Data-Led Methods for the Analysis and Interpretation of Eddy Covariance Observations

Vanessa Juliane Stauch

Dissertation
zur Erlangung des akademischen Grades
"doctor rerum naturalium"
(Dr. rer. nat.)
in der Wissenschaftsdisziplin "Geoökologie"

eingereicht an der
Mathematisch-Naturwissenschaftlichen Fakultät
der Universität Potsdam

Potsdam, den 11.09.2006

Institut für Geoökologie

und

Helmholtz-Zentrum für Umweltforschung – UFZ

Only two things are infinite, the universe and human stupidity, although I'm not sure about the former.

(Albert Einstein)

Acknowledgements

This work would have been impossible without the help and support of a number of people. I am particularly grateful to

- Prof Dr. Helmut Elsenbeer for the support of this PhD thesis at the University of Potsdam.
- PD Dr. Karsten Schulz for his constant support and motivation particularly over the last two years. He introduced me into the world of visions and strategies and made always sure that there is plenty of scope for the future.
- Dr. Andrew Jarvis for his friendship and uplifting support throughout. He taught me to think, to take a look over a cliff and not to lose sight of the most important things in life. Working with him is wearying for sure but definitely not to miss.
- Florian for the green penguin and particularly for his technical support when I became desperate with the use of the HPC and Matlab; Paul for being the best English teacher; Sascha for his support; Renata and Peter for stimulating scientific discussions.
- Annelie for her mental support and food supply in particular towards the end; Carsten for stimulating discussions particularly about statistics and the difference between Matlab and R; Ralf for his constant optimism; Carola for her mental support; Sylvia for the flowers.
- Dorle, Petra and Ursula for their eternal friendship.
- My parents, my grandma, Susanne and Oliver for their indispensable support and their boundless faith in me.

Summary

The terrestrial biosphere impacts considerably on the global carbon cycle. In particular, ecosystems contribute to set off anthropogenic induced fossil fuel emissions and hence decelerate the rise of the atmospheric CO_2 concentration. However, the future net sink strength of an ecosystem will heavily depend on the response of the individual processes to a changing climate. Understanding the makeup of these processes and their interaction with the environment is, therefore, of major importance to develop long-term climate mitigation strategies.

Mathematical models are used to predict the fate of carbon in the soil-plant-atmosphere system under changing environmental conditions. However, the underlying processes giving rise to the net carbon balance of an ecosystem are complex and not entirely understood at the canopy level. Therefore, carbon exchange models are characterised by considerable uncertainty rendering the model-based prediction into the future prone to error. Observations of the carbon exchange at the canopy scale can help learning about the dominant processes and hence contribute to reduce the uncertainty associated with model-based predictions. For this reason, a global network of measurement sites has been established that provides long-term observations of the CO_2 exchange between a canopy and the atmosphere along with micrometeorological conditions. These time series, however, suffer from observation uncertainty that, if not characterised, limits their use in ecosystem studies.

The general objective of this work is to develop a modelling methodology that synthesises physical process understanding with the information content in canopy scale data as an attempt to overcome the limitations in both carbon exchange models and observations. Similar hybrid modelling approaches have been successfully applied for signal extraction out of noisy time series in environmental engineering. Here, simple process descriptions are used to identify relationships between the carbon exchange and environmental drivers from noisy data. The functional form of these relationships are not prescribed *a priori* but rather determined directly from the data, ensuring the model complexity to be commensurate with the observations. Therefore, this data-led analysis results in the identification of the processes dominating carbon exchange at the ecosystem scale as reflected in the data. The description of

these processes may then lead to robust carbon exchange models that contribute to a faithful prediction of the ecosystem carbon balance.

This work presents a number of studies that make use of the developed data-led modelling approach for the analysis and interpretation of net canopy CO_2 flux observations. Given the limited knowledge about the underlying real system, the evaluation of the derived models with synthetic canopy exchange data is introduced as a standard procedure prior to any real data employment. The derived data-led models prove successful in several different applications. First, the data-based nature of the presented methods makes them particularly useful for replacing missing data in the observed time series. The resulting interpolated CO_2 flux observation series can then be analysed with dynamic modelling techniques, or integrated to coarser temporal resolution series for further use e.g., in model evaluation exercises. However, the noise component in these observations interferes with deterministic flux integration in particular when long time periods are considered. Therefore, a method to characterise the uncertainties in the flux observations that uses a semi-parametric stochastic model is introduced in a second study. As a result, an (uncertain) estimate of the annual net carbon exchange of the observed ecosystem can be inferred directly from a statistically consistent integration of the noisy data. For the forest measurement sites analysed, the relative uncertainty for the annual sum did not exceed 11 percent highlighting the value of the data. Based on the same models, a disaggregation of the net CO_2 flux into carbon assimilation and respiration is presented in a third study that allows for the estimation of annual ecosystem carbon uptake and release. These two components can then be further analysed for their separate response to environmental conditions. Finally, a fourth study demonstrates how the results from data-led analyses can be turned into a simple parametric model that is able to predict the carbon exchange of forest ecosystems. Given the global network of measurements available the derived model can now be tested for generality and transferability to other biomes.

In summary, this work particularly highlights the potential of the presented data-led methodologies to identify and describe dominant carbon exchange processes at the canopy level contributing to a better understanding of ecosystem functioning.

Zusammenfassung

Der Kohlenstoffhaushalt der Erde wird maßgeblich von der bewachsenen Landoberfläche beeinflusst. Insbesondere tragen terrestrische Ökosysteme dazu bei, den Anstieg der atmosphärischen Kohlenstoffdioxid- (CO_2-) Konzentration durch anthropogen verursachte Emissionen fossiler Brennstoffe zu verlangsamen. Die Intensität der Netto-CO_2-Aufnahme wird allerdings in einem sich verändernden Klima davon abhängen, wie einzelne Prozesse auf Änderungen der sie beeinflussenden Umweltfaktoren reagieren. Fundierte Kenntnisse dieser Prozesse und das Verständnis ihrer Wechselwirkungen mit der Umwelt sind daher für eine erfolgreiche Klimaschutzpolitik von besonderer Bedeutung.

Mit Hilfe von mathematischen Modellen können Vorhersagen über den Verbleib des Kohlenstoffs im System Boden-Pflanze-Atmosphäre unter zukünftigen Umweltbedingungen getroffen werden. Die verantwortlichen Prozesse und ihre Wechselwirkungen mit der Umwelt sind jedoch kompliziert und bis heute auf der Ökosystemskala nicht vollkommen verstanden. Entwickelte Modelle und deren Vorhersagen sind deshalb derzeit mit erheblichen Unsicherheiten behaftet. Messungen von CO_2-Austauschflüssen zwischen einem Ökosystem und der Atmosphäre können dabei helfen, Vorgänge besser verstehen zu lernen und die Unsicherheiten in CO_2-Austausch-Modellen zu reduzieren. Allerdings sind auch diese Beobachtungen, wie alle Umweltmessungen, von Unsicherheiten durchsetzt.

Ziel dieser Arbeit ist es Methoden zu entwickeln, die physikalisches Prozessverständnis mit dem dennoch großen Informationsgehalt dieser Daten vorteilhaft zu vereinigen. Dabei soll vereinfachtes Prozessverständnis dazu genutzt werden, Zusammenhänge zwischen dem CO_2-Austausch und den umgebenden Umweltbedingungen aus den Beobachtungen abzuleiten. Das Besondere hierbei ist, dass diese Zusammenhänge direkt aus den Daten geschätzt werden, ohne vorher Annahmen über ihre funktionale Form zu machen. Die Daten als Ausgangspunkt der Modellentwicklung zu wählen gewährleistet, dass die Komplexität der Modelle dem Informationsgehalt der Messungen entspricht. Auf diese Weise lassen sich diejenigen Prozesse identifizieren, welche für den CO_2-Austausch mit der Atmosphäre dominant sind. Die gewonnenen Erkenntnisse können dann in robuste CO_2-Austauschmodelle für Ökosysteme überführt werden und zur Vorhersage von Kohlenstoffbilanzen beitragen.

In der vorliegenden Arbeit werden diese entwickelten, datenbasierten Methoden zur Analyse und Interpretation von Netto-CO_2-Flüssen eingesetzt. Die erste Studie führt ein datenbasiertes Modell ein, das unvermeidliche Lücken in Messzeitreihen zuverlässig interpoliert. Dies ermöglicht erweiterte Anwendungen der Daten. In einer nächsten Studie wird ein Verfahren vorgestellt, mit dem die Unsicherheiten in den Beobachtungen charakterisiert werden können. Dies ist nötig, um jährliche Kohlenstoffbilanzen von Ökosystemen unter Berücksichtigung der Messungenauigkeiten direkt aus den Daten herzuleiten. Dabei liegt die Unsicherheit in den betrachteten Waldstandorten bei maximal 11% des Jahreswertes. In einer weiteren Studie werden dieselben Modelle genutzt, um die Netto-CO_2-Flüsse in Einzelkomponenten der CO_2-Assimilation und -Abgabe zu bestimmen. Diese Komponenten sowie die Nettobilanz sind zusammen mit ihren Ungenauigkeiten für Vorhersagen über das Kohlenstoffsenkenpotential eines Ökosystems von besonderer Bedeutung und können Abschätzungen des globalen Kohlenstoffhaushaltes maßgeblich unterstützen. Abschließend zeigt die letzte Studie ein Beispiel für die datenbasierte Entwicklung eines Modells, das die dominanten Prozesse des Kohlenstoffaustausches in Waldökosystemen beschreibt und erfolgreich vorhersagen kann.

Dies unterstreicht insbesondere das Potenzial des vorgestellten Modellierungsansatzes, vorherrschende Prozesse zu identifizieren, zu beschreiben und damit zum verbesserten Verständnis des CO_2-Austauschs zwischen Ökosystem und Atmosphäre beizutragen.

Contents

I. Introduction

Terrestrial ecosystems play a major role in controlling the global carbon cycle through their uptake of carbon dioxide from the atmosphere via photosynthesis, the storage of this reduced carbon in plant and soil matter and its loss due to respiration. Understanding the mechanisms regulating these carbon exchange processes is particularly important when investigating the ecosystems potential to offset fossil fuel emissions (mitigation) or when trying to predict impacts of potential changes in climate on the fate of ecosystems (adaptation). In order to address these issues, mathematical models are being developed that are designed to describe the ecosystems behaviour under changing environmental conditions. However, ecosystem carbon fluxes are the result of multiple complex interactions on different temporal and spatial scales rendering their qualitative and quantitative description particularly challenging.

I.1 Modelling ecosystem carbon fluxes

Figure I-1 illustrates the dominant carbon fluxes in an ecosystem. Canopies trade CO_2 for water through their stomata. The rate of this exchange primarily depends on the amount of incident radiation, the ambient temperature, the CO_2 concentration and the vapour pressure deficit of the surrounding air and the water and nutrient availability in the system. Once CO_2 is assimilated in the mesophyll, complex physical and biochemical processes transform this reduced carbon to intermediate organic structures for further use within the plant. They are either invested into new plant tissue being allocated to roots, shoots and leaves, or they are oxidised back to CO_2 to support plant maintenance. Subsequent litter fall adds to the organic soil carbon pool and stimulates the activity of soil mircoorganisms, releasing CO_2 back to the atmosphere, particularly in the top layer of the soil. The individual processes giving rise to the carbon budget of an ecosystem obviously operate on a variety of scales and at different locations within the soil-canopy system.

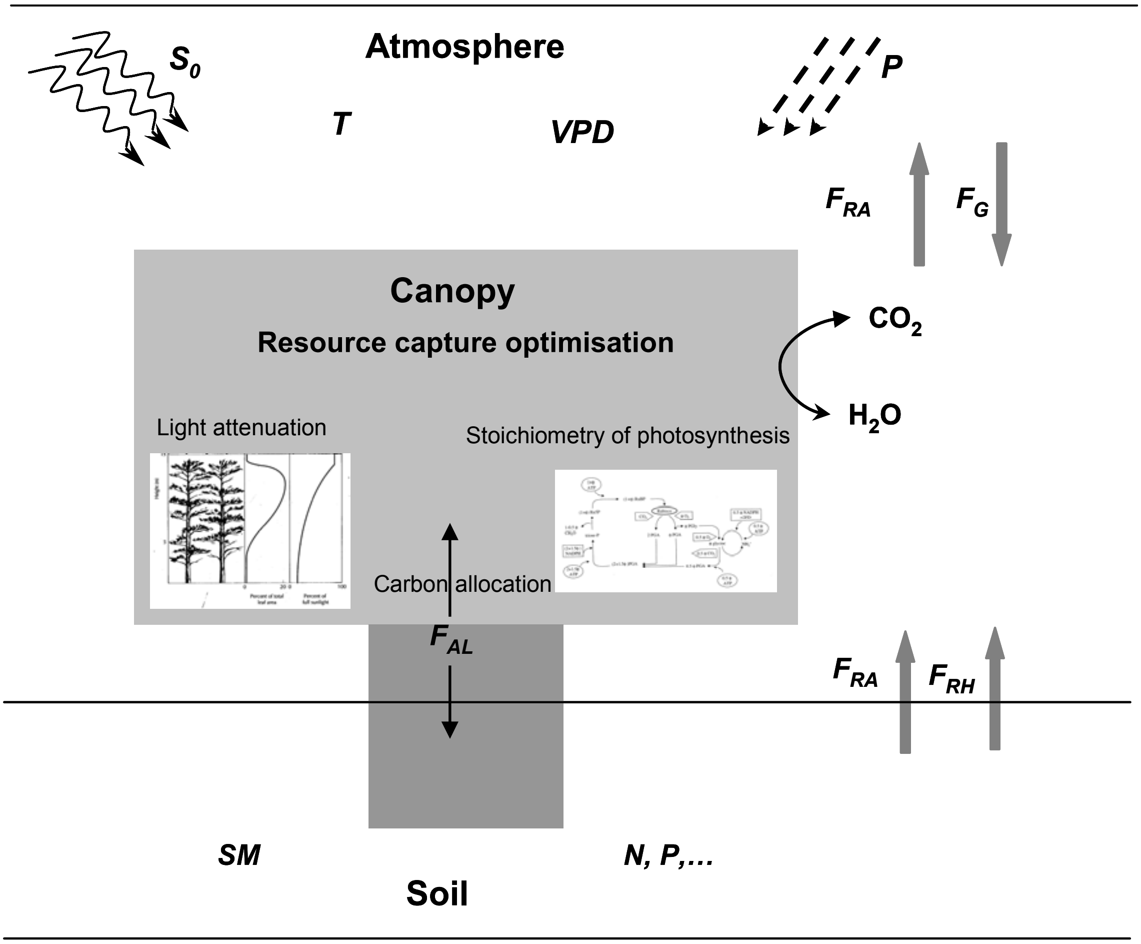

Figure I-1: Simplified illustration of carbon fluxes in an ecosystem (grey arrows) and controlling environmental conditions. Incident solar radiation (S_0), precipitation (P), vapour pressure deficit (VPD), temperature (T), soil moisture (SM), nutrient supply (N: nitrogen, P: phosphorus as representatives) are the most dominant environmental factors. Major carbon fluxes are assimilation via gross photosynthesis (F_G), autotrophic respiration by leaves, stems and roots (F_{RA}), heterotrophic respiration by soil micro-organisms (F_{RH}) and carbon allocation for maintenance and growth (F_{AL}). See text for further explanation.

Despite the complexity of the physiological processes in an ecosystem, many processes can be studied separately in controlled environments particularly for plants at the cell and leaf scale or for soils in columns or chambers. This way, a thorough understanding of the mechanisms regulating carbon assimilation and respiration at small scales has been accumulated (Jarvis 1995) and converted into sophisticated process models (e.g., Farquhar *et al.* 1980; von Caemmerer 2000; Ball *et al.* 1987; Lloyd & Taylor 1994). However, the representation of these processes at the plant and ultimately at the community level is subject to substantial uncertainty (e.g., Baldocchi *et al.* 2001*b*) because of spatial complexity, heterogeneity, and aggregation effects. As a result, scaling to the canopy level receives much attention in ecophysiology research and many different approaches are under investigation.

Two somewhat opposed approaches to scale up physiological processes from a leaf to the canopy have been developed and widely applied for describing canopy behaviour. The 'big leaf' models consider the canopy as one operating unit and assume canopy photosynthesis to be a constant fraction of the single unshaded leaf photosynthesis. In an attempt to address the main criticism of such a big leaf approach, “two-leaf” models have been developed that consider sunlit and shaded leaves separately (de Pury & Farquhar 1997; Wang & Leuning 1998). However, the parameters used to describe canopy photosynthesis are usually not measurable and the model’s validity heavily relies on the homogeneity of the canopy and the availability of information for the determination of remaining unknown parameters (e.g., Friend 2001). In contrast, ‘bottom up’ models are built in an attempt to thoroughly integrate the gas exchange over multiple layers of sunlit and shaded leaves to account for the vertical profile of the environmental conditions and the canopy architecture (e.g., Leuning *et al.* 1995; Williams *et al.* 1996; Knorr 2000). Provided the individual process descriptions and mutual interactions are correct and the parameters used to specify these descriptions are known, these models would deliver an entirely process-based simulation of the canopy behaviour under changing environmental conditions and could predict the response of ecosystems to possible future changes in climate. However, despite the complexity of the resulting models, their development still implies a number of simplifying assumptions and omissions, the impacts of which are impossible to quantify. On the other hand, it is the complexity of these systems (‘big leaf’ as well as ‘bottom up’ models) which are comprised of predominantly nonlinear process descriptions, in conjunction with a large number of uncertain parameters, that makes them suffer from considerable prediction uncertainty when compared with canopy observations (Franks & Beven 1997; Franks *et al.* 1997; Schulz *et al.* 2001).

Interestingly, a good model for describing ecosystem carbon exchange does not necessarily involve a detailed description of leaf processes. In fact, the behaviour of an ecosystem might well be characterised by a less complex model system which traded on the possibility of simplifying effects of community organisation and resource optimisation, process aggregation and averaging over space and/or time (e.g., Canadell *et al.* 2000). For example, resource use efficiency models for light, water and nutrients (Monteith 1972, 1977; Dewar 1997) make use of the assumption that canopies behave as a functional unit that optimises the capture of available resources (Monteith *et al.* 1989). This leads to simple model structures with the efficiency parameters being downregulated by resource limitations. A popular example is the model for light utilisation with the conversion efficiency (light-use efficiency) defined as the ratio of dry matter production and absorbed radiation by the foliage. Evidence for this ratio to be conservative for well watered ecosystems during the growing period has been accumulating since the observations for a crop field by Montheith (1977).

The light-use efficiency concept in conjunction with the advent of remote sensing information on the spectral properties of vegetated surfaces, has paved the way for the generation of terrestrial productivity maps delivering a key component for the calculation of regional and global carbon budgets (e.g., Running *et al.* 2000; Lobell *et al.* 2002; Leuning *et al*. 2005). However, the resolution of routinely available satellite information is still rather coarse and the derived estimates imply several assumptions and uncertainties with respect to homogeneity, data processing and model structure and parameterisation. Therefore, an evaluation of such approaches, preferably with corresponding ground measurements, is required. This could reveal errors, suggest model modifications and/or reduce the uncertainty associated with these estimates.

The success and limitations of the various approaches to modelling ecosystem carbon exchange highlight the importance of observations at the ecosystem scale. Long term continuous measurements can serve to rigorously evaluate simulation models, to test up and down scaling hypotheses, or to derive canopy responses to environmental forcings directly from the data. The latter aspect is particularly relevant when studying the dominant processes and regulations of carbon exchange at the canopy scale in order to derive robust models which have a level of complexity being in sympathy with the observations. Such an approach will be elaborated and discussed in the presented work.

I.2 The FLUXNET database

In the past two decades, the eddy covariance (EC) method has emerged as a suitable measurement technique of carbon, water and energy exchange processes at the canopy level. Provided a set of conditions for the study site and the atmosphere are met (see next section), the EC technique can be used to continuously record mass and energy fluxes between the terrestrial biosphere and the atmosphere over long time periods. The resulting data series consider the canopy as a single functional unit and represent an aggregate of the complex interactions between organisms in an ecosystem. Therefore, EC time series provide continuous information on the net carbon, water and energy exchange between the ecosystem and the atmosphere. With the growing network of eddy flux measurement stations around the world (FLUXNET, e.g., Aubinet *et al.* 2000; Baldocchi *et al.* 2001*b*) a considerable database is becoming available to help learn about ecosystem exchange processes in varying vegetation zones and climate conditions. The EC method is consistently used at all sites to measure the ecosystem response to short-term and long-term environmental variations. To date, more than 250 EC towers deliver continuous half hourly to hourly time series of mass and energy exchange fluxes along with a range of micrometeorological variables. FLUXNET sites are distributed fairly equally with respect to vegetation cover and climate across the United States (Hargrove *et al.* 2003) and to forests in Europe (Aubinet *et al.* 2000), whereas regional tower networks on the remaining continents are less mature. Nearly half of the EC stations are installed above forests, reflecting the assumed importance of these ecosystems in the terrestrial carbon cycle (Schimel 1995; Steffens *et al.* 1998). Standard instrumentation and methodology for data post processing (Aubinet *et al.* 2000; Baldocchi *et al.* 2001*b*) together with a common data archive (Oak Ridge National Laboratory Distributed Active Archive Center; http://www.ornl.gov) strengthens the integral network character and provides open data access for the scientific community and the public.

I.3 Theoretical background of EC measurements and instrumentation

Under turbulent conditions, mass and energy exchange between the surface and the atmosphere is dominated by eddies of different sizes within the surface boundary layer. Assuming horizontal homogeneity of the surface and atmospheric stationarity[1] and that molecular diffusion is a negligible contributor to the flux[2], the conservation equation for a given quantity simplifies to the covariance between the vertical wind velocity and the scalar concentration averaged over a specific time interval. Based on these theoretical principles, the eddy covariance (EC) technique measures the vertical flux densities of CO_2, water vapour and temperature between the vegetation and the atmosphere by sampling the turbulent motions along with their scalar concentrations over a time integral (Baldocchi *et al.* 1988; Baldocchi *et al.* 1996). Because the integral frequency spectrum of the fluctuations is limited by the observation duration and the measurement instrument response, EC data need to be corrected for frequency response losses (e.g., Aubinet *et al.* 2000; Baldocchi *et al.* 2001*b*). Data post processing also includes corrections for potential violation of stationarity assumptions and fluctuations in the air density due to temperature variations (Aubinet *et al.* 2000; Baldocchi *et al.* 2001*b*). However, due to a combination of both data recording and post processing errors and the stochasticity of the processes EC platforms observe, EC measurements contain a stochastic noise component (Mahrt 1998; Hollinger & Richardson 2005) that needs to be accounted for when making use of these data. A characterisation of this noise based on first

[1] To sample over the range of eddy sizes, an averaging time period of usually 30 to 60 minutes is necessary to derive representative flux values. This implies the assumption that the atmospheric turbulence conditions do not change over this averaging period.

[2] Obviously, when the boundary layer is in a tranquil state, this assumption may become invalid because the relative contribution of the diffusive pathway will become more important. Such conditions are often associated with nocturnal fluxes when turbulence in the boundary layer is no longer driven by surface warming from solar radiation.

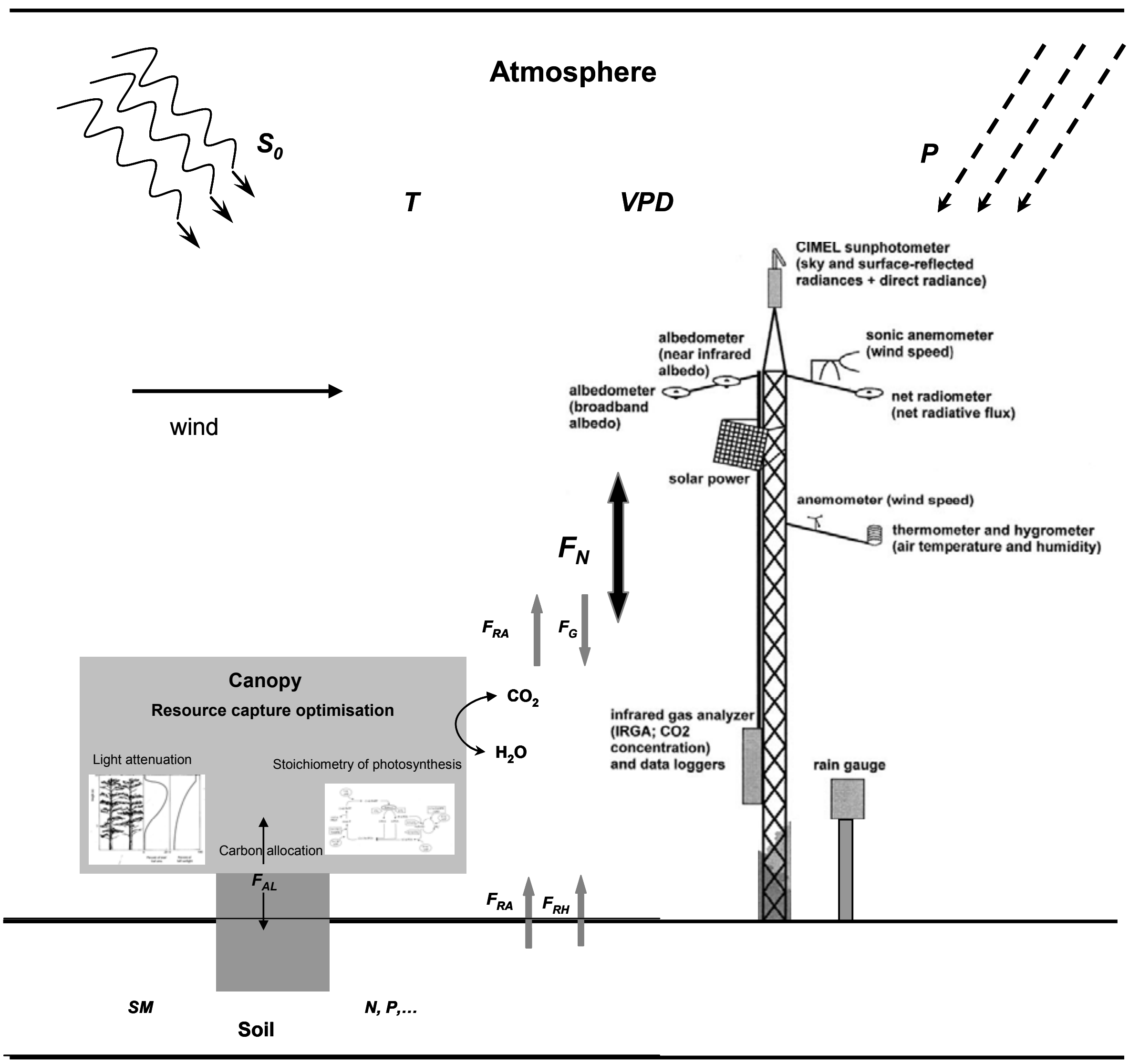

Figure I-2: A typical setup of an eddy flux station adapted from Running *et al.* (1999). The net carbon exchange flux F_N as the sum of all uptake and release fluxes is measured.

principles accounting for the contribution of all single sources is impractical and this work will suggest an alternative approach (see Chapter III).

Invariably, EC systems consist of a sonic anemometer for wind observations in three directions; a fast frequency response infrared gas analyser for measuring the concentrations of the scalars of interest (e.g., CO_2, water vapour); and a suite of software for data processing (Aubinet *et al.* 2000, Baldocchi *et al.* 2001*b*). The measurement ensemble is usually mounted on a tower above the top layer of the canopy (Figure I-2). It is accompanied by a set of instruments measuring micrometeorological variables (e.g., temperature, radiation, pressure, saturation deficit, precipitation) to characterise the meteorological conditions in which the mass and energy fluxes have been recorded.

I.4 Scientific use of EC data

The validity and applicability of the EC measurement technique is still an active area of research in its own right. In particular, stable conditions predominantly occurring at night, imply no turbulent mixing of the atmospheric boundary layer and hence zero flux. However, diffusive exchange within the boundary layer persists, particularly for CO_2, resulting in a systematic underestimation of the CO_2 efflux from the canopy (Aubinet *et al.* 2000). Commonly used approaches to limit this underestimation are to add a CO_2 storage term within the canopy (e.g., Wofsy *et al.* 1993) or to replace the EC measurements with simulations of a temperature dependent respiration function derived from nighttime data collected during turbulent conditions (e.g., Goulden *et al.* 1996*a*). However, both methods are prone to distorting the measured carbon budget (Lavigne *et al.* 1997, Law *et al.* 1999) as CO_2 stored over night will be either detected by the EC tower in the morning as a 'flush out' of the system, or will be readily assimilated by the canopy after sunrise. A standardised methodology for how to treat EC data collected under stable conditions has not been established yet and even its necessity is still under debate (Baldocchi 2003). Similarly, the validity of the EC towers in inhomogeneous terrain has been questioned (Aubinet *et al.* 2002). Fluctuations in wind speed and direction result in variations of the footprint of the tower blurring the separate contributions to the flux measured at the sensor (Schmid 2002). A large number of footprint models have been developed and applied to a range of site properties but there is still much scope for further investigations (Schmid 2002; Reithmaier *et al.* 2006).

As already mentioned above, EC data are uncertain and it is important to understand the makeup and the characteristics of this noise when making use of these time series. Only recently, attention has been drawn to the EC observation uncertainty and its significance for any use of the data, in particular when calibrating parametric models (Hollinger *et al.* 2004; Medlyn *et al.* 2005; Hollinger & Richardson 2005; Richardson *et al.* 2006; Hagen *et al.* 2006), or when extrapolating EC observations in space (Oren *et al.* 2006). As a result, the core of the EC data applications reviewed in the following paragraphs does not explicitly address the stochastic nature of the observations. The effect of this noise on inferences for annual carbon budgets directly from EC data will be studied in Chapter III and IV in this work.

A global network such as FLUXNET offers the opportunity for cross-site analyses to further enhance understanding of the role of terrestrial ecosystems in the global carbon cycle. Many studies have examined the differences in the effects of location, climate, and vegetation cover on ecosystem functioning (e.g., Valentini *et al.* 2000; Falge *et al.* 2001; Baldocchi *et al.* 2001*a*; Falge *et al.* 2002; Law *et al.* 2002). Besides the spatial distribution of stations over the globe that furnish data for global carbon budget studies, this network concept also provides a framework for a potential confirmation of biome specific findings (e.g., Williams *et al.* 2000; Curtis *et al.* 2002; Churkina *et al.* 2003).

EC observations represent an intermediate between leaf and single plant measurements and regional remote sensing information. As a result, their interrelation has been extensively investigated in order to gain insight into the effects of spatial and temporal scale on the effective description of carbon metabolism. Comparisons of EC data with smaller scale observations such as leaf cuvettes, soil chambers and biometric data and small scale model parameterisations highlight the differences in descriptions of biochemical process being dominant from leaves to the canopy and from hours to years, and emphasise the value of multi-scale observations for model derivation (e.g., Lavigne *et al.* 1997; Law *et al.* 1999; Barford *et al.* 2001; Curtis *et al.* 2002; Rayment *et al.* 2002).

Likewise, how EC measurements relate to larger scale observations is investigated to assess the potential of extrapolating mass and energy fluxes beyond the footprint to larger regions and ultimately to the globe (e.g., Desjardins *et al.* 1997; Reich *et al.* 1999; Running *et al.* 1999; see Friend *et al.* 2006 for a comprehensive review). Given remote sensing information and EC net CO_2 data provide information on different carbon components of an ecosystem, models are required to transform available data into comparable quantities. Usually, vegetation area indices, land cover and solar radiation data as deduced from remote sensing techniques are used within the above mentioned production efficiency model framework to estimate gross ecosystem production (Running *et al.* 1999). The resulting estimates can be compared to gross uptake derived from the EC net flux (e.g., Waring *et al.* 1995; Leuning *et al.* 2005). The two different estimates show moderate agreement that only improves when aggregated monthly values are considered, suggesting that errors due to model simplifications and heterogeneity somewhat cancel (Waring *et al.* 1995). The analysis of EC data might therefore reveal information that sheds light particularly on model errors in large scale applications. This supports the role of EC data contributing to carbon accounting efforts demanded by the Kyoto protocol and the potential of improving the estimation of the carbon source-sink strength of the terrestrial biosphere (Steffen *et al.* 1998; Hutley *et al.* 2005).

The net CO_2 flux at an EC tower represents a measure of the sum of carbon assimilation and respiration of the ecosystem. Several methodologies have been developed to disaggregate the measured flux into its major components to facilitate further model testing and comparison with remote sensing information (e.g., Goulden *et al.* 1996*a*; Reichstein *et al.* 2005; Hagen *et al.* 2006). However, a thorough evaluation of the results is still missing due to the lack of comparable observations of the two components at the corresponding scale. One way to overcome this restriction could be the use of synthetic data as will be demonstrated in Chapter IV.

