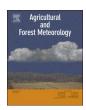
# ARTICLE IN PRESS

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# Surface-atmosphere exchange in a box: Making the control volume a suitable representation for in-situ observations

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#### ABSTRACT

Using the eddy-covariance (EC) method to determine net surface-atmosphere exchange relies on extensive simplifications of the mass balance concept. Among others, it is assumed that the 3-D flux field within a control volume is divergence-free, which is shown to be violated e.g. from large-eddy simulations. To practically evaluate the severity of these assumptions, case studies have monitored the surrounding of an EC tower, so the control volume can be represented more explicitly. Alternatively, diagnostic tests during data processing can be used to subset the EC data for periods that more likely fulfill the underlying assumptions. However, these existing methods are constrained either by their degree of realism, resource demand, temporal coverage, varying spatial representativeness, or combinations thereof.

It is hypothesized that these deficiencies can be overcome by using the environmental response function (ERF) technique: Relating flux observations at very high spatio-temporal resolution to meteorological forcings and surface properties, and utilizing the extracted relationships to map a single, regular and stationary control volume explicitly in 3-D space and time. Here, the novel ERF virtual control volume (VCV) concept and its implications are derived, and Xu et al. (this issue) are presenting its first practical application.

Initial results show that even from a single EC tower, ERF-VCV reduces advective errors by at least one order of magnitude, and incorporates net low-frequency flux contributions. In the same process tower location bias is treated through attaining a fixed-frame, thus equitable and time-invariant representation of the net surface-atmosphere exchange across a target domain. With regard to the frequently observed non-closure of the surface energy balance, this offers the potential for reconciling "spatial heterogeneity" and "storage term" theories. In extension, ERF promises a rectifying observational operator for unbiased model-data comparison, assimilation, and process representation at model grid scale.

#### 1. Introduction

Earth system models of surface-atmosphere interactions, including the carbon, water, and energy cycles, provide key tools for improving our ability to understand and forecast biosphere responses from local to continental scales. This is especially important in the context of global climate change, already resulting in a 0.85 °C  $\pm$  0.20 °C increase in mean global temperature (IPCC, 2013), a ~2% increase in mean global precipitation over land (Hulme et al., 1998), and an intensification of the hydrologic cycle (Hayhoe et al., 2006; Huntington, 2006). The National Academy of Sciences (2013) as well as the IPCC (2013) highlight the need for confronting these models with distributed observations, such as those made by the NEON, AmeriFlux, and ICOS flux tower networks.

However, the spatial mismatch between predictions and

observations is complicating the model improvement process (Fig. 1). Specifically, the eddy covariance (EC) method, in which the vast majority of flux tower observations are made, relies on extensive simplifications of the mass balance concept, including assumptions of surface homogeneity and constant sample characteristics with time. As a confounding factor, the flux tower measurement footprint represents only a small fraction of the model grid cell, and the location of this fraction changes with time. As a result, EC flux observations are subject to transient location bias (Nappo et al., 1982; Schmid and Lloyd, 1999) and energy imbalance (Foken et al., 2011; Wilson et al., 2002). These biases are each on the order of tens of percent, one order of magnitude larger than typical sensor errors. The question of scale is underlying both of these challenges, but rigorous testing of methods for scaling land-atmosphere exchange to regular areas and periods relevant for

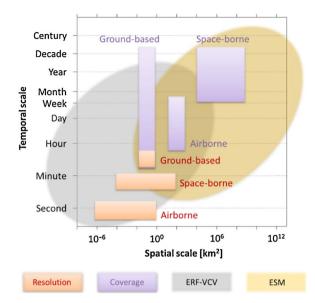
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**Fig. 1.** Space-time scope diagram for a hierarchy of environmental observations in relation to two principal approaches for scaling to an information continuum: Environmental response function virtual control volume (ERF-VCV) and earth system model (ESM).

atmospheric processes and models is limited, and efforts to date have been inconclusive (e.g., Desai et al., 2010).

EC flux tower observations such as those collected by AmeriFlux, ICOS, the forthcoming NEON and the global umbrella network FLUXNET have become available at unprecedented temporal duration and distributed spatial extents: Near continuous data on carbon, water, heat and momentum fluxes and their climate and biological drivers are collected across many eco-climatic domains. The longest running towers are now approaching two decades of observations (Baldocchi, 2008). Significant progress has been made on quality control metrics (Mauder et al., 2013) and addressing systematic biases (Foken et al., 2011). As a consequence, syntheses of flux-tower data have documented age-related changes in carbon flux in forests (Luyssaert et al., 2008), global photosynthetic potential (Beer et al., 2010), global carbon turnover times (Carvalhais et al., 2014), controls of temperature and dryness on latitudinal variations (Yi et al., 2010), and more. However, fundamental challenges remain to adequately integrate EC flux observations into the earth system model improvement process. To date virtually all model-data intercomparisons and regional to global syntheses have neglected uncertainties in EC flux observations resulting from location bias and energy balance non-closure.

