B42D MCC: 3014 Thursday 1600h

Estimating Terrestrial Carbon, Water, and Energy Fluxes From Site to Region II *(joint with A, H)*

Presiding: **H Schmid,** Indiana University**; C M Brown-Mitic,** SAHRA, University of Arizona

B42D-01 1600h INVITED

Carbon Fluxes Assessment Using Artificial Neural Networks

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The feed-forward backpropagation artificial neural networks (ANNs), used in this application, are non-linear models able to reproduce non-linear functions. Unlike process based and multiple constrain models, to use ANNs it is not necessary to know the relationship between input and output variables, because this is found directly by the neural network. To do this and also to set the values of the parameters, the ANNs have to be trained using examples with the input values and also the correct output (supervised approach). We used eddy covariance carbon flux measurements to train artificial neural networks to simulate carbon fluxes at different scales. ANNs showed good performances when applied to gap-fill and correct the flux datasets at site level. The input variables used are meteorological data (air and soil temperatures, photosynthetic photon flux density, air humidity etc.) and four fuzzy values for the seasons, while the output is the carbon dioxide flux. An intercomparison between different gap-filling techniques showed that ANNs are able to reconstruct the annual trend of fluxes better than the others classic methods (regressions, look-up tables, mean daily values...). Another ANNs possible application is the NEE spatialization at regional and continental scales. After a first methodological experiment where NEE data from the Euroflux sites were used to obtain NEE maps of Europe with weekly time resolution and 1 km of spatial resolution (Papale and Valentini 2003), other analysis showed the potentiality of this approach to generalize from site to region. The GLOFLUX initiative (http://gaia.agraria.unitus.it/gloflux.html), lunched one year ago, has the aim to combine the available datasets into an artificial neural networks system to spatialize carbon fluxes at global scale.

URL: http://gaia.agraria.unitus.it/gloflux.html

B42D-02 1620h

Parameter Estimation in Biogeochimical Surface Model Using Nonlinear Optimization With Eddy-Covariance Measurements Over Pine Forests.

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Global models of carbone, water, and energy exchanges between the biosphere and the atmosphere are usually validated and calibrated with intensive measurements made over specific ecosystems like those of the fluxnet networks. However the nonlinear dependance between fluxes and model parameters generally complicates the optimization of the major parameters and the assessment of their uncertainty. In this study, we estimate key parameters of the Land-surface ORCHIDEE model, using the seasonal and diurnal information from latent heat flux, sensible heat flux, net CO2 flux and net radiation measurements over pine forest (Landes, France). We first present the inverse methodology, the complications linked to the non linearity, and an approach to derive parameter uncertainties in this context. We optimize the major parameters controlling the rate of carbon assimilation, the carbon autotrophic and heterotrophic respiration, the aerodynamic resistance, and the surface energy balance. The results will be discussed in term of model to data fit and parameter estimation. Most parameters appear to be significantly changed from their a priori estimate. A detail analysis of the posterior covariance matrix will be performed including the correlation terms (which are high between certain parameters). This optimisation approach helped us to highlight discrepancies of the ORCHIDEE model and to improve some parametrizations. The results of the inverse procedure using measurements at other sites with similar ecosystem will be compared.

B42D-03 1640h

Scalar Profile Assimilation Into a Multi-Layer Model of Canopy-Atmosphere Exchange: Toward Optimal Estimation of Net Ecosystem Exchange

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A major focus of current research efforts in land-atmosphere exchange is the modeling and quantification of carbon dioxide, water vapor and energy fluxes between forested ecosystems and the atmosphere. Mechanistic models of the coupled physical and biological processes that determine the magnitude of scalar fluxes have been developed and tested at many sites under a variety of environmental conditions. High frequency eddy covariance measurements of scalar fluxes are often used to test these canopy exchange models. Concurrent observations of carbon dioxide concentration profiles within the canopy airspace are frequently left unutilized in such modeling studies. We explore the assimilation of the information contained in these concentration profile measurements to constrain forward model estimates of net ecosystem exchange (NEE). A high-resolution, one-dimensional multi-layer model of canopy-atmosphere dynamics, including turbulent transport, vertical radiation interception, photosynthesis, stomatal conductance and respiration, is implemented and tested against eddy covariance flux measurements taken at the Duke Forest. A simple assimilation scheme is used to compare the results of forward model integrations both with and without the assimilated profile information. Implications are discussed for the optimal merger of data and models for the estimation of NEE.