One of the major objectives identified with the setup of the global network of flux measurement sites was to provide data to test and parameterise simulation models, these being seen as a key tool for predicting the regional and global terrestrial carbon balance (Baldocchi *et al.* 1996). A large number of models varying in complexity and spatial and temporal resolution have been evaluated against EC time series with varying levels of success (e.g., Aber *et al.* 1996; Williams *et al.* 2000; Churkina *et al.* 2003). Best agreement of model predictions and observations is achieved when comparing temporal aggregates or short time periods. As already mentioned above, Schulz *et al.* (2001) pointed to the problem of insensitive parameters in complex simulation models not being supported by observations and demonstrated the large prediction uncertainties arising from these uncertain parameters. As a result, data assimilation techniques are being investigated for their capacity to help constraining simulation models (Williams *et al.* 2005; Knorr & Kattge 2005; Raupach *et al.* 2005).

An alternative to assimilating the observations into pre-defined models is to explore what systematic/process behaviour can be observed within EC data. This data based modelling approach is receiving increasing attention in the FLUXNET community. Purely data based approaches such as artificial neural networks have been explored particularly in the context of gap filling EC measurements or flux partitioning (Aubinet *et al.* 2000; Papale & Valentini 2003; Leuning *et al.* 2005). They also show potential to serve as diagnostic tools to identify dominant factors controlling the system under study as a first step of model building (e.g., van Wijk & Bouten 1999) although they lack transparency in this respect. An alternative approach would be to exploit simple model structures such as radiation and water use efficiencies (Monteith 1977) because these linear structures are particularly amenable to estimation from EC data. Despite their simplicity and notable success on the canopy level (e.g., Dewar 1997; van Wijk & Bouten 2002; Chapter V), light and water use models are only hesitantly incorporated in ecosystem simulation models and so far have rather served the utilisation of satellite data (Running *et al.* 2000). The reason for this reservation is the lack of faith in their predictive capacity under climate change scenarios. However, such approaches have much to offer and deserve further investigation.

A somewhat hybrid approach is introduced in the present work and has been adopted by others (Gove & Hollinger 2006). It is based on the interactive combination of mechanistic process understanding with data led analyses. Here, novel time series analysis techniques are applied to approach EC data with minimal prior assumptions. For this, simple model structures representing basic process understanding are used to help constrain the estimation problem. The objective of this modelling approach is to explore the information content of EC data that might lead to canopy carbon exchange models with a maximum complexity needed to explain the signal in the observations.

I.5 The modelling concept

Mechanistic simulation models for the carbon and water exchange of an ecosystem with the atmosphere play a particular role when trying to predict future ecosystem responses under climate change scenarios. However, given the temporal and spatial complexity of the underlying processes in an ecosystem, these upscaling approaches are inevitably prone to substantial uncertainty (e.g., Schulz *et al.* 2001). As a result, predictions will also be characterised by large uncertainties due to errors in the model structure, uncertainty in the parameters and the complex error propagation through (nonlinear) process descriptions.

One way of tackling this problem could be to reduce the complexity of the model to an extent such that the remaining calibration parameters can be well defined from the data (e.g., Wang *et al.* 2001). In contrast, the modelling approach applied in this work (see Figure I-3) starts off with an 'oversimplified' model structure based on common ecophysiological process understanding with a minimum of prior functional assumptions. The available observations are then interrogated to constrain the model, i.e. the level of additional complexity is determined from the data directly. This procedure adopts many aspects of the data based mechanistic modelling (DBM) concept developed by Young and co-workers (Young 1999; Young & Pedregal 1999; Young 2000) that has been successfully employed for a diverse range of environmental research questions (e.g., Young & Beven 1994; Young *et al.* 1996; Schulz & Jarvis 2004).

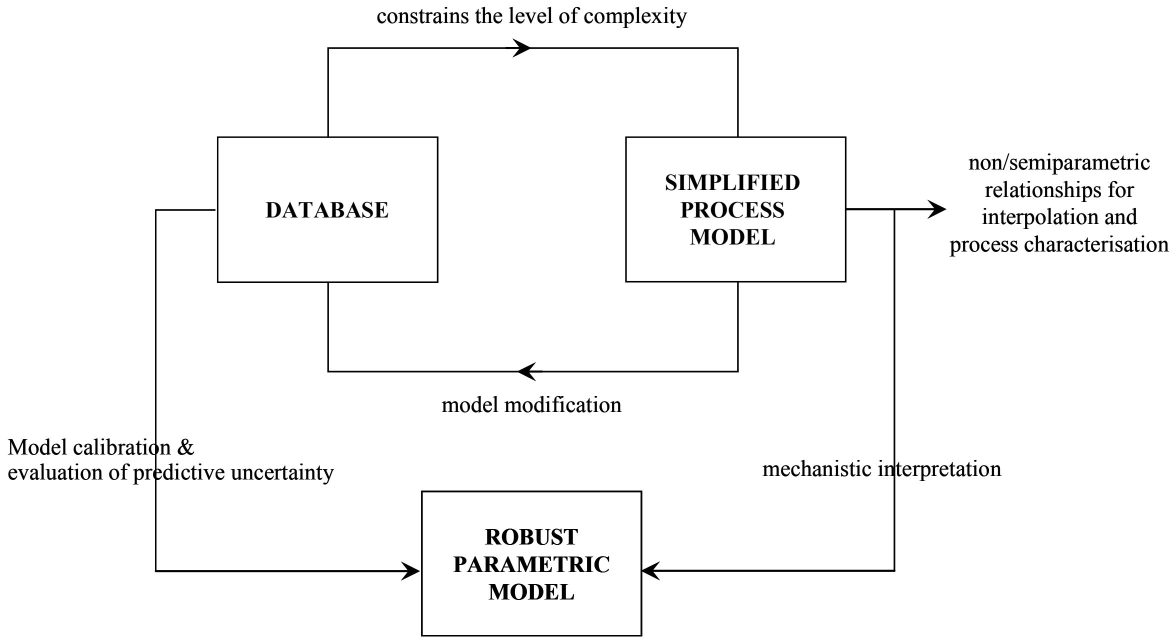

Figure I-3: Flowchart diagram of the modelling procedure as applied in the present work.

Given the enormous extent of observations from the EC tower network and the limited understanding of carbon processes at the canopy level, such a data led approach appears logical to complement the considerable efforts already put into the development of canopy simulation models, and ultimately one would hope to see convergence between these top-down inductive and bottom up reductionist modelling paradigms (Monteith 1995).

Two alternative modelling techniques are presented, differing in their underlying mathematical foundation but, as they are employed here, being driven by the same objective. The concept of time (TDP) and state dependent parameter (SDP) estimation (see Chapter V) has been developed for the analysis of nonlinear and nonstationary time series (Young 1999; Young 2000) forming a central part of the DBM approach for modelling nonlinear and nonstationary data. Here, parameters are allowed to vary with time or a specified driver(s) of the system under study in order to address dynamics that are not accounted for in the current model formulation. The estimation of these varying parameters is based on the recursive Kalman filter formulation that explicitly addresses noise in environmental observations as well as the stochastic nature of the system under study. The resulting (nonparametric) time or state dependencies are then to be interpreted based on mechanistic understanding and ultimately formulated as a function of the driver(s) found to dominate the behaviour of the system. Finally, a parametric model could be specified from these relationships and then calibrated and evaluated against the data in order to explore its validity and predictive capacity. To date, the use of TDP and SDP estimation is limited to the sum of one-dimensional responses, hence applying to only a subsample of environmental systems.

While being statistically less sophisticated, piecewise polynomials (see Chapters II-IV) allow for the simultaneous multidimensional estimation of dependencies. In the following this approach is referred to as being semi-parametric. Here, the values of the nodes joining the polynomials are optimised against the available data by minimising an appropriate objective function. The level of complexity allowed for the relationships can be controlled by varying the number of nodes. Similar to the TDP/SDP approach, the identified semi-parametric relationships could then be subject to mechanistic interpretation and ultimately parameterisation.

Because environmental measurements are corrupted with noise and, as a result, the true signal of the observed ecosystem is usually not known, the efficacy of any inductive data led modelling paradigm has to be checked in some way. One approach is to make use of synthetic data series. Complex simulation models that are well established in the scientific community can be used to simulate the net CO_2 flux under realistic environmental conditions thereby representing the behaviour of a virtual canopy. A known (synthetic) noise component can then be added to the simulated data to give rise to synthetic EC observation whose composition is known perfectly. From this any data analysis framework can be tested rigorously for both its capability to distinguish between signal and noise and its representation of the systematic behaviour of an ecosystem. This approach is novel in the analysis of EC data and is utilised in Chapters II-IV of this work.

I.6 General objective

This work is an attempt to contribute to the understanding of ecosystem carbon processes giving rise to carbon exchange fluxes between the terrestrial biosphere and the atmosphere. It aims to explore the information content on the systematic behaviour in the observations of these fluxes and to augment the data value for further carbon exchange studies. The following chapters are concerned with research questions directly arising from the general objective. These are:

- Can the dominant factors regulating canopy carbon exchange be extracted objectively from EC data?
- How can missing data in EC time series be overcome?
- How should uncertainty inherent in EC observations be dealt with?
- Can EC data contribute to carbon budget estimations given their limitations?

- Do the data allow for disaggregation into separate components?
- Do EC data allude to generic functional relationships that could represent canopy carbon processes?

These research questions shall be addressed by thoroughly interrogating the co-variations of EC net CO_2 time series data and concurrent micrometeorological measurements recorded above canopies following the modelling approach introduced above. As will be seen, the development and use of such hybrid statistical-mechanistic methodologies allow for a data-led identification of dominant systematic behaviour at the canopy scale as expressed in EC observations, whilst appreciating the stochastic nature of the observations. Based on the gained insights into canopy behaviour, the work sets out to explore simple model structures as representations of aggregated canopy carbon processes.

I.7 Chapter overview

The following work consists of four chapters each of which addresses different aspects of the overall objective elaborated above. The central product of this thesis forms a semi-parametric model for net CO_2 fluxes above canopies that estimates the simultaneous response of the CO_2 fluxes to light, temperature and time from EC time series data, making use of multidimensional cubic splines. Chapters II – IV present different applications of this model highlighting the insights into this system opened up by such a hybrid modelling approach.

In Chapter II it is shown that this model proves successful when estimating the systematic behaviour of the canopy net CO_2 flux even if calibrated against noisy and patchy data where much of valuable information is corrupted and/or missing. An analysis of the effect of missing data on the model performance is facilitated by the use of synthetic data produced by several canopy simulation models. Based on the results, the semi-parametric model is introduced as a suitable methodology to fill missing information in the underlying deterministic component of CO_2 flux time series provided by eddy flux towers.

As will be seen in the course of this work, to faithfully replace missing values in real observations an additional noise model is required to account for the stochastic component in EC data. Therefore, Chapter III presents an attempt to characterise this noise in EC data. Here, the spline model from Chapter II serves as a means to partition the deterministic part of the EC data from the stochastic component, hence facilitating their separate analysis. Synthetic data support the success of this method to reproduce the stochastic behaviour of EC data. Using a nonparametric method to derive the properties of the noise, the effects of its propagation through flux integration are assessed within a Monte Carlo simulation framework. It is shown how this application augments the value of the observations for annual carbon sequestration studies.

In Chapter IV, the ability of the spline model to disaggregate the deterministic net CO_2 flux into the carbon assimilation and respiration counterparts is assessed. Again, synthetic data is used to test the performance of the model. Compared to commonly applied parametric separation methodologies, the proposed scheme performs remarkably well while also accounting for observation uncertainty and error propagation in flux integrations. It is demonstrated how these estimates provide scope for the investigation of inter-site relationships with environmental site conditions.

Finally, Chapter V presents a study on how nonparametric relationships derived directly from the data can guide to physically meaningful parametric models as an ultimate example application of hybrid data-led analyses. Here, simple functional relationships are used to predict daily gross photosynthesis and ecosystem respiration of two deciduous forests by accounting for nonlinear effects of temperature and time. This chapter can be viewed as an initial step towards the development of regional models for carbon exchange between a diverse range of terrestrial ecosystems and the atmosphere.

An overall discussion (Chapter VI) integrates the four individual studies into the context of the general objective of the work and concludes with suggestions for further research and potential spin offs from the presented findings.

II. A Semi-Parametric Gap-Filling Model for Eddy Covariance CO_2 Flux Time Series Data

Vanessa J Stauch   Andrew J Jarvis

An edited version of this manuscript is published as

Stauch VJ, Jarvis AJ (2006) A semi-parametric gap-filling model for eddy covariance CO_2 flux time series data. Global Change Biology, 12, 1707-1716.

Abstract

This paper introduces a method for modelling the deterministic component of eddy covariance CO_2 flux time series in order to supplement missing data in these important data sets. The method is based on combining multi-dimensional semi-parametric spline interpolation with an assumed but un-stated dependence of net CO_2 flux on light, temperature and time. We test the model using a range of synthetic canopy data sets generated using several canopy simulation models realised for different micrometeorological and vegetation conditions. The method appears promising for filling large systematic gaps providing the associated missing data do not over-erode critical information content in the conditioning data used for the model optimisation.

II.1 Introduction

Quantitative descriptions for the exchange of energy and mass between the land surface and the atmosphere rely on the availability of suitable quality data for model identification, calibration and evaluation. The supply of data from the growing global network of tower measurements (FLUXNET; Baldocchi *et al.* 2001*b*) has become central to this model building process. The aim of these field campaigns is to provide long-run (multi-year) time series measurements of surface-atmosphere CO_2, H_2O and sensible heat fluxes, along with measures of the associated micrometeorological conditions, at a sampling interval of 30 to 60 minutes. However, due to a combination of the limitations on the applicability of the measurement techniques and the robustness of the measurement platforms, data rejection and missing data are inevitable leading to on average 65-75 percent data coverage across the season (Baldocchi *et al.* 2001*b*; Falge *et al.* 2001; Law *et al.* 2002). The resultant gaps in the time series measurements limit the use of these data in, for example, integrations to give seasonal carbon, energy and water balances.

To overcome the restrictions imposed by missing data a number of 'gap-filling' procedures have been developed. The term 'gap-filling' is somewhat misleading as it implies a temporal interpolation procedure where the available time series data adequately sample the full range of behaviour of the system. This is probably true for small, randomly distributed gaps, but is not necessarily the case for more systematic gaps. The more the missing data are associated with conditions that are poorly sampled by the available data, the more gap-filling becomes an extrapolation and the greater the uncertainty will become in the predicted response if it is based on the available observations alone. Because of this, it is important that there is an opportunity to include supplementary information to help constrain gap-filled predictions, particularly in the poorly sampled regions of the data set in question. However, in wanting to preserve the integrity of these valuable data we are wary about over-imposing our preconceptions about the underlying behaviour too strongly given the nonstationary and nonlinear nature of these systems and the uncertainties associated with the eddy covariance (EC) measurement technique (e.g. Goulden *et al.* 1996*b*; Moncrieff *et al.* 1996; Hollinger & Richardson 2005).

This paradox is a good example of the environmental modellers dilemma, how to attach appropriate weights to uncertain observations and prior knowledge about the system when making predictions. To a certain extent, the range of gap-filling procedures developed to date reflects these concerns. This range includes the use of moving averages (Falge *et al.* 2001; Reichstein *et al.* 2005); look-up tables (Falge *et al.* 2001; Law *et al.* 2002; Reichstein *et al.* 2005); artificial neural networks (Aubinet *et al.* 2000; Papale & Valentini 2003); multivariate correlation (Hui *et al.* 2004); nonlinear regression (Goulden *et al.* 1996*a*; Grünwald & Bernhofer 2000; Falge *et al.* 2001; Pilegaard *et al.* 2001; Suyker & Verma 2001), Fourier regression (Hollinger *et al.* 2004) and mechanistic simulation models (Law *et al.* 2002).

In what follows we devise a gap-filling scheme that attempts to address the problem of blending current observations and supplementary information when predicting the deterministic component of missing data in net CO_2 flux time series. The starting point for this approach is to assume light, temperature and time as the dominant driving forces controlling the net canopy CO_2 flux (Monteith & Unsworth 1973, 1990; Lloyd & Taylor 1994). The challenge then is to extract the relevant linear or nonlinear relationships between net CO_2 flux and each of these drivers, simultaneously, and without having to assume their parametric form a priori. Here, we achieve this by optimising a three dimensional hypersurface for net CO_2 flux within the CO_2 flux, light, temperature, time space. This hypersurface is constructed using piece-wise polynomials (cubic splines), hence allowing a certain degree of control over the rates of change within the hypersurface (i.e. the surface is smooth) whilst retaining the objectivity of the semi-parametric approach[3].

The use of semi-parametric and non-parametric optimisation to model EC data is not new. For example, Jarvis *et al.* (2004) used a sorting and kernel smoothing procedure to identify the functional form of the seasonal evolution of photosynthetic capacity and bulk respiration in EC net CO_2 flux time series. Adopting a hybrid approach, Yi *et al.* (2004) used a kernel smoothing technique to estimate the temporal evolution of parameters within a specified light saturation function in addition to the temperature dependency of bulk respiration. These methods contrast with the more subjective approach of optimising fixed parametric relationships based on prior assumed model structures such as light response functions for photosynthesis (e.g. Goulden *et al.* 1996*a*; Aubinet *et al.* 2000; Falge *et al.* 2001) or Arrhenius and Q_{10} functions for respiration (e.g. Lloyd & Taylor 1994; Grünwald & Bernhofer 2000; Falge *et al.* 2001). The semi-parametric estimation in the flux-light-temperature-time space being advocated in this paper is intermediate between gap-filling methods based on nonlinear regression of functional relationships (e.g. Grünwald &

[3] Here, semi-parametric is used to distinguish cubic splines, which involve an internodal parameterisation of a cubic polynomial, from kernel smoothing where no such parameterisation is prescribed. For a good introductory text on this and related issues see Simonoff (1996).

Bernhofer 2000), and more statistical methods based on covariance analysis such as multivariate correlation (Hui *et al.* 2004). Another way of viewing this work is as an attempt to optimise a continuous look-up table in the light-temperature-time space, with the cubic splines acting as the interpolating condition, as opposed to a discrete look-up table derived from binning data (e.g. Falge *et al.* 2001).

We assess the performance of this method using various synthetic data sets by introducing periods of artificial systematic gaps and comparing the results with the simulated fluxes. This provides a good test for gap-filling procedures because the systematic component of the EC observations is known perfectly, unlike with real data. As a result, deficiencies in the gap-filling procedure can be evaluated unambiguously. By comparison, the often significant uncertainties associated with real EC observations introduce ambiguity over the source of failure of a scheme and hence whether to reject that scheme or not. This is important in the context of this work as we will attempt to demonstrate not only the efficacy of the approach but also its inability to capture the response if excessive extrapolation is required, hence, exposing the need for additional information.

II.2 Methods

Nonlinear and non-stationary CO_2 flux model

We start by assuming that light, temperature and time are the major controlling factors for the response of the net canopy CO_2 flux, F_N, to the surrounding environment. Here, the time dependency of F_N denotes 'change' and covers all observed variation not attributable to either light or temperature. Similarly, the temperature dependency of F_N is an aggregate that does not differentiate between effects on photosynthesis and respiration. Light, temperature and time impact on F_N in a manner dependent on a diverse range of physical, biochemical and physiological processes. These processes may be well characterised at the sub-canopy scale, but their aggregation to the canopy scale and associated expression within EC measurements entrains a significant degree of uncertainty (e.g. Baldocchi 1993; Jarvis & Dewar 1993). This leads to ambiguities when specifying both the structure and parameterisation of relationships for F_N that will be in sympathy with a particular data set. Therefore, to specify a model that is a faithful representation (and hence interpolator) of the relationships between light, temperature, time and F_N in EC data requires a degree of objectivity when both structuring and subsequently parameterising the model. Because of this we start by simply assuming

$$F_N = f\{S_0, T, t\} + e \qquad \text{(II-1)}$$

where S_0 is the incident solar radiation, T is temperature and t denotes time and $f\{S_0, T, t\}$ is an unknown three dimensional function in S_0, T and t which will be obtained by conditioning the relevant cubic spline hypersurface on the data. Speculating F_N as a function of S_0 is a convenient way of handling the commonly observed nonlinearity between S_0 and F_N within any particular day (Ruimy *et al.* 1995; Law *et al.* 2002). The model error, e, will include the stochastic behaviour of the system, the uncertainty of the EC observations (Goulden *et al.* 1996*b*; Moncrieff *et al.* 1996; Hollinger & Richardson 2005) and the inadequacy of the model being applied. The choice of S_0, T and t is not prescriptive and the reader is at liberty to suggest additional or alternative relationships they deem important in explaining their data, providing measurements of the relevant drivers are available to identify functionalities when performing the semi-parametric estimation and that the observations support the estimation of these relationships. An example response of F_N to S_0, T_S and t is shown in Figure II-1[4].

Spline estimation of $f\{S_0, T, t\}$

$f\{S_0, T, t\}$ is represented using a three dimensional hypersurface of piecewise cubic polynomials or splines. Piecewise cubic polynomials are popular because they provide a reasonable compromise between flexibility, smoothness and the number of parameters to be determined (Press *et al.* 1988, 1992). Each dimension in $f\{S_0, T, t\}$ is described by an interval $[x_1 \dots x_n]$ and is divided into n-1 subsections resulting in n node locations, each with node values $y_1 \dots y_n$. For each subinterval $[x_i \dots x_{i+1}]$, the polynomials $P(x_i)$ are estimated as cubic *Hermite* interpolating polynomials based on four interpolation conditions (de Boor 1978, 2001),

$$\begin{aligned} P(x_i) = y_i, P(x_{i+1}) = y_{i+1} \\ P'(x_i) = d_i, P'(x_{i+1}) = d_{i+1} \end{aligned} \qquad \text{(II-2)}$$

[4] It is interesting to note that the estimate for the F_N, S_0, T_S, t hypersurface captured by $f\{S_0, T_S, t\}$ would provide a valuable means of characterising the simultaneous response(s) of F_N to S_0, T_S, t in eco-physiological and inference based modelling studies.

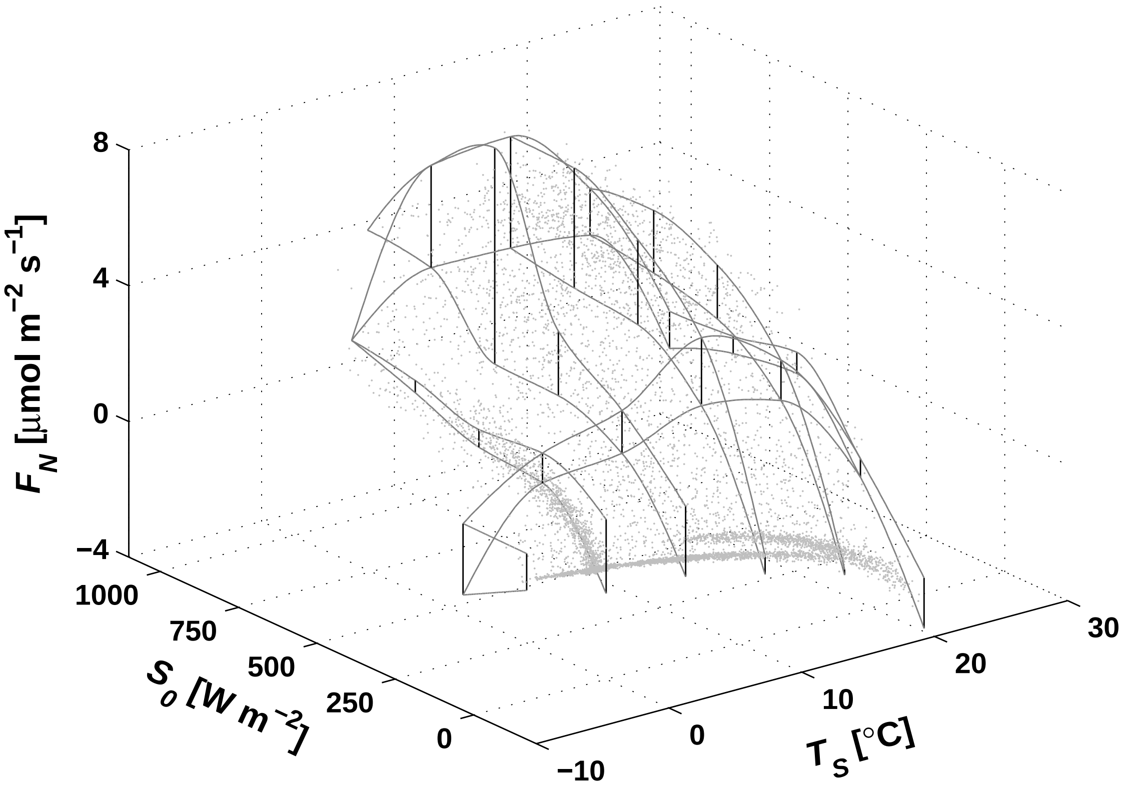

Figure II-1: 3D visualisation of the response of F_N to S_0, T_S and t for the synthetic SPA data set. F_N is plotted as grey dots in the S_0-T_S space. The vertical black lines indicate the temporal evolution of the $f\{S_0,T_S\}$ surface as estimated in model (1). The remaining grey lines are illustrative interpolations of internodal splines lying in the hypersurface.

where $P'(x_i)$ denotes the first derivative of the interpolant P at x_i, and d_i denotes the local slope at x_i. Here, we use a shape-preserving interpolation proposed by Fritsch & Carlson (1980) because it is stiff enough to prevent an overshoot of the cubic polynomials between the nodes (i.e. they are only continuous up to the first derivative, Mohr 2004). This interpolation determines the slope at a node as the harmonic mean of the slopes in the two adjacent nodes. In case of opposite signs of the slope in the adjacent nodes, x_i is a discrete local extremum and hence d_i is set to zero. The values of the nodes y_i in each relationship are then optimised against the data through non-linear least squares minimisation of the prediction error model $e = F_N - f\{S_0, T, t\}$ using Levenberg-Marquardt nonlinear least squares optimisation of the relevant node values $y_1 \ldots y_n$ at locations $[x_1 \ldots x_n]$ simultaneously in all three dimensions (S_0, T and t). Note that this optimisation weighs all observations equally and does not account for factors such as the night-time fluxes being more uncertain when using real data (Goulden *et al.* 1996*b*; Moncrieff *et al.* 1996). To account for this, prior knowledge of bias and/or uncertainty would be required, and the observations weighted accordingly.

Optimising (II-1) for the synthetic data sets used in this study results in residual colour in e. This is expressed as a small but significant autocorrelation reflecting the spline model's inability to reproduce the diurnal variation in the synthetic data that is not related to variations in S_0 or T (i.e. $e = e(t)$). This mainly reflects small diurnal hysteretic effects in the simulation models used. Where appropriate, we address this by estimating an autoregressive model from $e(t)$ and adding the systematic serial correlation to $f\{S_0, T, t\}$. In addition, the least squares optimisation used here ideally implies Gaussian residuals, whereas this is seldom the case for this application. However, any bias this introduces is not important for this application as we are only interested in fitting and not in interpretation.

The choice of the number of nodes and their allocation will obviously depend on the properties of the data. One is tempted toward a high node density because, in the extreme, if there were as many nodes as data points one could have an exact recreation of the available data. However, although introducing more nodes increases the flexibility of the model, this is at the cost of the semi-parametric relationships becoming increasingly sensitive to noise, hence making the predicted fluxes for the gap-filling increasingly uncertain. Therefore, as gap lengths increase so the node density has to fall in order to ensure nodes within gaps are constrained by adjacent available data. We use a six by six equidistant node matrix to represent the F_N-S_0-T space when estimating $f\{S_0, T\}$ as this number of nodes (36) proved sufficient. Only nodes lying within the dynamic range for S_0 and T are optimised as estimates outside this range will be associated with no data. Given this range changes through the year the node allocation in the F_N-S_0-T space is changed accordingly. The choice of the location of nodes in time provides an opportunity to the modeller to intervene when accounting for medium term 'changes' in $f\{S_0, T\}$. For example, the occurrence of a known 'event' could merit allocating nodes around this event whereas long periods of inactivity would not. Therefore, we advocate interrogating the data beforehand and exercising prior judgement when allocating the number and location of nodes in t, particularly in relation to gaps.

It is important to appreciate that the optimisation of the node values and the resulting hypersurface is carried out against the data sorted with respect to the magnitude of S_0, T and t. It is, therefore, the evolution of the sorted F_N giving rise to the shape of the smoothed changes of the interpolant P in the F_N-S_0-T-t space and not a direct function of S_0, T or t (see Young 2000). Not only does this facilitate the estimation, it also has the additional benefit of shuffling temporally ordered systematic gaps, making them somewhat more random.

Evaluation of the gap-filling model

To evaluate the performance of the gap-filling scheme we have elected to use synthetic data sets where we have full control over the nature of the missing data and the systematic and stochastic components of the observations. For this test we have simulated the canopy net CO_2 flux for four different biomes using three different simulation models. Each data set is comprised of one year of hourly F_N samples where $F_N = F_{Ns} + e_S$, with F_{Ns} being the deterministic simulation model output and e_S a synthetic noise component.

For a temperate coniferous forest under seasonal rainfall biome we have used the Soil-Plant-Atmosphere (SPA) model of Williams *et al.* (1996). The meteorological driving variables are taken from the Metolius FLUXNET site in Oregon (old-young ponderosa pine) for the year 2000 (Law *et al.* 2001; Anthoni *et al.* 2002; see also Williams *et al.* 2001 for a test of SPA against ponderosa pine EC data). In addition, soil respiration is described as an exponential function of soil temperature with a soil moisture dependent activation energy (Black *et al.* 1996; Goulden *et al.* 1996*a*; Lindroth *et al.* 1998; Fang & Moncrieff 2001). The relevant model outputs include F_{Ns} and 'surface' temperature, T_S and are shown together with associated model input data in Figure II-2a.

For a temperate deciduous forest under uniform rainfall we have used the Biosphere Energy-Transfer and Hydrology model (BETHY, Knorr 2000) applied to the Hainich FLUXNET site, Germany for the year 2000 (Knohl *et al.* 2003; Anthoni *et al.* 2004; see Knorr & Kattge 2005 for BETHY parameterisation). The relevant BETHY model inputs and outputs are shown in Figure II-2b.

A tropical, high productivity biome and an artic low productivity biome were simulated using the model described in Leuning *et al.* (1995). The meteorological driving variables for the tropics are taken from the typical meteorological year database (TMY2, 2006) for Honolulu, Hawaii and the leaf area index (LAI) has been set to 6 m^2/m^2 (Figure II-2c). For the simulation of an arctic site we reduced the maximum catalytic activity for rubisco and the temperature maximum of the potential rate of the electron transport (von Caemmerer 2000). Input variables are taken from the TMY2 database for Yakuta, Alaska, US (Figure II-2d).

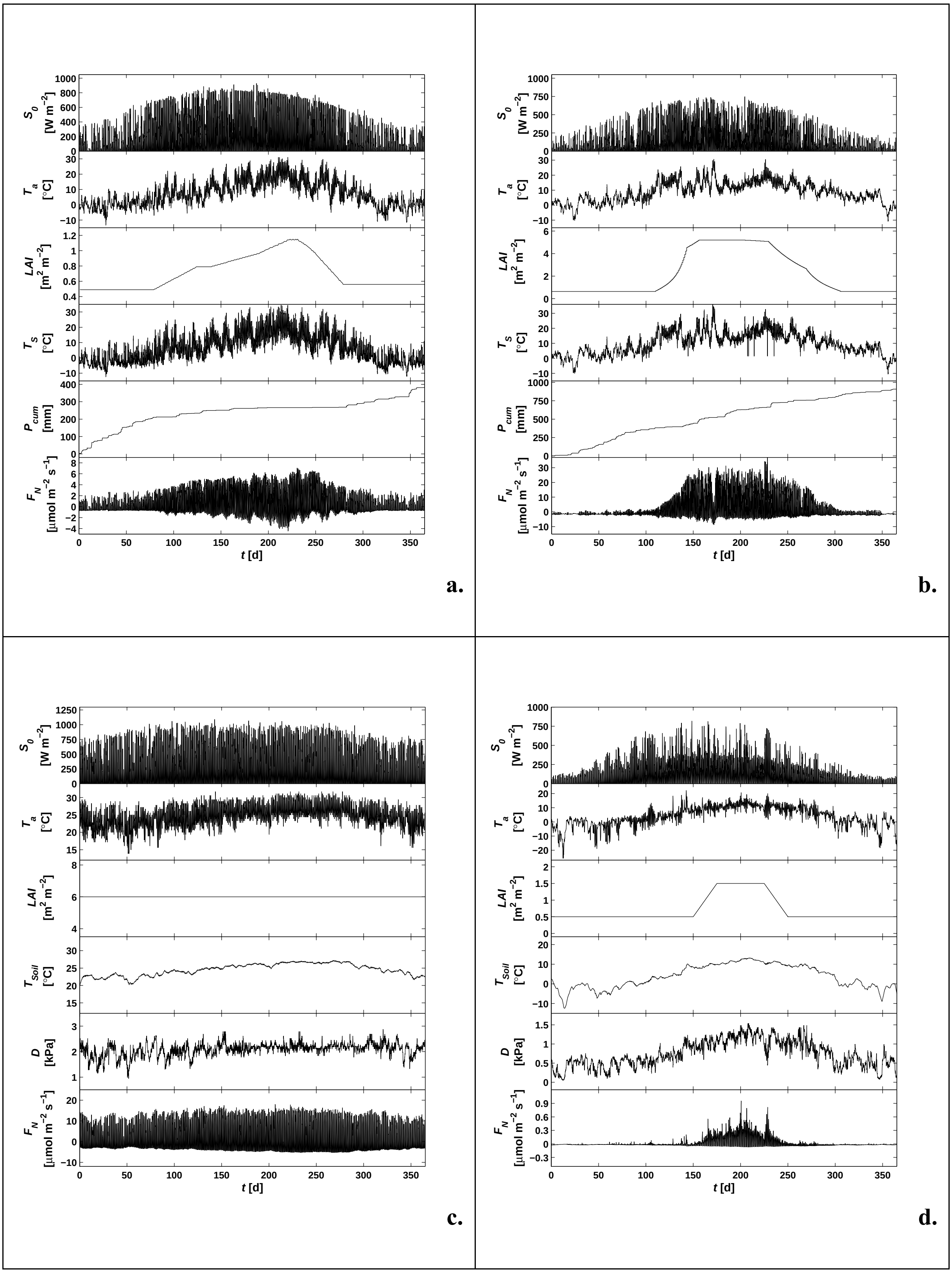

Figure II-2. Selected input and output series for the various simulations. **a**. SPA at the temperate coniferous forest site with seasonal rainfall. **b.** BETHY at the temperate deciduous forest site with uniform rainfall. **c.** Leuning *et al.* (1995) model at a high productivity tropical site. **d.** Leuning *et al.* (1995) model at a low productivity artic site. S_0 denotes incident radiation, T_a is air temperature, LAI is the leaf area index, T_S and T_{Soil} are surface and soil temperature, respectively. P_{cum} is cumulative annual rainfall, D is saturation deficit and F_N is the synthetic net CO_2 fluxes above the canopy (model plus noise).

