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Deliverable D2.5 “Simulations with vegetation coupled to the carbon and nitrogen cycles in EC-EARTH and COSMOS”

1 INTRODUCTION

Atmosphere-biosphere exchange of reactive carbon and nitrogen compounds and their reaction products plays a pivotal role in the Earth system through regulation of atmospheric- and biogeo-chemistry. Atmosphere-biosphere exchange is also relevant to past, present and future climate through its role in the tropospheric ozone (O_3), the third most important greenhouse gas (GHG), production of biogenic aerosol, and regulation of the oxidizing capacity. The latter determines the efficiency of chemical destruction of pollutants and GHG's such as methane and, consequently, their atmospheric residence time and contribution to radiative forcing.

The global biosphere emits about 1.3 PgC yr^{-1} of reactive carbon in the form of Volatile Organic Compounds (VOCs), e.g. isoprene and terpenes (Guenther et al., 2006). The biogenic emissions are thought to exceed anthropogenic emissions by a factor of 10 and are important to atmospheric chemistry and climate through formation of O_3 and Secondary Organic Aerosols (SOA) (Kanikadou et al., 2005). Soils are a large source of nitric oxide (NO), a reactive nitrogen compound which controls the NO_x ($NO+NO_2$) budget in remote and rural areas while emissions from fossil fuel combustion dominate the NO_x budget in

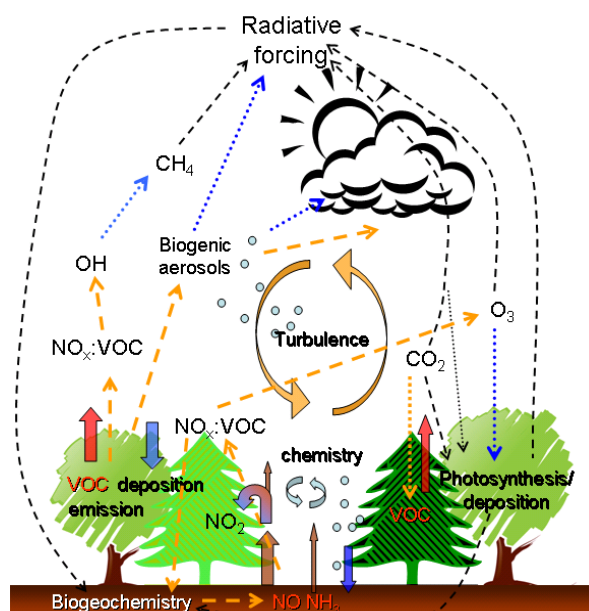


Figure 1: Earth system feedback mechanisms associated with atmosphere-biosphere reactive exchange processes. Long-dashed orange arrows and dotted blue arrows denote positive and negative process linkages, respectively. Other important linkages between processes already implemented in ESMs are denoted by dashed black arrows.

industrialized areas (Ganzeveld et al., 2004). Reactive nitrogen emissions in the form of ammonia (NH_3) are dominated by agriculture. NH_3 is involved in rain- and cloud-water chemistry, the formation of N-containing aerosols, acidification of ecosystems (de Vries et al., 2007) and is essential to assess the role of sulfate aerosol in climate (Luo et al., 2007). The biosphere also poses a large sink of many reactive compounds and aerosols due to active uptake by leaf stomata, soils and other canopy surfaces. For example, global dry deposition removes an estimated 600-1000 Tg O_3 yr^{-1} , an amount comparable to the source of tropospheric O_3 associated with stratosphere-troposphere exchange (Ganzeveld et al., 2002b)

There are important Earth system feedback mechanisms associated with atmosphere-biosphere reactive exchange (Figure 1). Biogenic aerosols play an important role in coupling the physical, chemical and biological components of the climate system and may therefore have a large impact on climate (Andreae and Crutzen, 1997). A change in radiation associated with cloud-biogenic aerosol interactions can have important consequences for vegetation uptake of CO_2 , VOC emissions, and, consequently, in turn for biogenic aerosol formation. Increased biogenic emissions of reactive nitrogen and carbon due to climate and land use change would result in elevated concentrations and deposition of nutrients and oxidants (e.g. nitrogen and O_3). This affects ecosystem functioning (Sitch et al., 2007) and, consequently, atmosphere-biosphere reactive exchange.