B42D-04 1700h

How Complex Must the Parameterization of Canopy Turbulent Transport Be to Capture Biophysical Sources and Sinks?

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The exchange of scalars and momentum through canopy volume exerts control over almost all aspects of the canopy microenvironment, which in turn, plays a significant role in regulating biologically controlled scalar sources and sinks. This study is the first to rigorously explore how detailed the parameterization of the turbulent transport mechanism must be to accurately predict source-sink and flux profile distributions within the canopy across a wide range of leaf area density, climatic, and environmental variables. Towards this end, detailed ecophysiological and radiative transfer schemes are coupled to higher-order closure models to capture the two-way interaction between the canopy and its microclimate. The turbulent transport schemes consider range from first- to third-order closure approximations assuming both thermally stratified and neutral flows. The data sets used in the model calculations include long-term within-canopy scalar concentration, and temperature profiles collected along with sensible heat, latent heat, and CO2 fluxes above the canopy. These measurements, collected from September 1998 to date, are part of an on-going long-term flux monitoring initiative (AmeriFlux) in an even-aged pine forest near Durham, North Carolina. Current model results suggest that first-order closure model, corrected for atmospheric stability, are sufficient to capture much of the scalar source-sink variations within the canopy as well as fluxes above the canopy; second-order closure models are necessary to accurately reproduce the scalar profiles within the canopy; and third-order closure models are no better than second order in terms of overall predictive skills for scalar profiles and fluxes. Our model calculations also suggest that accounting for atmospheric stability is more important than increasing the closure order for improving source-sink, flux, and scalar concentration predictive skills.

B42D-05 1715h

Estimation of the Net Ecosystem CO2 Exchange of Chaparral Using Eddy Covariance, remote sensing and Biome-BGC

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The chaparral ecosystem ranges from California to Arizona, USA, and into Nuevo Leon and Tamaulipas, eastern Mexico. Tower-based eddy covariance and measurements above the canopy of a young stand (10 years old) and an old stand (>100 years old) have been conducted at Sky Oaks Biological Field Station, San Diego, USA, for 5 years to quantify the seasonal and annual variation in the net ecosystem CO2 exchange (NEE) of the chaparral ecosystem. Both stands are a C sink on an annual basis. Surprisingly, and contrary to the hypothesis by Odum, the old, mature, "scenscent" stand was as large of a C sink as the young stand. The stands tended to be net sinks during the wet seasons, and net sources during the dry seasons. Seasonal changes in carbon flux reflected changes of light use efficiency and were well correlated with two remote sensing indices of leaf pigment composition (NDVI and PRI). This implied the possibility of using remote sensing to estimate ecosystem CO2 balance. Two practical tram systems with optical sensors were set within the footprint of each eddy covariance tower in the young stand and old stand at Sky Oaks. This comparison between data from the eddy tower and spectral reflectance from remote sensing presented a good correlation between CO2 flux and NDVI corrected to a constant solar angle, which indicated that remote sensing is a very promising tool for the estimation of carbon fluxes in a chaparral ecosystem. To develop methods for scaling eddy flux measurements to the surrounding region, Biome-BGC model and MODIS results were introduced into the analysis. The eddy covariance data illustrated sink NEE patterns during wet seasons and source patterns during dry seasons, while the data simulated from Biome-BGC presented a net sink pattern throughout the whole year. The GPP simulated from Biome-BGC was lower than the estimate from MODIS, and their GPP yearly patterns were also different. Peak GPP from Biome-BGC was around June, while MODIS showed the peak GPP around March and April. Further data collection, analysis and comparison are required to explain these differences. Key words: chaparral, carbon dioxide, eddy covariance, remote sensing, global change

B42D-06 1730h

Investigation of Relationships between Canopy Conductance, Carbon Exchange and Evapotranspiration using FLUXNET data

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Using FLUXNET data from a wide range of ecosystems, from tropical to arctic flux tower sites we investigate relationships between canopy conductance, ecosystem CO_2 exchange and evapotranspiration. By inverting the Penman-Monteith Equation we calculate the canopy conductance g_s for the canopy seen as a big leaf. The leaf level relationship between stomatal conductance and net assimilation can be rewritten for the whole canopy as $g_s = a + b$ NEE RH_s / C_s where g_s is the canopy conductance, NEE the half-hourly net

ecosystem exchange of CO_2, RH_s surface relative humidity and C_s surface CO_2-concentration. We are especially interested to see whether this leaf-level relationship holds true on a canopy scale for a wide range of different canopies and ecosystems as it could be used to scale tower measurements across larger spatial scales with the aid of remote sensing products. For our calculations mid-day data were used for the whole year in evergreen and for growing season only in deciduous and crop canopies. The resulting relationships were highly linear with an average slope a = -10.45 and intercept b = 0.32 with some degree of variation for different types of ecosystems and functinal types.

