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TESIS DOCTORAL

Remote sensing and ecosystem modeling to simulate terrestrial carbon fluxes

Autor: Sergio Sánchez Ruiz
Directores: Dra. Mª Amparo Gilabert y Dr. Fabio Maselli
Lugar: Universitat de València
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Abstract: The main goal of this thesis is the establishment of a framework to analyze the forest ecosystems in peninsular Spain in terms of their role in the carbon cycle. In particular, the carbon fluxes that they exchange with atmosphere are modeled to evaluate their potential as carbon sinks and biomass reservoirs. The assessment of gross and net carbon fluxes is performed at 1-km spatial scale and on a daily basis using two different ecosystem models, Monteith and BIOME-BGC, respectively. These models are driven by a combination of satellite and ground data, part of the latter being also employed as a complementary data source and in the validation process.

Key words: Carbon fluxes (GPP, NEP), forest, water stress, Monteith, BIOME-BGC.

Simulación de flujos de carbono terrestres mediante teledetección y modelización de ecosistemas

Resumen: El objetivo principal de esta tesis es el desarrollo de una metodología operativa para analizar las zonas forestales de la península a través de los flujos de carbono que intercambian con la atmósfera. En concreto se ha evaluado la producción primaria bruta y la producción neta, ambas a escala diaria y a 1 km de resolución espacial, con la aproximación de Monteith y el modelo BIOME-BGC, utilizando datos de satélite y diversos tipos de medidas en superficie. Estas últimas se emplean también en el proceso de validación.

Palabras clave: Flujos de carbono, bosques, estrés hídrico, Monteith, BIOME-BGC.

* *Corresponding author: sergio.sanchez@uv.es*

The main goal of this thesis is the establishment of a framework to analyze the forest ecosystems in terms of their role in the carbon cycle. In particular, the carbon fluxes that they exchange with atmosphere are modeled to evaluate their potential as carbon sinks and biomass reservoirs. Carbon flows between the atmosphere, land, and ocean in a cycle that encompasses nearly all life and sets the thermostat for Earth's climate. Plants in general, and forests in particular, play a crucial role in the carbon cycle. It can be considered (Waring & Running, 2007) that carbon begins its cycle through forest ecosystems when plants assimilate atmospheric CO_2 through photosynthesis into reduced sugars. The flux of carbon that is fixed by photosynthesis is called gross primary production (GPP). Part of it is released back into atmosphere by means of the plant autotrophic respiration (R_a), for the synthesis and maintenance of living cells, and by the heterotrophic respiration (R_{het}) from soil organisms other than plants. The net primary production (NPP) equals to GPP – R_a, whereas the net ecosystem production (NEP), also known as net ecosystem exchange (NEE), accounts for R_{het} too (NPP – R_{het}). In this thesis, the GPP is considered as positive (a gain to the system) and the respiration fluxes as negative (a loss to the system): the ecosystem may lose carbon if photosynthesis is suddenly reduced or when organic materials are removed as a result of disturbances.

Forests currently cover about 40% of Earth's ice-free land surface (Waring & Running, 2007), and around the 50% of the peninsular Spain, which constitutes the study area. The assessment of the aforementioned carbon fluxes is performed using two different ecosystem model types driven by a combination of satellite and ground data, part of the latter being also employed as a complementary data source and in the validation process. Considering the peculiarities of the study area, *i.e.*, the diversity of the vegetation type dynamics and its spatial heterogeneity, the algorithm was developed to run the models on a daily basis and 1 km × 1 km spatial resolution (to assure that the spatial resolution of the remotely sensed carbon flux estimates is comparable to the footprint of ground flux estimates in the validation process). Thus, the inputs of the models were retrieved at these temporal and spatial resolutions.

The first model used in the study is a production efficiency model (PEM) relying on the well-known Monteith approach (Monteith, 1972), which considers GPP –the daily GPP in this case– as proportional to the absorbed amount of photosynthetically active radiation through a conversion efficiency factor ε (also known as light-use efficiency factor). Thus, GPP is the product of the incident photosynthetically active radiation (PAR), the fraction of this flux absorbed by vegetation (f_{APAR}), and ε. In previous studies within our research group (Moreno, 2014; Gilabert *et al.,* 2015), the three terms in Monteith's equation were obtained following procedures optimized for the study area, peninsular Spain. The «optimized model» was driven by meteorological and satellite data (MODIS/TERRA and SEVIRI/MSG).