These findings indicate the potential importance of atmosphere-biosphere reactive exchange in atmospheric and biogeo-chemistry and climate. However, due to large uncertainties in biogenic sources and sinks, chemical processing and impacts, more quantitative assessments, e.g. of the relevance of biogenic aerosols in climate forcing, still contain a large uncertainty. In addition, use of empirical models, which do not consider the dependence of reactive exchange on key drivers, limits qualitative assessments of the importance of feedbacks associated with reactive exchange.

2 MODEL SYSTEM DEVELOPMENT & APPLICATION: BVOC EXCHANGES AND RELATED CHEMISTRY

2.1 Site-scale feedbacks involved in reactive N and C exchanges

A canopy model to simulate explicitly atmosphere-biosphere reactive trace gas and aerosol exchanges had been coupled to the representation of energy, water and CO_2 exchanges in a single column model ESM, the 1-D chemistry and climate model SCM (Ganzeveld et al., 2002a, 2008). One particular feature of the coupling between the SCM and the canopy exchanges model has been the coupling of transpiration and surface deposition to CO_2 exchanges.

The SCM has been coupled to the dynamical global vegetation model (DGVM) LPJGUESS. The latter DGVM simulates the biogenic emissions of Volatile Organic Compounds (VOC) from vegetation properties, the

atmospheric CO₂ concentration, and the SCM's meteorology. In addition, the SCM's simulation of the O₃ surface layer concentrations are used to consider O₃ deposition impacts on net primary production and, consequently, on VOC emissions as simulated by LPJGUESS. These VOC emissions are not only affecting the SCM's photochemistry but also SOA formation. As such the established coupling between the multi-layer canopy exchange model, the SCM and LPJGUESS allows to assess the role of reactive carbon and nitrogen in vegetation feedbacks, to assess site-scale ecosystem exchanges including biogenic emissions and wet and dry deposition of gases and aerosols.

The coupled SCM-LPJGUESS system has been deployed to first analyse the significance of these interactions between atmospheric- and biogeochemistry at the measurement site Hyytiala, Finland, where long-term and intensive field campaign observations are available to assess the potential existence and relevance of the proposed vegetation feedback mechanisms. Regarding intensive field campaign data for Hyytiala we use observations collected during the HUMPPA-COPEC intensive field campaign, July-August 2010. Since LPJGUESS requires a long spin-up to actually reach a quasi-steady state in terms of vegetation properties as a function of climate the system is based on a 105-year offline simulation with LPJGUESS constrained with CRU meteorological input data for the specific site until the starting date of available site-scale observations (or ECMWF data). As of this starting date, online simulations are conducted covering the growing season at Hyytiala with the vegetation dynamics of LPJGUESS being constrained with the online simulated meteorology in the SCM as well as O₃ concentrations determining the deposition impact. N-deposition impacts on atmosphere-biosphere reactive exchange are not yet considered also since the development of this N-cycle component in LPJGUESS has been delayed. However, the established coupling between the SCM including the multi-layer canopy exchange model and LPJGUESS will allow to further incorporate this coupling whenever an updated version of LPJGUESS including this representation of the N-cycle will become available. The current representation of reactive N exchanges in the SCM involves soil-biogenic emissions as a function of temperature, moisture and precipitation as well as canopy deposition or/and emissions as a function of foliage nitrate deposition and a leaf-scale NO_x and NH₃ compensation point (concentration threshold above which leaf-scale deposition occurs whereas for lower ambient concentrations leaf-scale emissions occur)

2.2 Development of stand-alone version of multi-layer reactive N and C exchange model

Another model activity that contributed to COMBINE's WP2.5 has been the development of a stand-alone model version of the Multi-layer Canopy Chemical Exchange Model (MLC-CHEM). This model system is applied for the simulation of the exchange of reactive compounds and aerosol inside and above vegetation canopies. A main specific feature of this canopy model that distinguishes this model from other existing canopy exchange models is that MLC-CHEM can be applied for both site-scale analysis of observations, as previously presented in 2.1, as well for explicit simulation

of atmosphere-biosphere exchanges in ESMs such as COSMOS and EC_EARTH. Actually, MLC-CHEM is based on the implementation of canopy exchange processes in the Earth system model EMAC (ECHAM5/MESSy Atmospheric Chemistry model, e.g., Ganzeveld et al., 2010). The main specific feature of MLC-CHEM is that, in contrast to the canopy modeling system implemented in the SCM, MLC-CHEM is a simple offline modeling system that allows flexible use by both experimentalists and modelers for the following activities:

- Use the model to analyze surface layer observations of tracer concentrations (and fluxes) as a function of the observed micro-meteorology and vegetation cover
- Introduce new model representations of biogenic emissions, dry deposition, chemistry or turbulence and to evaluate the impact of these new models on the simulations of atmosphere-biosphere exchanges
- Study the main set-up of the modeling system in support of the further deployment of the model in other large-scale models than EMAC

MLC-CHEM consists of a number of different sub-modules that are used to calculate the different relevant processes that ultimately determine atmosphere-biosphere fluxes of reactive compounds and aerosols. In most state-of-the-art chemistry and transport models atmosphere-biosphere exchange processes are represented by separate models of biogenic emissions and dry deposition without considering interactions that occur within the canopy. This commonly applied approach (the so-called "big leaf" approach) is applicable for compounds that are inert at the timescale of turbulent exchanges (seconds – minutes – hours), e.g., exchange of N_2O and CH_4 . However, for more reactive species such as NO_x , VOCs and O_3 , canopy interactions involving emissions, chemical transformations, dry deposition and turbulence ultimately determine the effective exchange between the canopy and overlying atmosphere, being the lower boundary conditions for the ESMs that do not consider explicitly these canopy interactions.

This recent model development substantially facilitates the introduction of these canopy interactions relevant to the exchange of reactive N and C in ESMs. The actual coupling has not yet been established because of the fact that site-scale analysis, as presented below, revealed that there are still a number of essential issues to be resolved on vegetation N- and C-cycle chemical interactions. In addition, delays in getting EC_EARTH running on the WUR HPC system has further hampered progress.

3 RESULTS AND OUTLOOK

3.1 Simulations of biogenic aerosol precursors in SCM-LPJGUESS

Analysis with the coupled SCM-LPJGUESS system indicates that the model simulates realistically the site-scale micro- and boundary layer meteorology. This is essential to assess the atmosphere-biosphere exchanges of reactive carbon and nitrogen as simulated by the coupled

system since it reflects the explicit simulation of emission, dry deposition, chemistry and canopy turbulence as a function of these meteorological drivers. A realistic simulation of the on-site meteorology is consistent with previous studies with the SCM being constrained with the ECMWF re-analysis data to consider the role of advection in this 1-D ESM (Ganzeveld et al., 2006). However, from Figure 2, which shows a comparison of the simulated and observed mixing ratios of the monoterpene α -pinene, a biogenic SOA precursor, it can be inferred that the model does not capture the observed large temporal variability in α -pinene mixing ratios. The coupled model system, which has demonstrated its merits in many studies of surface and boundary layer reactive trace gas exchanges, apparently does not reproduce this particular feature of the observed short time scale variability in SOA precursors. Explaining this poor representation of the locally observed monoterpene mixing ratios would require to first analyse in detail the simulations of day-to-day variability in monoterpene emission factors as simulated by LPJGUESS and resulting canopy-scale monoterpene emission fluxes by comparison with field observations. Unfortunately, canopy-scale monoterpene emission fluxes have not been

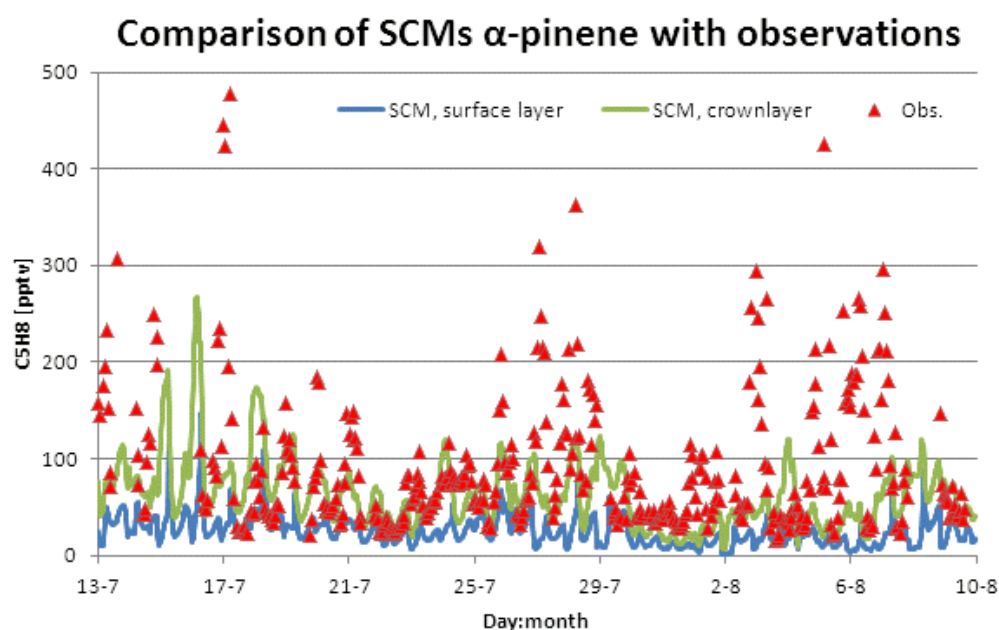


Figure 2: Comparison of simulated (surface layer, blue line, and crown layer, green line) and observed (red triangles) α -pinene mixing ratios during the HUMPPA-COPEC intensive field campaign, July 2010, Hyytiälä, Finland.