B42D-07 1745h

A Challenge to the Flux-Tower Upscaling Hypothesis? A Multi-Tower Comparison From the Chequamegon Ecosystem-Atmosphere Study

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The “flux-tower upscaling hypothesis” asserts that flux tower measurements of representative ecosystems can be upscaled to regional fluxes via ecosystems mapping and process models. Collecting an integrated set of measurements to attempt upscaling is challenging. The required sampling density is also uncertain, and at minimum depends on local soil and vegetation cover, land use patterns, and climate gradients. Measurements that can be used to evaluate upscaling efforts are similarly difficult to obtain. Thus the basic hypothesis behind the flux tower approach of studying regional and global carbon (and hydrologic) cycles remains difficult to implement and test. The Chequamegon Ecosystem-Atmosphere Study (ChEAS) has endeavored to create a distributed set of stand-level flux tower and supporting measurements that can be used to upscale carbon and water flux measurements to the regional scale. The flux measurements collected at the 447m WLEF TV tower are proposed as a regional integral that can be used to evaluate the stand-level upscaling. Though more exhaustive analyses are warranted, the results to date bear a mixed message for tower-based upscaling. The absolute magnitude of the fluxes from two stand-level towers cannot be simply aggregated to explain the observations from the WLEF tower. Decomposition implies that while photosynthesis may upscale, respiration does not. Potential explanations will be discussed, including comparisons to chamber respiration data, wetland water table, and flux measurements across young, mature and old-growth stands. The data from WLEF show a regional source of carbon to the atmosphere, counter to most temperate forest data and counter to the stand-level towers in the region. Upscaling interannual variability, however, appears to be a more tractable problem. Though the temporal extent of the multiple flux tower system is limited, a tent caterpillar outbreak in 2001 provides an example of a strong, coherent perturbation to the regional ecosystem that is captured by the available sampling. Stand-level measurements upscale reasonably well to explain the changes in regional fluxes measured at WLEF. Climatic variability from more recent data will also be presented, in addition to recommendations for future upscaling efforts.

B42E MCC: 3010 Thursday 1600h

Aqueous Microbial Geochemistry III
(joint with H, OS, V)

Presiding: **E Shock ,** Arizona State University**; L A Warren,** School of Geography and Geology, McMaster University

B42E-01 1600h

Pyrite oxidation by microbial consortia

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Acid mine drainage (AMD) is formed through pyrite oxidation, which produces acidity and releases toxic metals associated with pyrite and other sulfide minerals. Microbes accelerate pyrite oxidation markedly, thereby playing a major role in the production of AMD. Here, we probe pyrite oxidation by consortia of Thiobacillus ferrooxidans and thiooxidans using surface-sensitive photoelectron spectroscopy and X-ray absorption spectroscopy and compare them with surfaces oxidized through chemical and single species cultures. Microbial oxidation resulted in the formation of distinct oxidized surface species distributed nonuniformly over the pyrite surface; consortia produced a surface both more heterogeneous and more oxidized. In contrast, chemical oxidation proceeds without the build-up of passivating oxidation products. Surface morphology was not correlated with sites of nucleation or oxidation in any obvious manner. These results demonstrate that microbial oxidation occurs through a similar mechanism to chemical oxidation, but that the presence of complex microbial communities may impact the manner by which pyrite oxidation proceeds.

