Optimization of an Ecosystem Model through the Assimilation of Eddy Flux Observations using a Smoothed Ensemble Kalman Filter

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Abstract

The parameters of ecosystem models are conventionally optimized through nonsequential inversion methods, which treat observations as a whole and lack the flexibility to investigate possible temporal evolution of the model parameters. This research developed a smoothed ensemble Kalman filter (SEnKF) to assess to what extent the parameters and state variables of an ecosystem model can be simultaneously optimized through the assimilation of eddy flux observations. The performance of the SEnKF was demonstrated in one case study: the assimilation of measurements of carbon exchange between a mixed forest and the atmosphere at Niwot Ridge Forest (Colorado, USA) from 2000 to 2004 into a carbon flux partition model. Our analyses demonstrated that some model parameters, such as light use efficiency and respiration coefficients, were highly constrained by eddy flux data at daily to seasonal time scales. Light use efficiency was strongly seasonal. Model predictions based on parameters modified by the SEnKF were much improved, compared to predictions made without progressive data assimilation. The SEnKF reduced the variance of state variables that is caused by uncertainties of parameters and driving variables. The analysis of net ecosystem exchange of carbon between the forest and the atmosphere was improved.

1. INTRODUCTION

The accuracy of our measurement and modelling of ecosystem carbon dynamics is limited by many factors. Measurements of carbon in the environment are often patchy in space and discontinuous in time. The modelling of carbon dynamics is built on principles that must be coupled with assumptions and crafted with parameters that can only be imperfectly defined. Advanced data assimilation techniques based on statistics or optimization theory can mitigate these limitations by combining a series of measurements with dynamic models. To date, much of the effort spent in developing data assimilation methods for carbon dynamics analysis has focused on estimating optimal values for either model parameters [e.g. Braswell et al., 2005; Knorr and Kattge, 2005; Wang et al., 2006] or state variables [Bond-Lamberty et al., 2005], but only rarely both [Gove and Hollinger, 2006]. Methods that focus on estimating parameter values alone (i.e., without considering state variables) generally attempt to minimize long-term prediction error by using a historical set of data that assumes time-invariant parameters. The procedures used to process the historical data as a whole lack the flexibility to investigate the possibility that model parameters change over time. Although there have been some attempts to partition data into a number of subsets in time order, such partitions are inevitably subjective [Reichstein et al., 2005b]. The weakness of their approaches is that all errors from input, output, and model structure are attributed solely to model parameter uncertainties. Sequential data assimilation procedures such as the ensemble Kalman filter (EnKF) have the potential to overcome this drawback by explicitly taking all sources of uncertainty into account [Evensen, 2003; Nichol et al., 2002]. However, the successful application of the EnKF focuses primarily on estimating time-varying state variables under the typical presumption that the parameters are to be specified in advance. For example, Williams et al. (2005) successfully used the EnKF to improve analysis of forest carbon dynamics in a young ponderosa pine stand. Because the ecosystems are too complex to guarantee the time-invariance of the model parameters, we have developed a novel sequential data assimilation procedure that will provide simultaneous estimates of time-varying model states and parameters.

A conventional method of model calibration is to construct artificial parameter evolution at each time step by adding small random perturbations [Todini et al., 1976]. The drawback of such parameter sampling is the over-dispersion of parameter samples. We now describe a smoothed ensemble Kalman filter (SEnKF) to estimate simultaneously system states and model parameters of forest carbon dynamics. The aim of applying a kernel-smoothing algorithm to an ensemble Kalman filter is to overcome the dramatic, sudden change of parameter values in time and the loss of continuity between two consecutive points in time. This paper first describes the methodology of the SEnKF and builds up the mathematical formulation. The SEnKF is

then used to assimilate AmeriFlux tower measurements into a carbon flux partitioning model to estimate simultaneously the model states and parameters. Finally, the simulation results are displayed and analyzed.

