**Soil Functions in Earth’s Critical Zone – key results and conclusions**

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**Abstract**

This chapter summarises the methods, results and conclusions of a 5-year research project (SoilTrEC: soil transformations in European catchments) on experimentation, process modelling and computational simulation of soil functions and soil threats across a network of European, Chinese and USA Critical Zone Observatories (CZOs). The study focussed on the soil functions of biomass production, carbon storage, water storage and transmission, water filtration, transformation of nutrients and maintaining habitat and genetic diversity.

The principal results demonstrated that soil functions can be quantified as biophysical flows and transformations of material and energy and simulated with mathematical models of soil processes within the soil profile and at the critical zone interfaces with vegetation and atmosphere, surface waters and the below-ground vadose zone and groundwater. A new dynamic model for soil structure development, together with data sets from the CZOs, demonstrate both seasonal fluctuations in soil structure dynamics related to vegetation dynamics and soil carbon inputs, and long-term trends (decade) trends in soil carbon storage and soil structure development.

Cross-site comparison for 20 soil profiles at 7 field sites with variation in soil type, lithology, land cover, land use and climate demonstrated that sites can be classified using model parameter values for soil aggregation processes together with climatic conditions and soil physical properties, along a trajectory of soil structure development from incipient soil formation through productive land use to overly-intensive land use with soil degradation.

A new modelling code, the Integrated Critical Zone Model, was applied with parameter sets developed from the CZO site data to simulate the biophysical flows and transformations that quantify multiple soil functions. Process simulations coupled the new model for soil structure dynamics with existing modelling approaches for soil carbon dynamics, nutrient transformations, vegetation dynamics, hydrological flow and transport, and geochemical equilibria and mineral weathering reactions. Successful calibration, testing and application of the model with data sets from horticulture plot manipulation experiments demonstrate the potential to apply modelling and simulation to the scoping and design of new practices and policy options to enhance soil functions and reduce soil threats worldwide.

**Introduction**

 Increasing human population and wealth are placing unprecedented pressure on Earth’s soil and water resources. Drivers for resource demand are a projected increase in human population to 9.7 billion by 2050 (Pison, 2013) with an associated quadrupling in the global economy (Manders et al., 2012) and projected doubling in demand for food (World Bank, 2008) and fuel (Manders et al., 2012) and a more than 50% increase in demand for clean water (Leflaive et al., 2012). These resources will be required during a period of accelerating impacts from predicted changes in global climate with the Intergovernmental Panel on Climate Change (IPCC) 5th report projecting decreasing water availability in major global agricultural regions of Asia, Africa and Latin America (IPCC, 2014), and with increasing global biodiversity decline driven by land use intensification for agriculture and urbanisation (Newbold et al., 2011). The United Nations (UN) Environment Programme (UNEP) report on Global Land Use summarises evidence that by 2050 the demand for productive land will increase by 320-850 Mha which is estimated to be 10-45% greater than the environmental capacity for the sustainable use of Earth’s land resources (UNEP, 2014).

 Policy responses to these pressures on global soils define soil functions as environmental goods and services and identify global soil threats that degrade soil functions ((EC, 2006a,b; Banwart, 2011)). European Commission policy (EC, 2012) defines soil as all unconsolidated material from the land surface to the bedrock and considers the role of water flow and transport to expose the deeper subsurface to contamination and other inputs from the land surface. This conceptualisation of the soil system is coherent with scientific advances in the study of Earth’s critical zone (CZ). The CZ is the thin surface layer that extends from the top of vegetation to the bottom of groundwater circulation and supplies humans with most life-sustaining resources (NRC, 2001; Anderson et al., 2004; Brantley et al., 2007). The study of Earth’s CZ defines a new field of integrating environmental science that combines theory and observation methods from many fields of science. CZ science is largely congruent with other integrating sciences of the natural environment (Richter and Billings, 2015), but places a relatively greater emphasis on understanding the vertical integration through the full depth of the CZ and on the mechanistic understanding of CZ processes across physical scales from nanometric to global and across temporal scales from sub-second to those of tectonic forcing. A major research challenge for the study of soil functions within CZ science is addressing the sharp vertical gradients in physical, chemical and biological conditions within the CZ, from the oxic, rapid circulation of the atmosphere to the anoxic, slow-flowing circulation of aquifers, often encountered over depths on the order of only 5-10m and including the full genetic and functional biodiversity of Earth’s terrestrial surface.