B42E-02 1615h

Sulfur Oxidation, Microbes And Acidity In A Mine Tailings Lake

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Disposal of tailings (waste rock) aqueously is a common approach at mine sites to minimize oxidation of the associated sulfur minerals (pyrrhotite, pyrite) and the associated generation of acidity that accompanies this process. The study site, Moose Lake, receives tailings runoff at a nickel mine in Northern Ontario, which has rendered the lake highly acidic (surface pH values less than 3.5) with high metal loads and on-going acid export to off-site, downstream systems. To investigate the potential influence of microbial processes for acid generation, as well as characterizing any attendant influences for metal behaviour, the biogeochemistry of Moose Lake was characterized on a seasonal and a diel basis during the summer of 2002. Physico-chemical profiles were used to identify the area of strong redox gradient across the thermocline (typically 1 to 2 metres across this zone) on each sampling day. Samples at five depths within this redox gradient, were then collected for Fe^{3+}/Fe^{2+}, $SO_4{}^{2-}/H_2S$, metal and microbial samples, in addition to more highly resolved Hydrolab profiling. Samples were collected both during the lighted portion of the day (10am-12pm) and at dusk (6pm-8pm) to evaluate any contributions to S and Fe cycling attributed to photosynthetic activity. Results indicate a clear seasonal increase in acidity in the upper waters of the lake: pH values dropped from 3.19 in May to 2.90 in September. Further, a strong diel trend of increasing acidity (lower pH) from mid morning to dusk was also observed for each sampling period. Biotic control on S processes appears to be important associated with the thermocline region of the lake, whilst surficial processes occurring in the upper one to three meters are more consistent with a dominant abiotic control. Both pathways contribute to acidity generation, however the controls and rates differ. These results and implications for mitigation strategies will be presented.

B42E-03 1630h

Effects of Long-Term Acid-Mine Drainage Contamination on Diversity and Activity of Sulfate-Reducing Bacteria in a Natural Salt Marsh.

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Constructed wetlands have been studied as sites or analogs for *in situ* bioremediation of metal contaminants from acid mine drainage (AMD) or industrial sources (e.g. Webb et al. 1998). Wetlands bioremediation necessarily invokes the ubiquity and robustness of sulfate-reducing bacteria (SRB) to sequester dissolved metals into various poorly soluble metal-sulfides (e.g. PbS, CdS). However, few studies of natural wetlands under long-term ecological forcing by AMD or other contaminant sources are available for context. We are investigating the microbial diversity, mineralogy and geochemistry of a highly contaminated salt marsh along the East Central San Francisco Bay. For nearly a half-century, areas within this marsh have received acidic and/or metal-rich groundwaters from near-surface pyrite tailings (transported there from Iron Mountain Mine, near Redding, CA) and local industrial sources (e.g. paint and explosives manufacturers). Sediment cores (30-40 cm long) were taken from six contaminated sites in the marsh with pH range of $\sim$2 to $\sim$8. Previous analyses (URS Corp. 2001) reported As, Cd, Cu, Se, Zn, and Pb present in sediments at extremely high concentrations (100s of ppm), yet our ICP-AES analyses of pore waters showed only As present at concentrations of 10-50 ppb. We infer, from high-resolution transmission electron microscope (HRTEM) studies of biogenic (SRB biofilm) ZnS (Moreau et al. 2003, in review) and marsh sediments, that contaminant metals have been sequestered into aggregates of nanocrystalline metal-sulfides. Continuous-flow isotope ratio mass spectrometer (CF-IRMS) analyses of pore-water sulfate and sedimentary sulfides allow resolution of contributions to dissolved sulfate and sulfide from tailings oxidation and dissimilatory sulfate reduction. Sulfate analyses from subsections of three cores (pH 2-3, 6-7, 7-8, respectively) all yield $\delta^{34}S$ values consistent with bacterial sulfate reduction. We note that all three cores also contain very fine-grained black muds that are distinguishable from coarser pyrite cinders, and exhibit a noticeably strong sulfide odor. Aero- and halo-tolerant SRB were enriched from circumneutral pH cores, and we hypothesize that acido-tolerant SRB may also be present. Analysis of restriction fragment length polymorphism of whole community 16S rDNA extracted from each core shows an expected increase in diversity between acidic and circumneutral sediments, and clone libraries from both contaminated and uncontaminated marsh sediments are being compared to assess the impact of long-term contamination. *References:* Webb et al. 1998, *J. Appl. Microbio., 84,* 240-248; Moreau et al. 2003, *Amer. Min.*, in review; URS Corp. 2001, *Report 51.09967067.00.*

B42E-04 1645h

Sulfur Isotopic Analysis of Water and Sediment From Lake Hoare, Antarctica

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