolved and unresolved fractions of a turbulent flux are demonstrated.

Because the effect of damping is predictable and mostly affects the statistically well covered high frequencies, the unresolved fraction of the flux can be estimated using widely known corrections such as those by [8,19,17,11]. For example, in a time series measured with 20 Hz resolution, $f_{\text{cutoff}}$ is statistically represented by 72,000, while the low frequency where only few data points per time interval are available (e.g. $f=0.01$ is represented by only 72 data points) are almost unaffected by the slow response of an instrument. This is important since the low-frequency variation in turbulent motions is much less understood than the variation at high frequencies which obeys the physical laws of decaying turbulence (inertial transport of turbulent energy from larger to smaller eddies).

![Fig. 5](image-url)  
Fig. 5. Influence of various examples of damping on flux measurement. The area under each of the thin lines in relation to the area under the bold line (the ideal cospectrum) is equal to the fraction of resolved turbulent flux that can be achieved by a given combination of damping constant $\tau$ and $z/u$ (both in s).
5. Conclusions

Dynamic models are explicit in time and therefore need time series of greenhouse gas flux measurements for validation and improvement. The eddy covariance method provides experimental data that fulfill this basic requirement. However, in practice, not all greenhouse gases of interest can be measured directly with eddy covariance. Here we discussed how comparatively slow sensors could be used for direct flux measurements if a careful assessment of the environmental conditions (namely the magnitude of prevailing wind speed and the possibility to choose a measuring height that is not too close to the surface) together with the temporal resolution of a gas analyser is made.

References