The stochastic component e_S comprise a zero mean white noise series with a standard deviation of ten percent of F_{Ns} (i.e. constant relative error) to simulate the measurement errors (Moore 1986; Hollinger & Richardson 2005) and the stochastic nature of the underlying processes (Wesely & Hart 1985). Similarly, a realistic quantity of constant variance white noise is added to S_0 and T to represent measurement error.

We evaluate the model performance by comparing the final deterministic estimates of F_{Ns} with $f\{S_0, T, t\}$ for the four synthetic data sets, a privilege afforded by using synthetic data. The analysis will focus on two related aspects, the statistical properties of the error series $e^* = F_{Ns} - f\{S_0, T, t\}$ and, related to this, a comparison of the cumulative F_{Ns} and $f\{S_0, T, t\}$ fluxes across the years. This must be viewed as a particularly harsh evaluation given normally the model inadequacies exposed in e^* would be obscured in the more common analysis of e by the significant observational uncertainty.

The success of the scheme is tested against a gap-free scenario and a gap scenario for all four data sets. For the gap scenario we introduce regular, 20 day gaps interspersed by 13 day data series resulting in 60 percent of the entire data set missing. The choice of a uniform gap length of 20 days derives from the gap frequency spectrum in Falge *et al.* (2001) in that this length had an estimated probability of occurrence of just three percent and gap durations less than this did not prove very challenging to the estimation.

For an intercomparison of this and other gap-filling methods using measured EC data sets from a range of FLUXNET sites see Moffat *et al.* (2006).

II.3 Results and Discussion

For all eight scenarios e^* is free from any cross-correlation with T, but still shows a slight cross-correlation with S_0 highlighting some inadequacies in (II-1). This is not surprising given the strong autocorrelation of S_0 driving the simulation model in conjunction with the complexity of the simulation model(s) in comparison to (II-1). This does however highlight some scope for improvement.

Table II-1 shows the estimates of the mean and two standard deviation values of e^* derived from 10^5 random sub-sample draws for the eight scenarios. For the day-night data e^* is zero mean except for the tropical and artic biome 60 percent gap scenarios. For the day data e^* is also largely zero mean, whereas the model appears to miss-estimate the night fluxes slightly. This feature is only exposed when analysing the noise-free response and is probably due to a bias towards the larger daytime fluxes in the estimation given day and night fluxes are not

Table II-1: Summary of the model evaluation for the four synthetic data series and two artificial gap scenarios. The statistical properties (mean and twice the standard deviation) of the deterministic model error e^* are calculated from 10^5 randomly drawn sub-samples of e^* where a 10 percent sample is drawn each time. Estimates have been normalised to the mean F_N for the sample for comparison and are expressed as percentages. For the gap free scenario e^* is calculated for all N = 24x365 data, whereas for the 60 percent gap scenario e^* is only calculated for the missing data, i.e. N = 0.6 x 24 x 365.

Scenario	$\overline{e^*}$ ($2\sigma_{e^*}$) [%]		
	Day	**Night**	**Day-Night**
Temperate, coniferous forest (SPA), all data	-1.8 (1.8)	-6.4 (1.3)	0.3 (2.7)
Temperate, coniferous forest (SPA), 60% missing	1.9 (5.2)	-5.8 (2.6)	5.4 (7.8)
Temperate, decid. forest (BETHY), all data	-1.6 (2.4)	-4.4 (1.4)	-0.4 (3.4)
Temperate, decid. forest (BETHY), 60% missing	-4.7 (6.3)	-1.5 (3.5)	-5.7 (8.7)
Tropical, non-seasonal (Leuning et al. 1995), all data	-1.3 (2.2)	-3.1 (0.8)	-0.3 (3.5)
Tropical, non-seasonal (Leuning et al. 1995), 60% missing	5.4 (6.1)	-3.6 (0.7)	10.5 (9.6)
Arctic, low production (Leuning et al. 1995), all data	0.03 (5.6)	2.1 (3.3)	-0.6 (7.6)
Arctic, low production (Leuning et al. 1995), 60% missing	-17.6 (12.8)	9.1 (4.7)	-27.2 (17.4)

handled separately in the optimisation. Given the uncertainty in real EC flux observations this bias is not significant (Moffat *et al.* 2006) but again suggests room for improvement in the current model.

Figure II-3 shows the cumulative deterministic fluxes. It would be appealing at this stage to have an estimate for the propagation of parametric uncertainty through the integration. However, given just one realisation of the spline hypersurface took approximately 7 minutes, the computing effort had to be directed solely at the optimisation. A Monte Carlo simulation that adequately sampled the distributions of the 6x6x9 nodes in the hypersurface exceeded the capacity of the computing resource used in this study[5].

[5] The 3D interpolation was performed using INTERP3 in MATLB v6 running on a 3.8 GHz PC. In addition, the hypersurface has to be evaluated incrementally due to memory constraints (2 GB RAM).

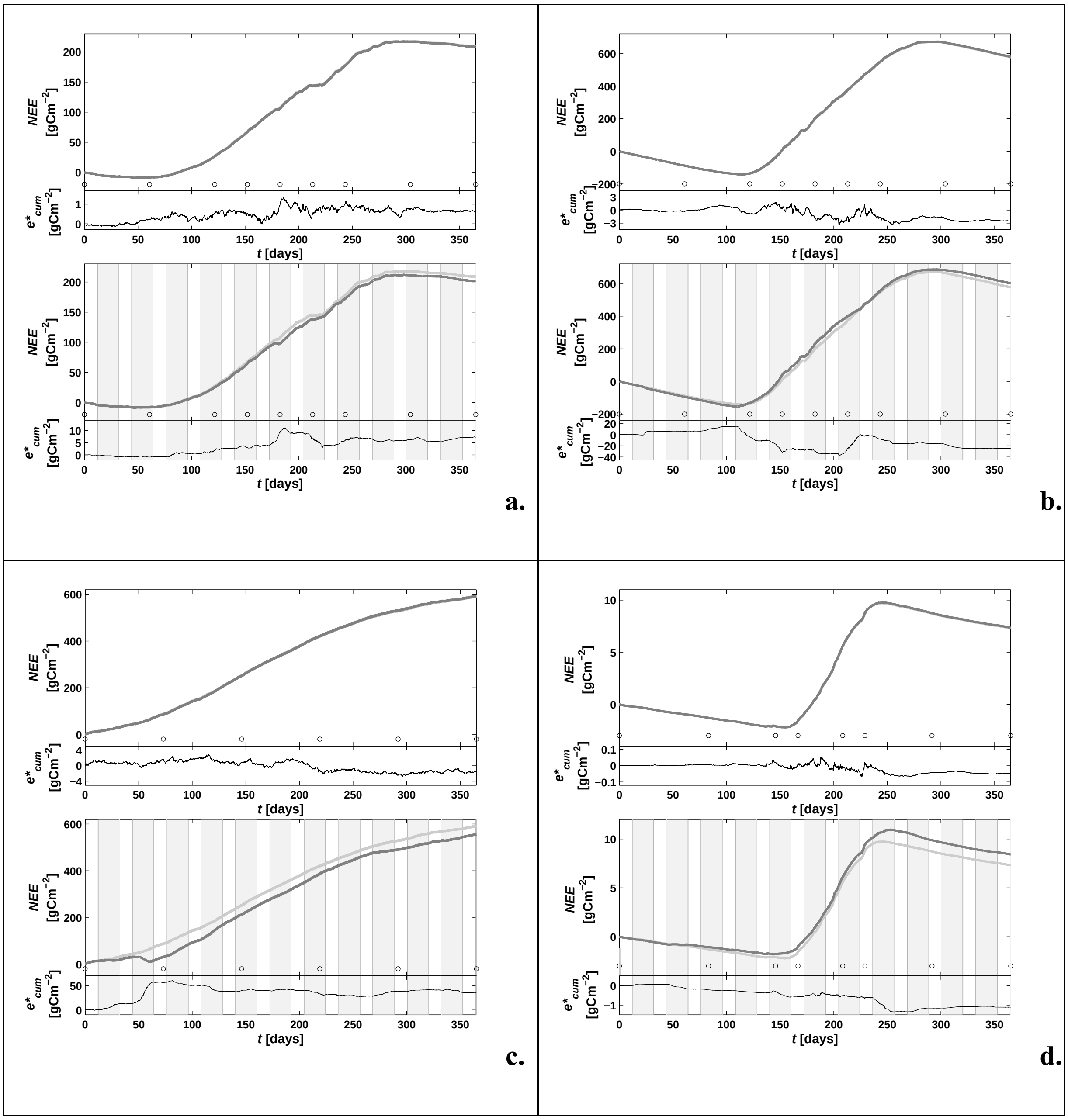

Figure II-3: Cumulative sum of the deterministic simulation data (light grey) and the output of (1). The circles underneath the graph denote the nodes in *t*. The upper panels show the results estimating (1) from the entire data series, the bottom panels show the results of the gap scenario (60% of the data missing, gaps indicated by light grey patches). Cumulative e^* is shown underneath each panel. **a.** Results for the temperate coniferous forest (SPA) **b.** Results for the temperate deciduous forest (BETHY) **c.** Results for the tropical biome (Leuning *et al.* 1995) **d.** Results for the arctic biome (Leuning *et al.* 1995).

As can be seen, not surprisingly the optimisation of model (II-1) based on all data results in no significant bias in the estimate of the cumulative flux on time scales from days to year end for all four synthetic data sets. In addition, the results in Figure II-3 show that it is not the amount of missing data that controls the performance of the scheme but instead, it is the coincidence of gaps with periods that contain important information for constraining the estimation correctly. For example, the response of $\hat{F}_N$ to (rare) low temperatures in the

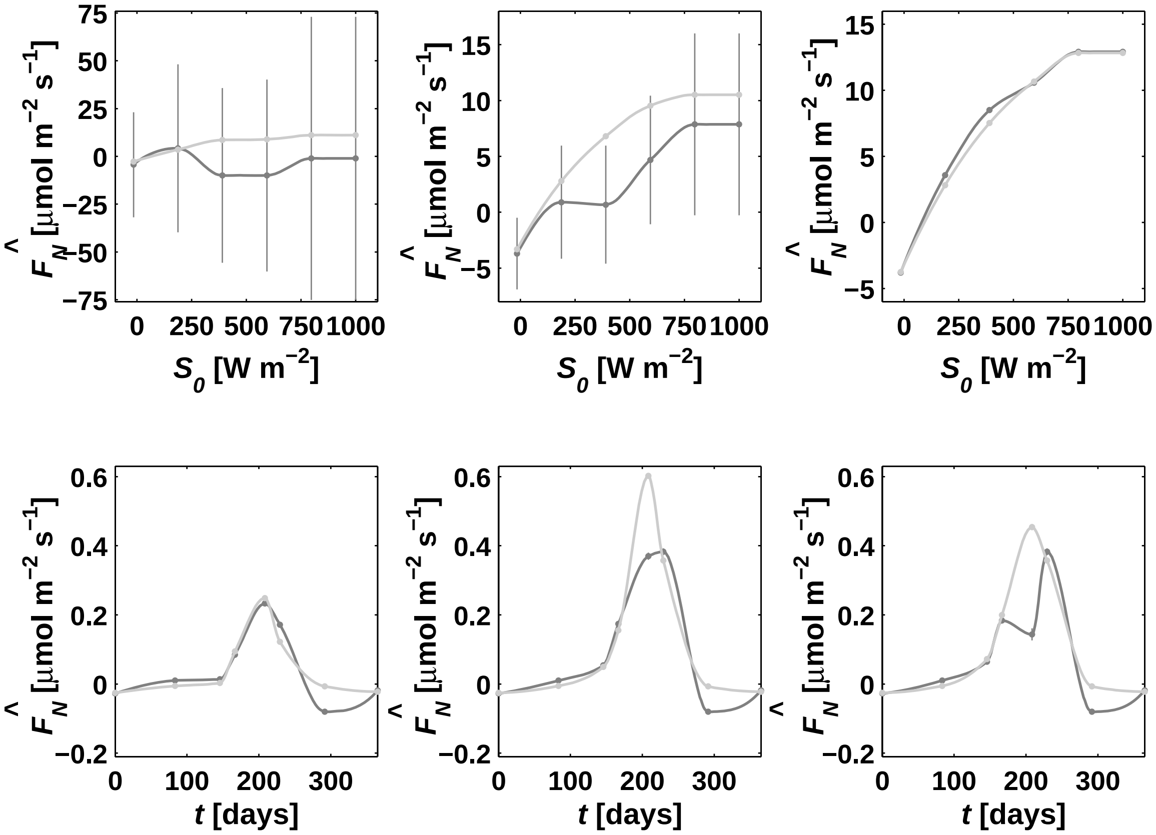

Figure II-4: Differences in the node values (and hence the interpolating polynomials) for the optimised model (1) using either all data (light grey) or the 60 percent gap scenario (dark grey). The upper series of panels show the estimated response to light at t = 73 days and T_S = 19.9, 21.4 and 22.9 °C. The bottom series of panels show the estimated response to time at T_S = 8.1 °C for S_0 = 322, 487 and 652 Wm^{-2}. The vertical lines denote the confidence intervals for the estimated parameters. Note that the actual interpolating polynomials will have a somewhat different shape depending on the nature of the covariation of S_0, T_S and t in this sector of the hypersurface.

tropical simulation shown in Figure II-3c has been completely removed by the second gap period resulting in an unconstrained and hence uncertain extrapolation in $f\{T\}$ (see Figure II-4 and cv Figure II-2c and II-3c).

Figure II-4 shows some example estimated responses of $\hat{F}_N$ to S_0 and t. As can be seen in the top panels, the significant parametric uncertainty for $f\{S_0\}$ decreases rapidly with increasing temperature and the shape of the estimated relationship converges on its gap-free counterpart. Similarly, much of the information on the timing of senescence during the short vegetation period in the artic simulation together with the response of $\hat{F}_N$ to a series of bright sunny days in late summer has been lost in gap period seven and eight (cv Figure II-2d and II-3d). As a result, the model picks up the temporal changes rather poorly, as well as the $f\{S_0\}$ being poorly defined for high S_0 during this period (Figure II-4, bottom panels). The low parametric uncertainty of these estimates probably reflects the fact that this is a (temporal) interpolation which gives rise to confident, but wrong node value estimates.

By way of contrast, the model performance for the two temperate biomes appears satisfactory despite 60 percent of the data being missing for the estimation (see Figure II-3a and b). This is a result of the seasonal distribution of S_0, T and phenology being more uniform (see Figure II-2a and b) and hence the probability of loosing information on these responses being less than in systems subject to more rapid changes. Therefore, when missing data cover periods of significant change in boundary conditions then clearly more reliance on additional information is required. Ideally this would be supplemented by also characterising $f\{S_0, T, t\}$ on data taken from adjacent years at the same site.

The reader will no doubt want to exercise their own judgment as which drivers to include when conditioning (II-1) to the observations. For example, we have not considered the effect of non-seasonal variations in water limitation (e.g. Hanson *et al.* 1993; Davidson *et al.* 1998; Reichstein *et al.* 2002) in the current analysis. It is important to appreciate however that in order to account for such effects, one would need a measure of that driver that related directly to the F_N observations (i.e. was applicable at the canopy scale). This need not be accurate measures but only need to reflect changes in the appropriate designated state given these measures will only be used to sort F_N into the relevant order for the spline estimation.

II.4 Conclusions

With gap-filling, we are generally in a 'data rich' situation compared to, for example, extrapolation to ungauged sites. As a result, gap-filling methodologies need to lean more toward the data, and use supplementary information to constrain the gap-filled predictions when data coverage in that area of the data space is sparse. Although there is no unique solution to this problem, we believe that estimating the semi-parametric relationships needed to reconcile simple model structures to the available data is a suitable hybrid methodology for achieving this compromise in many situations.

Clearly, the performance of the scheme used here will, in part, depend on the number and location of nodes. Although one important benefit of using splines is that the coefficients of the polynomials are determined non-locally (Press *et al.* 1988, 1992), nodes located in sparsely sampled areas of the data set/model space will be less constrained by the data whilst still being potentially important for determining the response. It is, therefore, reasonable to assume that the node density should reflect the local density of the available data and an automated procedure for this is currently being developed and evaluated by the authors.

It is important to underscore the advantages of using synthetic data sets to evaluate gap-filling procedures. To date, schemes have been exclusively evaluated on real data. However, the partitioning between the systematic and stochastic properties of real data is not known and as a result any evaluation is somewhat restricted by the significant uncertainties associated with EC flux data. In contrast, the components of synthetic data are known perfectly. This allows for a more comprehensive evaluation as one is in full control over the nature of the system giving rise to the observations, as well as which observations are missing. The same can be said for evaluating methods for partitioning fluxes between their photosynthetic and respiratory components or for exploring the expression of the aggregation of sub-canopy scale processes in canopy scale observations.

Finally, if we are going to faithfully synthesise missing EC data then it is essential that we realise both the systematic and the stochastic components when filling gaps. The analysis here has focused on an assessment only of the noise free response in order to see how successfully the systematic components could be captured by the proposed method. However, when integrating fluxes to give estimates of annual sums the uncertainty that results from noise needs to be computed if inferences on annual sums are to be drawn. This would require the characterisation of a noise model for EC data. Interestingly, adding an appropriate noise signal to gap-filled data series appears to have been notably absent from gap-filling strategies to date and the gap-filled data sets produced as a result must be characterised by highly truncated noise sequences.

Acknowledgements

VJ Stauch was supported by NERC project NER/M/S/2002 and later by a UFZ, Department of Applied Landscape Ecology research studentship. Data from Metolius were provided by the AmeriFlux web data archive and were supported by the U.S. Department of Energy Terrestrial Carbon Program (DOE grant # FG0300ER63014). Input and output data for BETHY were kindly provided by Jens Kattge and the CarboEurope Integrated Project. Finally, we are grateful for the valuable comments of two anonymous referees and the subject editor.

III. Estimation of Net Carbon Exchange Using Eddy Covariance CO_2 Flux Observations and a Stochastic Model

Vanessa J Stauch   Andrew J Jarvis   Karsten Schulz

An edited version of this manuscript is currently under review with the Journal of Geophysical Research – Atmospheres.

Abstract

In this paper we use a stochastic model to estimate annual Net Carbon Exchange (NCE) from eddy covariance data taken from various sites. The stochastic model is comprised of a signal and a noise component. The signal component is characterized using a semi-parametric model relating CO_2 flux to light, temperature and time fitted to the eddy covariance observations. The noise component is characterized from the resultant model residuals using empirical cumulative probability distribution. The estimates for NCE are then derived from multiple runs of the joint signal-noise model within a Monte Carlo framework. This model based approach to estimating NCE is evaluated using synthetic stochastic data and found to give a reasonable partitioning of the signal and noise in these data. Building on this, we derive estimates of NCE from observed annual eddy covariance data sets for various sites. The distributions of the annual NCE estimates appear relatively Gaussian despite the highly non-Gaussian nature of the stochastic model giving rise to the estimates. For the six sites analyzed the noise to signal ratio for the annual NCE estimates exceeded 11 percent only once highlighting the value of eddy covariance observations for this application.

III.1 Introduction

The land surface plays an important role in determining the fate of carbon in the global carbon cycle, but our understanding of the functioning of the terrestrial biosphere at this scale is subject to considerable uncertainty, especially with respect to the impacts of climate change (Janssens *et al.* 2003). One attempt to reduce this uncertainty is offered by the growing network of tower based observations of surface to atmosphere CO_2 exchange located in a broad spectrum of biomes (Baldocchi *et al.* 2001*b*). These eddy covariance measurements, in conjunction with carbon stock observations, are central to constraining the estimates for carbon sequestration by terrestrial ecosystems (Steffen *et al.* 1998; Papale & Valentini 2003). However, like all environmental time series data, eddy covariance net CO_2 flux observations are characterized by significant levels of noise which can impair its use. Therefore, knowing the makeup of the noise component within eddy covariance CO_2 flux observations is important not only for the use of these valuable data for model identification, calibration and evaluation (Medlyn *et al.* 2005; Hollinger & Richardson 2005) but, possibly more so, when integrating these flux data to derive the estimates of the daily, monthly and annual Net Carbon Exchange (NCE) used in carbon inventory studies. This is because such integrations necessarily involve the summation of both signal and noise, the latter having profound effects on the level of cumulative uncertainty attached to the final NCE estimate. Therefore, quantifying this uncertainty is important if inferences on NCE are to be made.

Noise in eddy covariance CO_2 flux observations has many sources (Mahrt 1998; Goulden *et al.* 1996*b*; Hollinger & Richardson 2005). Firstly, the observations are of a complex ensemble of sources and sinks within the canopy whose underlying properties are both heterogeneous and stochastic (Oren *et al.* 2006). Secondly, the turbulent exchange that connects the source-sink footprint region of a tower to the sensing platform on the tower is by definition stochastic. Thirdly, the ability of the sensing platform to measure this turbulent exchange is imperfect and subject to measurement error. Fourthly, the data pre-processing methodology that derives the flux estimates from the relevant measured variables is an imperfect approximation of the turbulent transfer it seeks to represent and hence is also subject to uncertainty. Any investigation into the effects of noise on the derivation of NCE estimates from eddy covariance data relies in part on the characterization of the aggregate noise.

There are several ways to approach noise characterization. Hollinger *et al.* (2004) and Hollinger & Richardson (2005) differenced parallel measurements made by adjacent towers at the same site in order to eliminate the systematic component from flux data, assuming this to be identical in the two time series they analyzed. However, recently Oren *et al.* (2006) have attributed half of the variability in high temporal (half-hourly) resolution EC data to spatial heterogeneity in a uniform pine forest. This suggests that a significant element of the systematic signal will be likely to be left in the difference of two adjacent tower measurement series. Hollinger & Richardson (2005) and Richardson *et al.* (2006) differenced successive draws of flux observations collected under similar conditions at the same tower at the same times of the day, again as an attempt to eliminate the systematic signal leaving the noise. However, to get a large enough pool of data in each similar condition bin required quite coarse grouping of data which inevitably involved inclusion of signal in the noise estimates whilst also limiting the number of random draws possible before significant repeat draws were encountered. For both of these purely data based methods the resulting noise series were found to be heteroskedastic with a variance being dependent on wind speed and the magnitude of the CO_2 flux itself, in line with the theoretical predictions of Lenschow *et al.* (1994), Mann & Lenschow (1994) and Finkelstein & Sims (2001). Based on these findings, Hollinger & Richardson (2005) and Richardson *et al.* (2006) approximated a parametric double exponential distribution for the noise probability density, although it was unclear from these studies to what extent the data were distributed in this way once the flux dependent variance had been accounted for.

Apart from the study by Hagen *et al.* (2006) who used binned model residuals as a pool from which they derived the uncertainties associated with their gap-filled estimates, it appears that model-based noise characterization has been somewhat overlooked. The reason for this is that the results are likely to be model dependent and hence biased by the choice of the model (Richardson & Hollinger 2005). However, such an approach has been used in related areas such as hydrology (e.g., Sorooshian & Dracup 1980) and climatology (e.g., Grieser & Schönwiese 2001). If found to be robust, this approach could offer certain advantages. Firstly, it is not limited to sites where replicate tower observations have been made. Secondly, it does not rely on coarse grouping of observations with particular sets of boundary conditions but instead yields an estimate of the error for each observation. Thirdly, it is also important to appreciate that, at some stage in the derivation of NCE estimates from eddy covariance observations, use has to be made of some kind of model to fill the inevitable missing data gaps. Given this requirement, it appears sensible to postulate the need for sympathy between supplementing these missing data using a model in the derivation of the NCE estimates and their uncertainties i.e. NCE estimation is necessarily a model-data fusion exercise (Williams *et al.* 2005; Gove & Hollinger 2006).

In what follows we fit a semi-parametric model to eddy covariance data to approximate the deterministic signal component. We then use the resultant model residuals to characterize the noise and hence derive a stochastic CO_2 flux model for the data set. To evaluate this approach we make use of a suitable synthetic data set (Stauch & Jarvis 2006) where the signal and noise characteristics are fully known beforehand. Having evaluated this method we then apply it to six real data sets covering various different biomes and climate regimes in order to give NCE estimates with uncertainty for these systems.

III.2 Methods

Half hourly eddy covariance observations of net CO_2 flux, $y(t)$, are comprised of a signal, $x(t)$, and some noise, $n(t)$, i.e. $y(t) = x(t) + n(t)$. The aim is to first obtain an estimate of $n(t)$ using the observations $y(t)$ and a model for $x(t)$ and then characterize $n(t)$ in the form of a suitable stochastic model. This allows us to produce multiple realizations of these two models in order to derive an ensemble estimate of annual NCE where the i'th annual estimate is given by

$$NCE(i) = \sum_{t=1}^{N} \left\{ \hat{x}(t,i) + \hat{n}(t,i) \right\}. \qquad \text{(III-1)}$$

Signal characterisation

The model we apply for the signal $x(t)$ is a three-dimensional spline model used to describe the relationships between $x(t)$ and light, I, temperature, T, and time, t (Stauch & Jarvis 2006). All that is assumed about these relationships is that they are relatively smooth. The forms of these relationships are described by semi-parametric Hermite splines whose shape in relation to I, T and t is conditioned through optimizing the model output $\hat{x}(t)$ against the observations $y(t)$ through adjusting the spline node values within a four dimensional hypersurface. This optimization involves minimizing the model prediction error $e(t) = y(t) - \hat{x}(t)$ using weighted least squares in order to account for any potential heteroskedacity of $n(t)$ (Hollinger *et al.* 2004; Hollinger & Richardson 2005; Medlyn *et al.* 2005; Richardson *et al.* 2006). Here, we apply an iterative optimization procedure that converges on weights which are the estimated flux dependent variance of the residuals. Providing $\hat{x}(t) \approx x(t)$ then $e(t) \approx n(t)$ and the characterization of the model for $n(t)$ can be based on $e(t)$ post optimization. This approach will be tested using the synthetic data where $n(t)$ is known.

The dependency of $y(t)$ on I, T and t is simply obtained by sorting $y(t)$ with respect to the magnitude of these three factors. Therefore, it is only the sorted indexing of *I*, *T* and *t* that is being used when fitting the spline hypersurface to $y(t)$ (Young 2000; Jarvis *et al*, 2004; Stauch & Jarvis 2006). As a result, the spline hypersurface is analogous to a lookup table linking $y(t)$ to individual values of *I*, *T* and *t* (Stauch & Jarvis 2006). As a result, this approach has parallels with the data-based differencing approach to this application advocated by Hollinger & Richardson (2005) and Richardson *et al.* (2006). However, because the spline hypersurface is continuous, there is no course grouping of 'like' data into discrete bins, thereby avoiding the sampling issues this causes, but at the cost of having to employ a model.

Noise characterisation

In order to simulate $n(t)$ and hence estimate the uncertainty in NCE we need to generalize its characteristics in the form of an appropriate stochastic model. Given the observations of Hollinger & Richardson (2005) that the probability density of $n(t)$ is likely to be non-stationary, this stochastic model needs to account for this type of behaviour. To do this in as an objective a fashion as possible we have elected to use a nonparametric statistical model (as opposed to a parametric statistical model) in order to avoid model structure biases.

Because Hollinger & Richardson (2004) identified the dominance of the effects of $x(t)$ on the variance of $n(t)$ our analysis will focus on this effect, although this assumption is not a restriction of the methodology and needs to be evaluated for each annual data set. Having derived the optimal estimates for $e(t)$ and assuming $e(t) \approx n(t)$, $e(t)$ is sorted with respect to the magnitude of $\hat{x}(t)$. Then discrete local estimates of the non-parametric cumulative probability of $e(\hat{x}(t))$ in the neighbourhood of differing levels of $\hat{x}(t)$ are derived using the numerical method of Weibull (1939) and Kaplan & Meier (1958). For the synthetic data, a square data window of the width of 0.6 µmol $m^{-2}\,s^{-1}$ within $\hat{x}(t)$ was used to sub-sample $e(\hat{x}(t))$. The step size for this moving window was 0.06 µmol $m^{-2}\,s^{-1}$ since this was found to give robust estimates of the local cumulative probability distribution, although this should be evaluated for individual data sets especially in relation to the distribution of missing data. An approximation of the equivalent continuous cumulative probability is obtained by linear interpolation of the local discrete cumulative probability. Having estimated the local continuous cumulative probability distributions we are then able to draw our stochastic estimate of $\hat{n}(\hat{x}(t))$ from this distribution. An illustration of this stochastic model is shown in Figure III-1 for an example window of $-0.75 < \hat{x} < -0.15$.

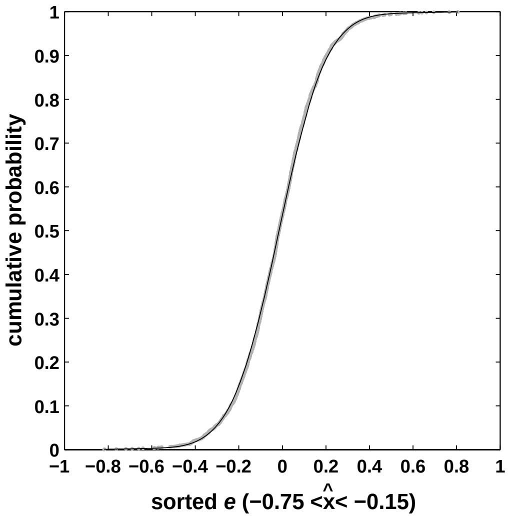

Figure III-1: An example cumulative probability distribution for the model error $e(t)$ in the range of $\hat{x}(t)$ of -0.75 to -0.15 (grey dots). The solid line is the linearly interpolated continuous spline which is used for further random draws from this distribution.

NCE estimates

Having characterized $x(t)$ and $n(t)$ we are now in a position to produce annual time series which can be integrated to give daily, monthly or annual NCE estimates with their associated uncertainties using (III-1). Obviously one annual realization of $x(t)$ and $n(t)$ will only result in one estimate of NCE. Therefore we need multiple realizations of $x(t)$ and $n(t)$ within say, a Monte Carlo (MC) framework, in order to construct the distribution for the NCE estimates. This MC simulation needs to account for both the stochastic model for $n(t)$ derived from the noise characterization and also the uncertainty associated with the optimized node values in the model for $x(t)$ as reflected in the node value parameter covariance matrix derived from the weighted nonlinear least-squares optimization.

For each MC run, $\hat{x}(t)$ is predicted using $I(t)$, $T(t)$ and t and the associated parameter covariance matrix for the spline node values. $\hat{x}(t)$ is then used to determine which cumulative probability distribution to use when drawing values for $n(t)$. The i'th estimate of annual NCE using half hourly sampled data is then given by (III-1).

Note the observations $y(t)$ are only used to condition the models for $x(t)$ and $n(t)$ and play no further role in the estimation of NCE after this. This is because we need multiple realizations as opposed to the single realization offered by $y(t)$. In this study we used 10^3 MC realizations because it was found that beyond this further MC realizations did not have a significant impact on the final distribution of the annual NCE estimates.