In the present study, the emphasis is put in ε. It is usually modeled as the product of a maximum value ε_{max} depending on the vegetation type and another term, which can be factorized in contributions that account for the reduction in efficiency due to different types of stress. In particular, the inter-annual variations of ε in Mediterranean ecosystems are significantly influenced by the water stress. A deep insight is carried out to evaluate the possibility of quantifying the dependence of this input on water stress using operational remotely sensed products exclusively. This constitutes the first objective.

Therefore, the capacity of six water stress factors (ε'_i) to track daily light-use efficiency of water-limited ecosystems is evaluated. These factors are computed with remote sensing operational products and a limited amount of ground data: ε'_1 uses ground precipitation and air temperature, and satellite incoming global solar radiation (MDSSF product from SEVIRI); ε'_2 uses ground air temperature, and satellite actual evapotranspiration and incoming global solar radiation (DMET product from SEVIRI); ε'_3 uses satellite actual and potential evapotranspiration (MOD16A2 product from MODIS); ε'_4 uses satellite soil moisture (L4SMv3 product from SMOS); ε'_5 uses satellite-derived photochemical reflectance index (calculated from MODIS MODOCGA product); and ε'_6 uses ground vapor pressure deficit. These factors are implemented in the PEM in order to assess their performance for modeling daily GPP. Estimated GPP is compared to reference GPP from eddy covariance (EC) measurements (GPP_{EC}) in four sites. Although the best results are shown by ε'_1, the study concludes that both ε'_3 and ε'_4 are robust options to estimate daily GPP using exclusively satellite data (Sánchez-Ruiz *et al.,* 2017). Nevertheless, ε'_1 has been used to obtain a time series of daily GPP images from 2005 to 2012 over the whole study area and used as the reference GPP throughout the thesis since input data were available. The other two inputs of the PEM (f_{APAR} and PAR) were obtained following the procedures adopted by our research group in the frame of previous projects (Moreno, 2014; Gilabert *et al.,* 2015).

The analysis of changes in the long-term estimates of the CO_2 terrestrial fluxes between ecosystems and atmosphere is important to establish the global carbon balance, especially in forest ecosystems, the main sinks of atmospheric carbon in the biosphere. However, obtaining long time series of annual GPP from daily GPP values is a time-consuming process that requires a huge number of inputs that might be unavailable, especially in retrospective studies. For this reason, a theoretically sound semi-empirical model, based on a linear relationship between the annual GPP and a PAR-weighted vegetation index (VI), is derived from the Monteith approach (second objective). This semi-empirical model can be used to estimate the annual GPP from commonly available VI images and a representative PAR, which does not require actual meteorological data. A cross validation procedure is used to calibrate and validate the model predictions against reference data. As the calibration/validation process depends on the reference GPP product, the higher the quality of the reference GPP, the better the performance of the semi-empirical model. Using the semi-empirical model, the annual GPP has been estimated at 1-km spatial resolution from MODIS NDVI and EVI images for eight years (from 2005 to 2012). On the one hand, MODIS NDVI is included since it is referred as the "continuity index" to the existing 30+ year NOAA-AVHRR derived NDVI time series, which can be extended to provide a longer-term data record required in climatic studies. On the other hand, EVI has been shown to improve NDVI sensitivity in dense vegetation regions and a better performance to minimize soil and atmosphere influences. Two reference data sets have been used to calculate reference annual GPP: the time series of daily GPP from 2005 to 2012 mentioned above for the study area and the MOD17A3 product. Different statistics show a good agreement between the estimated and the reference GPP data, with coefficient of determination around 0.8 and relative RMSE around 20%. The annual GPP is overestimated in semiarid areas and slightly underestimated in dense forest areas. With the above limitations, the model provides an excellent compromise between simplicity and accuracy for the calculation of long time series of annual GPP (Gilabert *et al.,* 2017).