measured during this campaign. Anyhow, such a poor representation of monoterpene concentration variability poses a major limitation to assess biogenic aerosol-cloud-vegetation feedback mechanisms at a site like Hyytiälä and, likely, at many other locations.

3.2 Analysis with MLC-CHEM of observed atmosphere-biosphere exchange fluxes

The stand-alone version of the multi-layer canopy chemical exchange system has been made available to the wider research community through a couple of activities and presentations including a workshop

presented at the Max-Planck Institute for Chemistry, Mainz (January 2013) as well as presentations at the General Assembly of the EU-FP7 project ECLAIRE (Effects of Climate Change on Air Pollution Impacts and Response Strategies for European Ecosystems), October 2012. As a result MLC-CHEM is now used by a number of experimentalist's also to analyse their observations of atmosphere-biosphere fluxes and concentrations. This will support further improvement of the key components of this representation of atmosphere-biosphere chemical interactions and exchanges for implementation in ESMs. One of those site-scale analysis with MLC-CHEM focused on observed O_3 deposition at a German forest site (Linda Voss, MPI-C, Mainz, Germany, personal communications). This study highlights the importance of properly considering the role of short-term moisture impacts as illustrated by the shown dependence of the discrepancies between the measured and observed O_3 deposition flux as a function of relative humidity in Figure 3 (the colors reflect the time of the day). Including the presence of canopy wetness as a function of humidity, which results in an enhanced non-stomatal uptake as well as consideration of the vapour pressure effect, resulted in a significantly improved simulation of both nocturnal and daytime O_3 deposition fluxes. This is also relevant for assessments of the O_3 deposition impact on ecosystems since these short-term (hours) moisture impacts determine the partitioning between the stomatal and non-stomatal uptake of O_3 where only the stomatal component is believed to be mainly responsible for inducing foliage damage and resulting impacts (see Section 3.3).

