Modeling of the carbon and water balance of agroecosystems

The main point of the thesis

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BACKGROUND AND AIM OF THE STUDY

It has been proven that human activity influences the climate of the Earth by changing the chemical components of the atmosphere. Power generation, industry, agriculture and transportation release a huge amount of greenhouse gas into the atmosphere. Any change in the quantity of atmospheric greenhouse gases can unbalance the energy budget of the Earth-atmosphere system and can trigger global warming (IPCC, 2007). The most important anthropogenic greenhouse gas is carbon dioxide (CO_2); its concentration has increased by about 40% from its preindustrial value (IPCC, 2007).

The biosphere-soil system is a sensitive carbon pool: the terrestrial carbon budget can change rapidly and significantly by the changing environmental conditions (rainfall, temperature, radiation, nutrition status), and can interact with the climate through the greenhouse effect. While in the last 10,000 year the terrestrial carbon budget has been balanced, in the past few decades the biosphere turned into a net CO_2 sink. Nevertheless, we can not preclude the possibility that the further increase of temperature will turn this labile carbon pool into a net CO_2 source. Until the behavior of the biosphere is not known, the changing of CO_2 concentration in the atmosphere (and therefore climate change) is not predictable. This requires the determination of the possible causes of carbon budget changes at the ecosystem level. Since the terrestrial carbon budget is influenced by many factors, it is essential to understand their biogeochemical processes (CIAIS ET AL. 1995).

In order to accomplish this task, numerical models are the most convenient instruments beyond the measurements, using mathematical description of the processes. There are several types of models that may be used in ecosystem analysis. Regression models are based on empirically derived statistical relationships between biometric parameters and production of the biomes. Such models are useful to predict stand development under stable conditions, but they cannot be used to incorporate changing environmental condition and spatial extrapolation. Therefore process-based models were employed which simulate mechanistically the ecosystem functioning as a result of ecophysiological processes. This type of model is able to incorporate the effect of environmental change on ecosystem development. Process-based ecosystem models usually use many ecophysiological and site parameters to describe the development and interaction of soil and biomass components. Therefore a critical step of using these models is the parameterization (RAJKAI ET AL. 2004).

Temperate grasslands cover large areas of the Earth's surface. Typically they are located in arid regions where the effects of global climate change are predicted to be high. Temperate grasslands represent about 10% of the global carbon pool (most of the carbon content is in the soil organic matter and the below-ground plant parts); therefore it is important to examine its functioning. Furthermore grasslands are able to adapt to the changing environmental conditions and thanks to their diversity they can store more carbon than arable lands. Croplands are small carbon sink or source. The nature, frequency and intensity of management play a key role in carbon balance of managed ecosystems (SOUSSANA ET AL. 2007).

The European Union has started several research projects (Carboeurope-IP, Carboocean-IP, GEOMON, IMECC) in order to describe the greenhouse gas exchange, mainly the sink and source characterization of ecosystems, among others grasslands and croplands. Most recently research focused on managed ecosystems human intervention has an important role in the formation of the land surface through e.g. agricultural practices, land use change, erosion, irrigation, grazing, etc. I is an important problem that current biogeochemical models are unable to adequately quantify managed ecosystem carbon dioxide exchange processes. Therefore it is an important task to create process-based models which can simulate the carbon and water exchange of the disturbed ecosystem (CIAIS ET AL. 2009).

The possibilities of the modeling of the Hungarian agroecosystems' carbon and water balance, the problems encountered during modeling and their results, the advantages and the difficulties of the model-method are detailed in present study.

The aims of the study

The main aim of my work is to examine the carbon and water exchange of agroecosystems, analyze the relationship between environmental conditions and functioning of the ecosystem and investigate the short- and long-term effect of the human activities through implementing the following methodological improvements:

- adaptation of a process-based ecosystem model: building the required input database using measured and modeled meteorological data
- development of Biome-BGC model's phenology and soil water sub-model
- development of a process-based model, CarbonISO, in order to simulate the temporal variation of atmospheric $^{13}CO_2$ concentration and ^{13}C content of plant material
- development of a novel calibration method based on Bayesian theorem in order to parameterize the process-based models mentioned above

MATERIALS AND METHODS

Study sites

Two of the most important steps of any modeling activity are the preparation of the input database and the validation (the examination of the model output data and the control of the functioning of the model). During validation the model output data are compared to measured data.