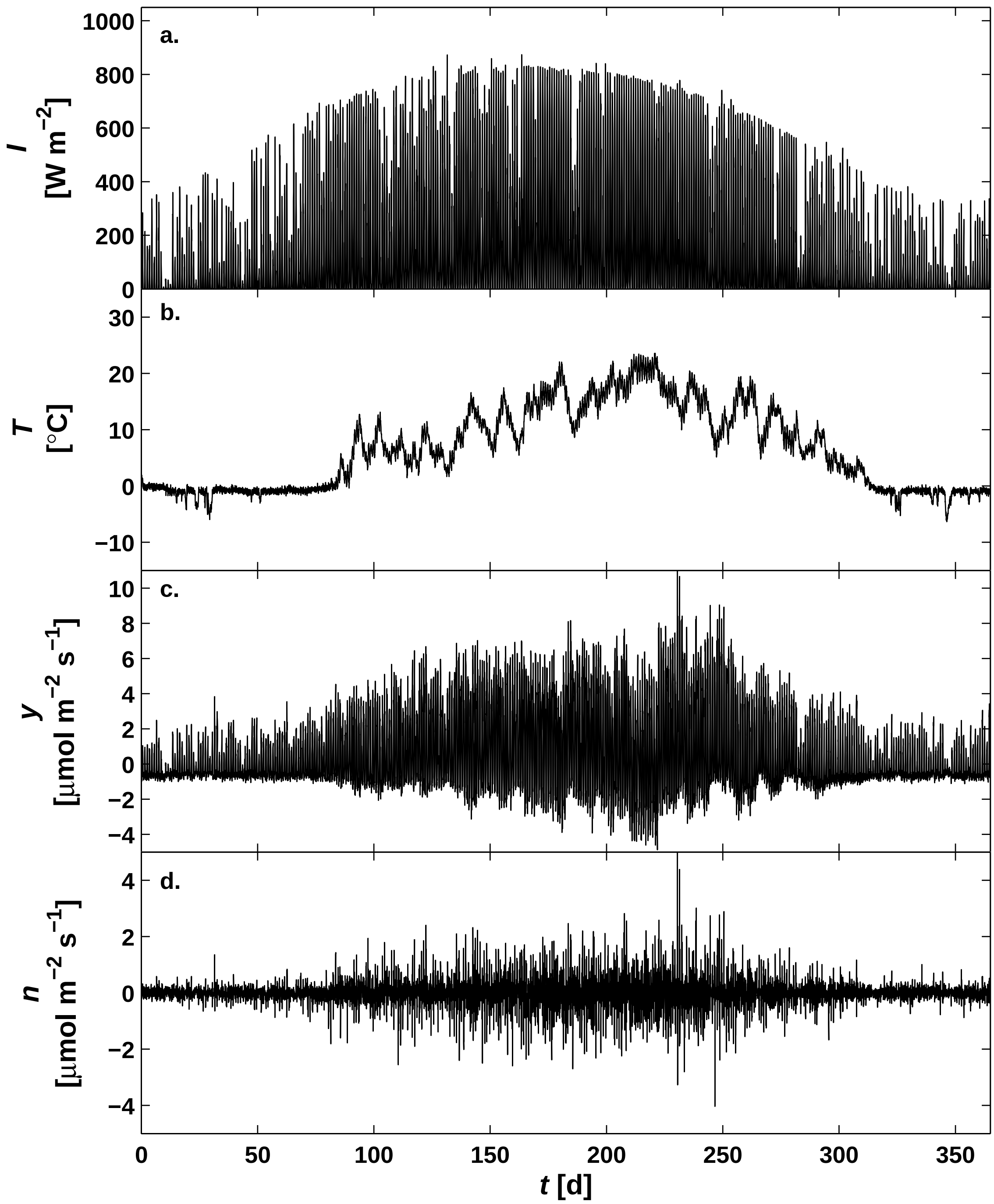

Figure III-2: The synthetic data used in the evaluation exercise. The relevant SPA model inputs are incident radiation, I (**a**.) and surface temperature, T (**b.**) and output net CO2 flux output y(t) is shown in **c.**. The simulated measurement error series $n(t)$ is shown in **d.** Positive fluxes for I and $y(t)$ denote mass or energy transfer from the atmosphere to the canopy.

Evaluation using synthetic and real data

Our synthetic evaluation data set is generated by the soil-plant-atmosphere (SPA) model (Williams *et al.* 1996) calibrated for the Metolius FLUXNET site in Oregon (Ponderosa pine) for the year 2000 (Law *et al.* 2001; Anthoni *et al.* 2002; see also Williams *et al*. 2001 for a test of SPA against ponderosa pine EC data). Following the analysis of Richardson *et al.* (2006), we elect to simulate $n(t)$ as a normally distributed random variable with a variance of $0.2x(t)$ and $0.05u(t)$ where $u(t)$ is wind speed. Similarly, a white noise series with a constant variance of two and five percent of the annual mean of $I(t)$ and $T(t)$ are added to these two input series to simulate measurement error. The input and output data used for the optimization of the model for $x(t)$ are shown in Figure III-2. For reference, Stauch & Jarvis (2006) have demonstrated the performance of this three dimensional spline model for several sample synthetic data sets. In that analysis they focused on an evaluation of $\hat{x}(t)$. Here, the evaluation will focus on the success of the noise characterization, which is in effect the other side of the same coin.

Clearly, the aim of the methodology is to estimate NCE from real flux data. Therefore we have chosen six different sites, i.e. four forests, a grassland and a crop site, to demonstrate the application on (see Table III-1 for a summary). The Hainich site in Germany (Knohl *et al.* 2003; Anthoni *et al.* 2004) is a deciduous forest with beech as the dominant species in a temperate continental climate with a mean annual air temperature of 6.8 °C and an average annual precipitation of 775 mm. The Hesse site in France (Granier *et al.* 2000) is a young beech forest in a temperate oceanic climate with a mean annual air temperature of 9.9 °C and an average annual precipitation of 975 mm. The Puechabon site in France (Rambal *et al.* 2003) is an evergreen oak forest in a Mediterranean climate with a mean annual air temperature of 13.5 °C and an average annual precipitation of 872 mm. The Yatir site in Israel (Grünzweig *et al.* 2003) is a pine forest in a semi arid climate with a mean annual air temperature of 18.2 °C and an average annual precipitation of 280 mm. The Shidler site in Oklahoma, USA (Suyker & Verma 2001; Suyker *et al.* 2003) is a (C4) grassland prairie in a temperate continental climate with a mean annual air temperature of 15.4 °C and an average annual precipitation of 835 mm. Finally, the Bondville site in Illinois, USA (Meyers & Hollinger 2004; Hollinger *et al.* 2005) is a crop land with maize and soybean in rotation in a temperate continental climate with a mean annual air temperature of 11.2 °C and an average annual precipitation of 990 mm. The selected year 1997 is under maize.

Table III-1: Fluxnet sites used in this analysis with their site specific vegetation cover and climate conditions.

Site (year)	Vegetation cover	Climate	References
Hainich, Germany (2001)	beech forest	temperate, continental	Anthoni et al. (2004); Knohl et al. (2003)
Hesse, France (2001)	young beech forest	temperate, oceanic	Granier et al. (2000)
Puechabon, France (2002)	oak forest	Mediterranean	Rambal et al. (2003)
Yatir Forest, Israel (2002)	pine forest	semi arid	Grunzweig et al. (2003)
Shidler, Oklahoma (1999)	grassland prairie	temperate, continental	Suyker & Verma (2001); Suyker et al. (2003)
Bondville, Illinois (1999)	agriculture (corn)	temperate, continental	Meyers & Hollinger (2004); Hollinger et al. (2005)

III.3 Results and Discussion

Optimizing the spline model $\hat{x}(t)$ against the synthetic SPA output $y(t)$ captures 98 percent of the variance in the SPA signal $x(t)$ (see also Stauch & Jarvis 2006). A comparison of the properties of the model residual series $e(t)$ with the synthetic noise $n(t)$ is given in Figures III-3 and III-4. The grouped probability distribution for $e(t)$ and $n(t)$ are shown in Figure III-3a. Note how the non-stationary variance for the underlying Gaussian distribution results in the elevated tails for the grouped distribution and hence the appearance of a double exponential type distribution (Hollinger & Richardson 2005). Figure III-3b shows how accounting for the flux dependency of the variance transposes back to quasi-Gaussian distributions whose properties vary as a function of $\hat{x}(t)$ as expected. Figure III-4 reveals $e(t)$ and $n(t)$ have similar properties in terms of mean and standard deviation for any given level of $\hat{x}(t)$ other than for values of $\hat{x}(t)$ close to zero (see also Figure III-3b). This reflects a small bias in $\hat{x}(t)$ resulting from an inadequate description of diurnal non-stationarity in the light response characteristics of SPA indicating the need for some increased flexibility in the spline model for $\hat{x}(t)$. It must be stressed however that this effect is small and has little impact on the final NCE estimates (see below).

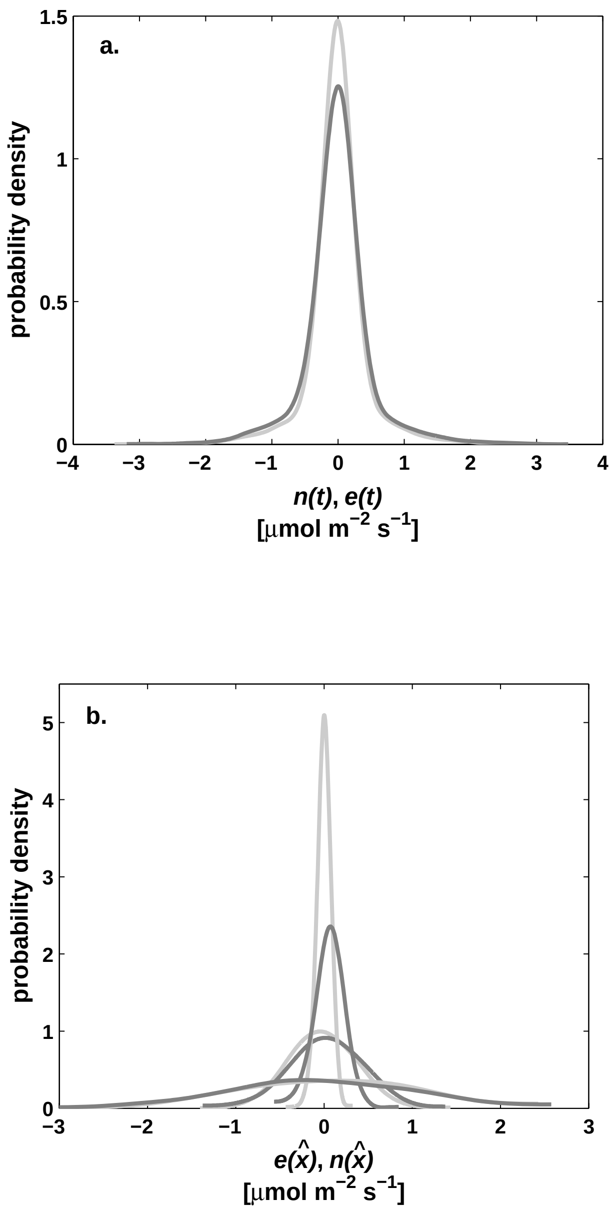

Figure III-3: a. The en bloc probability distributions for $n(t)$ (light grey) and the model error proxy $e(t)$ (dark grey). **b.** The probability distributions for $n(t)$ (light grey) and the model error proxy $e(t)$ (dark grey) for three different ranges of $\hat{x}(t)$, [-2.3 -1.7], [-0.3 0.3] and [4.9 5.5] μmol m^{-2} s^{-1}.

From Figures III-3 and III-4 we see that the variance of $e(t)$ slightly overestimates the variance of $n(t)$ over a range of values for $\hat{x}(t)$. This is not surprising given the modelled uncertainties reflect a complex combination of the effects of the input noise processed through the spline model, the parametric uncertainty inherent in $\hat{x}(t)$ as well as any structural error in the spline model. Also, the small effects of wind speed on $n(t)$ is not accounted for in the current noise characterization. However, the relatively close correspondence between the stochastic properties $e(t)$ and $n(t)$ in Figures III-3 and III-4 suggest that the characterization of

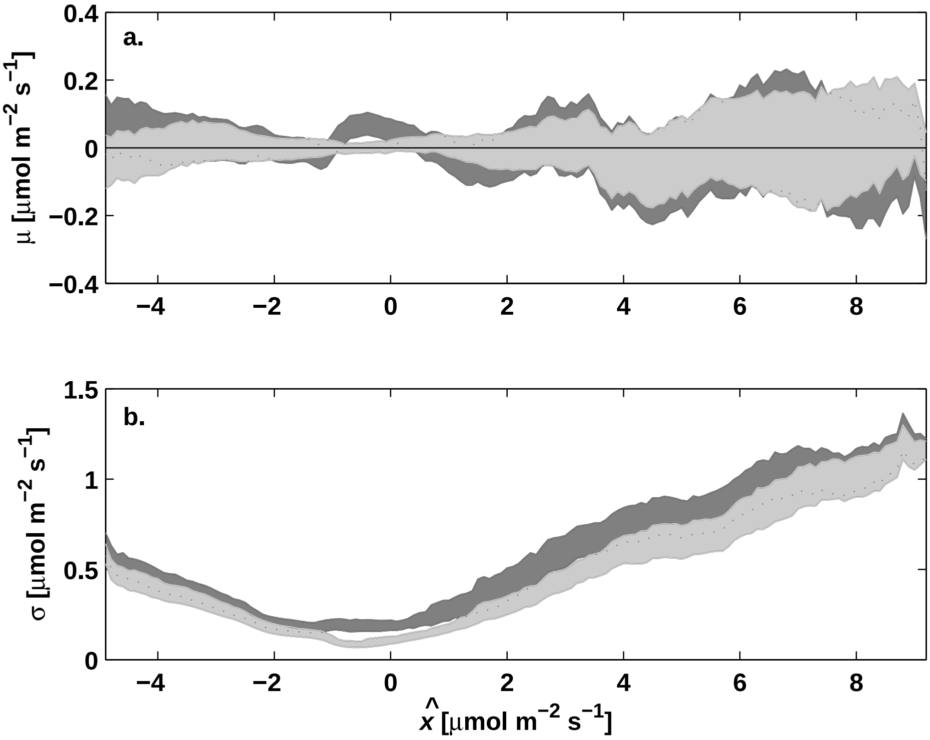

Figure III-4: Mean (**a.**) and standard deviation (**b.**) of $n(t)$ (light grey) and $e(t)$ (dark grey) as a function of $\hat{x}(t)$ for the synthetic SPA evaluation. Shown are the 95 percent confidence bounds derived from sub-sampling data with replacement (bootstrapping). A window width of 0.6 μmol m^{-2} s^{-1} was used here, moved at increments of 0.06 μmol m^{-2} s^{-1} in $\hat{x}$ (t) (see Methods).

$n(t)$ based on $e(t)$ is valid providing it is acknowledged that this is likely to yield a slight overestimate of the uncertainty in the associated NCE estimates. This is shown in Figure III-5 which compares the 95 percentile NCE envelopes for the true and estimated cases. Note how the estimated envelope embraces the true envelope highlighting the lack of significant bias despite the slight overestimation of $\hat{x}(t)$ for fluxes in and around zero. Note also how the NCE envelope grows slightly faster in the estimated case because of the slight overestimation of noise variance as discussed above. The small inset figure in Figure III-5 compares the year end NCE distributions again mirroring the various effects of the model based noise characterization discussed above. The range of accumulated carbon over the year is estimated to be 201.7 – 211.8 gC m^{-2} compared to the simulated range of 205.6 – 212.8 gC m^{-2}.

Figure III-6 shows the characterization of $n(t)$ from $e(t)$ for our six selected measurement sites. The mean is mostly insignificantly different to zero at all sites. Significant deviations from zero are found for low and high positive levels of $\hat{x}$ (cv Figure III-6 b, e, f) indicating that the pattern of model bias is not systematic across sites. The variance increases with the

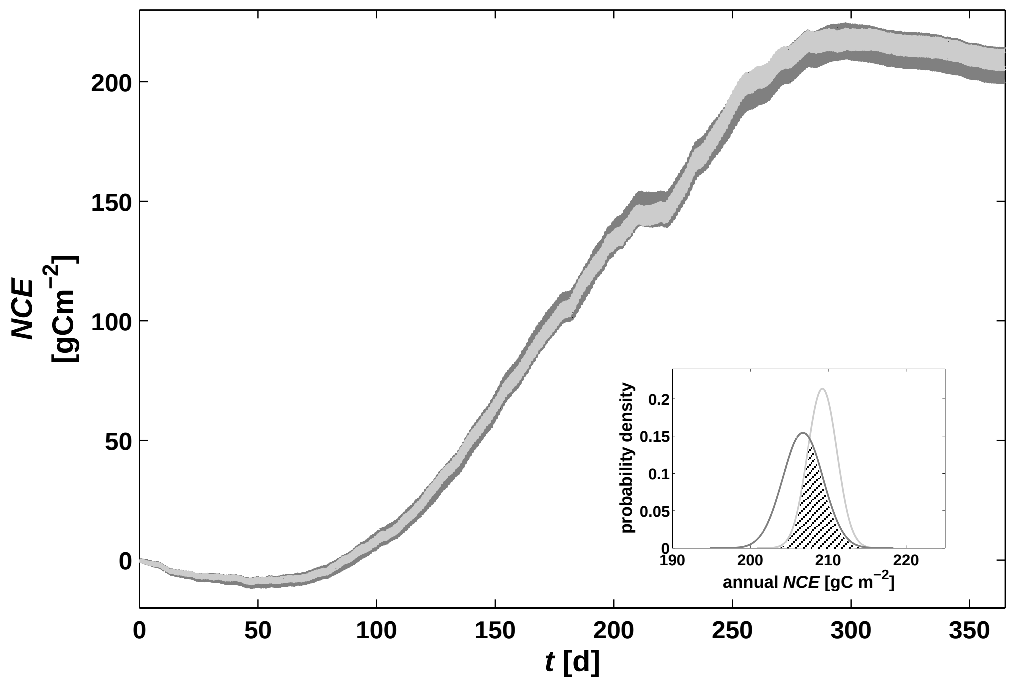

Figure III-5: Cumulative *NCE* with 95 percent confidence bounds for the synthetic SPA data (dark grey) and the stochastic model estimate of this (light grey). The inset panel shows the year end distributions for these two.

magnitude of $\hat{x}$ for all sites as expected[6]. As an aside, one would expect a higher relative uncertainty associated with nighttime eddy covariance observations due to low turbulence conditions (Richardson *et al.* 2006) or spatial heterogeneity (Oren *et al.* 2006), but this does not appear to be born out in the noise characteristics shown in Figure III-6.

The propagation of the estimated uncertainty into the NCE estimates and the year end NCE distribution for each site are shown in Figure III-7 and their 95 percent confidence intervals are given in Table III-2. Not surprisingly, the width of the confidence intervals is different for each site highlighting the site-specific nature of the noise pattern not least due to the differing distribution and magnitude of $x(t)$ across the year. Also shown in Figure III-7 is the single realization summation of a gap-filled observation series at each site for reference.

[6] It is interesting to note that the differences in the variances of $e(t)$ at different sites might give a valuable insight into the influence of site specific characteristics such as surface roughness, wind patterns, topography and spatial heterogeneity on flux uncertainties.

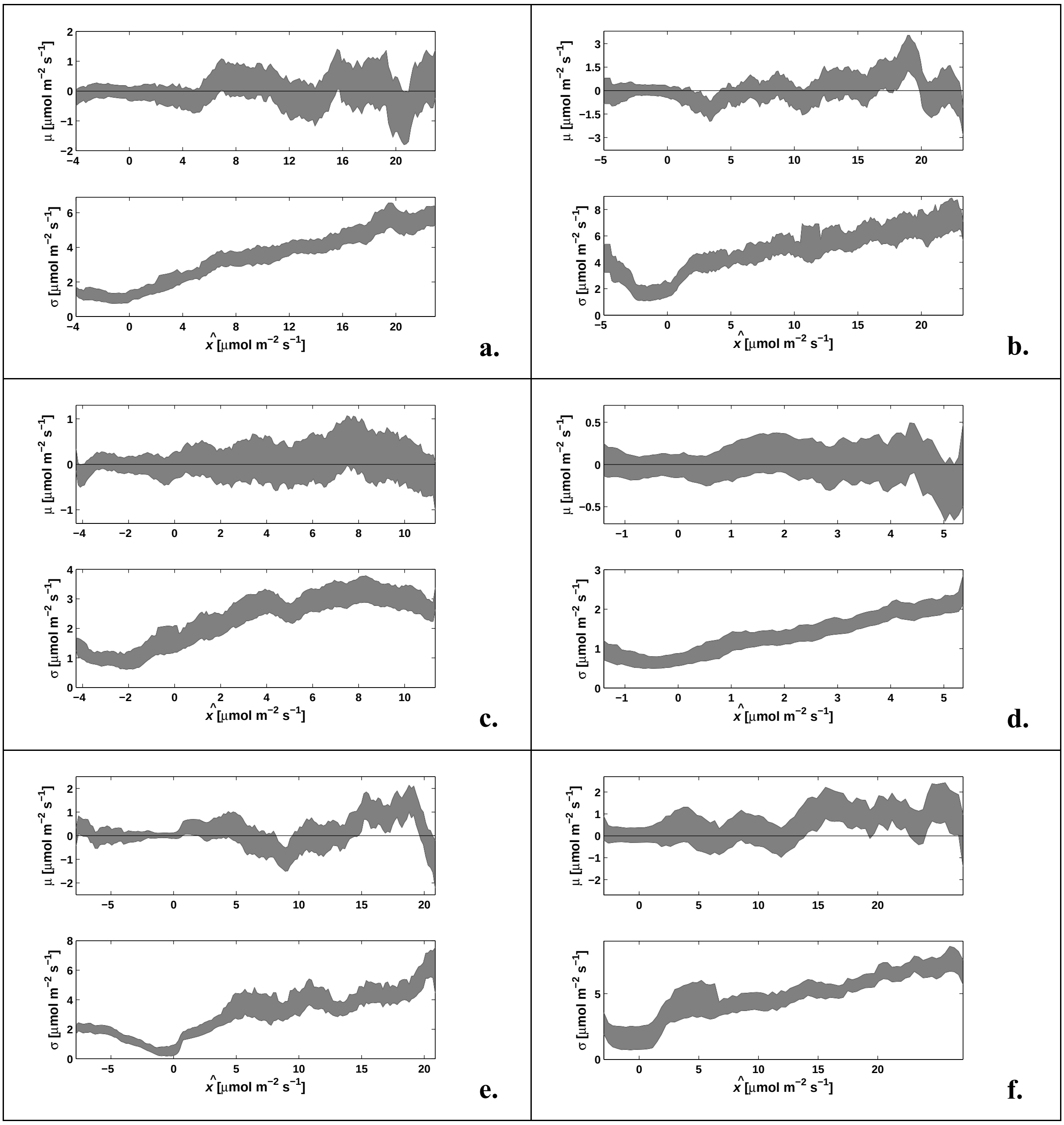

Figure III-6: Same as Figure III-4 for the selected real data examples. **a.** Hainich, Germany; **b.** Hesse, France; **c.** Puechabon, France; **d.** Yatir Forest, Israel; **e.** Shidler, OK; **f.** Bondville, IL.

Table III-2 additionally lists NCE values published by the principle investigators at each site. Not surprisingly, most NCE estimates lie within the ranges calculated in this study provided the estimates are based on EC data from the same year. Note that, unlike the other estimates the NCE estimates for the Puechabon site are based on measurements of the radial growth increments and allometric relationships (Rambal, personal comm.).

Table III-2: Estimated annual NCE range expressed as the 95 percent confidence intervals compared to previously published NCE estimates at these sites. The relative uncertainty is given by the ratio of the cumulative noise to signal at year end.

Site (year)	Published annual NCE [gC m^{-2}]	Estimated annual NCE [gC m^{-2}]	Rel. uncertainty [%]
Hainich, Germany (2001)	490 (2001) [Knohl et al 2003]	[506 535]	5.6
Hesse, France (2001)	68 (1998); 296 (1999) [Granier et al. 2002]	[543 592]	8.6
Puechabon, France (2002)	280 (2000-2002) [Rambal, unpublished data]	[327 353]	7.8
Yatir Forest, Israel (2002)	130-240 (10/2000-09/2001) [Grünzweig et al. 2003]	[160 178]	11.0
Shidler, Oklahoma (1999)	124 (04/1999-03/2000) [Suyker et al. 2003]	[117 142]	19.3
Bondville, Illinois (1997)	532 (1997) [Hollinger et al. 2005]	[502 544]	8.0

Clearly, the range of the uncertainty at the end of the flux summation period will heavily depend on the length of time the summation is performed over, but for the annual NCE estimates considered here it is interesting to see that, using the data as given, these estimates are relatively well defined highlighting the value of eddy covariance data for this application. This is especially true if we consider that the estimated distributions for NCE we have derived are likely to be more uncertain than in reality given the effects of parametric uncertainty and model input uncertainty associated with the observations of I and T. The maximum noise to signal ratio for the annual forest NCE estimates was just 11.0 percent for the Yatir site and 19.3 percent for the grassland site (see Table III-2).

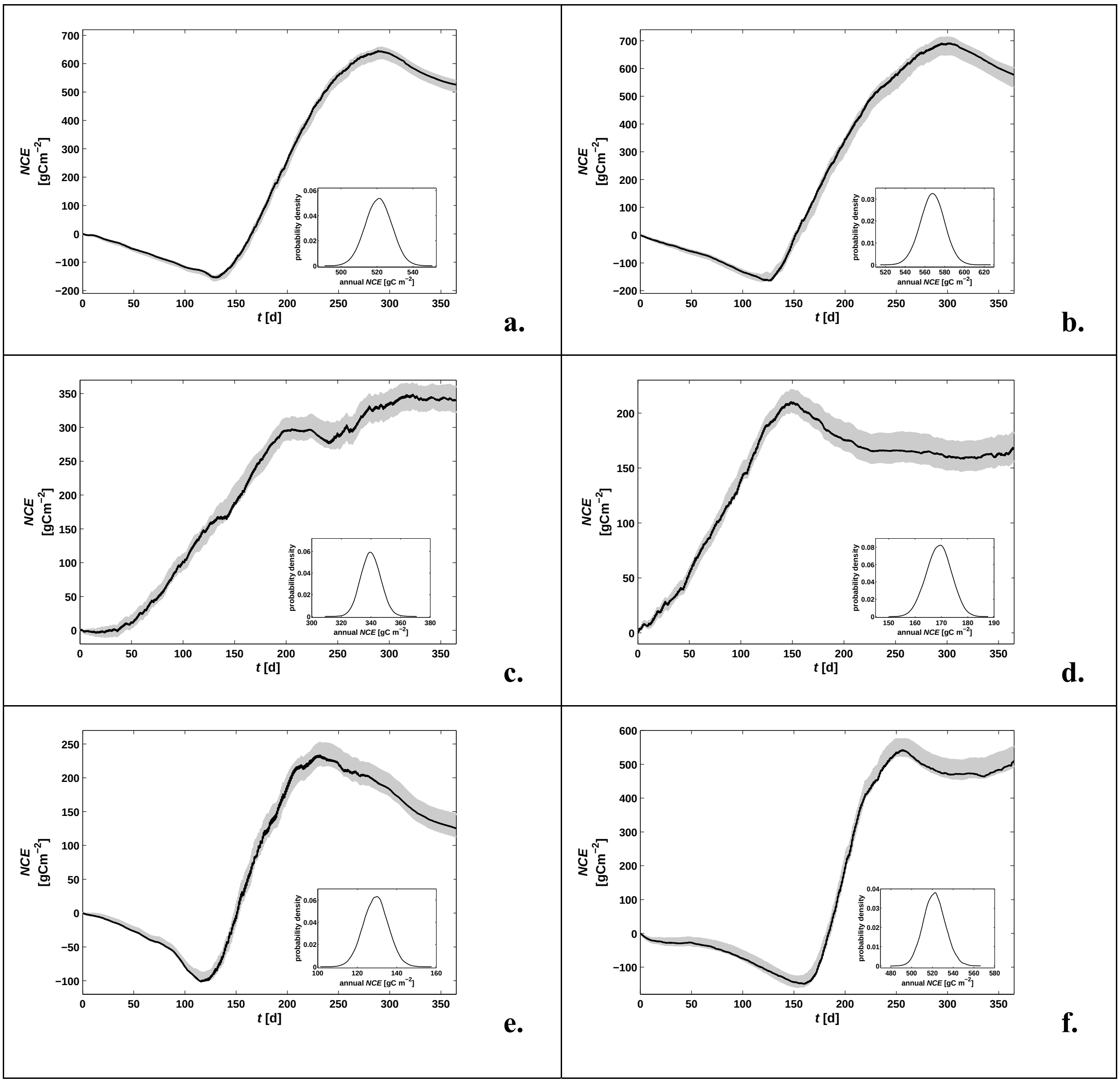

Figure III-7: Same as Figure III-5 for the selected real data examples. a. Hainich, Germany; b. Hesse, France; c. Puechabon, France; d. Yatir Forest, Israel; e. Shidler, OK; f. Bondville, IL. The solid black line in each case is constructed using a combination of the available data where possible in addition to one realization of the stochastic model for the gap-filling where required.

III.4 Conclusions

Eddy covariance flux time series contain a significant stochastic component which we have referred to as noise. Therefore, even in the absence of missing data, an observed annual flux data set reflects just one realization of the underlying stochastic process leading to just one estimate of annual NCE with no information on the uncertainty of this estimate. However, this data set can be used to characterize the signal and noise components giving rise to these observations, leading to the generation of the multiple realizations required to construct the distribution of annual NCE estimates needed to draw inference for carbon inventory studies.

In this study we have used a data led modelling approach to do this characterization and subsequent estimation in an attempt to minimize model structure biases. However, we have seen that because of model error and input uncertainties it is impossible to exactly recreate the noise component in the observations given the input uncertainties will always be processed through the core model in a complex way. The only alternative would be to attempt to minimize input uncertainties in some way (e.g., Kavetski *et al.* 2002). However, for the synthetic case we considered here it appears these distortions are not sufficient to abandon this methodology. Indeed, we would argue that, because of the need to assume a model to supplement missing data in the first place, a stochastic model based approach such as this is a logical step when extracting NCE estimates from eddy covariance flux observations.

Finally, the value of the evaluation based on synthetic data is again born out here (Stauch & Jarvis 2006) and we would argue that such evaluations should become commonplace in order to demonstrate the efficacy of model-data fusion exercises in this area.

Acknowledgements

VJ Stauch was supported by a UFZ – Department of Computational Landscape Ecology research studentship. Data from Metolius were provided by the AmeriFlux web data archive and were supported by the by the U.S. Department of Energy Terrestrial Carbon Program (DOE grant # FG0300ER63014). The measurements made at the Shidler AmeriFlux site were part of a project supported by the Office of Science, Biological and Environmental Research Program (BER), U.S. Department of Energy, through the Great Plains Regional Center of the National Institute for Global Environmental Change (NIGEC) under Cooperative Agreement No. DE-FC03-90ER61010. Data from the Bondville site were kindly provided by Tilden Meyers. Data from the Puéchabon site were supported by the DREAM CEFE-CNRS and were kindly provided by Jean-Marc Ourcival and Serge Rambal. We thank Werner Kutsch and Corinna Rebmann for providing the data from the Hainich site, Bernard Longdoz and André Garnier for providing the data from the Hesse site and Dan Yakir and Eyal Rotenberg for providing the data from the Yatir site.

IV. Objective Disaggregation of Eddy Covariance Observations to Infer Annual Carbon Uptake and Release

IV.1 Introduction

Understanding the fate of carbon in the terrestrial biosphere is important when speculating on regional carbon inventories within say the context of the Kyoto protocol (Steffen *et al.* 1998). Regional estimates of the net carbon balance in terrestrial ecosystems can help when identifying the potential carbon sink strength and its role in compensating for anthropogenic carbon emissions. At present, carbon accounting methods are based on national carbon stock estimates along with remote sensing information on changes in vegetation cover and land use (Steffen *et al.* 1998). The resulting estimates are prone to considerable uncertainty and an independent standard evaluation method is required, in particular when the objective is to establish a reliable carbon trading system (Schulze *et al.* 2002). The eddy covariance (EC) technique delivers (near) continuous observations of the net carbon exchange between the atmosphere and the land surface at the canopy scale. Given the global distribution of EC measurement sites organised under the umbrella FLUXNET, these data can contribute substantially when evaluating satellite-based estimates for the terrestrial net carbon exchange, hence reducing the uncertainties therein (e.g., Hutley et al. 2005; Friend *et al.* 2006). In addition, these multi-year time series provide a valuable data source to enhance the understanding of the underlying dominant physical processes at the canopy level. This aids the development of more faithful means for extrapolating to ungauged sites and/or changes in conditions at gauged sites.

The net carbon balance is composed by carbon uptake via photosynthesis and carbon release due to plant and soil respiration[7]. Each component responds differently to variations in environmental drivers. Prediction relies on characterising these dependencies. Although satellite data provide information on photosynthetic activity (e.g., Running *et al.* 1999), global estimates for the respiratory activity have to rely either on the extrapolation of local soil carbon inventories and/or on predictions from carbon exchange models (Steffen *et al.* 1998). The advent of the EC method has provided a direct measure of the net CO_2 flux above canopies, F_N. Therefore, provided a suitable disaggregation methodology is available, these data can help to derive scale consistent estimates for canopy carbon assimilation, F_G and ecosystem respiration, F_R.