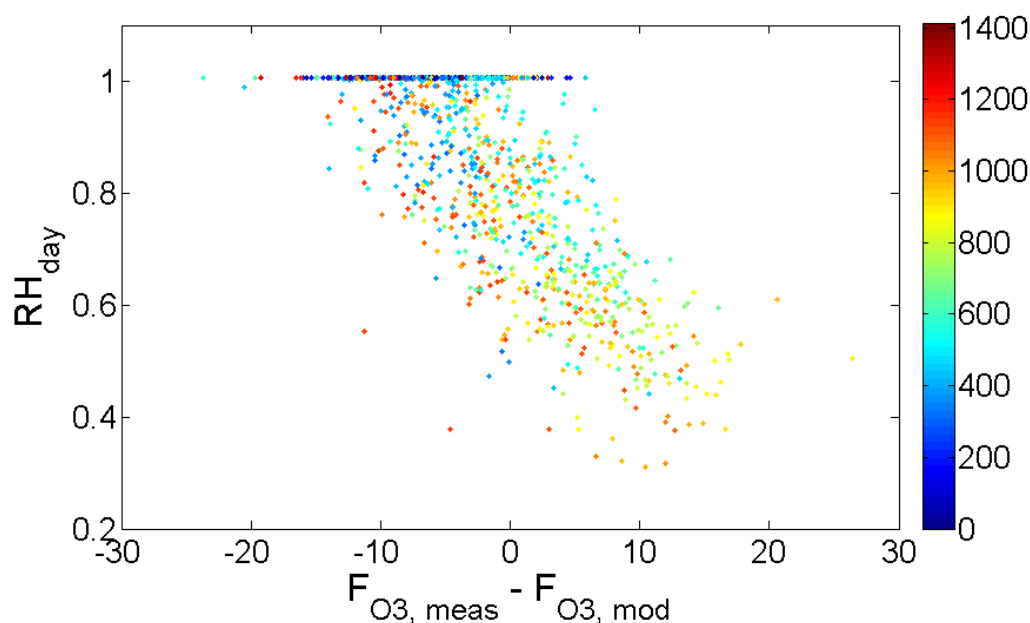


Figure 3: Difference between the measured ($F_{O_3, \text{meas}}$) and simulated ($F_{O_3, \text{mod}}$) O_3 dry deposition flux [$\text{nmol m}^{-2} \text{s}^{-1}$] as a function of relative humidity. The colors reflect the time of the day expressed in minutes (0=midnight, 720=noon). The observations were collected at a German forest site during the ExchanGE processes in mountainous Regions (EGER) - IOP3 intensive field campaign. The simulated O_3 fluxes initially ignored the role of enhanced uptake by wet vegetation and the vapour pressure deficit effect.

3.3 Feedbacks associated with reactive carbon and nitrogen exchanges: O₃ deposition impact

As has been indicated in the introduction; a main component involved in the potentially important feedback mechanism including reactive carbon and nitrogen exchanges is ozone (O₃). Biogenic emissions of reactive carbon and nitrogen affect O₃ production, which in turn feed back on the biogenic emissions through the impact of O₃ deposition on plant photosynthesis. The SCM-LPJGUESS system allows assessing this feedback mechanism through the online simulation of photo-chemistry, resulting O₃ deposition and its impact on LPJGUESS's VOC emissions. In addition, the O₃ deposition affects transpiration and CO₂ uptake through a reduced net primary production which affect boundary layer growth and

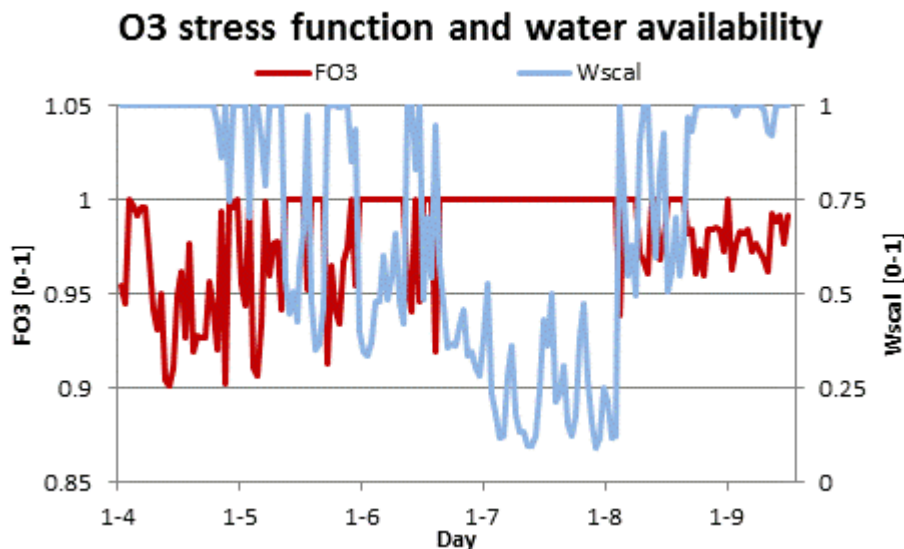


Figure 4: ozone stress value (FO_3 , 0-1, red dashed line) and water availability stress function (W_{scal} , 0-1, blue line). A value of 1 for the ozone and water stress functions reflects no ozone stress and optimal water availability, respectively.

entrainment of O₃ through changes in surface energy balance. However, assessment of the significance of this feedback mechanism by direct comparison of the involved main components with observations appears to be limited by the fact that LPJGUESS does not properly simulate the impact of soil moisture on summer transpiration. According to LPJGUESS, the July precipitation and high temperatures result in the occurrence of significant water stress resulting in a strong decrease of evapotranspiration through stomatal closure. Figure 4 shows the simulated O₃ stress and water stress expressed by the O₃ and water (soil moisture) stress functions. A value of 1 expresses no stress whereas values smaller than 1 reflect a simulated decrease in plant activity associated with these stresses. It can be inferred that especially in July-August 2010, when the HUMPPA-COPEC field campaign was conducted, the simulated water stress function in LPJGUESS indicates a substantial decrease in vegetation activity due to simulated low soil moisture conditions. Because of the direct coupling of O₃ deposition to plant-photosynthesis, the decrease in transpiration also results in strongly reduced O₃ deposition and, consequently, deposition impact exactly at the moment that observed O₃ concentrations were relatively elevated also

associated with the advection of air masses from Russia affected by strong biomass burning events. However, observations of CO₂ fluxes (shown in Figure 5) and latent heat fluxes (not shown) at the site do indicate that the forest at Hyytiala was apparently not affected by soil moisture stress during the field campaign.