Carbon-dioxide (CO_2) exchange was measured at three grassland sites by eddy covariance technique in Hungary. The first of these sites was established in 1999 in the relatively wet western part of the country, near Hegyhátsál (BARCZA ET AL. 2003; HASZPRA ET AL. 2005). The second one is located in the dry central region of Hungary, in Kiskunság National Park, near Bugac, where the measurements were started in July, 2002 (TUBA ET AL. 2004). The third one is in the north eastern region in Mátra Mountains where the study site was set up in June, 2003 (TUBA ET AL. 2004).

The presented research was conducted based on carbon exchange and meteorological measurements from these three different Hungarian measurement sites: managed, semi-natural grassland on silt soil (Hegyhátsál), a sand pasture (Bugac) and a dry mountain meadow on heavy clay soil (Szurdokpüspöki). The mean annual temperature and mean annual sum of the precipitation are 8.9 °C and 750 mm at Hegyhátsál (silt soil), 10.4 °C and 562 mm at Bugacpuszta (sandy soil) and 10.2 °C and 622 mm at Szurdokpüspöki (clay soil) respectively. Summer drought is typical at Bugacpuszta, but the climate is quite similar at the different sites. Soil types cover a wide range of nutrient and clay content (TUBA ET AL. 2004).

Description of Biome-BGC

Biome-BGC v4.1.1 was developed from the Forest-BGC family of models in order to simulate the functioning of the ecosystem. The Biome-BGC model is an extended version for use with different vegetation types. In the latest version the Biome-BGC used daily time step, and was driven by daily values for maximum and minimum temperatures, precipitation, solar radiation, and air humidity (RUNNING ET AL. 1993). Spatial variability is neglected by model because the model simulations regard to unit ground area.

Biome-BGC is a mechanistic model that simulates the storage and fluxes of water, carbon, and nitrogen within the vegetation, litter, and soil components of terrestrial ecosystems. State variables (pools) have three groups: normal pool, storage pool and transfer pool. Normal pools are the amount of carbon or nitrogen that displays on the actual simulation day; storage pools store the amount which will appear next year (like a core) and transfer pools store the whole amount of storage pool after the end of the actual transfer period until the next one and in the next transfer period will be transferred gradually into the leaf carbon pool (like a germ) (RUNNING ET AL. 1987; RUNNING AND COUGHLAN, 1988).

The most important blocks of the model are: carbon flux block, phenological block and soil flux block. In the carbon flux block the gross primary production of the biome is calculated using Farquhar photosynthesis routine. Phenological block calculates the foliage development and accumulation of carbon and nitrogen in leaf, stem, root and litter. Soil block describes the decomposition of litter, soil carbon and nitrogen. The simulation has two steps: the first is the optional spinup simulation which starts with very low initial level of soil carbon and nitrogen and runs until a steady state is reached in order to estimate the initial values of the state variables. The second, normal simulation uses the results of spinup simulation (initial carbon and nitrogen pools) and runs for a given predefined time period (RUNNING AND GOWER 1991).

Biome-BGC uses at least three input files. Initialization file includes information about the model run (input and output file names, first simulation year, etc) site and scenario parameters (elevation, soil texture, effective soil depth). Meteorological file contains daily climate data and the definition of several essential climate-, vegetation-, and site characteristics. This file can be prepared manually or using climate models C2W (which generates daily data from monthly means), and MTCLIM (which estimates the radiation and the dew point temperature on a daily scale) (BÜRGER, 1997). To carry out the long-term spinup-simulation standard meteorological data were combined with the high-resolution gridded datasets of the University of East Anglia Climate Research Unit. Biome-BGC is provided with default ecophysiological parameter sets for the major biome types (deciduous forest, evergreen forest, shrub, grassland). Besides these data elevated atmospheric CO_2 concentration and increased nitrogen deposition can be also taken into account in the model (WHITE ET AL. 2000).