Apart from some studies that used additional field observations (e.g., Baldocchi *et al.* 1987; Williams *et al.* 1997), most studies have derived partitioned estimates of the two components within EC CO_2 flux data by making use of models. Most commonly, a temperature dependent respiration model is fitted to nighttime EC data to extract F_R (e.g., Goulden *et al.* 1996*a*; Falge *et al.* 2002; Morgenstern *et al.* 2004). Other studies have applied nonlinear regression of different functional forms for the light response of F_N (e.g., Ruimy *et al.* 1995; Gilmanov *et al.* 2003). Some applications address the change of these relationships over the season by temporally binning the data (e.g., Falge *et al.* 2002) or by explicitly estimating the temporal evolution of selected fitting parameters (Yi *et al.* 2004; Reichstein *et al.* 2005). Recently, Hagen *et al.* (2006) pointed to the importance of explicitly addressing observation noise and parametric uncertainty when inferring flux components from EC data.

Interestingly, a comprehensive evaluation of the success of these partitioning methods has been notably absent from any analysis, due to the limited availability of suitable observations. An initial attempt to relate the estimated ecosystem respiration to chamber measurements of soil respiration was presented in Reichstein *et al.* (2005) but suffered from the scale mismatch of the two observation techniques. Unless reliable scale consistent observations become available, the use of canopy simulation data for model testing appears the only alternative to gain confidence in flux partitioning schemes (Chapter II, III).

In the following, F_N observations are disaggregated by making use of a semi-parametric hypersurface model for F_N as introduced in Chapter II. For this, F_R is derived from the light independent signal in the hypersurface. This approach does not rely on prior functional

[7] apart from additional non-respiratory losses, e.g., from fire, harvest or transport of dissolved organic carbon into groundwater.

assumptions about the underlying carbon exchange processes and explicitly accounts for continuous seasonality of carbon assimilation and respiration in an ecosystem. First, the performance of the semi-parametric model to disaggregate F_N is evaluated by using synthetic EC data derived from several deterministic, process based canopy exchange models. Following on from this, the hypersurface based estimates of F_R and F_G along with their associated uncertainties are used to calculate annual carbon uptake and release for eight FLUXNET sites in order to study their relative contributions to the net carbon budget at these sites.

IV.2 Methods and Material

Disaggregation of F_N into carbon assimilation and respiration

Owing to a range of different error sources, EC data are uncertain (e.g., Mahrt 1998) and therefore, we need a model to first determine the systematic signal of the net CO_2 flux measurements prior to any further decomposition. Here, the semi-parametric spline model (in the following referred to as the spline model) introduced in Chapter II is used to characterise the relevant response hypersurface and to derive a stochastic model for the EC data set in question (Chapter II). The resulting hypersurface describes the simultaneous response of F_N to the major environmental drivers, light, I, temperature, T, and time, t. The shape of the four-dimensional hypersurface is conditioned directly from the data by estimating the values of nodes for cubic splines within a weighted least-squares optimisation procedure. As a result, any environmental condition described by I_i and T_i at a particular point in time of the i'th year can be assigned a value provided this combination lies within the boundary of the interpolating hypersurface, i.e. within the range of observations used for the optimisation (see Chapter II).

Given that photosynthesis does not operate in the absence of light, ecosystem respiration can be characterised from the estimated hypersurface for I = 0. The resulting respiration component, F_R is therefore a two-dimensional function of temperature and time, the form of which is determined by the entire set of data as opposed to the derivation of F_R from nighttime observations alone (e.g., Goulden *et al.* 1996*a*). The estimated F_R time series is deduced from the two-dimensional interpolated surface conditioned on the temperature range recorded over the year. F_G is then calculated as the difference between the estimated F_N flux derived from the hypersurface and the simulated F_R, i.e.,

$$\begin{aligned} &F_N = f\{T, I, t\} + e_{F_N} = \hat{F}_N + e_{F_N}, \\ &\hat{F}_R = f\{T, t\}\big|_{I=0}, \\ &\hat{F}_G = \hat{F}_N - \hat{F}_R, \end{aligned} \tag{IV-1}$$

where e_{F_N} is the spline model residual series and the hats denote the spline model estimates for the different carbon flux components. Here, a positive sign denotes a carbon flux into the ecosystem and a negative sign indicates carbon loss to the atmosphere. Note, that the disaggregation in (IV-1) is based on the model results alone after having constrained the hypersurface for F_N with the data. Therefore, provided the signal extraction with the spline model was successful, observation noise should not obscure the derivation of F_G and F_R. The stochastic integration to annual estimates for carbon uptake, *ACU* and release, *ACR* result instead from a noise characterisation based on the F_N observations following the method proposed in Chapter III. A nested Monte Carlo simulation framework ($N = 10^5$) accounts for both, the parametric uncertainty derived from the optimisation of the hypersurface and the multiple realisation of the characterised noise for the corresponding F_N observation (cv equation III-1),

$$\begin{aligned} ACU(i) &= \sum_{t=1}^{N} \left\{\hat{F}_G(t,i) + \hat{n}_{F_N}(t,i)\right\} \\ ACR(i) &= -\sum_{t=1}^{N} \left\{\hat{F}_R(t,i) + \hat{n}_{F_N}(t,i)\right\} \end{aligned} \tag{IV-2}$$

where $\hat{n}_{F_N}$ denotes the estimate for the observation noise as derived from the model residuals e_{F_N} (see Chapter III). Here, the same uncertainty for both components as characterised for the corresponding F_N value is assumed, thereby doubling the overall variance of the noise distribution in the sum. One could argue that the observation noise should be partitioned in some way between the two components, for example according to their relative magnitudes (see Figure III-4). However, this approach requires assumptions on the stationarity of the relationship between the variance of the uncertainty and the magnitude of F_N and its transferability to F_G and F_R. Clearly, this ambiguity suggests scope for further investigation and it is currently being subject of further research.

Evaluation with synthetic data and application to FLUXNET sites

To test the performance of this disaggregation method, synthetic data sets of F_N produced by three different canopy exchange simulation models for four different vegetation and climate

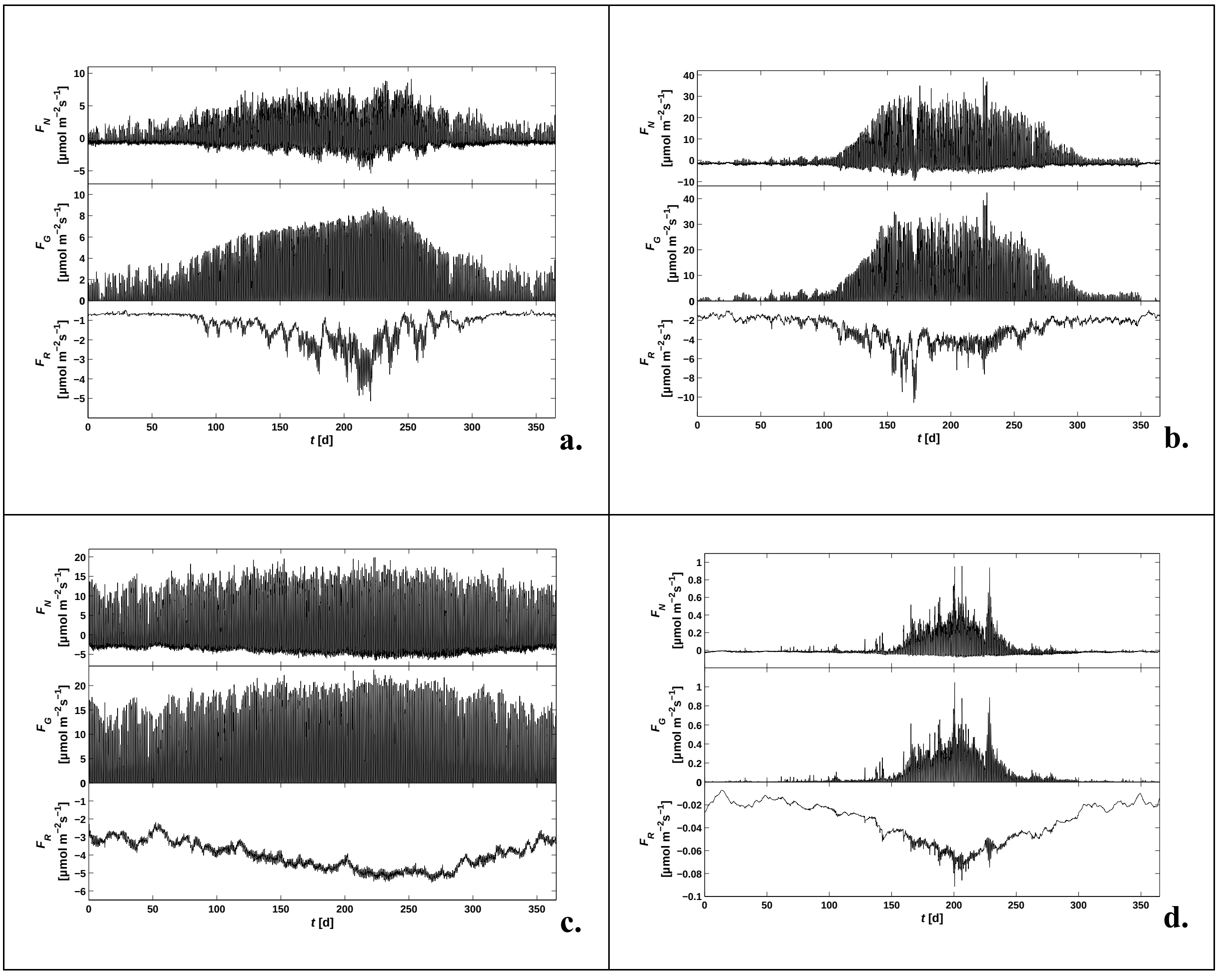

Figure IV-1: Simulated carbon exchange flux components at four sites with different vegetation and climate conditions. F_N is the net CO_2 flux, F_G is the gross carbon uptake and F_R is ecosystem respiration. **a.** SPA model simulations for a temperate coniferous forest site in Oregon, USA. **b.** BETHY model simulations for a temperate deciduous forest site in Hainich, Germany. **c.** Model simulations after Leuning *et al.* (1995) for a hypothetical tropical forest. **d.** Model simulations after Leuning *et al.* (1995) for a hypothetical low productive arctic ecosystem.

conditions are used (see Chapter III). This way, the estimates for F_G and F_R can be evaluated unambiguously against the known deterministic components from the simulation model outputs. Figure IV-1 shows F_N, F_G and F_R for one simulation year for (a) a coniferous pine forest in Oregon produced by the soil plant atmosphere model (SPA; Williams *et al.* 1996); (b) a deciduous forest in Germany produced by the biosphere energy transfer and hydrology model (BETHY; Knorr & Kattge 2005); (c) a low production arctic site produced by the model in Leuning *et al.* (1995); and (d) a high production tropic site produced by the model in Leuning *et al.* (1995). The sites and data sets are described in more detail in Chapter II and the references therein.

The performance of the decomposition is evaluated by means of the correlation coefficient, r, as a measure for how well the variations in the true fluxes are captured. Also, the cumulative error for the entire year relative to the annual fluxes is calculated to test for the

Table IV-1: FLUXNET sites used in this analysis with their site specific vegetation cover and climate conditions. T_{annual} and P_{annual} are mean annual air temperature and mean annual precipitation, respectively.

Site (year)	Vegetation	T_{annual} [°C]	P_{annual} [mm]	References
Hainich (HA), Germany (2001)	beech forest	6.8	775	Knohl et al. (2003); Anthoni et al. (2004)
Hesse (HE), France (2001)	young beech forest	9.9	975	Granier et al. (2000)
Puechabon (PU), France (2002)	oak forest	13.5	872	Rambal et al. (2003)
Yatir Forest (YA), Israel (2002)	pine forest	18.2	280	Grunzweig et al. (2003)
Howland Forest (HO), ME (2000)	spruce forest	6.6	1040	Hollinger et al. (2004)
University of Michigan Biological Station (UM), MI (2001)	mixed hardwood forest	6.2	750	Schmid et al. (2003)
Shidler (SH), Oklahoma (1999)	grassland prairie	15.4	835	Suyker & Verma (2001); Suyker et al. (2003)
Bondville (BV), Illinois (1997)	agriculture (corn)	11.2	990	Meyers & Hollinger (2004); Hollinger et al. (2005)

models' ability to identify the magnitudes of the two individual components from the net flux. For comparison, these measures are determined for three alternative partitioning methodologies commonly used in ecosystem studies based on EC data. The first two methods assume that ecosystem respiration responds as a parametric function of temperature (following either Lloyd & Taylor 1994: Falge *et al.* 2002, or Morgenstern *et al.* 2004). These functions are optimised against nighttime EC data for the entire year. To simulate the F_R series, this relationship is extrapolated to the range of temperatures occurring during the day. F_G is then calculated from the difference between the measured F_N flux and the estimated F_R series. A third method estimates canopy photosynthesis from a nonlinear regression of F_N against photosynthetically active radiation (PAR) and a constant respiration term (Ruimy *et al.* 1995). This function is fitted to data periods of 3 days to account for change in the relationship and the respiration (Gilmanov *et al.* 2003). For a more comprehensive intercomparison of current flux partitioning schemes the reader is referred to Moffat *et al.* (2006).

Obviously, the ultimate objective of this disaggregation technique is to deliver reliable estimates for carbon accumulation and respiration fluxes derived from real observations.

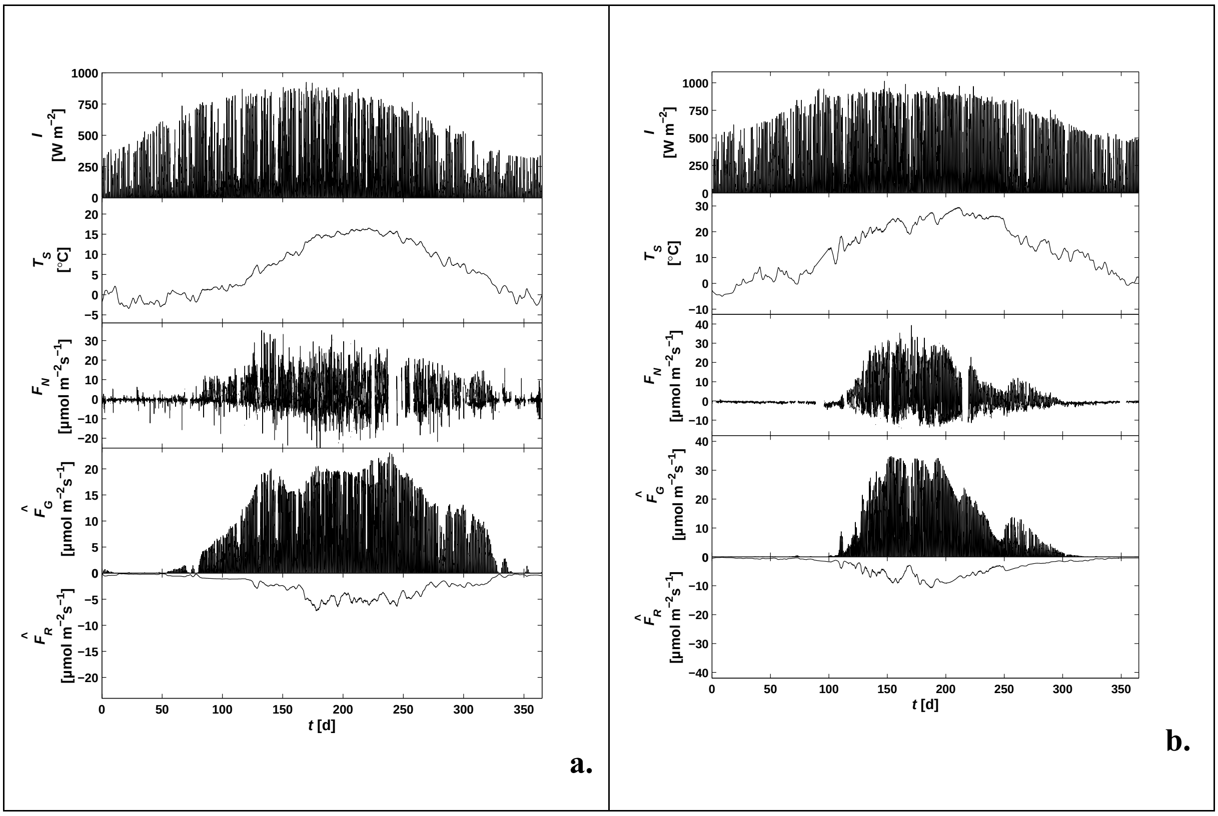

Figure IV-2: Real data examples for **a.** Howland Forest and **b.** Shidler. I is the incident radiation, T_S is the soil temperature, F_N is the net CO2 flux measured by the EC system, and F_G and F_R are the estimated carbon accumulation and respiration flux components using the semi-parametric model.

Eight different FLUXNET sites, six forests, a grassland and a crop site are chosen to apply the disaggregation method to. This must be seen as a rather provisional representation in attempting to cover a diverse range of biomes and climate conditions varying from 280 to 1040 mm annual precipitation and from 6.2 to 18.2 °C annual average temperature. Table IV-1 summarises the site characteristics and climate conditions for the considered measurement sites along with references for detailed descriptions. Figure IV-2 shows I, T_S and F_N for the Howland Forest site in the year 2000 and the Shidler site in the year 1999 as examples.

IV.3 Results and Discussion

Model performance

The correlation coefficients (r) for the two flux components F_G and F_R for the different synthetic data sets are given in Table IV-2. These results suggest that the spline model consistently performs well and outperforms the other three flux partitioning methodologies.

Table IV-2: Correlation coefficients, r for the two estimated true components F_G and F_R for the different data sets and methods. Splines as the method introduced here, L-T denotes the respiration model after Lloyd & Taylor (1994), Q10 denotes the respiration model with a Q_{10} function, and RH is the model for the assimilation with a rectangular hyperbola.

	SPA		**BETHY**		**Leuning tropic**		**Leuning arctic**	
	$r\ \{F_G\}$	$r\ \{F_R\}$	$r\ \{F_G\}$	$r\ \{F_R\}$	$r\ \{F_G\}$	$r\ \{F_R\}$	$r\ \{F_G\}$	$r\ \{F_R\}$
Splines	0.99	0.97	0.99	0.94	0.99	0.99	0.95	0.98
L-T	0.97	0.91	0.99	0.86	0.99	0.98	0.99	1.0
Q10	0.98	0.90	0.99	0.91	0.99	0.66	0.99	0.88
RH	0.99	0.77	0.99	0.73	0.99	0.54	0.96	0.35

Table IV-3: Relative cumulative error, Σe for the two estimated true components F_G and F_R for the different data sets and methods. The model notation is the same as in Table IV-1.

	SPA		**BETHY**		**Leuning tropic**		**Leuning arctic**	
	Σe_{FG} [%]	Σe_{FR} [%]	Σe_{FG} [%]	Σe_{FR} [%]	Σe_{FG} [%]	Σe_{FR} [%]	Σe_{FG} [%]	Σe_{FR} [%]
Splines	4.7	7.8	3.4	4.9	1.3	1.9	1.3	8.5
L-T	6.4	10.85	4.6	6.9	1.2	1.8	2.5	3.9
Q10	-8.5	-15.3	1.5	2.1	-10.4	-14.3	-3.4	-5.3
RH	4.3	7.2	2.0	2.9	0.5	0.8	8.2	12.9

Table IV-3 shows the relative cumulative error between the true and the modelled fluxes for the different data sets and modelling approaches. In general, the spline model identifies the relative magnitudes for the two components well and in particular, the cumulative error for F_G is consistently below 5% of the annual sum indicating a minor underestimation of carbon assimilation. The results for F_R are similarly satisfying despite some systematic underestimation of the magnitude of the flux especially for the SPA data and the low production site. Interestingly, the results for the other methods are more inconsistent suggesting a dependency of the models' performances on the data set and hence the underlying process descriptions in the simulation model being used[8]. This highlights the benefit of estimating flexible semi-parametric relationships as opposed to fixed parametric functions for this particular application.

[8] The three simulation models differ in the model formulation for the separate respiration fluxes in that some are based on a soil carbon content dependent Q_{10} function (e.g., BETHY, Knorr 1997), others are modelled with a temperature dependent exponential function after Lloyd & Taylor (1998) with an implemented discrete soil moisture dependence (SPA, Leuning model).

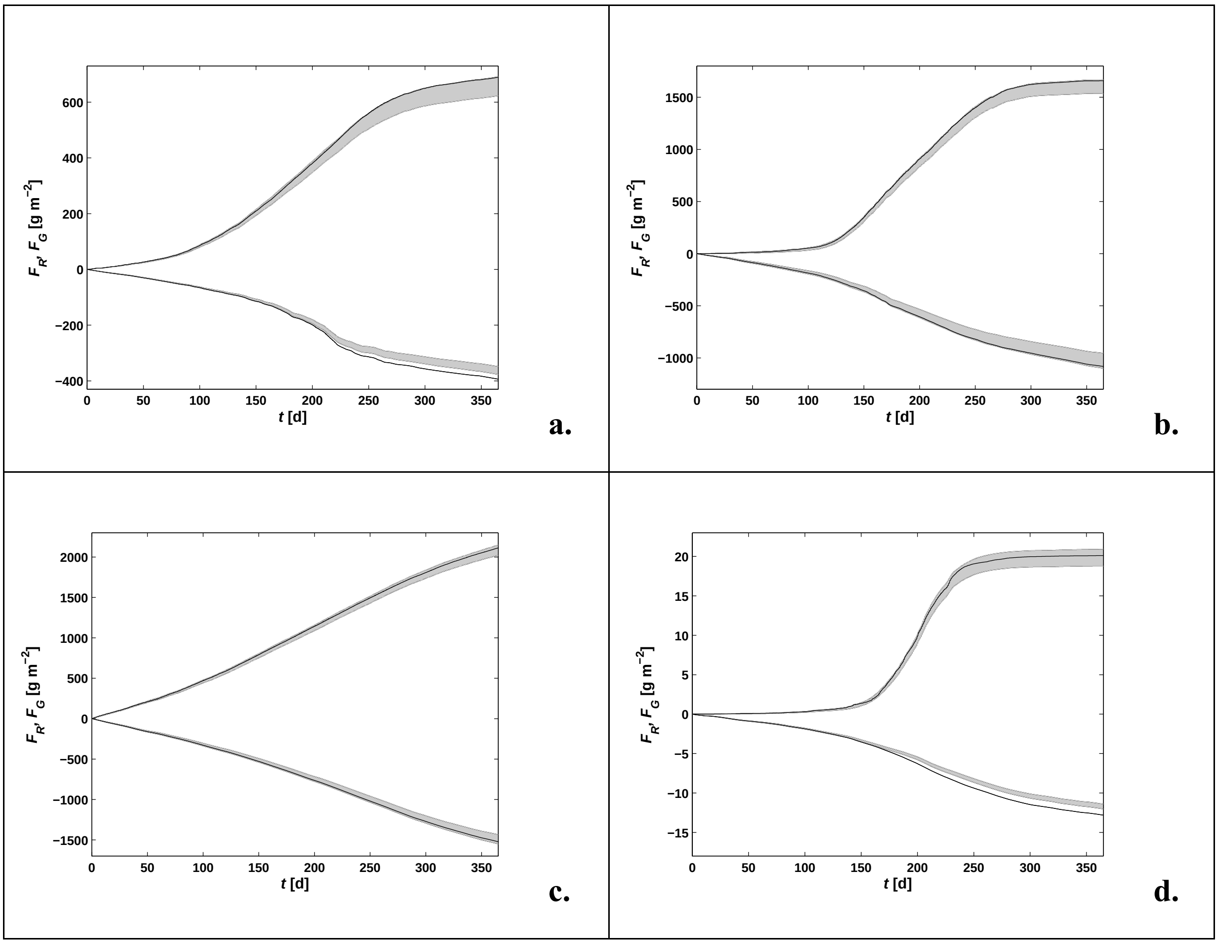

Figure IV-3: Annual cumulative evolution of the uptake (positive) and release (negative) fluxes for the four synthetic data sets. The grey envelopes show the propagation of the parametric uncertainty through the integration. The black line is the deterministic 'true' flux from the simulation model. **a**. SPA; **b**. BETHY; **c**. Leuning *et al.* (1995) high production; **d**. Leuning *et al.* (1995) low production.

Figure IV-3 shows the cumulative sum of F_R and F_G when accounting for the parametric uncertainties associated with the spline model calibration. The 'true' integrated fluxes in black are encompassed by the 95 percent quantiles except for the respiration component in the SPA data (Figure IV-3a) and the low production data (Figure IV-3d), as already indicated by the relative cumulative error (Table IV-3). Given the simple form of equation (IV-1), such model inadequacies are not surprising. For example, equation (IV-1) estimates the sensitivity of F_N to one temperature T, whereas in reality, the processes dominating F_G and F_R respond to different temperatures. F_G will predominantly be affected by the ambient air temperature mostly within the canopy, while the soil respiration share in F_R is driven by some superficial soil temperature diverging from air temperature (see Chapter V). It is interesting to note that, F_R is systematically underestimated predominantly during the summer daytime, indicating that the sensitivity of F_R to temperature is not sufficiently accounted for in the T-t surface. Again, this is not surprising given the summer daytime F_N fluxes will be dominated by

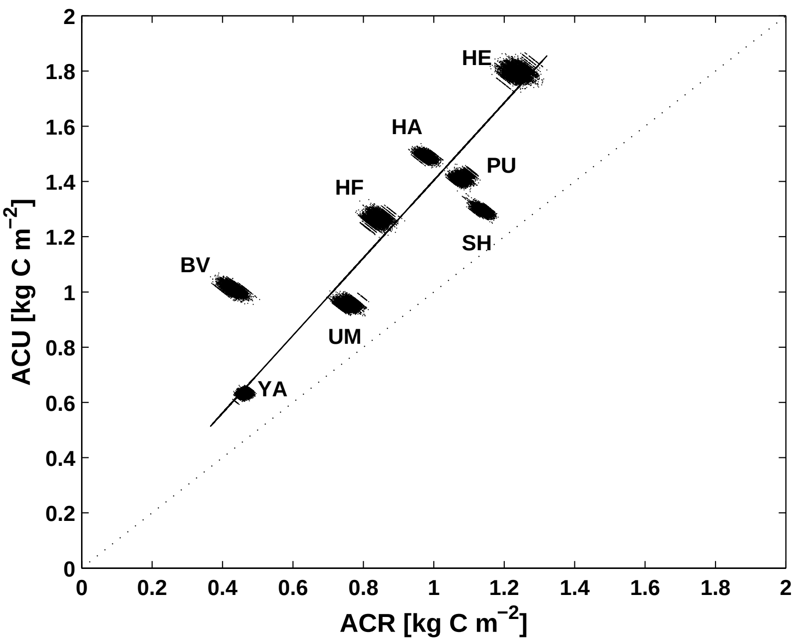

Figure IV-4: The relationship between annual carbon uptake, *ACU* and release, *ACR* for the six sites. BV: Bondville site; UM: University of Michigan Biological Station site; HF: Howland Forest site; HA: Hainich site; SH: Shidler site; HE: Hesse site. YA: Yatir site; PU: Puechabon site. The dotted line is the 1-to-1 line along which the ecosystem is carbon neutral. The black line is the result of a reduced major axis regression (Sokal & Rohlf 1995) minimising the Euclidean distance to a straight line through the origin.

assimilatory processes somewhat covering the respiration signal. Also, as already mentioned, the influence of canopy temperature on F_R (as opposed to soil temperature) will become increasingly important with a rising fraction of plant respiration. Finally, the smooth nature of the cubic splines in the temporal space might result in a slightly lower amplitude of the F_N flux and hence of the derived F_G and F_R. However, these inadequacies are small and will most likely become masked by the observation noise present in real EC data (Chapter III).

Carbon uptake and release for real data examples

The spline model in equation (IV-1) explains the variations in F_N well for all data sets at the eight FLUXNET sites (*r* between 0.9 and 0.95). The derived deterministic estimates for F_G and F_R at the Howland Forest site and the Shidler site are shown in Figure IV-2 as example representations of the disaggregation with the spline model. With the characterised observation noise and the parameter uncertainties associated with the estimated flux components, it is now possible to analyse the relative contributions of *ACU* and *ACR* to the annual net ecosystem carbon balance following equation (IV-2). In Figure IV-4, *ACR* is plotted against *ACU* for the eight FLUXNET sites. All sites acted as significant net carbon sinks in the selected year (see also Falge *et al.* 2002 for a similar result based on an analysis of EC data from northern hemispheric ecosystems). Furthermore, these two components appear to be strongly positively correlated as indicated by a reduced major axis regression (slope of 1.4 ± 0.002, $r^2 = 0.87$).

Clearly, given the rather small number of sites, these results have to be interpreted with care and a substantial expansion of the database is currently underway. However, these preliminary results provide scope for some interesting speculation. A positive annual net balance indicates that the ecosystem is acquiring more carbon than is lost due to respiration. Several reasons could be responsible for this observed trend. Firstly, as discussed briefly in chapter I, the EC measurements used for the analysis of the carbon balance could suffer from systematic errors. For example, stable atmospheric conditions occurring particularly at night prevent the turbulent mixing of the atmospheric boundary layer giving rise to a systematic underestimation of the EC nighttime fluxes as the surface boundary layer exchange becomes dominated by diffusion rather than turbulence (e.g., Moncrieff *et al.* 1996; Aubinet *et al.* 2000). As a result, on an annual basis, carbon neutral ecosystems might misleadingly appear as sinks. Secondly, net carbon uptake would be generally expected in forest sites covered with developing vegetation given they will not have reached equilibrium (Schimel *et al.* 2001). The ecosystems considered here were all fully closed and older than 90 years. As a result, it would be somewhat surprising if $ACU = 1.4ACR$ for this reason alone. Thirdly, $ACU > ACR$ could also originate from direct fertilisation effects of increased atmospheric CO_2 concentration on the photosynthetic activity (e.g., Ehleringer & Björkman 1977). Again however, although at the leaf level over short periods of time the effect of a 100 ppmv rise in CO_2 can be significant, the accommodated response of whole plants over longer intervals is invariably much less (Drake *et al.* 1997). However, what CO_2 fertilisation can induce is certain indirect effects such as the alleviation of nutrient and water limitations over longer timeframes (Drake *et al.* 1997). This, coupled to other global enhancements in productivity such as through enhanced nitrogen deposition (Schimel 1995) and increases in the diffuse component of down-welling solar radiation (Roderick *et al.* 2001) may go some way to explaining the degree of net accumulation expressed in Figure IV-4. This is supported by global studies that identified northern-hemispheric ecosystems as net carbon sinks (e.g., Tans *et al*. 1990; Keeling *et al.* 1996). In this context, the sensitivity of ACU and ACR to environmental conditions will be of particular interest for assessing the role of terrestrial ecosystems in the global carbon cycle in a changing climate.

Acknowledgements

Special thanks to the principle investigators for making available the eddy covariance measurements at the eight FLUXNET sites.

V. The Seasonal Temperature Dependency of Photosynthesis and Respiration in Two Deciduous Forests

Andrew J Jarvis   Vanessa J Stauch   Karsten Schulz   Peter C Young

An edited version of this manuscript is published as

Jarvis AJ, Stauch VJ, Schulz K, Young PC (2004) The seasonal temperature dependency of photosynthesis and respiration in two deciduous forests. Global Change Biology, 10, 939-950.

Abstract

Novel nonstationary and nonlinear dynamic time series analysis tools are applied to multiyear eddy covariance CO_2 flux and micrometeorological data from the Harvard Forest and University of Michigan Biological Station field study sites. Firstly, the utility of these tools for partitioning the gross photosynthesis and bulk respiration signals within these series is demonstrated when employed within a simple model framework. This same framework offers a promising new method for gap filling missing CO_2 flux data. Analysing the dominant seasonal components extracted from the CO_2 flux data using these tools, models are inferred for daily gross photosynthesis and bulk respiration. Despite their simplicity, these models fit the data well and yet are characterised by well defined parameter estimates when the models are optimised against calibration data. Predictive validation of the models also demonstrates faithful forecasts of annual net cumulative CO_2 fluxes for these sites.

V.1 Introduction

Through their interactions with the environment, plants modulate surface energy balance, geochemistry and hydrology, whilst acquiring atmospheric carbon to grow and reproduce. Concerns over the potential climatic impacts of increasing levels of atmospheric CO_2 have focused attention on the significance of the role played by plants in the modulation of land surface-atmosphere fluxes, especially since the relevant biochemical and physiological processes of the plant are themselves CO_2 sensitive (Sellers *et al.* 1996a). In an attempt to improve the representation of the control on land surface-atmosphere fluxes exerted by vegetation, models of the structure, biochemistry and physiology of plant gas exchange have frequently been incorporated into canopy scale flux schemes (Dickinson *et al.* 1986; Wang & Jarvis 1990; Sellers *et al.* 1996b; Cox *et al.* 1998).

Despite attempting to structure these models such that many of the associated model parameters can be specified a priori, there invariably remains a need for some parameterisation of the associated process descriptions to accommodate variations in scale, time and space. As a result, the parameterisation of models is often with reference to site and scale specific data, such as eddy covariance and associated micrometeorological measurements (e.g., see Lloyd *et al.* 1995; Baldocchi & Harley 1995; Cox *et al.* 1998; Hollinger *et al.* 1998). Recent studies have clearly demonstrated that the information content of such data is not rich enough to support the calibration of many components of current generation canopy scale flux models (Franks *et al.*1997; Franks & Beven 1997; Schulz *et al.* 2001). As a result, much of the model functionality being proposed is not constrained by the calibration process, rendering predictions from these schemes somewhat uncertain. This indicates that, to obtain robust descriptions of these systems, the level of complexity of the models being used needs to be commensurate with the information content of the calibration data being used.