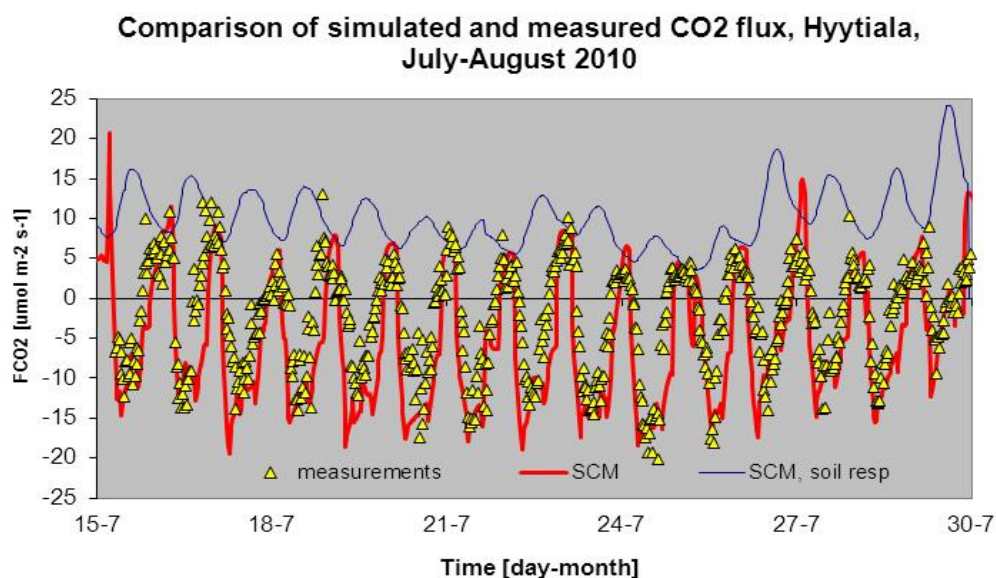


Figure 5: Comparison of the observed (yellow triangles) and simulated (red line) CO₂ fluxes during the HUMPPA-COPEC intensive field campaign, July-August 2010, indicating continuous CO₂ uptake in summer and no/limited soil moisture stress on plant-photosynthesis. Also shown is the soil CO₂ respiration flux (blue line) calculated from the SCM's soil temperature. Note that the simulated CO₂ flux is based on an alternative model simulation that uses another CO₂ photosynthesis/stomatal exchange model for non-soil moisture stress conditions compared to LPJGUESS's simulations which indicated a significant role of soil moisture stress.

These results were obtained from simulations with the coupled SCM-LPJGUESS system for the default settings on soil properties in LPJGUESS with a 1.5m deep soil moisture reservoir distinguishing two layers. To assess the sensitivity of the simulated evapotranspiration in this coupled 1-D ESM-DGVM to the representation of soil hydrology we have conducted a number of additional simulations changing the assumptions on soil hydrological properties in LPJGUESS. Two simulations actually used a substantially increased soil moisture depth of 4.5 and 7.5m, respectively, allowing for a larger storage of soil water and, consequently, a reduced sensitivity to soil moisture deficits.

Figure 6 shows the simulated normalized soil moisture (relative to the maximum soil moisture content) in the top layer for the 1.5m, 4.5 and 7.5m soil depth profile from 15th of May until the end of August. Note that the simulated soil moisture variability reflects simulations being constrained with the actual in-situ observed precipitation rates because the comparison of the observed and simulated precipitation indicates a substantial underestimation of precipitation by the SCM constrained with ECMWF re-analysis data. It can be inferred that over the growing season soil moisture is gradually decreasing except in the case of some

precipitation events. Especially after the middle of June, lack of significant precipitation results in the occurrence of very low soil moisture levels. These very low soil moisture conditions for the year 2010 resemble the simulated minimum top layer soil moisture levels for the month of July over the full 105 year period of the offline simulations with LPJGUESS for this site being constrained with CRU climate data.