2. METHODS

2.1. *SEnKF*

The SEnKF is a sequential data assimilation method with three components: (1) a dynamic model used to forecast system states as well as a parameter evolution process, (2) observation data and the relationship between the data and the model states, and (3) an assimilation scheme for model-data synthesis [Evensen and Van Leeuwen, 2000; Evensen, 2003; Raupach et al., 2005].

2.1.1. Dynamic Model

A dynamic model can be expressed as one or more discrete-time nonlinear stochastic processes:

$$X^{k+1} = f(X^k, U^k, \theta^k) + \varepsilon^k \tag{1}$$

where k denotes the time step, X^k is a vector of random state variables or object variables (such as carbon flux or storage attributes), f is the model operator as a propagation of model state (such as rates of change of net carbon fluxes), U^k is a set of externally specified time-dependent forcing variables (such as meteorological variables and soil properties), θ^k is a set of model parameters or auxiliary variables (such as light use efficiency and partition ratios), and the noise term ε^k accounts for both imperfections in model formulation and random variability in forcing variables and parameters.

To extend the applicability of the EnKF to simultaneous state-parameter estimation, we need to build an evolution of the parameters similar to that of the state variables:

$$\theta^{k+1} = g(\theta^k) + \tau^k \tag{2}$$

where g is a transition operator (such as a linear function,), and τ is a random error term. We will discuss their definitions below. Now we define $Y^k = (X^k, \theta^k)^T, M = (f, g)^T$ and $q^k = (\varepsilon^k, \tau^k)^T$, where T denotes transposition. Then (1) and (2) are changed into a standard state model

$$Y^{k+1} = M(Y^k, U^k) + q^k \tag{3}$$

2.1.2. Observation Data

The observation (Z^k) is related to the system state, external forcing variables, and parameters through an expression of the form

$$Z^k = H(X^k, U^k, \theta^k) + \delta^k \tag{4}$$

Or

$$Z^k = H(Y^k, U^k) + \delta^k \tag{5}$$

where the operator H specifies the deterministic relationship between the observation data and the model states. The noise term δ^k accounts for both measurement error (instrument and processing errors in the measurements) and representation error (errors in the model representation of Z, introduced by shortcomings in the observation model H), which is assumed to be Gaussian and independent of model error.

2.1.3. Assimilation Scheme

The EnKF is based on the Monte Carlo method and the Kalman filter formulation to mimic the probability distribution of the model state, conditioned on a series of observations of the model state. The probability density of the model state is represented by a large ensemble of model states, and these are integrated forward in time by the model with a stochastic forcing term representing the model errors [Evensen, 1994]. Each ensemble member evolves in time according to:

$$Y_{j-}^{k+1} = M(Y_{j+}^k, U_j^k), \ j = 1, \cdots, N \tag{6}$$

Where N denotes the number of model state ensemble members, Y_{j-}^{k+1} is the component of the jth ensemble member forecast at time k+1 and Y_{j+}^k is the jth updated ensemble member at time k. The noise term is not explicitly represented because the EnKF represents multiplicative model errors through forcing data perturbations [Evensen, 1997]. The forcing data perturbations are made by adding white noise (subject to Gaussian distribution with zero mean and covariance Q_j^k) to forcing data at each time step:

$$U_j^k = U^k + \eta_j^k, \ \eta_j^k \sim N(0, Q_j^k) \tag{7}$$

Now we discuss how to build an evolution of the parameters similar to that of the state variables. Conventional evolution of artificial parameters, which adds a small random

perturbation at each time step, results in over-dispersion of parameter samples and loss of continuity between two consecutive points in time. We used the kernel smoothing of parameter samples to remedy the problem, as described in West [1993]

$$\begin{cases} \theta_{j-}^{k+1} = a\theta_{j+}^{k} + (1-a)\bar{\theta}_{+}^{k} + h\tau_{j}^{k} \\ \tau_{j}^{k} \sim N(0, V_{+}^{k}),\ \bar{\theta}_{+}^{k} = \mathrm{mean}(\theta_{j+}^{k}), \\ V_{+}^{k} = \mathrm{var}(\theta_{j+}^{k}),\ a^2 + h^2 = 1 \end{cases} \tag{8}$$

where a is the shrinkage factor in (0,1) of the kernel location, which is typically around 0.45–0.49, h is the smoothing or variance reduction parameter, θ_{j-}^{k+1} is the component of the jth ensemble member forecast at time k+1, and θ_{j+}^{k} is the component of the jth updated ensemble member at time k.