Recognising the need for an appropriate level of parsimony in canopy model descriptions Monteith (1995) writes *“There are two complementary ways of moving forward – to remove routines from the complex models that contribute little to their predictive power, or to add routines to the simple models that will make them more robust.”* The obvious question is, what to omit or what to add? One strategy for tackling this question is to start by specifying a model of the canopy whereby the model parameters can be estimated unambiguously from canopy scale observations such as eddy covariance time series. Then, since the model parameters can be estimated for specified time periods, significant temporal evolution of these parameters, as conditioned by the measured time series data, can be used to objectively identify what additional complexity needs to be introduced to describe the system as observed. Obviously, changes in properties of the canopy that fall outside the domain of the observations e.g. defoliation, wind throw or fire, may lead to compromised predictive performance in such models. Therefore, it is important that the resultant inductive models are interrogated in order to identify the mechanisms they represent.

The procedure for model identification eluded to here parallels certain aspects of the data-based mechanistic model identification and estimation methodologies developed by Young and co-workers (see e.g., Young & Pedegral 1999; Young 1999; Young 2000) for modelling stochastic, non-stationary and nonlinear dynamic systems. This paper applies one such methodology known as State Dependent Parameter (SDP) estimation to deriving descriptions for annual carbon acquisition dynamics in two forest systems as expressed in eddy covariance time series. The starting point for this analysis is the following generic description for the canopy net CO_2 flux, F_N,

$$F_N = \varepsilon . S_0 - F_R \tag{V-1}$$

where S_0 is the incident down-welling solar radiation, F_R is the canopy-soil respiration rate and ε is the radiation capture and utilisation coefficient.

(V-1) can be viewed as the basis for terrestrial CO_2 flux modelling, with the differences between models being defined by the functional relationships assumed to describe ε and F_R. These range from relatively simple descriptions used in resource capture type models (e.g., Monteith 1972, 1977; Field *et al.* 1995) to the relatively complex descriptions used in photosynthetic bio-physical and biochemical models (e.g., Dickinson *et al.* 1986; Wang & Jarvis 1990; Leuning *et al.* 1995). In this paper the aim will be to extract the functional forms for ε and F_R directly from eddy covariance and micrometeorological measurements and assess the level of complexity in the functional relationships for ε and F_R that the observations support. Initially this will focus on accounting for the seasonal dynamics within cumulative daily data.

(V-1) is an obvious candidate model structure for SDP estimation and model identification procedures due to its simple regression-type format and the availability of time series measurements for F_N and S_0 at the canopy scale. As will be seen in this paper, (V-1) in conjunction with the SDP estimation procedure may provide a useful top-down framework for both identifying and estimating canopy models from eddy covariance and micrometeorological data, which, in conjunction with a priori knowledge of the relevant canopy processes could yield robust hybrid statistical-mechanistic models for canopy CO_2 exchange.

In similar work, Falge *et al.* (2002) applied a variant of (V-1) to eddy covariance measurements of CO_2 flux to derive time varying estimates for the parameters in predefined nonlinear descriptions for both ε and F_R estimated using a simple nonlinear least squares window function. The approach adopted here differs significantly from their approach principally in that the functional forms of ε and F_R do not need to be specified a priori, but instead can be objectively inferred directly from the observations. An additional benefit of this approach is that it provides an objective methodology for filling gaps in CO_2 flux data, through combining elements of current gap filling methodologies within a coherent, data-led framework.

V.2 Materials and Methods

Data sources and site descriptions

Two different FLUXNET (Baldocchi *et al.* 2001b) deciduous forest sites have been chosen for the illustration of the model development: Harvard Forest, Massachusetts (HF, 1994-1999, Barford *et al.* 2001; Wosfy & Munger 2003) and University of Michigan Biological Station, Michigan (UMBS, 1999-2001, Schmidt *et al.* 2003, Curtis 2003). The two sites differ especially in the mean annual precipitation (1066 mm at HF and 750 mm at UMBS) and the mean annual temperature (7.8 °C at HF and 6.2 °C at UMBS). The different climatic conditions are mirrored in the vegetation type. While HF is a temperate deciduous forest site, the vegetation at UMBS is characterised by an intermediate mix of temperate deciduous and boreal forest (Curtis *et al.* 2002). Both forests are of similar age and stage of maturity (70 years at HF, 90 years at UMBS).

State dependent parameter estimation

Young and co-workers (see e.g., Young & Pedegral 1999; Young 1999; Young 2000) have developed recursive parameter estimation algorithms, based on Kalman filtering and smoothing techniques. These allow for the evolution of parameters to be estimated directly from time series data and hence identification of any non-stationary and/or state dependency of these parameters. In particular, the State Dependent Parameter (SDP) algorithm, which is able to optimally estimate a broad class of non-stationary and nonlinear dynamic regression models, is well suited to the current study. This can be seen when expressing (V-1) in an equivalent SDP format (see Young 2000).

$$F_N(t) = \hat{\varepsilon}(x,t).S_0(t) + \hat{F}_R(x,t) + \xi_N(t) \qquad \text{(V-2)}$$

Here $\hat{\varepsilon}(x,t)$ and $\hat{F}_R(x,t)$ are estimates for the evolution of ε and F_R, $\xi_N(t)$ is the regression model error series and x is the state(s) on which ε and F_R are assumed to be dependent.

To objectively identify the nature of the functional relationships between the variations in ε, F_R and the relevant measured states of the system, the regression model (V-2) is implemented such that the incremental variations in $\hat{\varepsilon}(x,t)$ and $\hat{F}_R(x,t)$ are estimated using the paired measures of S_0 and F_N, but with these series sorted with respect to the ascending magnitude of x, where here x is the measured surface temperature, T_S. Surface temperature was found to be an appropriate state in this study where the focus is on the seasonal dynamics.

The stochastic evolution of each parameter in (V-2) is assumed to be described by the following random walk process (Young 1999),

$$\hat{\varepsilon}(x,t) = \hat{\varepsilon}(x,t-1) + \eta_{\varepsilon}(t) \qquad \text{(V-3a)}$$

$$\hat{F}_R(x,t) = \hat{F}_R(x,t-1) + \eta_R(t) \qquad \text{(V-3b)}$$

where η is a zero mean, white noise sequence allowing for stochastic variability in the parameters. Although apparently complex at first sight, the assumption that the model parameters evolve as non-stationary stochastic variables is simply a statistical device to allow for the estimation of parametric change. It ensures that the recursive parameter estimates at the t'th sample depend only on the data in the vicinity of this sample in the sorted state space. In the case of the random walk model (V-3), this weighting effect of the data on the parameter estimates has a Gaussian-like shape with maximum weight at the t'th sample and declining weight to either side (see Young & Pedregal, 1999). The 'bandwidth' of this Gaussian window function is characterised by the *Noise Variance Ratio*, *NVR* = $\sigma^2(\eta(t))/\sigma^2(\xi(t))$. As a result, a high value of the *NVR* means that only data in the immediate vicinity of the t'th sample are used for the t'th estimate. On the other hand, an *NVR* of zero ensures that the parameter is assumed constant across the entire observation interval (i.e., the same as in standard en bloc regression where all data have equal weighting in the estimation). The former case is particularly useful in the present context because it results in variations in the parameter estimates that are conditioned by the time series data being used. Of course, one of the keys to the employment of (V-2) and (V-3) when estimating the SDPs, is specifying the magnitude of the *NVR*s within the SDP model. Here, the methods of Young (1999) are used where the required *NVR*s are optimised via maximum likelihood prediction error decomposition.

Once the non-parametric (graphical) form of the state dependency has been identified from the observed relationship between $\hat{\varepsilon}(x,t)$, $\hat{F}_R(x,t)$ and x, a suitable parametric function can be specified to describe this form, and the resultant model can be parameterised using standard optimisation procedures such as nonlinear least squares or maximum likelihood (Young 2000). The selection of the parametric function may also be guided by relevant prior knowledge of canopy processes and so attempt to guard against spurious predictions made beyond the domain of the observations. The focus of this study was to derive descriptions for the seasonal dynamics of two forest systems, therefore, the SDP model identification procedure was implemented on the cumulative daily data.

Gap filling

A very useful property of the recursive SDP approach to parameter estimation is that missing values in the output series are readily interpolated in an objective, non-parametric manner, conditioned only by the properties of the model (V-2) and the available input-output data. As a result, not only does this approach facilitate the objective model identification, which forms the central theme to this paper, but also the objective gap filling of the hourly eddy covariance time series needed to derive the daily cumulative CO_2 fluxes utilised in this paper. Because this gap filling procedure is based on the recursive implementation of a Gaussian-like window function within a Kalman filter-regression framework, it can be viewed as a logical synthesis and extension of current gap filling methodologies (e.g., Goulden *et al.* 1996a; Anthoni *et al.* 1999; Grünwald & Bernhofer 2000; Falge *et al.* 2001; Pilegaard *et al.* 2001).

Utilising the SDP estimation procedure described above, $\hat{\varepsilon}(x,t)$ and $\hat{F}_R(x,t)$ are estimated out of temporal order (see the explanation in Young 2000) using hourly values for S_0 and F_N, with the ordering determined by the sorted order of T_S. Because of the sorting out of temporal order the systematic gaps in the time series become much smaller nonsystematic gaps in the sorted temperature space. These smaller gaps are readily traversed by a small estimation window that is able to pass the majority of the systematic variations in $F_N(t)$. The optimised *NVR*s for the hourly data are $5\ 10^{-6}$ for $\hat{\varepsilon}(T_S,t)$ and $5\ 10^{-5}$ for $\hat{F}_R(T_S,t)$. These *NVR*s are such that $\xi_N(t)$ are serially uncorrelated, and zero mean, but it is interesting to note that this error series demonstrates seasonality in its variance (see Figure V-1f). The estimates for $F_N(t)$ derived from realising (V-2) are then used to fill in the gaps in the measured $F_N(t)$ series to form a continuous time series which is resorted back into temporal order. It must be stressed that, although T_S is used to determine the sorted order of the SDP estimation, only paired values of $S_0(t)$ and $F_N(t)$ are used in the estimation itself. Also, the *NVR*s used are such that the gap filling procedure is not constrained by a linear model. Indeed, $\hat{\varepsilon}(x,t)$ and $\hat{F}_R(x,t)$ are free to vary such that $\xi_N(t)$ are serially uncorrelated, and zero mean.

Example hourly estimates for $\hat{\varepsilon}(x,t)$ and $\hat{F}_R(x,t)$ are shown in Figure V-1c and d, the latter of which providing the estimates for the daily $\hat{F}_R$ and hence gross canopy photosynthesis, $\hat{F}_G$, used later in the model identification. Corrections of F_N under quiescent atmospheric conditions (see Aubinet *et al.* 2000; Falge *et al.* 2001) are not considered here. Instead, the available flux series are treated as accurate, if somewhat uncertain, measures of the underlying canopy-atmosphere exchange processes.

For the gap filling of the input series (light and temperature; see later), measurement gaps of three hours or less were filled using a random walk procedure identical to (V-3). For gaps greater than three hours, values from the Typical Meteorological Year (TMY2) data set (Renewable Resource Data Center 2003) from the nearest meteorological station were inserted.

V.3 Results

Model identification

Non-parametric Variations in $\varepsilon(t)$ and $F_R(t)$

Figures V-1a and b show a one-year time series of hourly S_0 and F_N measured above HF (1996) along with the associated gap-filled estimates. The estimates of $\hat{\varepsilon}(x,t)$, $\hat{F}_R(x,t)$ and hence $\hat{F}_G(t)$ are shown in Figures V-1c, d and e, respectively. It is worth noting that, here, estimates of $\hat{F}_R$ are based on all hourly data, as opposed to deriving estimates from the most uncertain night time fluxes (see e.g., Aubinet *et al.* 2000; Grünwald & Bernhofer 2000). As a result, the SDP estimates of $\hat{F}_R$ are well defined and are used here to define ecosystem respiration. Close inspection of the estimates of $\hat{\varepsilon}(x,t)$ reveals that, although some within day variation is observed, this is dominated by the seasonal variations (Figure V-1c). Therefore, one would anticipate that attempts to estimate any nonlinear relationship between S_0 and F_N, using blocked hourly data, would be prone to significant uncertainties (see e.g., Grünwald & Bernhofer 2000), especially as it is unclear to what extent these variations in $\hat{\varepsilon}(x,t)$ within

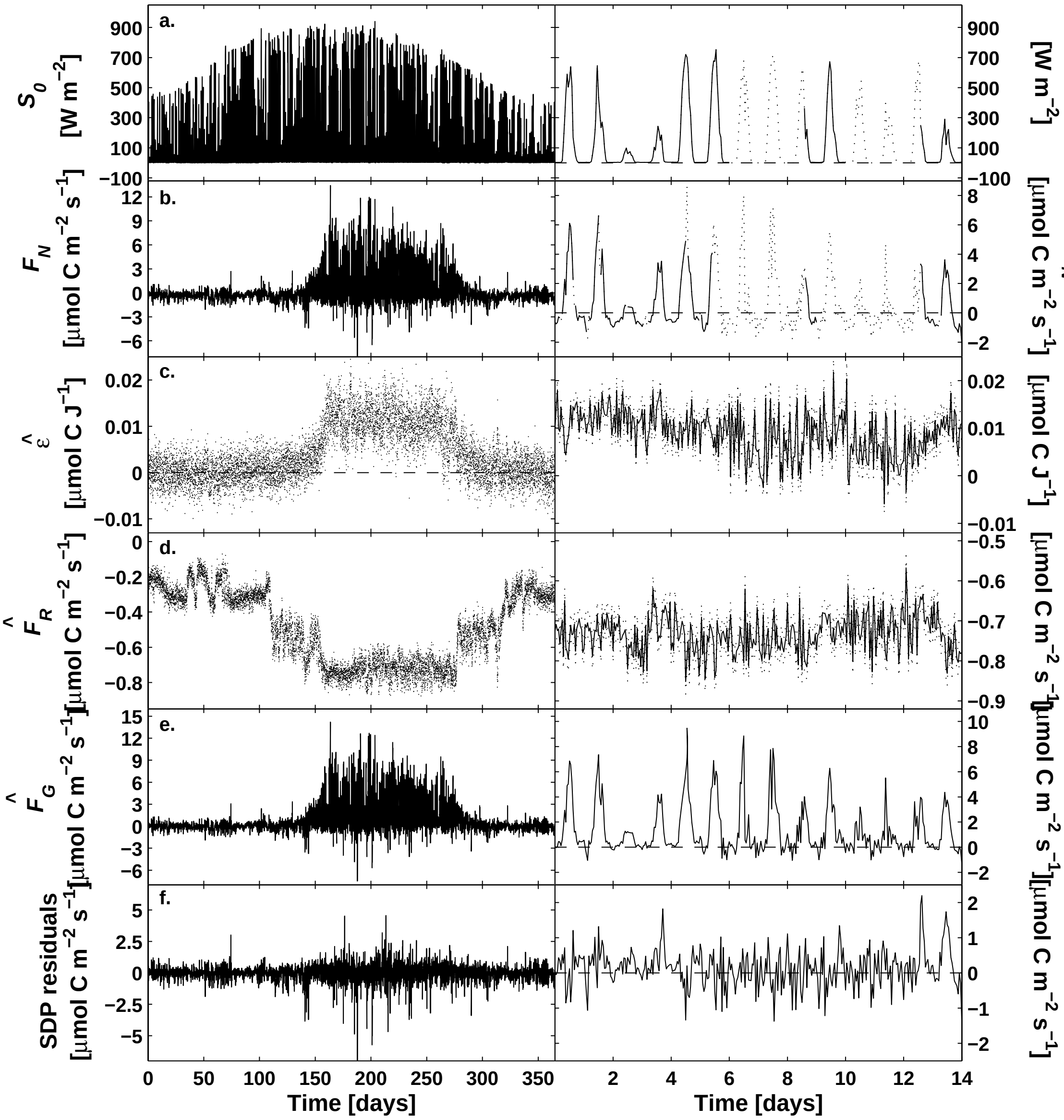

Figure V-1. Hourly data for HF in 1996. The appended plots on the right are sections of 14 days chosen to elucidate associated gap filled periods (dashed lines). Panels **a** and **b** show the interpolated hourly measurements of total downwelling solar radiation, S_0, and net CO_2 flux, F_N. Panels **c** and **d** show the temporal evolution of radiation use, $\hat{\varepsilon}$, and bulk respiration, $\hat{F}_R$, estimated using (1) (*NVR*s = 5 10^{-6} and 5 10^{-5} respectively). Panel **e** shows the resulting gross photosynthesis, $\hat{F}_G$, estimated as $F_N - \hat{F}_R$. Panel **f** shows the error series between the SDP fit of (1) and the F_N measurements shown in panel **b**.

any particular day are attributable to light saturation kinetics or other processes. The underlying causes of the observed seasonal variations in $\hat{\varepsilon}(x,t)$ are likely to be complex, incorporating the effects of the emergence, development and senescence of the vegetative canopy (Waring *et al.* 1995). Similarly, from Figure V-1d we observe that the significant variations in $\hat{F}_R$ are also dominated by seasonality, which likewise aggregates multiple sources of variation through its dependency on soil and canopy respiratory CO_2 sources.

Parameterisations for ε and F_R

Because it appears that both ε and F_R are dominated by seasonal variations we have elected to analyse the cumulative daily flux data derived from summing the hourly fluxes. This is likely to have the additional benefit of linearising the relationship between daily F_N and S_0 on timescales of weeks (Ruimy *et al.* 1995), hence simplifying the final model formulation. Figures V-2a/c and b/d demonstrate that the seasonal variations in $\hat{\varepsilon}(x,t)$ and $\hat{F}_R(x,t)$ can be represented as functions of the measured surface temperature, T_S. The use of surface rather than air temperature provided a superior descriptor for variations in both $\hat{\varepsilon}(x,t)$ and $\hat{F}_R(x,t)$, which is not surprising in light of the thermal inertia of the system allied to potential lag effects of plant and soil metabolism (Jones 1983; Linder & Flower-Ellis 1992; Su *et al.* 1996; Dewar *et al.* 1998; Baldocchi *et al.* 2001a).

The seasonal temperature dependency of ε was parameterised in sympathy with the SDP relationship shown in Figure V-2a/c using the following smooth transition relationship (e.g. Granger & Terasvirta 1993; Young *et al.* 2003):

$$\varepsilon = \frac{\varepsilon_{\max}}{1 + e^{k(T - T_{1/2})}} \qquad \text{(V-4)}$$

where k determines the rate of the transition between the lower (zero) and upper (ε_{max}) levels of ε and $T_{1/2}$ is the temperature at the inflection point where one half of the transition is experienced and hence, along with k, determines the temperature switching characteristics of the canopy between winter and summer. Consistent with the SDP result (Figure V-2a/c), the lower level of ε is set to zero, i.e. no photosynthetic activity at low temperatures. (V-4) can be viewed as a temperature scalar for ε (Field *et al.* 1995). The form of this scalar differs from those used by Field *et al.* (1995) since significant decreases in ε with increasing temperature were not identified in these particular data. For the two data sets analysed the relationship (V-4) was found to be relatively stationary across all years, irrespective of whether the canopy was dormant, emerging, fully expanded or senescing, implying a close correlation between variations in temperature, leaf area and photosynthetic capacity of the canopy across the season. This is somewhat fortuitous since it facilitates realisation of ε without having to specify a dynamic state description for, for example, leaf area. However, it was found that the response of ε to T_S was lagged by approximately five days. As a result, T_S was replaced by the lagged temperature, T_τ, in (V-4) with the magnitude of the lag being determined in the final

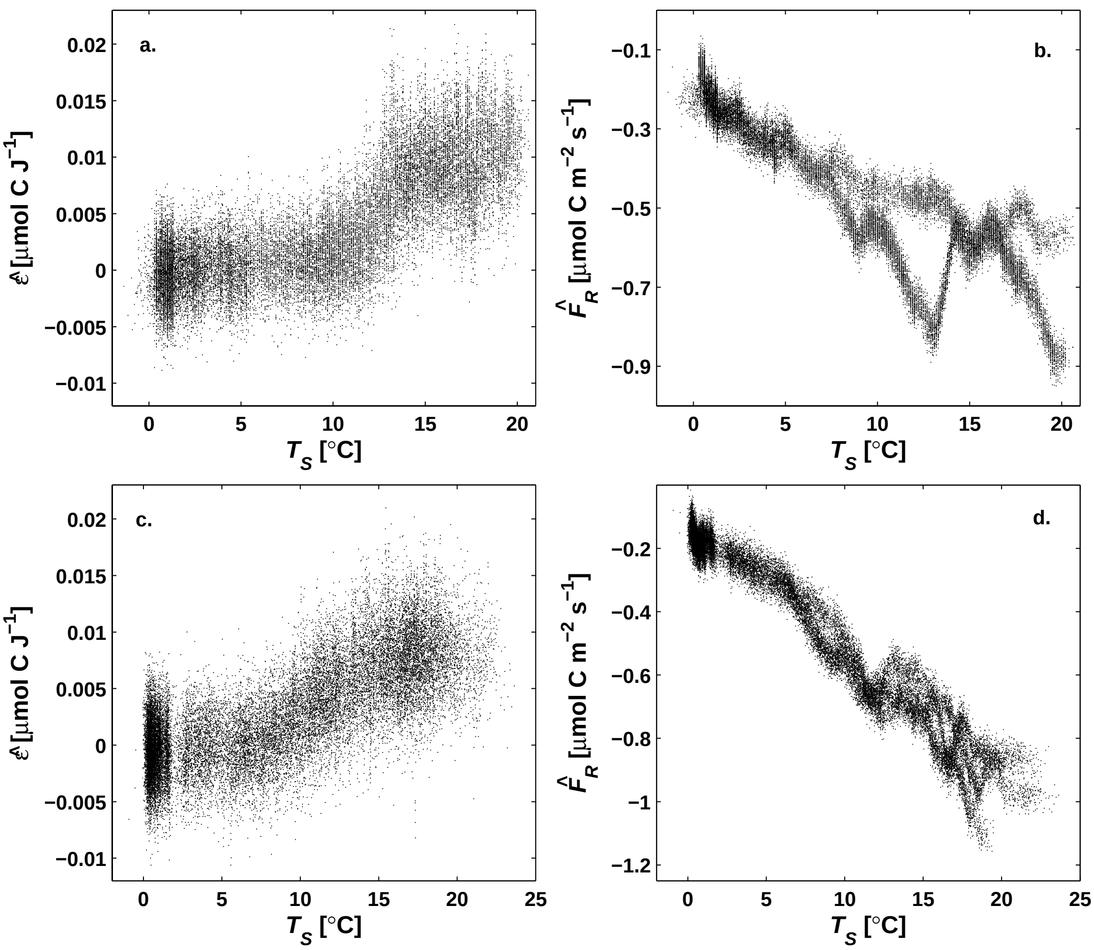

Figure V-2. The non-parametric relationships between **a**/**c** $\hat{\varepsilon}$ and **b**/**d** $\hat{F}_R$, and the surface temperature, T_S, at HF 1994 to 1996 (panels **a** and **b**), and at UMBS 1999 to 2001 (panels **c** and **d**) on an hourly time step. The estimates for $\hat{\varepsilon}$ and $\hat{F}_R$ are those shown in Figures 1**c** and **d** respectively.

parametric model optimisation.

The SDP relationship between T_S and $\hat{F}_R(x,t)$ is shown in Figure V-2b/d. This relationship is typically represented as an Arrhenius function, which may be justified for the UMBS data, but not for HF where non-stationarity in the data masks any potential nonlinearity, precluding the parameterisation of this type of function. Therefore, we have chosen a linear parameterisation so as to be able to compare the sensitivities of respiration to temperature for the two sites.

Model calibration

So far, we have used non-parametric parameter estimation to identify candidate parametric models to describe the daily variations in F_G and F_R as functions of S_0 and T_S (and hence T_τ). This leads to the following two stage parameter optimisation for F_G and F_R against three years

(HF 1994-1996; UMBS 1997-2000) of daily data:

$$F_G(t) = \left(\frac{\varepsilon_{\max}}{1 + e^{(T_\tau(t) - T_{1/2})}}\right) . S_0(t) + \xi_G(t) \qquad \text{(V-5a)}$$

where,

$$T_\tau(t) = (1-\alpha)T_S(t) + \alpha T_\tau(t-1) \qquad \text{(V-5b)}$$

and,

$$F_R(t) = aT_S(t) + b + \xi_R(t) \qquad \text{(V-5c)}$$

Interestingly, one stage optimisation of the full model (V-5) against the daily F_N data is not possible since the aggregation of the daily F_G and F_R within F_N masks the co-variation of ε and F_R with temperature. As a result, confident estimation of dependencies of ε and F_R on temperature is only facilitated by the partitioning of F_N into ε and F_G and ε and F_R afforded by the non-parametric procedures employed on the hourly data.

The optimised parameter sets for both the HF and UMBS are given in Table V-1. Here, Levenberg-Marquardt nonlinear least squares optimisation has been used. Both of the model error residuals $\xi_G(t)$ and $\xi_R(t)$ were found to be zero mean with no significant serial correlation, although some cross-correlation between $\xi_G(t)$ and the cumulative residual rainfall was found (see later). As can be seen in Figure V-1f, the $F_N(t)$ time series contains a strong seasonality in the residual variance, with the larger variance being associated with the summer measurements. Due to the low pass nature of the SDP estimates for F_R, this residual effect is only present in the F_G series. To make $\xi_G(t)$ constant variance, hence satisfying the assumptions of maximum likelihood estimation, an appropriate non-constant variance white noise signal was added to the daily F_G series to make the model residuals $\xi_G(t)$ constant variance.

Table V-1: Results of the model calibration for the two sites, HF 94-96 and UMBS 99-01 (r^2 of 0.86 and 0.84 for F_N at HF and UMBS respectively). Figures in brackets are standard deviations. Estimates have been made using Levenberg-Marquardt nonlinear least squares optimisation of model (4a, b and c) against continuous three year blocks of daily CO_2 flux data.

Parameters	Units	HF 94-96	UMBS 99-01
ε_{max}	g C MJ^{-1}	0. 39 (4.66 10^{-3})	0.34 (4.45 10^{-3})
k	°C^{-1}	-1.11 (8.72 10^{-2})	-0.70 (5.97 10^{-2})
$T_{1/2}$	°C	11.88 (8.31 10^{-2})	11.10 (1.08 10^{-1})
α	-	0.79 (2.27 10^{-2})	0.87 (9.82 10^{-3})
a (slope)	g C m^{-2} d^{-1}°C^{-1}	-0.10 (1.37 10^{-3})	-0.15 (8.39 10^{-4})
b (offset)	g C m^{-2} d^{-1}	-0.85 (1.48 10^{-2})	-0.51 (9.13 10^{-3})

Table V-1 shows that, because the model structures have been identified directly from the calibration data, the optimisation of the model leads to highly significant estimates of the model parameters, whilst also explaining the variations in F_N, F_G and F_R (r_T^2 of 0.86, 0.86 and 0.83 respectively for the full three year simulation of HF). The model proved similarly successful when optimised against three years of UMBS data (see Table V-1; r_T^2 of 0.84, 0.88 and 0.97 for F_N, F_G and F_R respectively). The parameterised models for ε (V-4) and F_R (V-5c) for both sites are shown in Figure V-3.

Model evaluation

An initial model evaluation was based on predictive validation over the full six-year period (1994-1999) at the HF site. This provided validation r_T^2 of 0.80, 0.75 and 0.82 to the daily F_N, F_G and F_R respectively (see Figure V-4a). To test for systematic errors within the model, forecast against the accumulated net flux were made as shown in Figure V-5a. The forecasting results presented in Figure V-5a must be viewed as a particularly stringent evaluation of the model for two reasons. Firstly, the parameter estimates used in the simulation have been derived from a two stage optimisation against F_G and F_R and not the net CO_2 accumulation series. Secondly, in integrating the daily flux predictions over six years small systematic errors will become amplified since the model is realised in a true predictive mode initiated at t = 0 and only driven by the input variables.

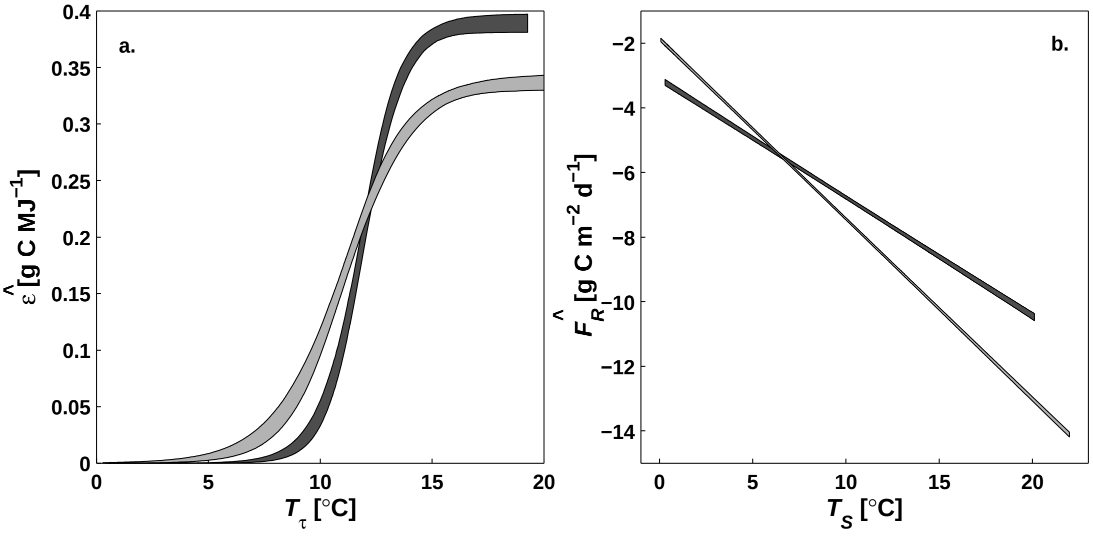

Figure V-3. Parameterised functions for $\varepsilon(T_\tau)$ (panel **a**) and $F_R(T_S)$ (panel **b**) at HF (dark grey) and UMBS (light grey). The patches in **a** indicate the 95 percent uncertainty bounds caused by the propagation of the uncertainties in the associated parameter estimates, as obtained by a Monte Carlo Simulation (N = 1000). For parameter values and associated uncertainties see Table V-1.

From Figure V-5a we see that the prediction envelope of the model largely encompasses that of the observations for the annual net CO_2 accumulation series ($r_T^2 = 0.99$). However, there are notable departures particularly in years 1994, 1997 and 1998. Investigation of the cause for the departures revealed that these arise from small but significant variations in ε_{max} over the six year period (see Figure V-5b). ε_{max} was then estimated as a non-stationary parameter within the model framework (V-5a and b) and variations in ε_{max} were found to be significantly cross correlated (peak correlation of 0.6 at a lag of 70 days) with perturbations in the accumulated residual rainfall (Σ(precipitation – evapotranspiration), compare Figures V-5b and c). Here, perturbations in the accumulated residual rainfall are used as an index of moisture availability (Wilson 1983). The apparent lag of 70 days between variations in water balance and ε_{max} probably reflects dynamic changes in water storage in the system.

The model evaluation also includes inter-comparison between the HF and UMBS optimised parameter sets given in Table 1. Figure V-3a illustrates that the principle difference in the description for ε is that HF experiences a significantly higher ε_{max} in summer (ε_{max}: HF: 0.39 g C MJ^{-1} ± 4.66 x 10^{-3}; UMBS: 0.34 g C MJ^{-1} ± 4.45 x 10^{-3}) and, hence, higher F_G, allied to a more marked transition in ε with temperature (k: HF: -1.11 ºC^{-1} ± 8.72 x 10^{-2}; UMBS: -0.70 ºC^{-1} ± 5.79 x 10^{-2}). This is consistent with the fact that, unlike UMBS, HF is predominately deciduous and hence experiences stronger seasonality in photosynthesis. With respiration we observe that UMBS experiences greater sensitivity to T_S (a: HF: -0.10 g C m^{-2}

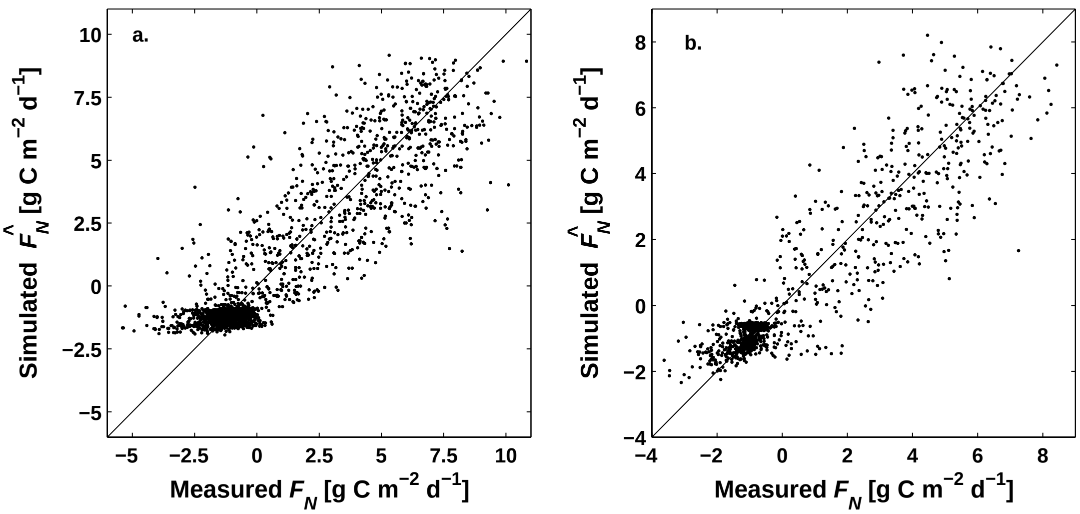

Figure V-4. Results of the model (4a, b and c) calibration and evaluation for F_N for HF 1994 to 1999 (panel **a**, r^2 = 0.80) and UMBS 1999 to 2001 (panel **b**, r^2 = 0.84) plotted against the F_N measurements. Note that the simulated F_N are the sums of the two separately calibrated (and forecasted) fluxes $\hat{F}_G$ and $\hat{F}_R$.

d^{-1} °C^{-1} ± 1.37 x 10^{-3}; UMBS: -0.15 g C m^{-2} d^{-1} °C^{-1} ± 8.39 x 10^{-4}). Finally, we note that the temperature lag for HF is slightly smaller than that for UMBS (4.2 ± 0.26 and 6.9 ± 0.21 days respectively). This presumably reflects the fact that the greater seasonality at the HF site requires a less persistent temperature cue.