The second modeling approach used in the study is not a PEM but an ecosystem process model or biogeochemical (BGC) model, the Biome-BGC (Running & Hunt, 1993; White *et al.,* 2000). BGC models are considered as an integral tool of ecosystem analysis (Waring & Running, 2007). Ecosystems are too complex to be described by a few equations; current ecosystem models have hundreds of equations, which present interaction in non-continuous and non-linear ways. Furthermore, these models provide the organizational basis for both interpreting ecosystem behavior and simulating system behavior under normal conditions by comparing with ground data. In particular, a forest ecosystem includes the living organisms of the forest, and it extends vertically upward into the atmospheric layer enveloping forest canopies and downward to the lowest soil layers affected by roots and biotic processes (Waring & Running, 2007). In addition to meteorological data, Biome-BGC requires a huge amount of ecophysiological and soil-related inputs that are not always available. By this reason, the model is run with the default values for most of them. However, there are two inputs especially crucial that can differ from the default values due to the relevant characteristics of Mediterranean areas: the stomatal conductance and the rooting depth, that is, the depth at which plants are able to grow roots. The first input was optimized by Chiesi *et al.* (2007) for Italy, an area presenting similar ecoclimatic features to our study area. The optimization of the rooting depth is the third objective of this thesis.

Then, a methodology for improving the application of Biome-BGC in the study area is developed focusing on the optimization of the rooting depth (z_{root}), which is not available for the study area on a spatially distributed basis. The optimal z_{root}

was identified by comparing daily GPP simulations from the Biome-BGC with varying z_{root} to daily GPP estimations from the PEM previously optimized for and validated in the study area (the time series of daily GPP from 2005 to 2012 mentioned above). The methodology was first tested in four EC sites representative of Mediterranean ecosystems and next applied at a regional scale to the whole study area. As a result, daily GPP simulated maps for the 2005–2012 period and an optimal z_{root} map were obtained. Optimal z_{root} in the four EC sites was shallower than the default one (100 cm) and led to better simulation results. Realistic, spatially distributed GPP estimates were obtained at regional scale. Withal, some discrepancies appeared both at local and regional scale emphasizing the difficulty to adequately simulate the site's water budget and the need for proper setting of inputs, including z_{root}, for the correct functioning of Biome-BGC. The performed optimization (Sánchez-Ruiz *et al.,* 2018) opens the door for using Biome-BGC to simulate other main vegetation processes, such as net carbon fluxes, in the study area.

Forest ecosystems are open systems in the sense that they exchange energy and matter with other systems (including the atmosphere). This exchange is essential for the continued persistence of the ecosystem. A forest ecosystem is never in complete equilibrium, a term appropriate only to closed systems in the laboratory (Waring & Running, 2007). However, the simulations of the Biome-BGC correspond to equilibrium conditions. Therefore, they have to be corrected to properly reproduce the ecosystem dynamics. The correction is applied using the growing stock volume GSV (*i.e.*, the volume of all living trees in a given area of forest or wooded land that have more than a certain diameter at breast height) as proposed by Maselli *et al.* (2009). The last objective of this thesis develops in this framework. It is twofold: first, a GSV map is obtained to take into account the non-equilibrium conditions of the forest ecosystem; second, all carbon fluxes are preliminarily estimated to show how the GSV will be inserted in a net carbon flux processing chain, which will be fully operationally developed in the near future.

On the one hand, a wall-to-wall GSV map over peninsular Spain is produced by the combination of Third Spanish National Forest Inventory (NFI3) data and Landsat-5 TM and Landsat-7 ETM+ imagery. Google Earth Engine was used, as a novelty, to deal with Landsat scenes covering more than 50 000 plots along the whole NFI3 period (1997-2007). 805 predictors were calculated by the combination of Landsat reflectance data, including time and texture metrics, vegetation indices, and band ratios. Guided regularized random forest (GRRF) was used to drastically reduce the dimensionality of the original partially correlated 805 predictors and identify the best performing ones, while maintaining the level of accuracy. Predictors involving short-wave infrared reflectance and texture metrics presented the highest importance. A standard random forest algorithm was then used to produce the wall-to-wall GSV map for the whole study area at 30 m spatial resolution with the 29 selected predictors. RMSE around 60 m^3ha^{-1} was obtained at plot level. The GSV map was finally aggregated at 1-km spatial resolution, its non-forest pixels were masked using Land Cover and Use Information System data for Spain provided by ©Instituto Geográfico Nacional, and validated against NFI3 estimations at province level. R^2 = 0.91 and RMSE = 15 m^3ha^{-1} were obtained. On the other hand, the GSV map was used to take into account the actual conditions of the forest ecosystems and to correct the carbon fluxes estimates corresponding to optimal ecosystem functioning. Preliminary results suggest that the aforementioned correction reduce the uncertainty of the estimates (as comparing with reference data). However, further research in relation to the implementation of this correction in the net carbon flux processing chain is proposed to improve the results.

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