Similarly, observation data are treated as random variables by generating an ensemble of observations from a distribution with the mean equal to the measurement value and a covariance equal to the estimated measurement error [Williams et al., 2005].

$$Z_{j}^{k+1} = Z^{k+1} + \delta_{j}^{k+1}, \delta \sim N(0, R^{k+1}) \tag{9}$$

Because the true state is generally unknown, we calculate a forecasted ensemble covariance matrix to substitute for the definitions of the error covariance matrix in the Standard Kalman filter.

$$P_{-}^{k+1} = \tfrac{1}{N-1}[M_{Y}^{k+1} - \bar{M}_{Y}^{K+1}][M_{Y}^{k+1} - \bar{M}_{Y}^{k+1}]^{T} \tag{10}$$

Where $M_{Y}^{k} = [Y_{1-}^{k} - \bar{Y}_{1-}^{k}, \cdots, Y_{N-}^{k} - \bar{Y}_{N-}^{k}]$ and $\bar{M}_{Y}^{k} = \frac{1}{N}\sum_{j=1}^{N} Y_{j-}^{k}$.

The updated scheme of the EnKF is as follows:

$$Y_{j+}^{k+1} = Y_{j-}^{k+1} + K^{k+1}(Z_{j}^{k+1} - H(Y_{j-}^{k+1}, U_{j}^{k+1})) \tag{11}$$

where K^{k+1} is Kalman gain

$$K^{k+1} = P_{-}^{k+1} H^{T} (HP_{-}^{k+1} H^{T} + R^{k+1})^{-1} \tag{12}$$

2.2. APPLICATION OF SENKF TO CARBON (C) MODELLING

2.2.1. FLUX PARTITION MODEL

We use a flux partition model [Reichstein et al., 2005b] as our test dynamic model for the SEnKF method. Our selection is based on two considerations. First, it is a widely used model for constructing bottom-up estimates of continental carbon balance components. Second, it is appropriate for testing the robustness of the SEnKF method because it is nonlinear, there are sufficient observations of state variables, and it has multiple unknown parameters. The flux partition model divides net ecosystem exchange (NEE) into gross primary production (GPP) and total ecosystem respiration (RESP), in which function expressions of GPP and RESP are introduced through mechanistic analysis and many data regression analyses as follows:

$$\begin{cases} NEE_{t} = GPP_{t} - RESP_{t} \\ GPP_{t} = LUE_{t} \cdot PAR_{t} \cdot NDVI_{t} \cdot D_{temp} \cdot D_{VPD} \\ RESP_{t} = R_{ref,t} \exp[E_{0}(\frac{1}{T_{ref,t} - T_{0}} - \frac{1}{T_{air,t} - T_{0}})] \end{cases} \tag{13a–c}$$

where subscript t denotes time-dependent, LUE_t is light use efficiency, PAR_t is photosynthetically active radiation, $NDVI_t$ is the normalized difference vegetation index, $R_{ref,t}$ is respiration when air temperature ($T_{air,t}$) equals reference temperature ($T_{ref,t}$, usually specified as 10 °C), E_0 is temperature sensitivity, and T_0 is a datum of temperature to avoid a denominator of zero in the model (13c), kept constant at –46.02 °C as in Reichstein et al., [2005a]. D_{temp} determines the effect of temperature on photosynthesis, and D_{VPD} expresses the decrease in leaf exchange from both photosynthesis and transpiration caused by vapor pressure deficit (VPD), according to