Earth’s soil layer is at the heart of the CZ, as a reactive layer that transmits mass, energy and biodiversity and which transforms within the soil volume the input flows and generates output flows, both downwards to the groundwater, upwards to the vegetation and atmosphere, and laterally to surface waters (Figure 1). Soil functions are defined as the sets of flows and transformations that provide benefits for humans and align with the broad concept of environmental good and services, most visibly articulated as the ecosystem services defined by the Millennium Ecosystem Assessment (MEA, 2005). The present study focuses on quantitative methods to understand the soil functions defined in Figure 1; i.e. biomass production, carbon and nitrogen storage associated with climate regulation, water storage and transmission, water filtration and attenuation of contaminants, transformation of nutrients for soil fertility, and maintaining habitat and genetic diversity.

 Within this framework, soil functions are degraded when the soil processes that maintain fluxes and transformations are altered such that the benefits derived from these soil functions are decreased or lost. Soil threats are defined as human pressures from land use that are known to degrade soil functions and include soil erosion, loss of soil organic matter, decline in soil biodiversity, soil acidification, mechanical compaction, sealing by infrastructure, salinization from irrigation water evapotranspiration and industrial contamination (EC, 2006a; FAO and ITPS, 2015). Recent compilations of scientific evidence for global soil decline include Amundson et al. (2015) who summarise current data and uncertainties on soil organic matter stocks and vulnerabilities for accelerated greenhouse gas emissions from soil, Banwart et al., (Eds., 2014) who compiled evidence on soil organic matter decline and the potential for innovation in land management practices and policy to improve soil carbon stocks, and the UN Food and Agriculture Organisation (FAO) report on the status of the World’s soils (FAO and ITPS, 2015).

 The aim of this study and outcomes reported in this volume are to provide independent scientific evidence and new methods of mathematical modelling of soil processes to quantify soil functions. The hypotheses and experimental design have been previously reported (Banwart et al., 2011) as have initial results of the research project (Banwart et al., 2012). Summarising briefly, the hypotheses are that the intensity of human land use defines a life cycle of soil function, where soil functions develop from parent material, support terrestrial ecosystems which humans utilise for agriculture, forestry and other productive land uses, and that soil functions decline under increasingly over-intensive land use, with the potential under conditions of extreme degradation to lose all soil functions through a complete loss of bulk soil by physical erosion of surface soils down to parent material.

 A secondary hypothesis builds on the concepts of Graham et al. (2010) and Brantley (2010) that development of the subsurface porosity structure through combined weathering and fluid circulation gives rise to soil functions. This view of pedogenesis places relatively greater emphasis on the definition of soil functions as the evolution of natural processes and their rates and physical extent. From this framework, the present study hypothesises that the development of soil pore structure and the soil aggregation strongly correlates with the development of soil functions (Banwart et al., 2011, 2012). The research design for this project thus focusses on quantifying through observation, and the development of mathematical models to simulate, the dynamics of soil structure in connection with the soil functions illustrated in Figure 1.

 The specific objectives of the full research project have been previously presented (Banwart, 2011, 2012). The focus of the studies presented in this volume are to:

1. Develop a conceptual model for soil structure dynamics and translate it into mathematical models,
2. Obtain data on soil functions from Critical Zone Observatories across gradients of land use intensity,
3. Study soil processes at field scale and gain data to test models for soil structure dynamics,
4. Develop a Critical Zone Integrated Model (ICZM) that quantifies soil functions (Figure 1) as flows and transformations of mass, energy and biodiversity and their dependence on soil structure, and
5. Apply field observations from Critical Zone Observatories (CZOs) and results from computational simulation in order to quantify soil functions, assess the economic value of selected soil functions, and assess soil threats at EU scale.

This chapter provides a summary of the key advances that were achieved and introduces the detailed experimental and modelling studies which comprised much of the project and are presented in subsequent chapters.

**Research Methods**

The overarching experimental design is to quantify soil structure and process at research field sites that are Critical Zone Observatories (CZOs) located along a gradient of land use intensity that defines a conceptual life cycle of soil functions (Banwart et al., 2011). Four European field sites were selected as CZOs that characterise key stages of land use intensity of relevance for soil management and policy innovation (site descriptions provided in Banwart et al., 2011).