Model calibration

In order to set up model simulations direct measurement data are used regarding to meteorological and soil specific data. The input parameters of the process-based models determine model output completely. However, our knowledge of the world is incomplete, which means that there are several input parameters for which values are hard to obtain directly from experiments or no local measurements are available. The exact values of these parameters are unknown; therefore they are referred as unknown model parameters (KENNEDY AND O'HAGAN ET AL. 2001).

Due to the uncertainty associated with the unknown model parameters significant bias can be experienced if the model is used to simulate the carbon cycle components at the eddy covariance measurement sites described above. In order to improve model performance the unknown model parameters has to be estimated or at least their uncertainty has to be constrained. The unknown model parameters can be estimated using inverse techniques based on measurement data, which means that the model is being calibrated (VAN OIJEN ET AL. 2005).

In order to determine the unknown model parameters which have strong effect on a given simulation it becomes necessary to perform sensitivity analysis. A possible solution for sensitivity analysis is the use of the least square linearization (LSL) which divides output uncertainty into its sources and can be conducted with the partial result of our calibration process. LSL is a multiple linear regression between the parameter deviation from the mean and the output (in our case: the likelihood value in the given iteration step). As result of the LSL method, the total variance of the model output and the sensitivity coefficient of each parameter can be determined. Sensitivity coefficient shows the percent of total variance for which the given parameter is responsible; it can be approximated using regression coefficients and the variations of the parameter uncertainties (RAUPACH ET AL. 2005).

Bayesian-approach is a global optimization method to estimate the optimal values of the unknown model parameters. Bayesian procedure begins with quantifying the variability of the unknown model parameters in the form of *a priori* probability distribution. Then measured data are compared with simulated data via calculating a likelihood function. Likelihood is the degree of goodness-of-fit between simulated and measured data. The next step is the construction of a random walk in the parameter space based on the Metropolis-algorythm. The optimization process is a quasi-random walk through the parameter space, which attempts to find parameter sets that minimize the model-data error defined in terms of likelihood function. Each unknown model parameters are varied randomly within their measured range of variability and the model is run several times using variable model parameters. Finally, the *a priori* distribution is updated with model information (distribution of the likelihood function) which means the convolution of the *a priori* distribution with the likelihood function provided by the large number of model simulations. If the calibration procedure is successful, the uncertainties of unknown model parameters (confidence intervals) decrease and the measured variable variances explained by the model increase (HOLLINGER AND RICHARDSON, 2005).

RESULTS

Methodological results

Improvement of soil water balance module of Biome-BGC model

The water supplied to the soil surface by precipitation can be transported in several ways. A part of the precipitation is intercepted on canopy and is evaporated without passing through the soil or the plant. The amount which is not intercepted reaches the soil. If the water is supplied to the soil surface faster than it can *infiltrate* (intensive raining) the excess water may be lost as *runoff*. The fraction which flows into the soil can be stored in root zone or lost by *deep percolation*. If the soil moisture content rises above the saturation point after a big precipitation event, the surplus flows out of the soil. Biome-BGC was primarily developed to simulate the carbon budget; the water balance sub-model is simple. The model takes into consideration the phenomenon of *interception* and *outflow*. I have integrated a *runoff* and *deep percolation* sub-module in order to improve the soil water balance simulation using empirical formula (CAMPBELL AND DIAZ, 1988).

Improvement of model phenology of Biome-BGC model

The phenological state of vegetation significantly affects the exchanges of carbon and latent heat between the ecosystem and the atmosphere. Growing season index is widely used to calculate the start and the end of the vegetation period (DORKA, 2005). These days can be set manually in ecophysiological file of Biome-BGC or model phenology can be used. The start of the growing season calculated by the model was experienced to be unrealistic late in case of herbaceous ecosystems; therefore a new phenology module was created. A new growing season index was defined: heatsum growing season index. This index is constructed with the combination of a common set of variables into an index for the estimation of growing season: minimum (suboptimal) temperature, vapor pressure deficit, daylength and 10-day heatsum with 5°C basic temperature were combined in the estimations. For each variable threshold limits were set, within which the relative phenological performance of the vegetation was assumed to vary from inactive (0) to unconstrained (1). The values of the limits regarding to the different variables can be set by the user. If on a given day the index is greater than a limit (can be set by the user) the start of the growing season is assumed to be found. After finding the start of the growing season the end day is searched: if on a given day the index is less than a limit the end of the growing season is assumed to be found.