$$D_{temp} = \max\left[\frac{(T_{\max} - Tair)(Tair - T_{\min})}{(T_{\max} - Tair)(Tair - T_{\min}) + (T_{opt} - Tair)^2}, 0\right] \tag{14}$$

$$D_{vpd} = 0.5\left[1 + \frac{1}{1 + v_{0} \exp(v_{1} VPD)}\right] \tag{15}$$

where T_{min}, T_{opt}, and T_{max} denote minimum, optimal, and maximum temperatures for photosynthesis, respectively, VPD is vapor pressure deficit, and v_0 and v_1 are two unknown coefficients. If we define state and driving force vectors as $Y_t = (NEE_t, GPP_t, RESP_t, LUE_t, T_{\min}, T_{opt}, T_{\max}, v_0, v_1, R_{ref}, E_0)$

and $U_t = (T_t, PAR_t, VPD_t, NDVI_t)$, then the model can be expressed in the form of (6).

2.2.2. FLUX DATA

Eddy flux estimates of net ecosystem exchange (NEE) are based on the covariance of high frequency fluctuations in vertical wind velocity and CO_2 concentration [Baldocchi et al., 1988]. We applied the SEnKF approach to data obtained at the AmeriFlux station at Niwot Ridge Forest (Colorado, USA). The used period was from 2000 to 2004 because there were sufficient hourly and daily data at the station for that time, and because NDVI data from the Moderate Resolution Imaging Spectroradiometer (MODIS) were not available before 2000. Field observations included hourly observations of NEE, humidity, photosynthetically active radiation (PAR), air temperature, air pressure, wind speed, and daily precipitation data. In our analysis, we used daily data of three state variables (NEE, GPP, and RESP) and four driving force variables (air temperature, PAR, VPD, and NDVI). NEE data were directly downloaded from the AmeriFlux Web station, in which NEE daily data were actually a composite of half-hour observations. RESP data were calculated from the temperature dependence curve of ecosystem respiration derived from nighttime NEE observations [Yuan et al., in press]. GPP data were pseudo-observations calculated as a total of NEE and RESP (13a). Gaps in carbon exchange and meteorological data were filled using multivariate nonlinear regression. Daily NDVI was calculated using linear interpolation of the MODIS 16-day composites. We assumed that data errors were subject to a Gaussian distribution with a zero mean and a variance of 20% of the average data based on uncertainty analysis in eddy covariance measurements [Hollinger and Richardson, 2005]. The transition operator (H) in (4) was taken as a 3 x N linear matrix with elements of 1 at diagonal nodes and 0 at other nodes.

To test the predictive power of the SEnKF, we held 80 percent of the data for model validation. Data assimilation was performed on only 20 percent of the observations.

3 RESULTS AND ANALYSIS

For 2000 to 2004, the total assimilated GPP, RESP, and NEE were 4970 ±21.7, 4137 ±16.8, and 833 ±22.3 gC m^{-2}, respectively. These compared well with observed GPP, RESP, and NEE of 5188 ±50.1, 4327 ±41.9, and 861 ±24.6 gC m^{-2}, respectively. The estimate of NEE clearly indicates that the system was acting as a C sink during this time period. The maximum daily root mean square errors of the ensemble means of GPP, RESP, and NEE were 0.28, 0.25, and 0.24 gC m^{-2} day^{-1}, respectively, which were small compared with their respective maximum daily means. Data assimilation effectively captured the temporal changes of GPP, RESP, and NEE over the four years (Fig. 1).