1. The Damma Glacier CZO, Switzerland, allows the study of incipient soil formation in the glacial forefield as the glacier retreats, exposing the underlying bedrock. A chronosequence on the order of centuries allows the earliest stages of soil formation to be observed.
2. The Lysina-Slavkov Forest CZO, Czech Republic, allows the study of soil processes during managed forest land use for intensive silvaculture.
3. The Fuchsenbigl-Marchfeld CZO, Austria, allows the study of soil processes during managed arable land use for production agriculture.
4. The Koiliaris River CZO, Crete, allows the study of highly degraded soils that have experienced millennia of intensive agricultural land use, including grazing, and is under additional threat from desertification due to modern climate change.

The research method was to select and characterise essential terrestrial variable across the 4 sites, and across different land cover and land use within the sites, at the physical scale of the soil profile. The selection of variables was prioritised in order to parameterise mathematical models of vegetation dynamics, soil structure dynamics, soil carbon dynamics, nutrient transformations, hydrological flow and reactive transport, mineral weathering, and a highly simplified model of the soil food web. Common soil variables are listed in Banwart et al. (2011, Table 1) and additional variables are presented in the individual studies within this volume or otherwise cited from the literature.

 Development of the conceptual model for soil functions as flows and transformations (Figure 1) utilised concepts of mass flux balance by physical flow and transport processes across flux planes which defined physical interfaces of the CZ; atmosphere-vegetation, vegetation-soil, soil-vadose, vadose- groundwater (Figure 2). Mass transformations were conceptualised within the plant-soil-water system as plant production of biomass, development of soil microbial biomass, aqueous chemical reactions and mass transfer processes between soil particles and fluids. Translation to mathematical equations utilised theory of fluid flow and advective transport, diffusion and dispersion; empirical rules for rates and stoichiometry of plant growth from known plant physiology and traits; thermodynamic and kinetic laws of mass action for geochemical reactions; phenomenological zero- or first-order rate laws for soil carbon degradation, soil structure dynamics, and soil N and P transformations.

 The terrestrial variables selected for experimental study were identified from the beginning of the study in order to support the parameterisation of the process models. A new model for soil structure was developed, the Carbon Aggregation and Structure Turnover (CAST) model (Stamati et al., 2013), and applied in a number of studies reported in this volume. In brief, the model considered soil structure to be defined by 3 size classes of soil aggregates, particle size (dp) < 53µm, 53µm < dp < 250 µm, and dp > 250µm, composed of mineral soil texture units (clay-, silt- and sand-sized particles), living organisms, decomposing biomass, and fluids and solutes. As the mass fractions of soil aggregates change, new values for soil properties of bulk density, porosity, and saturated hydraulic conductivity are calculated. The model defines first-order rate laws for mass transfer of organic carbon and mineral texture units between aggregate size classes, and for mineralisation of organic carbon within each size class, and calibrates the rate constants with site-specific data on organic matter inputs, soil texture, structure and organic carbon content in aggregate size classes (Stamati, et al., 2013). The code allows simulation of flows and transformations that define the soil functions of carbon storage and water transmission and storage.

 A new mathematical model for soil processes, the Integrated Critical Zone Model (ICZM) for computational simulation of multiple soil functions, in addition to those simulated with CAST, allowed calculation of process rates associated with water filtration, nutrient transformations, and biomass production. The ICZM embeds the CAST model within a reactive transport model at soil profile scale which is driven by inputs from models of vegetation dynamics and soil hydrology. These processes are coupled with a highly simplified model of the soil food web which includes dynamic representation of biomass growth from producers (plant roots and their mycorrhizal fungi), heterotrophic biomass decomposers (bacteria and fungi), and grazing pressure exerted by consumers (fauna).

As described by Kotronakis et al. (2016), the ICZM (Figure 3) integrates process descriptions from the CAST model for structure and carbon dynamics (Stamati et al, 2013) and existing codes for the simulation of vegetation dynamics (PROSUM, Giannakis et al., 2016), 1-D water flow, reactive transport and energy transfer (Hydrus 1-D, Šimůnek et al., 2009), geochemical speciation based on the BRNS model (Aguilera et al., 2005) and weathering kinetics based on the SAFE component of the ForSAFE model, Wallman et al., 2005). The 1-D ICZM has been added as a module within the Soil and Water Agriculture Tool (SWAT, Gassman et al., 2007) for 3-D dynamic simulation of soil functions at landscape scale.