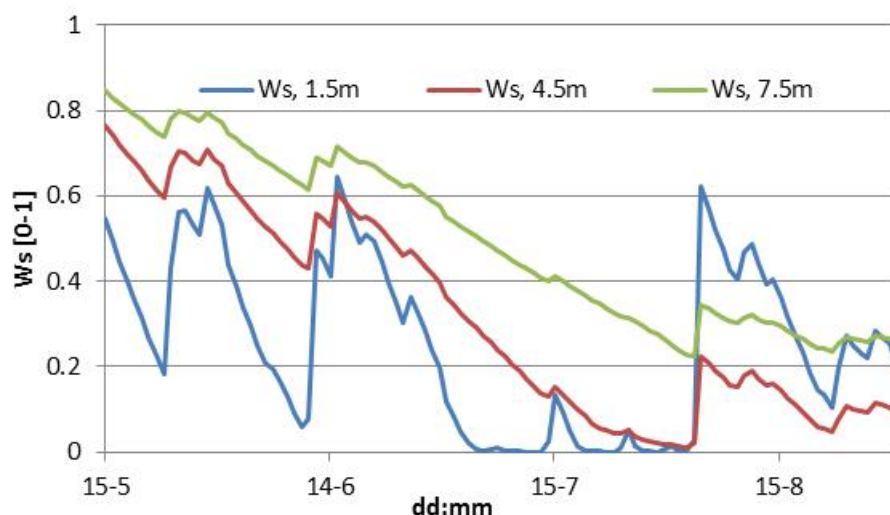


Figure 6: Simulated normalized soil moisture in top layer of LPJGUESS from 15th of May until the end of August, 2010.

The deep soil profile results in larger soil moisture content in July compared to the shallow soil profile simulations but there is still a soil moisture deficit effect that results in a negligible O₃ deposition impact due to stomatal closure over most of the measurement period (Figure 6).

The soil depth has an impact on the simulated VOC emissions: a near doubling in isoprene emissions is found in the period with a large soil moisture deficit according to LPJGUESS. There are other small changes in simulated VOC emissions due to, for example, differences in the canopy radiation regime due to differences in the simulated vertical biomass density profiles by LPJGUESS for the different soil depth assumptions. However, these differences in VOC emissions (that would be reflected in a similar difference in concentrations for an unchanged boundary layer depth) appear to be smaller compared to the discrepancies between simulated and observed VOC concentrations (see also Figure 2).

We have conducted one more sensitivity simulation in which we set the soil moisture level of both layers to 1. Figure 7 shows the simulated LAI over the 105-year period of the offline simulations comparing the default, deeper soil profile and maximum soil moisture simulations. Apparently, the annual LAI is not very sensitive to the representation of soil moisture conditions suggesting a dominating role of other drivers of NPP such as radiation and temperature. The results also show a similar small sensitivity of the annual AET and VOC emissions to the representation of soil hydrology. Thus, in contrast to the findings of the detailed analysis on

the short timescales in an effort to evaluate directly the feedbacks involved in atmospheric chemistry-vegetation interactions by comparison with observations, long-term interactions appear to be less dependent on the representation of soil hydrology.

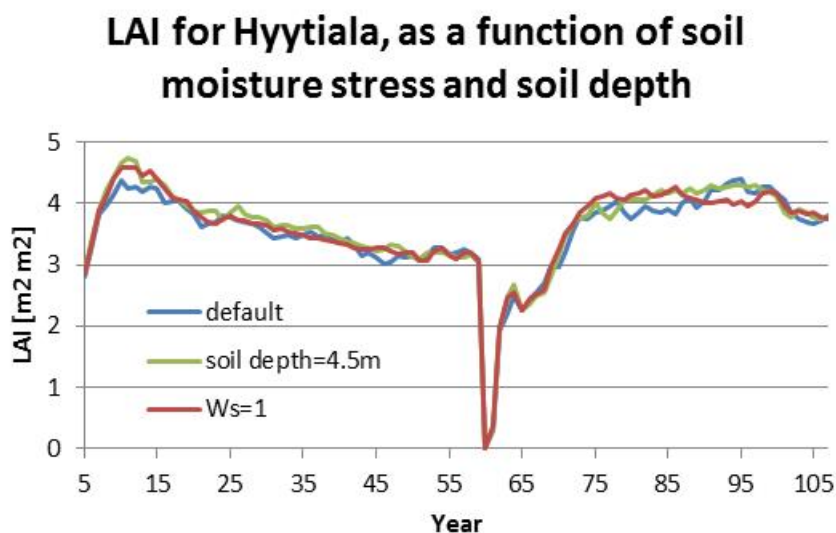


Figure 7: Simulated annual LAI for Hyytiala comparing the default model set-up of LPJGUESS with the version with a soil moisture depth of 4.5m and a simulation in which soil moisture has been set to its maximum ($W_s=1$)