Modeling the effect of drought on the functioning of the vegetation

The stomatal conductance calculation is based on environmental limiting factors in Biome-BGC model (similar to other process-based biogeochemical models). The most important limiting factor is the soil moisture content: if the moisture content decreases due to the low level of the precipitation, the stomatal conductance and therefore carbon uptake will decrease. Nevertheless if the stress ends, the limitation of the stomatal conductance ends, and the simulated carbon uptake returns to the previous stress value. Thus the original model ignores the phenomena of plant wilting caused by soil drying-up. In order to solve this problem a drying-up module was implemented to simulate the ecophysiological effect of the drought stress. If the soil water potential decreases below a critical value, the new module starts to calculate the number of the days under drought stress (stress days). A *drought coefficient* is calculated based on the number of the stress days which determines the ratio of the plant material (carbon and nitrogen content of leaf and fine root) which turns into the litter pool as results of drought stress.

Integration of management modules into Biome-BGC model

Biome-BGC has been developed to simulate the carbon, water and nitrogen cycles of undisturbed, unmanaged ecosystems. In order to use Biome-BGC to simulate the effect of agricultural management some new modules were integrated into the source code: *mowing*, *grazing*, *fertilizing*, *harvest*, *ploughing* and *sowing*. In order to simulate the effect of management activities on the carbon, nitrogen and water pools new fluxes were defined between the pools and between pools and the environment. In the present dissertation I used Biome-BGC to simulate the functioning of grasslands; the modeling of croplands was out of scope of the study. Therefore the modules of *mowing* and *grazing* (on grasslands) were validated using Hungarian measurement data. The modules of *fertilizing*, *harvest*, *ploughing* and *sowing* are only prepared to simulate the management activities on croplands and are only tested with synthetic data.

The main effect of *grazing*, *mowing* and *harvest* is the defoliation (SOUSSANA ET AL. 2007). In these cases the normal carbon and nitrogen pools are decreased. The rate of the plant material reduction depends on the management type: in case of *mowing* the leaf area index of the grass after mowing can be set by user (from the decrease of leaf area index the decrease of carbon content can be calculated); in case of *grazing* the daily ingested dry matter and the animal stocking rate determines the plant material decrease; in case of harvest the leaf area index of snag (remaining plant after harvest) can be determined by user. If the harvested plant material is transported away from the site the cut-down fraction (carbon and nitrogen) is net loss to the system; if it is left at the site plant material can return to the soil pools. Besides the defoliation effect of grazing (intake by animals) it is important that a fixed proportion of the above ground biomass flows to the litter compartment as result of trampling of excretal returns.

Ploughing means farming for initial cultivation of soil in preparation for sowing seed or planting. The primary purpose of ploughing is to turn over the upper layer of soil bringing fresh nutrients to the surface, while allowing the remains of previous crops to break down and return to the soil. Since the soil model of Biome-BGC is one-layered the effect of layers turning over is ignored. It is assumed that due to the plough all the plant material of snag (remaining after harvest) returns the litter pools.

Sowing is the process of planting seeds. In order to simulate the effect of sowing it is assumed that the plant material which is in the planted seed gets into the transfer pools. From the proportion of material of seed which produces leaf the proportion which produces root can be calculated easily, because C3 and C4 plant consists of leaf and root in Biome-BGC. The nitrogen content of leaf and root can be calculated using ecophysiological constants: carbon and nitrogen ratio of leaf and root.

The most important effect of *fertilization* is the increase of soil nitrogen (the other effects are ignored). A fixed proportion of the fertilizer enters the soil on a given day after fertilizing. Not all this fraction gets into the soil pools because a given proportion is leached; this is determined by the efficiency of utilization. Nitrate content of fertilizer can be taken up by plant directly, therefore we assume that flows the soil mineral pool. Ammonium content of fertilizer has to be nitrificated before being taken up by plant, therefore flows into the litter nitrogen pool. The carbon content of fertilizer gets into the litter carbon pool.