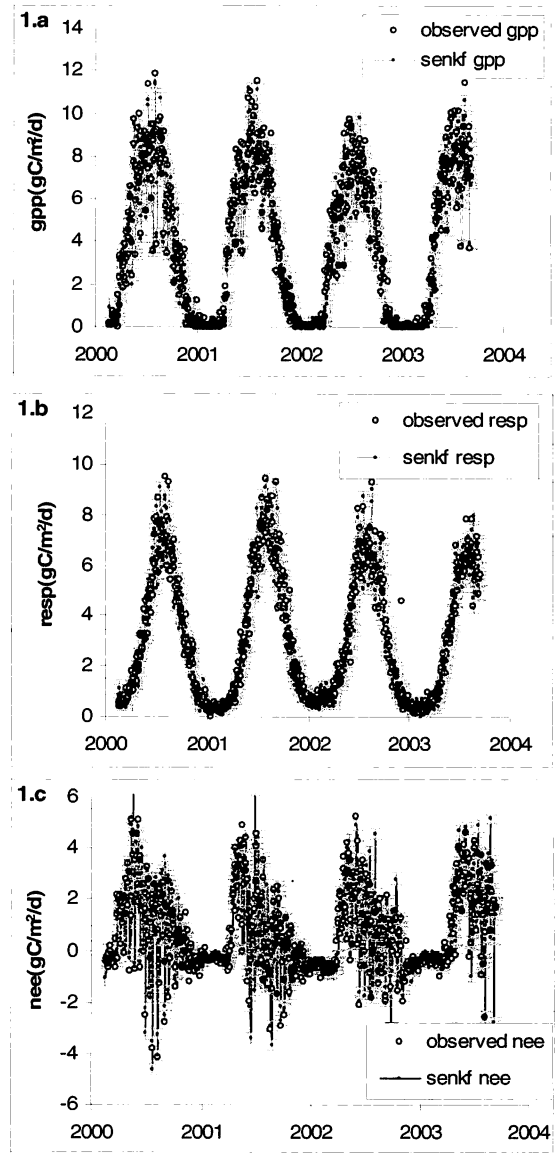

Figure 1. Time series of GPP, RESP, and NEE simulated by the SEnKF and assimilated data. The grey vertical lines indicate the corresponding standard deviation around the mean of ensembles.

We evaluated the performance of the SEnKF method, comparing results from the SEnKF with those generated by the conventional modelling approach. The conventional modelling approach had the same flux partition model, but a set of fixed optimal parameter values were obtained using the conventional nonlinear inversion procedures in the statistical analytical software package SAS (SAS, 1990).

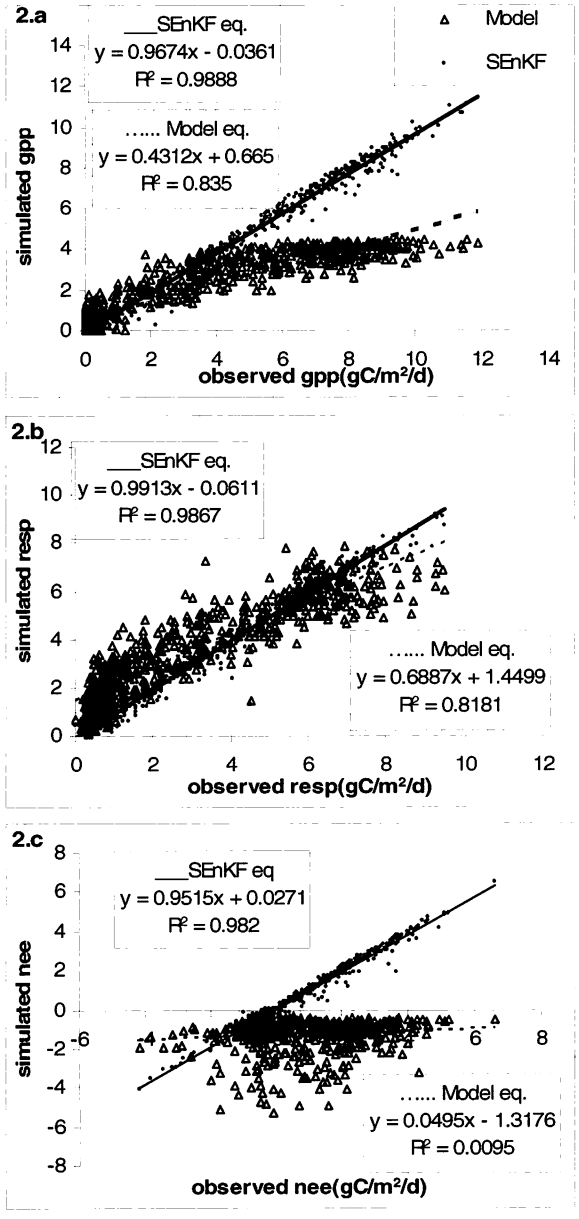

Figure 2. Comparison of estimates of GPP, RESP, and NEE generated by the SEnKF and the base model against 20 percent of the assimilated data.