The presented detailed analysis on some of these potentially important atmospheric chemistry-vegetation feedback mechanisms stresses that evaluation of the feedback mechanism based on this state-of-the-art 1-D ESM-DGVM, deemed to be representative for other (3D) ESMs-DGVMs, is largely limited by the skills of such coupled systems to actually reproduce some of the observed essential metrics involved in the feedback mechanism. It is conceivable that the results come out differently for Hyytiala for a moister and cooler summer or, for other sites with a different meteorology, hydrology and atmospheric chemistry regime. But none of those other sites do pose so many observational constraints as the Hyytiala site. Most favourably, one would want to redo the presented analysis for measurement sites more strongly impacted by high levels of pollution and being equipped comparable to the Hyytiala site.

3.3 Outlook and vision on land-atmosphere chemical and aerosol interactions in ESMs

We have presented a number of results on simulations with a 1-D ESM including a detailed representation of canopy process interactions to consider the exchange of reactive nitrogen and carbon compounds, also acting as precursors for SOA and O_3 formation and feedbacks involved in this surface and boundary layer exchange mechanism. For the latter, a coupling to the DGVM LPJ-GUESS has been established as well as to the Multi-Layer Canopy Chemical and aerosol exchange Model system (MLC-

CHEM) that facilitates implementation of these processes in 1-D and 3-D ESMs.

(1) The 1-D ESM (coupled to the DGVM and MLC-CHEM) approach is a much more sensible approach than what was originally planned (to use fully coupled 3-D ESMs) because we have now realized that it is necessary to assess and fully understand the interactions between chemical and aerosol exchange, vegetation biogeochemistry and the link with cloud processes, prior to attempting a 3-D coupling. The 1-D ESM approach should be based on dedicated studies for sites with optimal observations such as Hyytiala with the combined detailed and long-term information on chemical and aerosol exchange processes as well as micro- and boundary layer meteorological parameters involved in these feedback mechanisms. The presented detailed site-scale analysis with the 1-D ESM has revealed that we are still not capable to simulate at a satisfactory level some of the fundamental features involved in the feedback mechanisms that we are interested in. Consequently, we first need to find an optimal balanced representation of the components involved in the interaction mechanisms, an investigation that would further rely on the application of 1-D ESMs for Hyytiala and other measurement sites. This would be an essential step before we could even anticipate that introduction of improved representations of these vegetation carbon and nitrogen interactions would result in improved climate predictions with 3-D ESMs.

(2) It has been demonstrated with the 1-D ESM approach that an important issue on fundamental process understanding and representation appears to be the role of hydrological processes in these atmospheric chemistry and biogeochemistry interactions. This is based on a conducted detailed site-scale analysis for Hyytiala with the 1-D ESM system and an analysis with the stand-alone canopy exchange system MLC-CHEM for another forest site, which showed the significance of properly considering short-term moisture impacts such as canopy wetness and vapour pressure deficit effects to assess these interactions. It stresses that to allow further analysis of the proposed vegetation feedback mechanisms it is key to first improve the ESMs/DGVMs representation of site-scale hydrological processes and its role in atmosphere-biosphere exchanges of reactive compounds and aerosols. This would rely on more in-depth analysis with the SCM (or other 1-D ESMs), deemed providing results representative for global ESMs such as EC_EARTH, at a number of additional sites with detailed observations of atmosphere-biosphere exchanges as well as soil hydrological and plant physiology properties.

A second result of the presented analysis with the 1-D ESM is that it turns out that, for at least Hyytiala, where we have most optimal observations available to validate the various components involved in these feedback mechanisms, at the end the overall changes associated with the O₃ deposition appear to be very small. There are very little simulated changes in VOC emissions that would affect O₃ and its deposition impacts. Regarding this, Hyytiala is not an optimal site to study such pollution-climate feedback mechanisms since it is a relative clean site. Preferentially, we should redo the presented analysis for a more polluted

site. However, such sites that offer also such extensive observations of all relevant components are very limited.

Whenever these fundamental issues on some of the weak components involved in the presented feedback mechanisms have been resolved, availability of MLC-CHEM secures an efficient implementation in EC_EARTH (and a suite of other ESMS) to assess the global implications of the canopy- and boundary layer atmospheric chemistry and biogeochemistry interactions. In addition, the presented application of MLC-CHEM by the experimental community, to analyse in detail their observations of atmosphere-biosphere exchange, provides an optimal mechanism to apply the information gained from these observations for further improvement of the representation of vegetation interactions and feedback mechanisms in 3-D ESMS.

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