The development of CarbonISO

The stable carbon isotope content of carbon dioxide ($^{13}CO_2$) in air contains unique information on the biological and physical processes that govern the CO_2 budget of the atmosphere (since diffusion and carboxylation processes discriminate against the heavier isotope, plants preferentially use $^{12}CO_2$ in photosynthesis, therefore CO_2 in the atmosphere becomes relatively enriched in $^{13}CO_2$ during carbon uptake). It could help to understand the functioning of the vegetation and give information on the contribution of the anthropogenic sources to the atmospheric carbon budget. At Hegyhátsál weekly measurements of $^{13}CO_2$ has been performed. It is useful but costly; therefore a process-based model was developed in order to simulate the abundance ratio of atmospheric $^{13}CO_2$ ($\delta^{13}C_{air}$) based on eddy-covariance data.

The model domain is an air-column with the height of planetary boundary layer, forming a box on the surface (box-model). It is assumed that the air inside the box is well mixed, meaning that the atmospheric mixing ratio of CO_2 and its carbon isotope composition is uniform in space. An adiabatic temperature lapse rate and barometric vertical pressure gradient are assumed inside the box, which are used to calculate the average temperature and air pressure for the box. The height of the box varies in time; it is equal to the height of the boundary layer from the ECMWF data at any moment. Such a box model cannot handle the advection processes, which is an obvious limitation of this simple model type (HIDY ET AL. 2009).

The simulation time step was one hour. As initial condition the $^{13}CO_2$ content of the box was calculated from the measured CO_2 mixing ratio and atmospheric stable carbon isotope ratio ($\delta^{13}C_{air}$) (NOAA ESRL data). As a first approach it is assumed that the plant and soil carbon pools can be divided into two parts: short-term (carbon residence time is from a day to a week) and long-term (carbon residence time is greater than a week) pools. In every simulation step the atmospheric mixing ratio of CO_2 and its stable isotope ratio in the box were recalculated by taking into account the mixing with the upper atmospheric layers (when the box is expanding upward) as well as the source and sink processes at the surface. Using eddy covariance flux data and the simulated atmospheric mixing composition of CO_2, stable carbon isotope ratio of plant material were also recalculated. Changes in $\delta^{13}C_{air}$ in the model were driven by the change of the boundary layer height and by the ecosystem carbon exchange processes (HIDY ET AL. 2009).

Self-developed implementation of calibration procedure

A novel, n × m-step, multi-objective calibration method was implemented (n: the number of internal *model parameters* which determines the number of iteration sections; m: number of iteration steps in an iteration section) with a special likelihood function.

Uniform distribution is assumed to *a priori* distribution between their minimum and maximum values that are estimated from the literature. In present work likelihood includes the relative error of the simulation and the correlation between measured and simulated data. Relative error (RE) is the ratio of mean absolute error of the simulation and the maximal interval of the given measured data (difference between maximum and minimum measured data). This normalization is important in multi-objective calibration because the different misfit (errors regarding to different reference data) must be comparable. Correlations mean a further weighting factor to avoid labeling a given run that has small errors but poor correlation with the measured data, with good likelihood value. Therefore the meaning of likelihood is as follows: if an unreal parameter set generates a big difference or incoherence (large relative error and small correlation) between the simulated and the measured data, the likelihood is close to zero. If a good parameter set generates a small difference and strong relationship (small relative error and large correlation) between the simulated and the measured data, the value of likelihood will be close to one.

Gross primary production (GPP), total ecosystem respiration (TER) and latent heat flux (LE) are used as reference measurement data in case of Biome-BGC and CO_2 mixing ratio in case of CarbonISO. To achieve the combined likelihood in case of Biome-BGC, the likelihood of each variable were multiplied. In case of CarbonISO a simple, one-member likelihood was used.