**Overview of Results**

 Conceptual site models of the 4 CZOs (Figure 4a-d) incorporate information from existing site characterisation and monitoring data (Panakoulia et al., 2016) and new soil characterisation data from soil profile sampling across the CZOs (Rouseva et al., 2016). Mathematical models and parameter sets translated from these conceptual models using the CAST code quantified for soil profiles the biophysical flows and transformations that define the soil functions within and between CZOs (Panakoulia et al., 2016). Comparison of site characteristics and model results distinguish the state of soil functions between sites, exemplified by comparison of climate conditions, soil carbon flux balance and organic matter decomposition rate constants for the 4 CZOs (Figure 5).

Incipient soil formation at the Damma Glacier CZO correlates with low rates of biological productivity and organic matter input to the soil at the early stages (< 20 years age) but demonstrates around half of the input organic carbon is stored in the soil each year. The conceptual model for the Damma Glacier CZO (Figure 4a) demonstrates increasing mass of stored carbon in soil as an intensifying soil function at later stages of soil profile development within the chronsequence at the site. Comparison of the carbon flux balance for the Damma Glacier site with that of the Slavkov Forest CZO demonstrates a substantially greater input of organic matter to the soil resulting from the far greater biological productivity for the mature plantation forest, however, with a far smaller fraction of the organic carbon that is input to soil being stored, compared to the young soils of the Damma Glacier.

Comparison with the soil C flux results for the Marchfeld CZO (Figure 5c) demonstrates nearly equal rates of organic carbon input to soil and mineralisation, with a small loss of soil carbon calculated for the conditions of intensive mechanical agricultural practices on the arable farmland. The results for the Koiliaris CZO are substantially different, showing a significantly greater loss of soil organic C from mineralisation, compared to inputs from biological productivity, indicating a substantial, ongoing loss of soil organic C. From these results, the calculated rates of soil C accumulation serve to quantify the soil function of carbon storage and indicate a degraded soil function under arable land use, with indications of low rates of soil C loss. The results presented for the Koiliaris CZO represent intense arable agriculture and horticulture and demonstrate a severely degraded soil function with a loss of carbon storage function and an ongoing loss of soil organic C through mineralisation.

 Results of the ICZM model calibration for the Koiliaris CZO horticulture experiments, which are reported in detail by Giannakis et al. (2016), demonstrate the dynamics of soil structure development and the associated dynamics of organic C content within aggregate size fractions (Figure 6a,b). For the simulated 10-year period, corresponding to conventional horticulture practices utilising mineral fertiliser to supplement soil fertility, there are intra-annual fluctuations in soil organic carbon content and soil structure due to organic C inputs and removal during the cropping season, and a long-term decline in soil organic carbon (on the order of 10%) primarily associated to loss of carbon from macroaggregates (dp > 250 µm).

 Incorporation of the CAST model code into the ICZM allows bulk soil properties to be simulated dynamically at soil profile scale. The detailed results reported by Kotronakis et al., (2016) show how bulk density, porosity, water holding capacity and saturated hydraulic conductivity are calculated from changes in soil structure. These dynamic properties of soil are in turn utilised by the modelling code to quantify water and gas content, plant available water and uptake, infiltration flow and vertical advective transport velocity. From these calculations, the biophysical flows and transformations are quantified and define the multiple soil functions presented above.

 The detailed studies (summarised in Table 1) published previously or reported in this volume illustrate this methodology to implement soil characterisation and field experimental data (Rouseva et al., 2016; Regelink et al., 2015; Blaud et al., 2016; Wang et al., 2016a,b; Liu et al., 2016) in mathematical modelling studies to quantify changes in soil carbon and structure and the relation of soil structure changes to changes in soil functions (Stamati et al., 2013; Li et al., 2015; Andrianaki et al., 2016); synthesis of modelling results for soil C sequestration, soil aggregation and soil structure development across multiple sites in the USA, Europe and China (Panakoulia et al., 2016), application of parameter sets and model simulations to evaluate biophysical flows and transformations that define multiple soil functions (Kotronakis et al., 2016; Giannakis et al., 2016); and their translation into environmental service flows for economic valuation (Jónsson et al., 2016).