However, this set of parameter values was derived from a mixture of 15 AmeriFlux stations, covering a variety of ecosystem types [Yuan et al., in press]. As a result, these parameter values were not necessarily optimal for the Niwot Ridge station in this study. From Figures 2 and 3, we can see that predictions from the conventional modelling approach deviate from the observations at the Niwot Ridge site, caused at least partially by the use of time-invariant parameter values. In this paper, we refer to the conventional modelling approach as the base model. No further optimization of the parameter values was performed specifically for Niwot Ridge Forest in order to see whether or not the SEnKF could reduce the bias of the model stemming from parameter uncertainty.

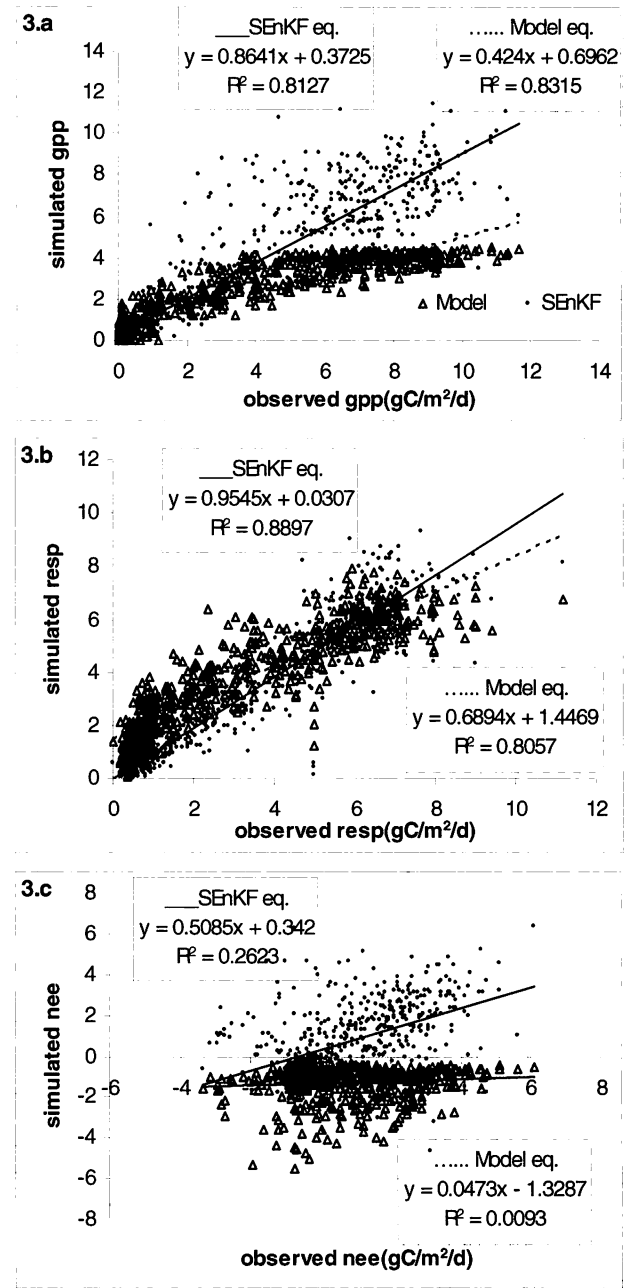

Figure 3. Comparison of the forecasted values of three state variables (GPP, RESP, and NEE) of the model modified by the SEnKF and of the original base model against unassimilated data (80 percent of total observations).