An important and well-known problem of the global optimization method is the *parameter equifinality*. It means that many different parameter combinations can produce similar good simulation results with respect to calibration data. In order to avoid *parameter equifinality* after the first iteration section only the most *important* parameter is set to its optimal value. *Important* is used here in the sense that the *important* parameter has strong effect on model outputs (and through this on goodness-of-fit). To determine *important* parameters sensitivity analysis is necessary. A possible solution to improve sensitivity analysis is the least square linearization (LSL) method which provides sensitivity coefficients of the given parameters. Parameters with high *sensitivity coefficient* are in strong relationship with the variance of likelihood values; they have convergence in their *a posteriori* probability density function. The parameter of which *sensitivity coefficient* is the highest is fixed on its optimal value. In the next iteration section, only *n*-1 parameters are varied randomly. The iteration section detailed above is repeated till each *model parameter* is set to its optimal value.

If the calibration procedure is successful, the uncertainties of model parameters (confidence intervals) are decreased and the measured variable variances explained by the model are increased.

Simulation results

Validation of the developed and calibrated Biome-BGC

As a result of the calibration and the incorporation of the management activities (referred as developed model) the simulation of the carbon and water fluxes of the three Hungarian grasslands has significantly improved. The success of calibration can be evaluated with the goodness-of-fit of the simulation and the decrease of the uncertainty of the model parameters. The simulation improved due to the model developments and the calibration: errors are smaller, square of correlations are higher than in case of the original model using original parameter set. RE is between 15-20%, R^2 between 0.65-0.80 regarding to the different sites and reference data using developed model using calibrated parameter set. The confidence intervals decreased regarding each parameters (on the average *a posteriori* intervals are the 40-70% of the *a priori* intervals). It means that the uncertainty of the *model parameters* decreased due to the calibration.

Effect of the site-specific conditions on simulated data of Biome-BGC

The model was applied to simulate the long term dynamics of the carbon cycle components at the eddy covariance sites. Because of the different ecophysiological parameters, different local climate and soil type the carbon exchange is different at the three measurement sites. For the simulations input meteorological data are used from 1997 to 2008 at Hegyhátsál, from 2002 to 2008 at Bugacpuszta and from 2003 to 2008 at Szurdokpüspöki. The multi-annual average of gross carbon uptake (GPP) is the highest at the managed grassland on silt soil (Hegyhátsál) and the lowest at the grassland on mountain heavy clay soil (Szurdokpüspöki). In case of respiration and latent heat flux the situations are similar. The amount of soil moisture necessary to the optimal carbon uptake processes depends on the soil type (plant available water) and the local climate (precipitation and temperature). The water holding capacity of the soil is the highest in silt soil and the lowest in heavy clay soil. Therefore the soil moisture limitation of carbon uptake is the lowest at Hegyhátsál (silt soil, low mean annual temperature, high mean annual sum of precipitation) and is the highest at Szurdokpüspöki (clay soil, medium mean annual temperature, medium mean annual sum of precipitation).

Net carbon uptake (NEE) is the difference between TER and GPP (positive if the ecosystem is net source). At Hegyhátsál and at Szurdokpüspöki the multi-annual average of GPP is higher than multi-annual average of TER (grasslands are usually net carbon sinks during all the growing season). In contrast, at the dry, managed grassland on sandy soil (Bugacpuszta) usually multi-annual average of GPP becomes lower than multi-annual average of TER (grassland usually became a net source) for circa a month in the growing season (from day 180 to 220; July and August). This is because the soil usually dries out, the soil moisture content decreases below the plant available water in July and August, but afterwards − owing to the precipitation in late August − the carbon uptake increases again. Important and well-known feature is this second growing period after drying-up (beginning from late August till early September) of the grassland at Bugac.

In summary, the annual carbon uptake is the highest at Hegyhátsál and the lowest at Szurdokpüspöki. These measurement sites are similar because the ecosystem is usually net carbon sink in the vegetation period, while there are two growing seasons at Bugacpuszta owing to drying-up of the soil in July and August. The agreement between simulated and measured data is good for all the measurement sites.

Analyzing the effects of management on the simulation results of Biome-BGC model

In order to analyze the effect of the management, Biome-BGC was run for a 38-year period (1971-2008). Meteorological data for that period are only available for Hegyhátsál therefore the simulations were tested here.