V.4 Discussion

Simplified models of canopy behaviour trade on fundamental ordering of biological processes at the organism to community level (Field *et al.* 1995) as well as the potential linearising effects associated with temporal and spatial aggregation. For example, nonlinear relationships observed between incident radiation and leaf photosynthesis can often be subsumed within a much simpler quasi-linear relationship at the whole plant-canopy level due to the optimal allocation of photosynthetic apparatus through the depth of the canopy in parallel with the distribution of light attenuation (Haxeltine & Prentice 1996). Here, the lack of any strong diurnal patterns in the estimated variations in ε would support this observation, and has focused this work on accounting for the more significant seasonal effects using daily data.

So far, we have extracted a site-specific model structure for canopy scale CO_2 fluxes directly from the relevant time series data and have calibrated and provisionally evaluated this model. Previously, calibration of canopy CO_2 flux models has tended to focus on short periods of data where much of the seasonality effects are not observed (e.g., Baldocchi &

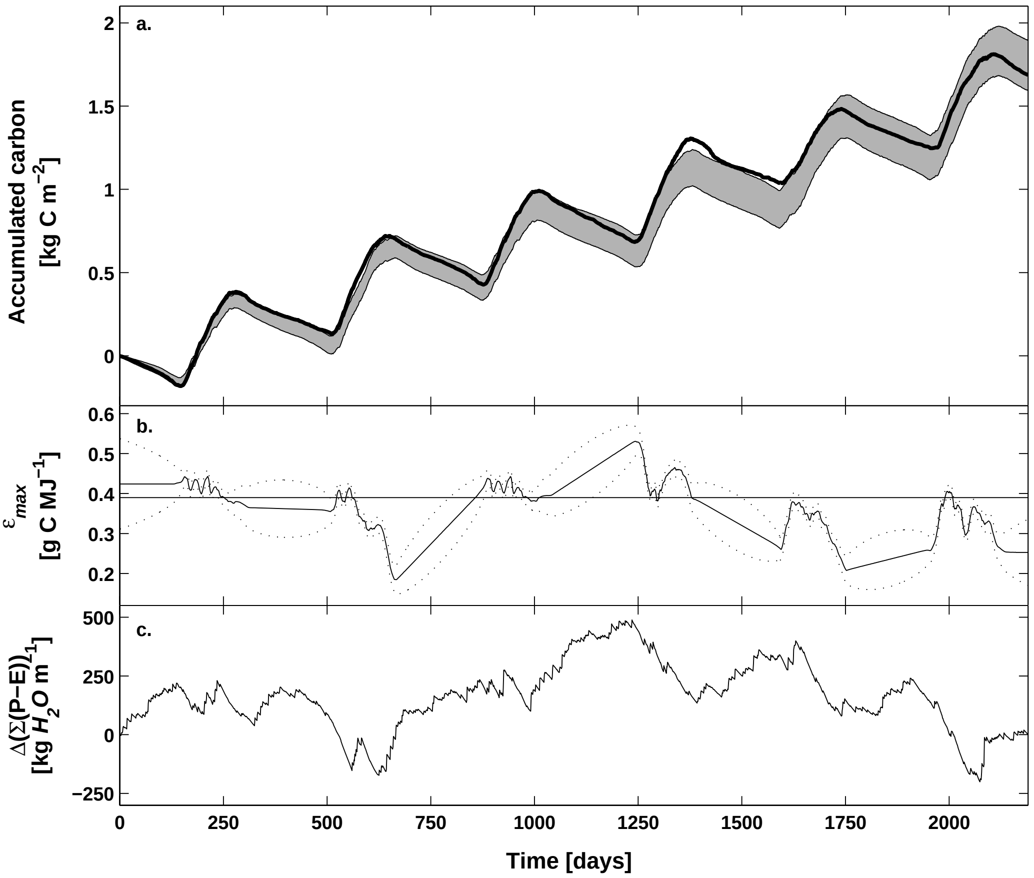

Figure V-5. Forecast of the net carbon accumulation at HF 1994-1999 (panel **a**). The thick solid line denotes the measured net carbon accumulation. The grey patch represents the 95 percent uncertainty band obtained by a Monte Carlo Simulation of (4a, b and c) accommodating both the parametric uncertainty given in Table 1 and the model residual uncertainty (N = 1000). The calibration interval is 1994-1996 whilst the validation interval is 1997-1999. Panel **b** shows the estimated temporal variation of maximum radiation use ε_{max} plotted along with the estimated 95% confidence band. Note the higher uncertainty in the winter estimates as expected. Panel **c** shows the accumulated residual rainfall with the mean trend removed. Here, this is used as an index for water availability as it reflects changes in storage and runoff from the site. Variations in ε_{max} shown in panel **b** are significantly cross-correlated with those in panel **c** with a peak correlation of 0.6 at a lag of 70 days.

Harley 1995; Cox *et al.* 1998; although see Aber *et al.* 1996). Although this may prove attractive when demonstrating the efficacy of a selected model representation, until robust representations for how the model parameters change over a season can be specified, practical implementation of these models to describe other time periods, even at the same site, prove impracticable. Here, despite retaining a credible, if somewhat simplistic, representation of the short-term response of F_N to light, the dominant seasonality effects are explicitly handled through treating them as functions of T_S. As a result, the calibrated model is able to capture a significant proportion of the annual variability in F_G, F_R and hence F_N. Also, because the model is well defined in relation to the calibration data, the associated parameters can be estimated with a known degree of certainty, and genuine probabilistic forecasts can be generated as seen in Figure V-5a.

The observation that (V-4) captures variations in ε that must, in principle, be dependent on variations in both leaf area and intrinsic photosynthetic capacity is interesting. Much of our initial research with this data focused on attempting to disaggregate these two components of ε with only limited success (Stauch 2002), hence the alternative approach is adopted here. One would anticipate that any fortuitous correlations between temperature, leaf area and photosynthetic capacity would only operate during the emergent phase of canopy development (Goudriaan & Monteith 1990) and that, as a result, a pronounced hysteresis could be observed in the relationship between T_S and ε during senescence. The fact that this is not observed for these data would suggest that both the development and senescence of leaf area and photosynthetic capacity are coordinated and strongly related to variations in temperature (Berry & Raison 1981; Sparks & Menzel 2002). This could be explored by disaggregating ε into its light interception and photosynthetic capacity components using, for example, remote sensing information on the fraction of absorbed radiation (Waring *et al.* 1995).

It is a common observation at the leaf scale that F_N falls when temperature exceeds a certain level, and this is a ubiquitous feature of most detailed canopy CO_2 flux models that is not included in (V-4). The fact that this is not observed in Figure V-2a/c may be due to the temperatures having not reached a level where this effect is observable. The response of the canopy being lagged behind surface temperature highlights the dynamic nature of the transduction of temperature signals by these canopies because one would assume that soil-surface temperature already reflects the thermal equilibrium of the canopy-soil system. Such lag effects would suggest that the temperature regulation of leaf development and photosynthetic metabolism involves some form of filtering mechanism (e.g., Berry & Raison 1981; Baldocchi *et al.* 2001a), presumably to remove any unwanted stochastic cues from the environment, hence guarding against the vagaries of the weather.

The annual CO_2 fluxes at both sites are somewhat similar ($\sum \hat{F}_G$: HF (n=6): 928.10 g C a^{-1} ± 8.61; UMBS (n=3): 917.95 g C a^{-1} ± 57.06; $\sum \hat{F}_R$: HF (n=6): -657.84 g C a^{-1} ± 52.08; UMBS (n=3): -663.98 g C a^{-1} ± 8.00). Therefore, the differences in the estimated parameter values represent the differences in how photosynthetic and respiratory activity is distributed over the season. Presumably, this distribution is itself a reflection of the composition of the canopy and its adaptation to the local climatology, hydrology and nutrient availability. Identifying these higher level controls may offer an opportunity to develop the current model beyond its somewhat restricted site specific form.

Obviously one needs to be cautious when using correlations like the ones shown in Figure V-2 to make more general predictions and it is important to understand the connections between these simple representations and the underlying canopy processes they represent if we wish to extend these models to different conditions. For example, it is clear from Figure V-5b and c that drought episodes are capable of affecting the relationship between T_S and ε and should be accommodated into the model structure to improve its predictive properties (Field *et al.* 1995). However, although we endorse the view that an understanding of the underlying processes is important for constructing robust predictions, we also stress the importance of the uncertainties associated with temporal and spatial scaling of processes descriptions (Beven *et al.* 2000) and, therefore, the need to also adopt an inductive model building paradigm that places appropriate emphasis on the observations at the scale of interest. The approach advocated here should not be viewed as purely black box exercise, but instead may be both data-based and mechanistic (Young 2000) through providing an opportunity to include process understanding but only to a level commensurate with the information content of the available data at that scale.

V.5 Conclusions

The proliferation of flux tower sites worldwide has resulted in the collection of large quantities of flux and associated micrometeorological times series data sets. Due to the seasonal nature of the behaviour of plant canopies, these data are often characterised by nonstationary and nonlinear dynamics. This, allied to the inherently uncertain nature of the measurements, results in data that can prove difficult to analyse, especially when it is punctuated by significant measurement gaps.

The novel nonstationary and nonlinear dynamic time series tools applied here appear well suited to both the objective interpolation of missing data and also the signal extraction needed for model formulation. Not surprisingly, the dominant modes of the behaviour of the canopy scale carbon fluxes identified here are clearly related to light and temperature, as it is in process based counterparts to this model. However, in focusing only on the seasonal functionality it is not surprising that the identified model resembles resource capture models such as CASA (Field *et al.* 1995). This does not appear to distract from either the ability to parameterise this model, or its predictive power. Indeed, one could argue that this model has distinct advantages over its process-based counterparts in both cases. The generality of these descriptions obviously needs to be investigated using flux data from a more diverse range of sites.

Even if ones preference is for more complex model formulations, the SDP interpolation over measurement gaps should be viewed as a significant advance over current gap filling practice given that it maximises the retention of information in the interpolated data conditioned only on the available data. However, it seems entirely reasonable to propose that gap filling and model derivation should be closely related as illustrated here, especially if the objective of any such modelling exercise is to provide a robust predictive framework for annual net carbon accumulation.

Acknowledgements

This study is funded by NERC research grant NER/M/S/2002/00074 and by a joint DAAD-British Council travel grant, 1208 awarded to AJ and KS. We would also like to thank Steven Wofsy (principle investigator for HF) and Peter Curtis, Hans Schmid and Christoph Vogel (principle investigators for UMBS) for use of the data, Dr. Eva Falge for stimulating discussions on an early version of this paper and one anonymous referee for their constructive comments.

VI. Discussion and Conclusions

This work set out to derive a modelling methodology that attempts to explore the information content of EC net CO_2 flux time series. In the previous chapters, the potential of this methodology to answer the research questions raised in Chapter I has been explored. In the following, the results of the separate studies shall be integrated into four somewhat overarching subjects to discuss them in a broader context. First, the capacity of the data-led modelling approach to serve as a multiple purposes tool for analysing noisy time series is discussed. Second, the way the data-led model can address limitations in the observations is examined with particular emphasis on data augmentation where data augmentation summarises; replacing missing data, the characterisation of observation noise and the subsequent probabilistic flux integration. Third, the potential of the data-led model to disaggregate the net CO_2 flux into carbon assimilation and respiration is elaborated. Finally, opportunities to derive canopy process understanding from the data with this modelling approach are discussed opening up interesting scope for further research.

VI.1 The data-led modelling approach: potentials and limitations

This thesis presented a modelling methodology that objectively approaches EC data in order to ensure the conservation of the information content for mechanistic interpretation. It is explicitly designed for signal extraction from noisy observation series based on a simplified model structures and minimal prior assumptions. The corresponding model development must be seen as an iterative learning procedure, adding constraints to the model structures incrementally when required. The tight interaction of system understanding and data interrogation leaves enough opportunity to adjust the model structures to the available information in the data as opposed to being committed to a prior assumed fixed parametric structure for the dependencies in question. On the other hand, both modelling techniques applied here allow for a substantial level of control over the nature of the investigated relationships, e.g., by the choice of the number and location of nodes when optimising multidimensional splines or, by the selection of the noise variance ratio, *NVR* when estimating time or state dependent parameters. As a result, this procedure allows for objective model building being in sympathy with the observations held at the particular scale of interest. In this way, prediction uncertainties that inevitably arise when having to constrain a model with observations remain traceable and can ultimately be quantified for e.g., model assessment.

However, such data-led modelling approaches unavoidably suffer from limitations. In line with their development, the derived models are largely only valid within the range of environmental conditions observed, rendering their extrapolation to conditions outside that range somewhat uncertain. Provided the identified relationships are smooth and there is evidence that they can be assumed smooth beyond the observed range, inference can be drawn from these models when employed with care. Obviously, as discussed in Chapter II, the success of this modelling approach will substantially depend on the quality of the data the model development is based upon. The performance of the derived model will therefore suffer from poorly sampled conditions or missing data for potentially important system behaviour. The database used here for model derivation is normally characterised by a dense sampling of current environmental conditions. Additionally, the EC measurement technique is subject to a comprehensive quality control overseen by a large scientific community.

Processes in an ecosystem occur continuously and the diverse factors controlling them naturally operate simultaneously in space and time. As a result, one dimensional data analyses of the response of a system to a selected driver will be disrupted by concurrent effects of other drivers. In Chapter II it was demonstrated that the multiple effects of dominant factors can be objectively extracted from EC data. The estimation of smoothing splines was shown to be particularly suitable for signal extraction because of its interpolating and multidimensional nature. In contrast, binning the relevant environmental data into classes of discrete sizes (e.g., Falge *et al.* 2001; Hollinger *et al.* 2004) will most likely leave dynamic behaviour within the classes being lost for further analyses.

A particular novelty of the data-led CO_2 exchange modelling approach applied here is the explicit consideration of time as a driver. So far, any dynamic in identified relationships such as the response of canopy photosynthesis to light has only been addressed by allowing selected parameters within prescribed model structures to change (Falge *et al.* 2002; Yi *et al.* 2004; Gove & Hollinger 2006). In contrast, the hypersurface approach presented in Chapter II acknowledges a more complex evolution of the dependencies with time whilst providing scope to subsequently infer parametric descriptions. Similarly, the SDP approach applied in Chapter V enabled the investigation of the response of CO_2 assimilation to drivers other than light.

As it is demonstrated particularly in Chapter V, such data based analyses initially resulted in restricted site specific models. A test of their general applicability obviously requires an extensive evaluation on a multiplicity of observation series. However, given the large data set available through FLUXNET we are in a good position to meet this demand. It should be noted that an expansion of the data base used might even elucidate additional controls being important when intending to generalise model structures.

A particular strength of the semi-parametric spline model is its ability to serve more than one application. Estimating the hypersurface from EC observations provides (i) the disaggregation into a systematic signal and a residual series for noise characterisation, (ii) consistent gap-filled estimates allowing for series aggregation to a coarser temporal resolution, (iii) stochastic estimates for ecosystem carbon assimilation, respiration and net exchange components from net flux observations and (iv) a diagnostic tool to objectively study ecosystem functioning and ultimately derive parametric process descriptions on the community level.

Although a detailed comparison is beyond the scope of this thesis, it is interesting to note that both techniques presented here for the hybrid stochastic-mechanistic model derivation produce very similar results when applied to the same model identification problem (e.g., the model structure in Chapter V). This can be viewed as an evaluation of the model structure confirmed by two independent methods showing the data to unambiguously reveal the same systematic behaviour.

It has to be stressed again that the use of synthetic data for rigorous model testing as a routine part of the model development exercise should receive further attention in canopy exchange modelling. In the particular applications presented here (Chapters II, III, IV), this approach proved indispensable as the different components of EC data are only known in this situation thereby facilitating rigorous evaluation.

VI.2 Data augmentation

The previous chapters highlight the substantial value of EC observations for carbon exchange studies and address only a small subsample of their possible applications. However, we have seen that we have to be aware of their stochastic properties when making use of these time series. As EC data represent the sum of two or more unknown components, additional information is by necessity required to determine those components. This work demonstrates that a suitable model can help to overcome this problem and hence to broaden the range of data applications whilst keeping track of the associated uncertainties.

The importance of explicitly addressing observation noise has been somewhat overlooked, although a few methods for noise extraction have been proposed recently (Hollinger *et al.* 2004; Hollinger & Richardson 2005; Richardson *et al.* 2006). These purely data-based approaches highlight the importance of the choice of an appropriate objective function when using these data for parameter optimisation. However, they suffer from coarse stationarity assumptions (Richardson *et al.* 2006) or limited applicability (Hollinger & Richardson 2005). The approach being advocated here (Chapter III) results in estimates of both the deterministic series as a representation of F_N and a semi-parametric characterisation of the stochastic properties of the uncertainty in the F_N observations. Clearly, this model-based characterisation will suffer from uncertainties due to model error and the propagation of input noise. However, as demonstrated in Chapter III, these errors appear to be small compared to the estimated observation noise. It is important to appreciate that this procedure is not restricted to the spline model used in Chapter III. The characterisation of the noise component can rather be based on any model provided no significant systematic signal is left in the model residuals. Therefore, if the spline model proved inappropriate for a particular site, alternative model structures could be applied for the estimation of F_N followed by a noise characterisation.

A characterisation of the observation noise is relevant when replacing missing data. For example, a complete series is required when inferring temporal integrals needed in model derivation, testing and evaluation studies. Given that the observations include one realisation of an unknown random variable, simply replacing missing data in the measurements with a deterministic model (e.g., Goulden *et al.* 1996*a*; Aubinet *et al.* 2000; Falge *et al.* 2001; Law *et al.* 2002; Reichstein *et al.* 2005) will result in a statistically inconsistent series. The derived semi-parametric model in Chapter II delivers a data-led estimate for the systematic F_N while the semi-parametric distributions from the model residuals (Chapter III) provide a means to produce a 'best' estimate for a statically consistent gap-filled time series.

As presented in Chapter III, a full noise characterisation allows us to derive probabilistic temporal (annual) flux integrals based on the estimate of the underlying deterministic flux component and the associated error distributions. In contrast, the straightforward integration of the (half-) hourly noisy measurements to deterministic temporal aggregates (e.g., Lee *et al.* 1999; Aubinet *et al.* 2002; Griffis *et al.* 2003) will give a false impression of accuracy whilst running the risk of significant error propagation. The significant uncertainties due to spatial variation in the turbulent fluxes however (Oren *et al.* 2006) highlight the scope for further research on the representativeness of EC observations for classified biomes (Hargrove *et al.* 2003), in particular when extrapolating the derived values to give regional estimates.

VI.3 Disaggregation of the net flux

The modelling approach introduced in this work facilitates the disaggregation of the EC net CO_2 flux time series into several components. As discussed above, the decomposition of the observations into a systematic signal and a stochastic component is crucial for any further use of these time series despite this having been somewhat overseen in the past. In contrast, the determination of an assimilation component and an estimate for ecosystem respiration from EC data has received a lot of attention, motivated by the demand for these quantities in regional to global ecosystem models and terrestrial carbon inventories. The methodologies applied so far primarily suffer from the oversimplification of the models used for flux disaggregation (Reichstein *et al.* 2005). Similarly, the assumption of a stationary temperature response of ecosystem respiration extrapolating from conditions in the absence of light to the daytime regime has surely to be questioned. Interestingly, the stochastic noise component in EC observations has not been consistently addressed in such studies. The approach presented in this work successfully addresses some of these limitations. Firstly, the semi-parametric model is constrained by all available data avoiding a somewhat truncated data analysis. The resulting hypersurface is then used to derive a light-independent seasonal response to temperature that is referred to as 'ecosystem respiration'. Secondly, the multidimensional nature of the spline model implicitly allows the components to evolve with several drivers simultaneously and, hence, includes the required additional complexity. Thirdly, given the characterised EC observation noise from Chapter III and the parameter covariance structure from the model optimisation, observation and parameter uncertainty can be traced throughout the disaggregation. The decomposed fluxes F_G and F_R may serve further disaggregation, signal extraction and model derivation, testing and evaluation (see next section). Alternatively, probabilistic flux integrals can be inferred from these quantities as is required for carbon budget studies and/or cross-site analyses (see Chapter III and IV). It will be interesting to compare the disaggregation scheme introduced in this study particularly with other nonparametric approaches such as artificial neural networks (Papale & Valentini 2004; Braswell *et al.* 2005). Such an intercomparison is currently underway (Moffat *et al.* 2006).

VI.4 Opportunities for inferences on canopy behaviour and parametric models

The semi-parametric hypersurfaces are unique in their multidimensional representation of the variations in the carbon exchange fluxes (e.g., F_N, F_G, F_R). Given that experiments on the canopy level in controlled environments inevitably accompany substantial financial investment, such set ups are rare and the data availability is limited as a result (e.g., Ellsworth *et al.* 1995; Osmond *et al.* 2004). Therefore, the semi-parametric modelling approach offers a readily available (cheap) alternative for a diagnostic analysis of the responses of carbon fluxes to separate drivers based on EC data, provided these signals can be extracted from the data.

Figure VI-1 shows the derived F_R surface and the remaining F_G hypersurface for the SPA simulation data set (see Chapters II-IV) that could provide a basis for further characterisation of the flux components. Obviously, a comprehensive analysis is beyond the scope of this thesis, but it is worthwhile pointing out scope for further investigation. It has to be noted again that these studies will only prove beneficial when initially working with an entirely known system, i.e. synthetic data from a simulation model. One obvious objective would be to explore the separate dependencies to light, temperature or time under fixed environmental conditions. Here, all the complexity and interaction implemented in the simulation model is unlikely to be uncovered by the simple spline model structure. Therefore, the investigation should focus on specific aspects of canopy carbon exchange. For instance, the F_G hypersurface in Figure VI-1a allows for the identification of the temporal evolution of the light response curve at different temperature levels. It would be interesting to investigate how this dynamic might be related to downregulations of photosynthesis due to environmental factors, e.g., as represented in production efficiency models (e.g., Potter *et al.* 1993; Runyon *et al.* 1994). Another aspect of interest related to this could be the investigation of the temperature optimum of photosynthesis at light saturation as deduced from the F_G hypersurface. Here, the temporal evolution of this value could provide information on possible downregulations due to limiting environmental conditions or the plasticity of this property in response to shifts in the background meteorological conditions (Berry & Bjorkman 1980). Obviously, this is only a small subsample of a wide range of research questions the hypersurfaces invite.

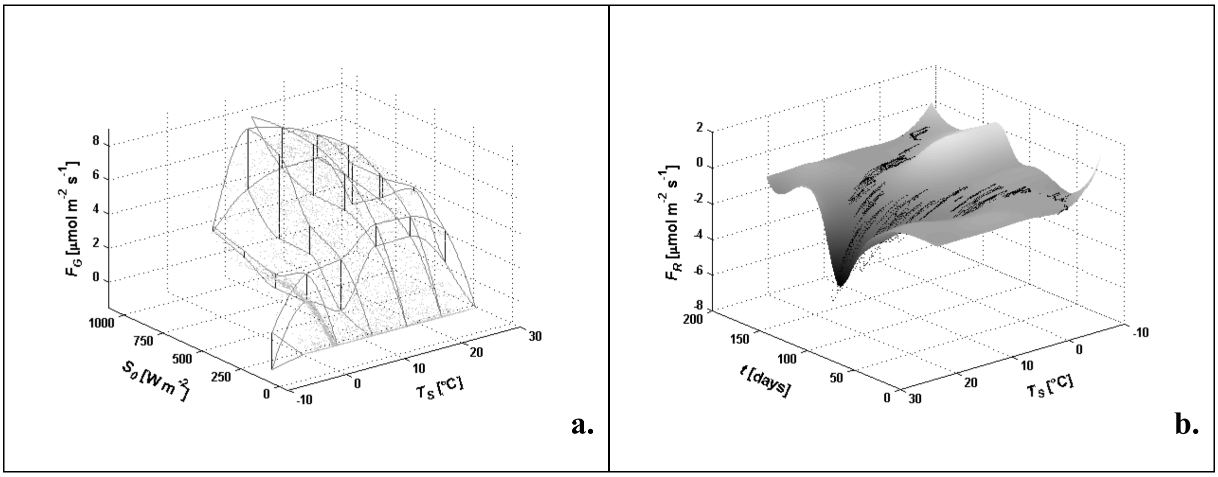

Figure VI-1: Gross photosynthetic uptake, F_G as a function of light, temperature and time (a) and ecosystem respiration, F_R as a function of temperature and time (b) derived from the SPA synthetic data. The simulated 'true' components are added as grey dots.

The success of the multidimensional spline model to explain the variations in F_N during the day and over the year endorses the three driving forces, light, temperature and time as being major regulating factors in many ecosystems. However, owing to the flexible nature of the splines, other controls might be confronted. Provided all variations in the response to incident radiation and temperature have been accounted for in the light and temperature dimension of the hypersurface, the variations in F_N in the temporal space will reflect a conglomeration of the effects of all other environmental drivers. For example, the semi-parametric spline model as implemented here does not explicitly account for the effects of water limitations over and above that of the climatic mean. As a result, any medium term effects of dry periods will be projected onto the estimated phenological evolution of the canopy. Such model inadequacies might become obvious when analysing the residuals similar to those shown in Chapter V for LUE_{max} when allowed to vary over time. Water limited sites have not been a particular focus of this study and the estimation of the splines from such data might suggest choosing different environmental drivers. Such changes of drivers could be readily incorporated into the spline framework and tested for appropriate data providing relevant measures of the drivers were available for the sites in question.

As has been demonstrated in Chapter V, semi- and nonparametric modelling techniques provide a promising framework for exploring the derivation of simple parametric model structures to explain the variations in ecosystem exchange data. While the nature of the modelling approach ensures the data support during the model derivation, the physical interpretation of the semi- or nonparametric relationships demands some considerable comprehension of the system. Fortunately, understanding of plant scale processes including resource use efficiency provide a valuable source to draw from. Therefore, this approach to model derivation can be seen as complementary to both purely process based modelling and simple ‘top down’ approaches, as they are commonly applied when assimilating remote sensing information. The tight coupling between CO_2 uptake and water loss through stomatal control for instance could be explored in a similar way while also making use of some products of this work as already indicated by the correlation of LUE_{max} and the index for water availability shown in Chapter V.

As we have seen, temporal aggregation of the observations is likely to result in simpler model structures. The daily model for the net CO_2 flux in Chapter V for instance, could be reduced to two dimensions compared to the three dimensional hypersurface based on hourly data (Chapters II, III, IV). On the other hand, valuable information might get lost due during data aggregation (van Wijk & Bouten 2002). This dilemma highlights the importance of defining research question(s) prior to any model development (Goldenfeld & Kadanoff 1999). The data being used for the analysis can then be chosen appropriately.

Given the data availability for FLUXNET sites in a range of vegetation and climate conditions, the generality of the derived model structures can be extensively tested in order to assess the predictive performance. Obviously, for a rigorous test of the temperature dependent light-use efficiency model presented in Chapter V, the available resources on different biomes were not exhausted. It is, therefore, appealing to evaluate the model for more EC tower locations and subsequently to relate the differences in the derived parameters to biome information and site characteristics. Such relationships might then pave the way for regionalised models for the CO_2 exchange between the vegetated surface and the atmosphere derived from EC observations.

Finally, it is worthwhile noting that, in line with the iterative model building philosophy used here, the semi-parametric modelling approach provides the framework to include more process information. This could be afforded by replacing selected parts of the spline model with particular parametric structures. In this way, physical process understanding would be linked with information in the data progressively, leading to full parametric models commensurate with the observations at the scale of interest.

VII. References

Aber JD, Reich PB, Goulden ML (1996) Extrapolating leaf CO2 exchange to the canopy: a generalized model of forest photosynthesis compared with measurements by eddy correlation. *Oecologia*, **106**, 257-265.

Amthor JS, Goulden ML, Munger JW, Wofsy SC (1994) Testing a mechanistic model of forest-canopy mass and energy exchange using eddy correlation: carbon dioxide and ozone uptake by a mixed-oak stand. *Australian Journal of Plant Physiology*, **21**, 623-651.

Anthoni PM, Law BE, Unsworth MH (1999) Carbon and water vapor exchange of an open-canopied ponderosa pine ecosystem. *Agricultural and Forest Meteorology*, **95**, 151-168.

Anthoni PM, Unsworth MH, Law BE, Irvine J, Baldocchi DD, Moore D (2002) Seasonal differences in carbon and water vapor exchange in young and old-growth ponderosa pine ecosystems. *Agricultural and Forest Meteorology*, **111**, 203-222.

Anthoni PM, Knohl A, Rebmann C *et al.* (2004) Forest and agricultural land-use-dependent CO_2 exchange in Thuringia, Germany. *Global Change Biology*, **10**, 2005-2019.

Aubinet M, Grelle A, Ibrom A *et al.* (2000) Estimates of the annual net carbon and water exchange of forests: the EUROFLUX methodology. *Advances in Ecological Research*, **30**, 113-175.

Aubinet M, Heinesch B, Longdoz B (2002) Estimation of the carbon sequestration by a heterogeneous forest: night flux corrections, heterogeneity of the site and inter-annual variability. *Global Change Biology*, **8**, 1053-1071.

Baldocchi DD, Verma SB, Anderson DE (1987) Canopy photosynthesis and water use efficiency in a deciduous forest. *Journal of Applied Ecology*, **24**, 251-260.

Baldocchi DD, Hicks BB, Meyers TP (1988) Measuring biosphere-atmosphere exchanges of biologically related gases with micrometeorological methods. *Ecology*, **69**, 1331-1340.

Baldocchi DD (1993) Scaling Water Vapor and Carbon Dioxide Exchange from Leaves to a Canopy: Rules and Tools. In: *Scaling Physiological Processes: leaf to Globe*. (eds. Ehleringer JR, Filed CB), pp. 77-114. Academic Press, San Diego, California.

Baldocchi DD, Harley PC (1995) Scaling carbon dioxide and water vapour exchange from leaf to canopy in a deciduous forest. II. Model testing and application. *Plant, Cell and Environment*, **18**, 1157-1173.

Baldocchi DD, Valentini R, Running S, Oechel W, Dahlman R (1996) Strategies for measuring and modelling carbon dioxide and water vapour fluxes over terrestrial ecosystems. *Global Change Biology*, **2**, 159-168.

Baldocchi DD, Falge E, Wilson K (2001*a*) A spectral analysis of biosphere-atmosphere trace gas flux densities and meteorological variables across hour to multi-year time scales. *Agricultural and Forest Meteorology,* **107**, 1-27.

Baldocchi DD, Falge E, Gu L *et al.* (2001*b*) FLUXNET: a new tool to study the temporal and spatial variability of ecosystem-scale carbon dioxide, water vapor and energy flux densities. *Bulletin of the American Meteorological Society*, **82**, 2415-2434.

Baldocchi DD (2003) Assessing the eddy covariance technique for evaluating carbon dioxide exchange rates of ecosystems: past, present and future. *Global Change Biology*, **9**, 479-492.

Ball JT, Woodrow IE, Berry JA (1987) A model predicting stomatal conductance and its contribution to the control of photosynthesis under different environmental conditions. In: *Progress in Photosynthesis Research*. (eds Biggens J), pp. 221–224, Martinus Nijhoff, CZ Zoetermeer, Netherlands.

Barford CC, Wofsy SC, Goulden ML et al. (2001) Factors controlling long- and short-term sequestration of atmospheric CO_2 in a mid-latitude forest. *Science*, **294**, 1688-1691.

Berry JA, Björkman O (1980) Photosynthetic response and adaptation to temperature in higher plants. *Annual Review of Plant Physiology and Plant Molecular Biology*, **31**, 491-543.

Berry JA, Raison JK (1981) Responses of macrophytes to temperature. In: *Physiological Plant Ecology I: Responses to the Physical Environment* (eds Lange OL, Nobel PS, Osmond CB, Ziegler H), **12A,** 277-338, Springer-Verlag, Berlin, Heidelberg, New York.