Figure 2 compares the results simulated by the SEnKF data assimilation and by the base model. Only 20 percent of the observations were used during data assimilation. The assimilated fluxes were very similar to the observations as indicated by the closeness of the points along the diagonal line, whereas the flux estimates generated by the base model contained systematic errors as indicated by the deviation of triangles from the diagonal line. Data assimilation accounted for more than 98 percent of the variation in the observations of GPP, REPS, and NEE, whereas the base model only explained 84, 82, and 10 percent of the variation for GPP, RESP, and NEE, respectively. All the linear regression equations between assimilated and observed GPP, RESP, and NEE indicated no significant bias ($\alpha<0.05$), whereas the base model generated strong biases.

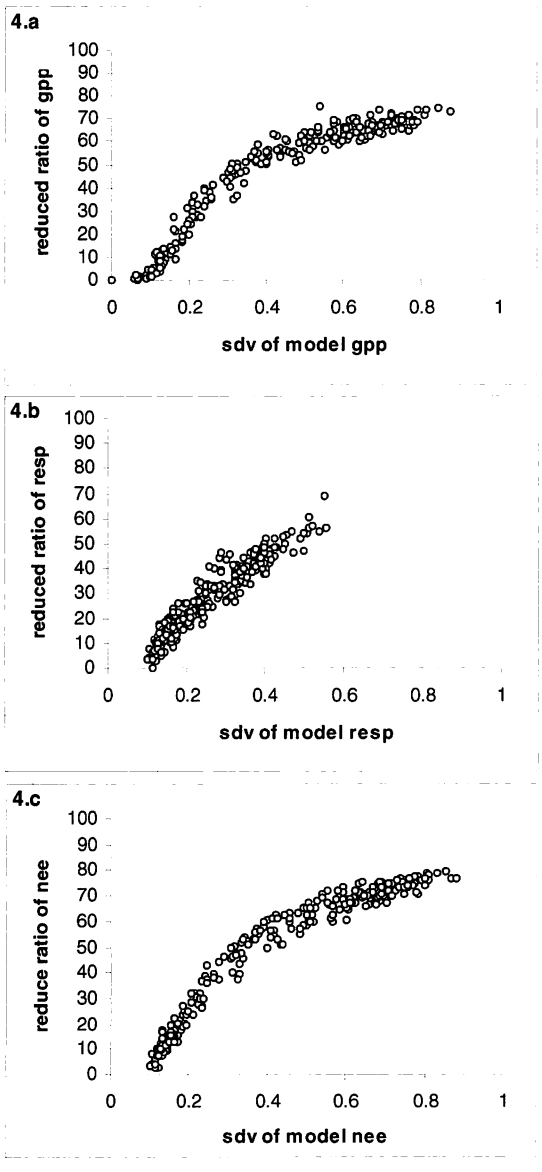

Figure 4. Reduced ratio of ensemble variances of GPP, RESP, and NEE generated by the SEnKF against that by the base model alone. The results show the SEnKF can more dramatically reduce variances of state variables than the ensemble based only on Monte Carlo technique.

The next step was to test whether the new parameter values derived from the SEnKF could be used to improve the prediction of system conditions. Figure 3 compares the model predictions (based on parameters derived from 20 percent of the observations using the SEnKF and by the base model) with the observations that were held for validation (i.e., the 80 percent of the observations that the SEnKF did not see). Comparing three pairs of corresponding linear fitting regression equations for GPP, RESP, and NEE, and their corresponding coefficients of determination (R^2), we see that the estimates of the three flux variables using the parameters (e.g., light use efficiency and reference respiration) modified by the SEnKF had less bias against observations than did the estimates using the base model (Fig. 3). This indicates that the SEnKF can extend the model parameter values generated from data assimilation to predictions when observations are not available. This capability could be valuable for filling data gaps caused by instrument failure.