Net biome production (NBP) shows the net gain or loss of carbon from an ecosystem or from a region where carbon loss/surplus caused by human activity is included (in contrast to NEE). NBP is positive when the ecosystem (taken into account the effect of disturbances) is net sink and negative if it is a net source. The annual sums of NEE are less (more negative NEE means higher CO_2 uptake) in case of the mowed grassland than in case of the undisturbed grassland despite of the decreasing plant material caused by mowing. The leaf area − which intercepts and evaporates a certain part of the precipitation − decreases to a fixed value twice a year, therefore more precipitation turns into the soil. This results in the increase of the soil moisture content which is the most important limitation factor of the stomatal conductance. If more soil moisture is available, the stomatal conductance is less limited; as a consequence higher carbon uptake is possible. In contrast, NBP is lower in case of the mowed grassland which means that if carbon loss by cutting and removal is taken into account the ecosystem is a net source in most of the simulation years. In case of the undisturbed grassland the soil carbon content increases; in case of mowed grassland it decreases continuously. The reason of this phenomena is that in case of mowing the ecosystem is a net carbon source (NBP is negative) in contrast of the undisturbed ecosystem (due the removed biomass).

The situation is similar in case of grazed grassland, but the changes are less, because the carbon loss (decrease of plant material) caused by grazing (animal intake) is less than caused by mowing (cutting) and animal intake is recovered partly by carbon and nitrogen surplus from excretal returns in contrast to mowing (cut-down fraction is transported which means net loss for the system).

Validation of CarbonISO model

CarbonISO simulates the atmospheric stable carbon isotope abundance ratio and variation of ^{13}C content in plant material using biosphere-atmosphere CO_2 flux and meteorological data. The physiologically based approach was successfully applied to calculate discrimination (Δ), ^{13}C content in plant material and in the air from measured eddy data (assimilation and transpiration) and atmospheric CO_2-concentration data. In this way, representation of the discrimination process became more reliable as opposed to other less realistic solutions as taking a constant value of Δ, for example. More importantly, modeling of ^{13}C of atmospheric CO_2 became also more reliable and the model can serve as an independent tool for calculation of biogenic ^{13}C fluxes and therefore may be used as a constraint in future investigations regarding fossil fuel CO_2 contributions. The model proved to be an appropriate tool to simulate $\delta^{13}C_{air}$ variation where eddy flux data were available. Correlation between the measured and simulated $\delta^{13}C_{air}$ was 0.72 with a relative error was 15% regarding the validation years (2001-2004). The corresponding values for atmospheric CO_2 mixing ratio were 0.74 and 13%. The correlation between the measured and the simulated values is statistically significant at $P < 0.01$ probability level.

Estimation of the fossil fuel combustion using CarbonISO model

Observed deviations between the measured and simulated $\delta^{13}C_{air}$ values were systematically negative in winters, while deviations were random in sign and smaller by an order of magnitude during periods when the vegetation was photosynthetically active. This difference is suggested to be influenced by anthropogenic emission of CO_2 strongly depleted in ^{13}C due to fossil fuel based winter heating and also by the lower boundary layer heights during winter periods.

In order to estimate the contribution of fossil fuel CO_2 to the concentration at the receptor station Hegyhátsál we used modeled values from the COMET Lagrangian transport model. As expected the fossil fuel contributions to the CO_2 concentration are high in winter time due to higher emissions and lower PBL heights.

The simulated contribution to atmospheric CO_2 concentration by fossil fuel combustion modeled by the COMET transport model significantly (at $P < 0.01$ probability level), although weakly, correlates with the difference between the measured and simulated $\delta^{13}C_{air}$ values, and this relationship is negative further supporting that the deviations may well be caused by anthropogenic contribution due to gas combustion during winter.

NEW SCIENTIFIC RESULTS

1. The process-based ecosystem model, Biome-BGC was adapted: the input database was created using measured meteorological and ecological data and using weather generator.

2. The original Biome-BGC model does not handle management activities therefore different management modules (mowing, grazing, harvest, ploughing, sowing, fertilizing) were integrated in order to analyze the functioning of a disturbed ecosystem. Mowing and grazing modules were validated using measurement data from the grassland at Hegyhátsál and Bugac.