These problems are well known, yet unified solutions remain elusive. Desai et al. (2008) significantly improved the comparison between a very tall flux tower and scaled stand-scale flux towers by "de-biasing" the tall tower footprint. Wang et al. (2006) demonstrated retrieval of land cover specific respiration and photosynthesis parameters by utilizing hour-to-hour variations in flux footprint. Overall, location bias diagnostics (Chen et al., 2011; Chen et al., 2012) or corrections (rectification) have been applied only in limited domains.

Solutions to the energy balance closure problem are even less developed: The surface energy balance at most EC sites is not closed, the available energy often 10–30% larger than the sum of the turbulent fluxes (e.g., Stoy et al., 2013; Wilson et al., 2002). Numerous reasons are proposed for the lack of energy balance closure. Recent studies evaluating sensor uncertainty and spatial scaling have ruled out radiation and ground heat measurements as the primary cause (e.g., Horst et al., 2015; Liu et al., 2011). Flawed measurement and interpretation of heat storage in soil, air column, and biomass below the EC measurement has shown promise in reducing the bias (Leuning et al., 2012; Lindroth et al., 2010). However, it does not apply similarly across sites: For example, over low stature ecosystems storage in air and biomass are

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typically of little relevance. Similarly, horizontal and vertical divergence terms can lead to a lack of closure, but in complex terrain it is difficult to attribute a systematic loss of energy since coupling should occur at least periodically (e.g., Barr et al., 2013; Zitouna-Chebbi et al., 2012). This leaves landscape heterogeneity and associated low-frequency mesoscale circulations (e.g., Foken, 2008; Panin et al., 1998) as suggested systematic source, with the bias largely attributed to simplifications of the mass balance concept upon which most EC studies depend (Finnigan et al., 2003).

To practically evaluate the severity of violated EC assumptions, case studies have monitored the surrounding of an EC tower to more explicitly represent a control volume (incl. storage and divergence terms, Aubinet and Feigenwinter, 2010; Foken et al., 2010; Oncley et al., 2007). Alternatively, diagnostic tests during data processing can be used to subset the EC data for periods that more likely fulfill the underlying assumptions (Foken et al., 2004; Mauder and Foken, 2006). However, these existing methods are constrained either by their degree of realism, resource demand, temporal coverage, varying spatial representativeness, or combinations thereof.

I posit here that surface heterogeneity and changing sample characteristics over time are not problems that necessarily require additional data filtering. Instead, they are characteristics whose inherent variability can be utilized to develop better flux data products for model evaluation, assimilation, and improvement. This shall be achieved through transferring EC flux observations from multiple mismatching, irregular and transient control volumes to a single matching, regular and stationary control volume. It is accomplished by expanding the temporally resolved but planar environmental response function (ERF) technique (Metzger et al., 2013a; Xu et al., 2017) to a virtual control volume (VCV).

The objective of this manuscript is to derive the theoretical background and requirements for ERF-VCV, and thus to provide a means for addressing the location and energy balance biases underlying EC flux measurements. I will test the hypothesis that the resilience of tower eddy-covariance measurements to advection errors can be improved by at least one order of magnitude through combining spectral averaging with source area modeling and spatio-temporally explicit ensembling. In the following sections the ERF-VCV concept and its implications are derived. Section 2 introduces the methodology, beginning from the control volume framework (Section 2.1), and then using ERF-VCV to formally interrelate point measurements to it (Sections. 2.2-2.4). Section 3 presents example results, beginning with performance requirements (Sect. 3.1), then discussing implications of representation and representativeness on energy imbalance (Section 3.2), as well as practical difficulties and proposed solutions (Section 3.3). Section 4 summarizes my findings and provides an outlook. In extension, Xu et al. (this issue) present the first practical application of ERF-VCV.

#### 2. Materials and methods

The exchange of momentum, heat, water vapor,  $CO_2$  and other scalars between the earth's surface and the atmosphere is often dominated by turbulent transport: Buoyancy as well as shear stress result in a turbulent wind field for most of the day (e.g., Stull, 1988). The EC technique utilizes these turbulence properties, making it a suitable method for the direct and continuous monitoring of surface-atmosphere interactions. However, questions arise from inherent theoretical assumptions of the EC method about relevant terms to the full mass balance, spatial scale and representativeness, and energy balance closure. All of these impact environmental inference and the efforts to develop and test model parameterizations.

In the following I will explore the foundation of EC, the formal control volume framework (Section 2.1). This is followed by deriving ERF-VCV, through relating point measurements to surface patches (Section 2.2), and subsequently surface patches to the control volume (Section 2.3). Section 2.4 provides the minimum requirements for applying ERF-VCV to flux towers.

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