Beven K, Schulz K, Franks S (2000) The use of generalised likelyhood measures for uncertainly estimation in high-order models of environmental systems. In: J. Feyen and K. Wiyo (Editors), Proceedings Leuven InternationalWorkshop: *Modelling of Transport Processes in Soils at Various Scales in Time and Space*. Institute of Land and Water Management. Katoliek University Leuven, Belgium. pp. 725 - 735.

Black TA, DenHartog G, Neumann HH *et al.* (1996) Annual cycles of water vapour and carbon dioxide fluxes in and above a boreal aspen forest. *Global Change Biology*, **2** (3), 219-229.

Canadell JG, Mooney HA, Baldocchi DD *et al.* (2000) Carbon Metabolism of the Terrestrial Biosphere: a Multitechnique Approach fro Improved Understanding. *Ecosystems*, **3**, 115-130.

Churkina G, Tenhunen J, Thornton P *et al.* (2003) Analysing the Ecosystem Carbon Dynamics of Fout European Coniferous Forests Using a Biogeochemistry Model. *Ecosystems*, **6**, 168-184.

Cox PM, Huntingford C, Harding RJ (1998) A canopy conductance and photosynthesis model for use in a GCM land surface scheme. *Journal of Hydrology*, **212-213**, 79-94.

Curtis PS (2003) UMBS Forest Carbon Cycle Research. UMBS research. Ameriflux network. UMBS data access. http://cdiac.esd.ornl.gov/ftp/ameriflux/data/us-sites/preliminary-data/UMBS (data accessed on February 14, 2003).

Curtis PS, Hanson PJ, Bolstad P, Barford C, Randolph JC, Schmid HP, Wilson KB (2002) Biometric and eddy-covariance based estimates of annual carbon storage in five eastern North American deciduous forests. *Agricultural and Forest Meteorology*, **113**, 3-19.

Davidson EA, Belk E, Boone RD (1998) Soil water content and temperature as independent or confounded factors controlling soil respiration in a temperate mixed hardwood forest. *Global Change Biology*, **4**, 217-227.

de Boor C (1978, 2001) *A Practical Guide to Splines*, rev. ed (eds Marsden JE, Sirovich L), Springer-Verlag, New York, Berlin, Heidelberg, 346 pp.

de Pury DGG, Farquhar GD (1997) Simple scaling of photosynthesis from leaves to canopies without the errors of big-leaf models. *Plant, Cell and Environment*, **20**, 537-557.

Desjardins RL, MacPherson JI, Mahrt L, Schuepp P, Pattey E, Neumann H, Baldocchi DD, Wofsy S, Fitzjarrald D, McCaughey H, Joiner DW (1997) Scaling up flux measurements for the boreal forest using aircraft-tower combinations. *Journal of Geophysical Research-Atmospheres,* **102**, D24, 29125-29133.

Dewar RC (1997) A Simple Model of Light and Water Use Evaluated for *Pinus radiata*. *Tree Physiology*, **17**, 259-265.

Dewar RC, Medlyn BE, Mc Murtrie RE (1998) A mechanistic analysis of light and carbon use efficiencies. *Plant, Cell and Environment*, **21**, 573-588.

Dickinson RE, Henderson-Sellers A, Kenedy PJ, Wilson MF (1986) NCAR Tech. Note NCAR/TN-275+STR, *National Center for Atmospheric Research*, Boulder, Colorado.

Drake BG, Gonzalez-Meler MA, Long SP (1997) More efficient plants: a consequence of rising atmospheric CO_2? *Annual Review of Plant Physiology and Plant Molecular Biology*, **48**, 609-639.

Ehleringer JR, Björkman O (1977) Quantum yields for CO_2 uptake in C3 and C4 plants – dependence on temperature, CO_2 and O_2 concentration. *Plant Physiology*, **59** (1), 86-90.

Ellsworth DS, Oren R, Huang C et al. (1995) Leaf and canopy responses to elevated CO_2 in a pine forest under free-air CO_2 enrichment. *Oecologia*, **104** (2), 139-146.

Falge E, Baldocchi DD, Olson R *et al.* (2001) Gap filling strategies for defensible annual sums of net ecosystem exchange. *Agricultural and Forest Meteorology*, **107**, 43-69.

Falge E, Baldocchi DD, Tenhunen J *et al.* (2002) Seasonality of ecosystem respiration and gross primary production as derived from Fluxnet measurements. *Agricultural and Forest Meteorology*, **113**, 53-74.

Fang C, Moncrieff JB (2001) The dependence of soil CO_2 efflux on temperature. *Soil Biology & Biochemistry*, **33**, 155-165.

Farquhar GD, von Caemmerer S, Berry JA (1980) A Biochemical Model of Photosynthetic CO_2 Assimilation in Leaves of C_3 Species. *Planta*, **149**, 78-90.

Farquhar GD, von Caemmerer S (1982) Modelling of Photosynthetic Response to Environmental Conditions. In: *Physiological Plant Ecology II, Water Relations and Cabon Assimilation.* (eds Lange OL, Nobel PS, Osmond CB, Ziegler H). Encyclopedia of Plant Physiology, New Series, Volume **12B**, pp. 549-587, Springer-Verlag, Berlin.

Field CB, Randerson JT, Malmström CM (1995) Global net primary production: combining ecology and remote sensing. *Remote Sensing of the Environment*, **51**, 74-88.

Finkelstein PL, Sims PF (2001) Sampling error in eddy correlation flux measurements. *Journal of Geophysical Research*, **106**, NO. D4, 3503-3509.

Franks SW, Beven KJ (1997) Bayesian estimation of uncertainty in land surface-atmosphere flux predictions. *Journal of Geophysical Research*, **102** (D20), 23991–23999.

Franks SW, Beven KJ, Quin PF, Wright IR (1997) On the sensitivity of soil-vegetation-atmosphere transfer (SVAT) schemes: equifinality and the problem of robust calibration. *Agricultural and Forest Meteorology*, **86**, 63–75.

Friend AD (2001) Modelling canopy CO_2 fluxes: are 'big leaf' simplifications justified? *Global Ecology & Biogeography*, **10**, 603-619.

Friend AD, Arneth A, Kiang NY *et al.* (2006) Fluxnet and modeling the global carbon cycle. *Global Change Biology*, **12**, doi: 10.1111/j.1365-2486.2006.01223.x

Fritsch FN, Carlson RE (1980) Monotone Piecewise Cubic Interpolation, *SIAM Journal on Numerical Analysis*, **17** (2), 238-246.

Gilmanov TG, Verma SB, Sims PL *et al.* (2003) Gross primary production and light response parameters of four Southern Plains ecosystems estimated using long-term CO2-flux tower measurements. *Global Biogeochemical Cycles*, **17** (2), art. No. 1071.

Goldenfeld N, Kadanoff LP (1999) Simple Lessons from Complexity. *Science*, **284**, 87-89.

Goudriaan J, Monteith JL (1990) A mathematical function for crop growth based on light interception and leaf area data. *Annals of Botany*, **66**, 695-701.

Goulden ML, Munger JW, Fan S-M, Daube BC, Wofsy SC (1996*a*) Exchange of Carbon Dioxide by a Deciduous Forest: Response to Interannual Climate Variability. *Science*, **271**, 1576-1578.

Goulden ML, Munger JW, Fan S-M, Daube BC, Wofsy SC (1996*b*) Measurements of carbon sequestration by long-term eddy covariance: methods and a critical evaluation of accuracy. *Global Change Biology*, **2**, 169-182.

Gove JH, Hollinger DY (2006) Application of a dual unscented Kalman filter for simultaneous state and parameter estimation in problems of surface-atmosphere exchange. *Journal of Geophysical Research*, **111** (D8), Art. No. D08S07, doi: 10.1029/2005JD006021.

Granger CWJ, Terasvirta T (1993) *Modelling nonlinear economic relationships*. Oxford University press, Oxford, 187 pp.

Granier A, Ceschia A, Damesin C *et al.* (2000) The carbon balance of a young Beach forest. *Functional Ecololgy*, **14**, 312-325.

Grieser J, Schönwiese C-D (2001) Process, Forcing, and Signal Analysis of Global Mean Temperature Variations by Means of a Three-Box Energy Balance Model. *Climatic Change*, **48**, 617-646.

Griffis TJ, Black TA, Morgenstern K et al. (2003) Ecophysiological controls on the carbon balances of three southern boreal forests. *Agricultural and Forest Meteorology*, **117**, 53-71.

Grünwald T, Bernhofer C (2000) Regression modelling used for data gap filling of carbon flux measurements. In: *Forest ecosystem modelling, upscaling and remote sensing.* (eds Ceulemans RLM, Veroustraete F, Gond V, Van Rensbergen JBHF), pp. 61-67. SPB Academic Publishing bv, The Hague, The Netherlands.

Grünzweig JM, Lin T, Rotenberg E, Schwartz A, Yakir D (2003) Carbon sequestration in arid-land forest. *Global Change Biology*, **9** (5), 791-799.

Hagen SC, Braswell BH, Linder E, Frolking S, Richardson AD, Hollinger AD (2006) Statistical uncertainty of eddy flux-based estimates of gross ecosystem carbon exchange at Howland Forest, Maine. *Journal of Geophysical Research*, **111**(D8), D08S03, doi:10.1029/2005JD006154.

Hanson PJ, Wullschleger SD, Bohlman SA, Todd DE (1993) Seasonal and topographic patterns of forest floor CO_2 efflux from an upland oak forest. *Tree Physiology*, **13**, 1-15.

Hargrove WW, Hoffman FM, Law BE (2003) New analysis reveals representativeness of the Ameriflux network. *EOS Transactions, American Geophysical Union*, **84** (48), 529-544.

Haxeltine A, Prentice IC (1996) A general model for the light-use efficiency of primary production. *Functional Ecology*, **10**, 551-561.

Hollinger DY, Kelliher FM, Schulze E-D et al. (1998) Forest-atmosphere carbon dioxide exchange in eastern Siberia. *Agricultural and Forest Meteorology*, **90**, 291-306.

Hollinger DY, Aber J, Dail B *et al.* (2004) Spatial and temporal variability in forest-atmosphere CO_2 exchange. *Global Change Biology*, **10** (10), 1689-1706.

Hollinger DY, Richardson AD (2005) Uncertainty in eddy covariance measurements and its applications to physiological models. *Tree Physiology*, **25**, 873-885.

Hollinger SE, Bernacchi CJ, Meyers TP (2005) Carbon budget of mature no-till ecosystem in North Central Region of the United States. *Agricultural and Forest Meteorology*, **130**, 59-69.

Hui D, Wan S, Su B, Katul G, Monson R, Luo Y (2004) Gap-filling missing data in eddy covariance measurements using multiple imputation (MI) for annual estimations. *Agricultural and Forest Meteorology*, **121**, 93-111.

Hutley LB, Leuning R, Beringer J, Cleugh HA (2005) The utility of the eddy covariance technique as a tool in carbon accounting: tropical savanna as a case study. *Australian Journal of Botany*, **53** (7), 663-675.

Janssens IA, Freibauer A, Ciais P *et al.* (2003) Europe's Terrestrial Biosphere Absorbs 7 to 12% of the European Anthropogenic CO_2 Emissions. *Science*, **300**, 1538-1542.

Jarvis PG (1995) Scaling processes and problems. *Plant, Cell and Environment*, **18**, 1079-1089.

Jarvis PG, Dewar RC (1993) Forests in the Global Carbon Balance: From Stand to Region. In: *Scaling Physiological Processes: leaf to Globe*. (eds. Ehleringer JR, Filed CB), pp. 191-221. Academic Press, San Diego, California.

Jones HG (1983) *Plants and Microclimate*. Cambridge University Press, Cambridge, 323 pp.

Kaplan EL, Meier P (1958) Nonparametric Estimation from Incomplete Observations. *Journal of the American Statistical Association*, 53 (282), 457-481.

Kavetski D, Franks SW, Kuczera G (2002) Confronting Input Uncertainty in Environmental Modelling, in *Calibration of Watershed Models*, *AGU Water Science and Applications Series*, vol. 6, edited by Q. Duan, H. V. Gupta, S. Sorooshian, A. N. Rousseau, R. Turcotte, pp 49-68, AGU, Washington, D. C.

Keeling RF, Piper SC, Heimann M (1996) Global and hemispheric CO_2 sinks deduced from changes in atmospheric O_2 concentration. *Nature*, **381**, 218-221.

Knohl A, Schulze E-D, Kolle O, Buchmann N (2003) Large carbon uptake by an unmanaged 250-year-old deciduous forest in central Germany. *Agricultural and Forest Meteorology*, **118**, 151-167.

Knorr W (1997) Satellite remote sensing and modeling of the global CO_2 exchange of land vegetation: a synthesis. PhD thesis, Max Planck Institute for Meteorology, Hamburg.

Knorr W (2000) Annual and interannual CO_2 exchanges for the terrestrial biosphere: process based simulations and uncertainties. *Global Ecology and Biogeography*, **9**, 225-252.

Knorr W, Kattge J (2005) Inversion of terrestrial ecosystem model parameter values against eddy covariance measurements by Monte Carlo sampling. *Global Change Biology*, **11**, 1333-1351.

Lavigne MB, Ryan MG, Anderson DE, *et al.* (1997) Comparing nocturnal eddy covariance measurements to estimates of ecosystem respiration made by scaling chamber measurements at six coniferous boreal sites. *Journal of Geophysical Research*, **102** (D24), 28977-28985.

Law BE, Baldocchi DD, Anthoni PM (1999) Below-canopy and soil CO_2 fluxes in a ponderosa pine forest. *Agricultural and Forest Meteorology*, **94**, 171-188.

Law BE, Falge E, Gu L *et al.* (2002) Environmental controls over carbon dioxide and water vapor exchange of terrestrial vegetation. *Agricultural and Forest Meteorology*, **113** (1-4), 97-120.

Law BE, Thornton P, Irvine J, Van Tuyl S, Anthoni P (2001) Carbon storage and fluxes in ponderosa pine forests at different developmental stages. *Global Change Biology*, **7** (7), 755-777.

Lee X, Fuentes JD, Staebler RM, Neumann HH (1999) Long-term observation of the atmospheric exchange of CO_2 with a temperate deciduous forest in southern Ontario, Canada. *Journal of Geophysical Research*, **104** (D13), 15975-15984.

Lenschow DH, Mann J, Kristensen L (1994) How long is long enough when measuring fluxes and other turbulence statistics? *Journal of Atmospheric and Oceanic Technology*, **11**, 661-673.

Leuning R, Kelliher FM, de Pury DGG *et al.* (1995) Leaf nitrogen, photosynthesis, conductance and transpiration: scaling from leave to canopies. *Plant, Cell and Environment*, **18**, 1183-1200.

Leuning R, Dunin FX, Wang Y-P (1998) A two-leaf model for canopy conductance, photosynthesis and partitioning of available energy. II. Comparison with measurements. *Agricultural and Forest Meteorology*, **91**, 113-125.

Leuning R, Cleugh HA, Zegelin SJ, Hughes D (2005) Carbon and water fluxes over a temperate *Eucalyptus* forest and a tropical wet/dry savanna in Australia: measurements and comparison with MODIS remote sensing estimates. *Agricultural and Forest Meteorology*, **129** (3-4), 151-173.

Linder S, Flower-Ellis JGK (1992) Environmental and physiological constraints to forest yield. In: *Responses of Forest Ecosystems to Environmental Changes.* (eds Teller A, Mathy P, Jeffers JNR), pp 149-164. Elsevier, London.

Lindroth A, Grelle A, Moren AS (1998) Long-term measurements of boreal forest carbon balance reveal large temperature sensitivity. *Global Change Biology*, **4** (4), 443-450.

Lloyd J, Taylor JA (1994) On the temperature dependence of soil respiration. *Functional Ecology*, **8**, 315-323.

Lloyd J, Grace J, Miranda AC *et al.* (1995) A simple calibrated model of Amazon rainforest productivity based in leaf biochemical properties. *Plant, Cell and Environment*, **18**, 1129-1145.

Lobell DB, Hicke JA, Asner GP, Field CB, Tucker CJ, Loss SO (2002) Satellite estimates of productivity and light use efficiency in United States agriculture, 1982-98. *Global Change Biology*, **8**, 722-735.

Mahrt L (1998) Flux Sampling Errors for Aircraft and Towers. *Journal of Atmospheric and Oceanic Technology*, **15**, 416-429.

Mann J, Lenschow DH (1994) Errors in airborne flux measurements. *Journal of Geophysical Research*, **99** (D7), 14519-14526.

Medlyn BE, Robinson AP, Clement R, McMurtrie RE (2005) On the validation of models of forest CO_2 exchange using eddy covariance data: some perils and pitfalls. *Tree Physiology*, **25**, 839-857.

Meyers TP, Hollinger SE (2004) An assessment of storage terms in the surface energy balance of maize and soybean. *Agricultural and Forest Meteorology*, **125**, 105-115.

Moffat A, Papale D, Reichstein M *et al.* (2006) http://www.bgc-jena.mpg.de/~antje.moffat/, gap filling comparison.

Mohr C (2004) *Numerical Computing with Matlab*, Society for Industrial and Applied Mathematics, Philadelphia, 354 pp.

Moncrieff JB, Mahli Y, Leuning R (1996) The propagation of errors in long-term measurements of land-atmosphere fluxes of carbon and water. *Global Change Biology*, **2** (3), 231-240.

Monteith JL (1972) Solar radiation and productivity in tropical ecosystems. *Journal of Applied Meteorology*, **9**, 747-766.

Monteith JL (1977) Climate and the efficiency of crop production in Britain. *Philosophical Transactions of the Royal Society*, Series B, **281**, 277–294.

Monteith JL, Huda AKS, Midya D (1989) Modelling Sorghum and Pearl Millet. RESCAP: A resource capture model for Sorghum and Pearl Millet. In: *Modelling the Growth and Development of Sorghum and Pearl Millet.* (eds Vilmani SM, Tandon HLS, Algarswamy G), ICRISAT Research Bulletin, Patanchern, India, pp. 31-34.

Monteith JL, Unsworth M (1973, 1990) *Principles of Environmental Physics*, 2nd ed., Butterworth- Heinemann, Oxford, 291 pp.

Monteith JL (1995) Accommodation between transpiring vegetation and the convective boundary-layer. *Journal of Hydrology,* **166**, 251-263.

Moore CJ (1986) Frequency response corrections for eddy covariance systems. *Boundary Layer Meteorology*, **37**, 17-35.

Morgenstern K, Black TA, Humphreys ER *et al.* (2004) Sensitivity of the carbon balance of a Pacific Northwest Douglas-fir forest during an el Niño/La Niña cycle. *Agricultural and Forest Meteorology*, **123**, 201-219.

Nemry B, Francois L, Gerard JC *et al.* (1999) Comparing global models of terrestrial primary productivity (NPP): analysis of the seasonal atmospheric CO_2 signal. *Global Change Biology*, **5** (Suppl. 1), 65-76.

Oren R, Hsieh C-I, Stoy P, Albertson J, McCarthy HR, Harrell P, Katul GG (2006) Estimating the uncertainty in annual net ecosystem carbon exchange: spatial variation in turbulent fluxes and sampling errors in eddy-covariance measurements. *Global Change Biology*, **12**, 883-896.

Osmond B, Ananyev G, Berry J et al. (2004) Changing the way we think about global change research: scaling up in experimental ecosystem science. *Global Change Biology*, **10**, 393-407.

Papale D, Valentini R (2003) A new assessment of European forests carbon exchanges by eddy fluxes and artificial neural network spatialization. *Global Change Biology*, **9** (4), 525-535.

Pilegaard K, Hummelshoj P, Jensen NO, Chen Z (2001) Two years of continuous CO2 eddy-flux measurements over a Danish beech forest. *Agricultural and Forest Meteorology*, **107**, 29-41.

Potter CS, Randerson JT, Field CB et al. (1993) Terrestrial ecosystem production: a model based on global satellite and surface data. *Global Biogeochemical Cycles*, **7** (4), 811-841.

Press WH, Flannery BP, Tenkolsky SA, Vetterling WT (1988, 1992) *Numerical Recipes in C: The Art of Scientific Computing*, 2nd ed., Cambridge University Press, Cambridge, New York, Port Chester, Melbourne, Sydney, 994 pp.

Rambal S, Ourcival J-M, Joffre R, Mouillot F, Nouvellon Y, Reichstein M, Rocheteau A (2003) Drought controls over conductance and assimilation of a Mediterranean evergreen ecosystem: scaling from leaf to canopy. *Global Change Biology*, **9** (12), 1813-1824.

Raupach MR, Rayner PJ, Barrett DJ et al. (2005) Model-data synthesis in terrestrial carbon observation: methods, data requirements and data uncertainty specifications. *Global Change Biology*, **11**, 378-397.

Rayment MB, Loustau D, Jarvis PG (2002) Photosynthesis and respiration of black spruce at three organizational scales: shoot, branch and canopy. *Tree Physiology*, **22**, 219-229.

Reich PB, Turner DP, Bolstad P (1999) An Approach to Spatially Distributed Modelling of Net Primary Production (NPP) at the Landscape Scale and Its Application in Validation of EOS NPP Products. *Remote Sensing of the Environement*, **70**, 69-81.

Reichstein M, Tenhunen JD, Roupsard O *et al.* (2002) Severe drought effects on ecosystem CO_2 and H_2O fluxes at three Mediterranean evergreen sites: revision of current hypothesis? *Global Change Biology*, **8** (10), 999-1017.

Reichstein M, Falge E, Baldocchi DD *et al.* (2005) On the separation of net ecosystem exchange into assimilation and ecosystem respiration: review and improved algorithm. *Global Change Biology*. **11** (9), 1424-1439.

Reithmaier LM, Gockede M, Markkanen T, Knohl A, Churkina G, Rebmann C, Buchmann N, Foken T (2006) Use of remotely sensed land use classification for a better evaluation of micrometeorological flux measurement sites. *Theoretical and Applied Climatology*, **84** (4), 219-233.

Renewable Resource Data Center (RreDC) (2003) National Renewable Energy Laboratory. Solar Radiation Resource Information, US Department of Energy. http://rredc.nrel.gov/solar/ (accessed on April 3, 2003).

Richardson AD, Hollinger DY (2005) Statistical modelling of ecosystem respiration using eddy covariance data: Maximum likelihood parameter estimation, and Monte Carlo simulation of model and parameter uncertainty, applied to three simple models. *Agricultural and Forest Meteorology*, **131**, 191-208.

Richardson AD, Hollinger DY, Burba GG *et al.* (2006) A multi-site analysis of random error in tower-based measurements of carbon and energy fluxes. *Agricultural and Forest Meteorology*, **136**, 1-18.

Roderick ML, Farquhar GD, Berry SL, Noble IR (2001) On the direct effect of clouds and atmospheric particles on the productivity and structure of vegetation. *Oecologia*, **129** (1), 21-30.

Ruimy A, Jarvis PG, Baldocchi DD, Saugier B (1995) CO_2 fluxes over plant canopies and solar radiation: a review. *Advances in Ecological Research*, **26**, 1-68.

Ruimy A, Kergoat L, Field CB, Saugier B (1996) The use of CO_2 flux measurements in models of the global terrestrial carbon budget. *Global Change Biology*, **2**, 287-296.

Running SW, Baldocchi DD, Turner DP, Gower ST, Bakwin PS, Hibbard KA (1999) A global terrestrial monitoring network integrating tower fluxes, flask sampling, ecosystem modeling and EOS satellite data. *Remote Sensing of Environment*, **70** (1), 108-127.

Running SW, Thornton PE, Nemani RR, Glassy JM (2000) Global Terrestrial Gross and Net Primary Productivity from the Earth Observing System. In: *Methods in Ecosystem Science*, Sala O, Jackson R, and Mooney H (Eds). Springer-Verlag, New York.

Running SW, Nemani RR, Heinsch FA, Zhao M, Reeves M, Hashimoto H (2004) A continuous satellite-derived measure of global terrestrial primary production. *Bioscience*, **54** (6), 547-560.

Runyon J, Waring RH, Goward SN, Welles JM (1994) Environmental limits on net primary production and light-use efficiency across the Oregon transect. *Ecological Applications*, **4** (2), 226-237.

Schimel DS (1995) Terrestrial Ecosystems and the Carbon Cycle. *Global Change Biology*, **1** (1), 77-91.

Schimel DS, House JI, Hibbart KA *et al.* (2001) Recent patterns and mechanisms of carbon exchange by terrestrial ecosystems. *Nature*, **414**, 169-172.

Schmid HP (2002) Footprint modelling for vegetation atmosphere exchange studies: a review and perspective. *Agricultural and Forest Meteorology*, **113**, 159-183.

Schmid HP, Su H-B, Vogel CS, Curtis PS (2003) Ecosystem-atmosphere exchange of carbon dioxide over a mixed hardwood forest in northern lower Michigan. *Journal of Geophysical Research – Atmosphere*, **108** (D14), 4417, doi: 10.1029/2002JD003011.

Schulz K, Jarvis AJ, Beven KJ, Soegaard H (2001) The predictive uncertainty of land surface fluxes in response to increasing ambient carbon dioxide. *Journal of Climate*, **14**(12), 2551-2562.

Schulz K, Jarvis AJ (2004) Environmental and biological controls on the seasonal variations in latent heat fluxes derived from flux data for three forest sites. *Water Resources Research*, **40**, W12501.

Schulze E-D, Valentini R, Sanz M-J (2002) The long way from Kyoto to Marrakesh: Implications of the Kyoto Protocol negotiations for global ecology. *Global Change Biology*, **8**, 505-518.

Sellers PJ, Los SO, Tucker CJ, Justice CO, Dazlich DA, Collatz GJ, Randall DA (1996b) A revised land surface parameterization (SiB2) for atmospheric GCMs. Part II: the generation of global fields of terrestrial biophysical parameters from satellite data. *Journal of Climate,* **9**, 706-737.

Sellers PJ, Randall DA, Collatz GJ et al. (1996a) A revised land surface parameterization (SiB2) for atmospheric GCMs. Part I: model formulation. *Journal of Climate,* **9**, 676-705.

Simonoff JS (1996) *Smoothing Methods in Statistics*. Springer Series in Statistics, Springer Verlag, 338 pp.

Sokal RR, Rohlf FJ (1995) *Biometry the principles and practice of statistics in biological research.* 3rd edition. W. H. Freeman and Co.: New York. 887 pp.

Sorooshian S, Dracup JA (1980) Stochastic parameter estimation procedures for hydrologic rainfall-runoff models: Correlated and heteroscedastic error cases. *Water Resources Research*, **16** (2), 430-442.

Sparks TH, Menzel A (2002) Observed changes in seasons: an overview. International Journal of Climatology, **22**, 1715-1725.

Stauch VJ (2003) Identification of a data-based canopy carbon balance model derived from agricultural eddy flux measurements. Diploma thesis. Technical University of Braunschweig, Germany, 77 pp.

Steffen W, Noble I, Canadell J *et al.* (The International Geosphere-Biosphere Programme Terrestrial Carbon Working Group) (1998) The Terrestrial Carbon Cycle: Implications for the Kyoto Protocol. *Science*, **280**, 1393-1394.

Su HB, Paw KT, Shaw RH (1996) Development of a coupled leaf & canopy model for the simulation of the plant-atmosphere interaction. *Journal of Applied Meteorology,* **35**(5), 733-748.

Suyker AE, Verma SB (2001) Year-round observations of the net ecosystem exchange of carbon dioxide in a native tallgrass prairie. *Global Change Biology*, **7** (3), 279-289.

Suyker AE, Verma SB, Burba GG (2003) Interannual variability in net CO_2 exchange of a native tallgrass prairie. *Global Change Biology*, **9** (2), 255-265.

Tans PP, Fund IY, Takahashi T (1990) Observational constraints on the global atmospheric CO_2 budget. *Science*, **247**, 1431-1438.

TMY2 (2006) http://rredc.nrel.gov/solar/old_data/nsrdb/tmy2/, accessed in January 2006.

Valentini R, Matteucci G, Dolman AJ *et al.* (2000) Respiration as the main determinant of carbon balance in European forests. *Nature*, **404**, 861-865.

Van Wijk MT, Bouten W (1999) Water and carbon fluxes above European coniferous forests modelled with artificial neural networks. *Ecological Modelling*, **120**, 181-197.

Van Wijk MT, Bouten W (2002) Simulating Daily and Half-Hourly Fluxes of Forest Carbon Dioxide and Water Vapor Exchange with a Simple Model of Light and Water Use. *Ecosystems*, **5**, 597-610.

Von Caemmerer S, Farquhar GD (1981) Some relationships between the biochemistry of photosynthesis and the gas exchange of leaves. *Planta*, **153** (4), 376-387.

Von Caemmerer S (2000) *Biochemical Models of Leaf Photosynthesis*, CSIRO Publishing, Australia, 165 pp.

Wang Y-P, Jarvis PG (1990) Description and validation of an array model - MAESTRO. *Agricultural and Forest Meteorology*, **51**, 257-280.

Wang Y-P, Leuning R (1998) A two-leaf model for canopy conductance, photosynthesis and partitioning of available energy I: Model description and comparison with a multi-layered model. *Agricultural and Forest Meteorology*, **91**, 89-111.

Wang Y-P, Leuning R, Cleugh HA, Coppin PA (2001) Parameter estimation in surface exchange models uising nonlinear inversion: how many parameters can we estimate and which measurements are most useful? *Global Change Biology*, **7**, 495-510.

Waring RH, Law BE, Goulden ML, Bassow SL, McCreight RW, Wofsy SC, Bazzaz FA (1995) Scaling gross ecosystem production at Harvard Forest with remote sensing: a comparison of estimates from a constrained quantum-use efficiency model and eddy correlation. *Plant, Cell and Environment*, **18**, 1201-1213.

Weibull W (1939) A Statistical Theory of Strength of Materials. *Proceedings of the Royal Academy of Science*, 15.

Wesely ML, Hart RL (1985) Variability of short term eddy correlation estimates of mass exchange. In: *Forest-Atmosphere Interaction: Proceedings of the Forest Environmental Measurements Conference*, (eds Hutchinson BA, Hicks BB), pp. 591-612. Reidel Publications, Dordrecht, Netherlands.

Williams M, Rastetter EB, Fernandes DN *et al.* (1996) Modelling the soil-plant-atmosphere continuum in a *Quercus-Acer* stand at Harvard Forest: the regulation of stomatal conductance by light, nitrogen and soil/plant hydraulic properties. *Plant, Cell and Environment*, **19**, 911-927.

Williams M, Rastetter EB, Fernandes DN, Goulden ML, Shaver GR, Johnson LC (1997) Predicting gross primary productivity in terrestrial ecosystems. *Ecological Applications*, **7** (3), 882-894.

Williams M, Eugster W, Rastetter EB, McFadden JP, Chapin FS (2000) The controls on net ecosystem productivity along an Arctic transect: a model comparison with flux measurements. *Global Change Biology*, **6** (Suppl. 1), 116-126.

Williams M, Law BE, Anthoni PM, Unsworth M (2001) Using a simulation model and ecosystem flux data to examine carbon-water interactions in ponderosa pine. *Tree Physiology*, **21**, 287-298.

Williams M, Schwarz PA, Law BE, Irvine J, Kurpius MR (2005) An improved analysis of forest carbon dynamics using data assimilation. *Global Change Biology*, **11**, 89-105.

Wilson EM (1983) *Engineering Hydrology*, MacMillan, 309 pp.

Wofsy SC, Goulden ML, Munger Jw, Faan SM, Bakwin PS, Daube BC, Bassow SL, Bazzaz FA (1993) Net exchange of CO_2 in a mid-latitude forest. *Science*, **260**, 1314-1317.

Wofsy SC, Munger JW (2003) Harvard University. Atmospheric Sciences. Forest and Atmospheric Measurements. Data exchange. NIGEC data archive. http://www-as.harvard.edu/data/nigec-data.html (accessed on June 23, 2003).

Yi c, Li R, Bakwin PS *et al.* (2004) A nonparametric method for separating photosynthesis and respiration components in CO_2 flux measurements. *Geophysical Research Letters*, **31**, L17107. doi:10.1029/2004GL020490.

Young PC, Beven KJ (1994) Data-based mechanistic modelling and the rainfall-flow nonlinearity. *Environmetrics*, **5** (3), 335-363.

Young PC, Parkinson S, Lees M (1996) Simplicity out of complexity in environmental modelling: Occam's razor revisited. *Journal of Applied Statistics*, **23** (2-3), 165-210.

Young PC, Pedregal DJ (1999) Recursive and en-bloc approaches to signal extraction. *Journal of Applied Statistics*, **26**, 103-128.

Young PC (1999) Nonstationary time series analysis and forecasting. *Progress in Environmental Science*, **1** (1), 3-48.

Young PC (2000) Stochastic, dynamic modeling and signal processing: time variable and state dependent parameter estimation. In: *Nonlinear and Nonstationary Signal Processing*, (eds Fitzgerald WJ, Smith RL, Walden AT, Young PC), pp. 74-114. Cambridge University Press, Cambridge, New York.

Young PC, Garnier H., Jarvis AJ (2003) The identification of continuous-time linear and nonlinear models: a tutorial with environmental applications, *Proceedings International Federation on Automatic Control (IFAC) SYSID Conference, Rotterdam, 2003*.