Predictions made by SEnKF with data assimilation matched observations substantially better (Fig. 2) than predictions made without data assimilation (Fig. 3). The SEnKF procedure becomes regular Monte Carlo analysis at the time steps when no observation data are available for assimilation. At the data assimilation points (20 percent of the data), observation data strongly constrained the three flux variables (Fig. 2), and the differences between SEnKF model simulations and observations increased when no data were assimilated (Fig. 3). This might mean that prior states of the model have a weak effect on subsequent states. It might also suggest that there were other controlling factors affecting these processes which were not included in the model, or that uncertainty existed in observations. Figure 4 compares standard ensemble variances by SEnKF data assimilation against those by Monte Carlo analysis without data assimilation. The SEnKF can reduce up to 70 percent of the variance of the ensemble without data assimilation. As the magnitude of the variance of the ensemble increases, the smoothing effect also increases. The variance measures the uncertainty stemming from parameters and driving forces.

Because the SEnKF can assimilate sequential observation data into the model, the SEnKF also revealed that the parameter values (e.g., light use efficiency and reference respiration) possessed strong seasonality or temporal variability (Fig. 5). This indicates that the base model has structural errors (manifested by non-optimal parameter values in this study) and results in bias in

prediction. The temporal change of parameter values was relatively smooth because a smoothing procedure was implemented in the SEnKF to control the over-dispersion of parameter sampling. These demonstrate that the SEnKF can be used to perform recursive model calibration to diagnose the adequacy of model structure.

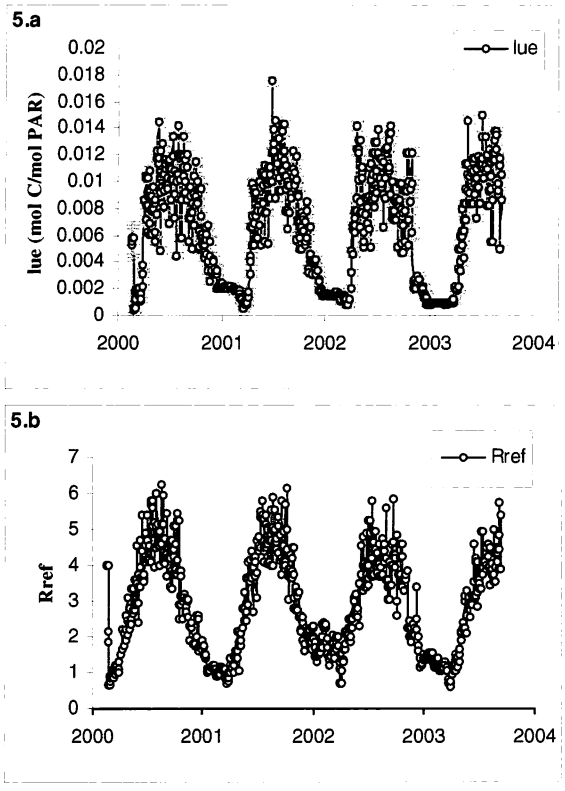

Figure 5. Temporal variations of two key parameters in the flux partition model: (a) light use efficiency (lue) and (b) reference respiration (Rref). The grey vertical lines indicate the standard deviation around the mean of ensembles.

4. CONCLUSIONS

The objective of this study is to assess to what extent the parameters and state variables of an ecosystem model can be simultaneously optimized through the assimilation of eddy flux observations. Our analyses demonstrated that some model parameters, such as light use efficiency and respiration coefficients, were highly constrained by eddy flux data at daily to seasonal time scales. Light use efficiency was strongly seasonal. Model predictions based on parameters modified by the SEnKF were much improved, compared to predictions made without progressive data assimilation. The SEnKF reduced the variance of state variables that is caused by uncertainties of parameters and driving variables. Simultaneous parameter estimation can use near real-time observations to improve the predictive ability of dynamic models. The model based on the SEnKF can be used to fill data gaps in observations. This research demonstrates that the SEnKF is a robust and effective algorithm for evaluating and developing ecosystem models, resulting in better quantification of model parameters and improving our understanding of carbon cycle processes.

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