3. The phenology and soil water module of Biome-BGC was developed. As result of the phenology corrections the Biome-BGC can well simulate the start and the end of the growing season for herbaceous ecosystems. Thanks to the soil water module developments the model can handle the process of runoff and deep percolation and the effect of summer drought became more realistic.

4. Another process-based ecosystem model, CarbonISO was developed in order to simulate the temporal variation of atmospheric $^{13}CO_2$ concentration and ^{13}C content of plant material. The model is driven by observed meteorological and measured biosphere-atmosphere CO_2 exchange data.

5. After adapting the Biome-BGC and developing CarbonISO the models were calibrated in order to decrease the difference between the measured and the simulated data using Bayesian approach. A novel calibration method with a special likelihood function was implemented. As results of the calibration the simulation of the models were improved and the uncertainty of the unknown model parameters were decreased.

6. CarbonISO model was validated using measurements from a Hungarian atmospheric monitoring station. The simulated atmospheric stable carbon isotope ratio data agreed well with the measured ratios considering both the magnitude and the seasonal dynamics. Observed deviations between the measured and simulated $\delta^{13}C_{air}$ values were systematically negative in winters, while deviations were random in sign and smaller by an order of magnitude during periods when the vegetation was photosynthetically active. This difference, supported by a significant correlation between the deviation and modeled fossil fuel contributions to CO_2 concentration, suggests the increased contribution of ^{13}C-depleted fossil fuel CO_2 from heating and the lower boundary layer heights during winter.

7. According to the simulation results the most influential factor of carbon uptake is plant available water and therefore the multi-annual average carbon uptake is the least at Szurdokpüspöki (mountain meadow on clay soil). Examining the effect of management activities it is pointed out that (despite of carbon loss by mowing and grazing) the net carbon uptake (NEE) is greater than in case of undisturbed ecosystem. However, if the human induced carbon loss (lateral carbon transport) is considered in the carbon balance the grassland become net carbon source.

CONCLUSIONS AND PROPOSITIONS

According to present study it is concluded that process-based Biome-BGC model is able to simulate the carbon and water exchange of grasslands and therefore it is an appropriate tool to examine the effect of the different environmental conditions and the human activity on the functioning of the grasslands. The calibrated, developed and validated Biome-BGC was used to estimate the carbon balance components at the three measurement sites. Using Biome-BGC we compared the carbon budget of the three Hungarian measurement sites with different site-specific conditions. We found that carbon fluxes are strongly affected by the type of the soil: carbon uptake is the highest at the managed grassland on silt soil, and the lowest at the grassland on mountain heavy clay soil. Thanks to the implementation of the management modules we can test the short-term and long-term effect of management activities (mowing and grazing). We pointed out that due to mowing and grazing the ecosystem is able to turn into net carbon source from net carbon sink if the carbon loss by human activity is taken into account.

A further goal is to improve the management modules to take into account the effect of human activity on soil properties not only on aboveground biomass.

An important future task is the development and implementation of a multilayer soil-submodel into Biome-BGC.

I am planning to improve Biome-BGC in order to simulate the budget of other greenhouse gases (N_2O, CH_4) based on the quantification of nitrogen budget.

In addition a further goal is using Biome-BGC to simulate the functioning of croplands (besides grasslands) including the validation of sowing, harvesting, ploughing, and fertilizing.

The self-developed CarbonISO model can simulate the ^{13}C ratio of the CO_2 in the air and in plant material using carbon flux data and provides further information on the functioning of the vegetation. Comparing the measured and simulated ^{13}C ratio of the CO_2 further information can be provided on the contribution of the anthropogenic sources to the atmospheric carbon budget.

Calibration of the Biome-BGC and CarbonISO was performed using Bayesian approach with measurement flux data from three Hungarian measurement sites (Hegyhátsál, Bugac, and Szurdokpüspöki). This new, self-developed calibration method is appropriate to optimize the unknown parameter of a non-linear process-based model regardless the simulated processes. Thanks to the calibration the correlation between simulated and measured data increases, the simulation error and the confidence intervals decrease.

The present study is important step towards the understanding and describing the functioning of grasslands under actual environmental circumstances. Further goal is to use Biome-BGC and CarbonISO under changing environmental circumstances to predict the change of the carbon and water exchange of the ecosystem.

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