**Discussion**

 This series of published results shows that the dynamics of soil structure are driven by temporal trends and fluctuations in soil organic matter input to soil including that from dynamic vegetation production, and land use practices such as tillage, fertilisation and irrigation. The detailed results demonstrate that the simulated biophysical flows and transformations that define soil functions are affected by, and in some cases sensitive to, the dynamic behaviour of soil structure. The mathematical models described here quantify the mechanistic linkages between physical, chemical and biological processes that determine the flows and transformations and define soil functions. Bulk soil physical properties, particularly pore size distribution and permeability, impact water holding capacity and drainage rates (Rouseva et al., 2016). Increasing soil aggregation increases both the potential for water storage within the micropores of aggregating soil (Regelink, 2015; Rouseva et al., 2016) and the potential for improved drainage through the larger resulting interaggregate pores (Kotronakis et al., 2016). Therefore, enhanced soil functions of water storage and transmission correlate with increased soil aggregation.

Changes in porosity distribution and permeability that arise from soil aggregation also influence O2 ingress for root respiration, water holding capacity, plant available water and hence vegetation production. The associated plant litter and below-ground biomass production determines the rate of input of soil organic matter in the absence of amendments and through the role of mass action, drives macroaggregate formation and turnover of nutrients from particulate organic matter decomposition. A portion of the decomposing biomass is processed as humic material and becomes associated with the clay-silt sized texture units, with the potential to stabilise soil carbon by formation of organo-mineral complexes and incorporation of basic texture units into microaggregates and macroaggregates which further offer physical and chemical protection (Stamati et al., 2013). Therefore, enhanced soil functions of nutrient transformation, biomass production and carbon storage correlate with increased soil aggregation.

Increased vegetation production and soil organic matter input also increases the flow of carbon and energy to support heterotrophic respiration as the base of the soil food web. The interior of soil aggregates can maintain anoxic conditions that select for anaerobic respiration processes that sit alongside the ingress of O2 in interaggregate pores which supports aerobic respiration at the exterior of macroaggregates. Hence, greater diversity of soil microhabitat and selection pressure for functional microbial diversity is expected to correlate with increasing soil aggregation, although this level of analysis of biodiversity is not addressed in the mathematical models. If this reasoning holds, then enhanced soil functions of maintaining habitat and gene pool correlate with vegetation production and increasing soil aggregation. Furthermore, as a consequence of maintaining functional biodiversity, the role of the soil microbiome in filtering water is supported, through functional guilds that degrade organic contaminants and process organic matter to release organic forms of N directly to plants rather than nitrification with transport to receiving waters as nutrient contamination. For these cases, enhancing the soil function of filtering water also correlates with increasing soil aggregation.

In conclusion, this series of studies builds on the framework of Earth’s critical zone where soil is a central reactive layer at Earth’s surface that receives inputs of energy, mass and biodiversity, transmits and transforms these across the reacting layer, and produces output flows both above- and below-ground. This concept of soil as a reactive layer with soil functions as biophysical flows and transformations establishes soil as a control point in Earth’s critical zone. Through measurement and quantitative analysis, represented by the data sets and modelling results of this study, human intervention can be planned in order to impact specific soil functions; i.e. to store more carbon, remove more contamination, produce more biomass, reduce greenhouse gas emissions and increase recharge to groundwater, to name a few.

Central to this framework is the development from regolith of porosity, fluid circulation, vegetation production, and resulting carbon, energy and water inputs to soil - to drive the flows and transformations of multiple soil functions. Analysis of the state of soil functions therefore requires information on the state of soil structure. A quantitative understanding of how human intervention can improve soil structure, for example through soil organic carbon amendment as studied by Kotronakis et al. (2016), holds the potential to positively influence multiple soil functions and through mathematical modelling and computational simulation to both scope potential interventions and to interpret experiments and field trials.

The results presented here and in the cited studies include new soil and site characterisation data sets across a range of field sites which represent substantial variation in lithology, soil type, climate and land use intensity that includes both natural and agricultural sites and experimental manipulations. The results include data to aid understanding of the interactions between soil structure and soil process rates, new modelling codes to interpret the data sets, model parameter sets for this range of sites and soil processes, and mathematical modelling results to quantify biophysical flows and transformations that define multiple soil functions at the field sites.

This approach of defining soil functions as flows and transformations is challenging. Model parameter values are often not available from first principles analysis and must be determined from extensive and thus potentially expensive site-specific data. Some soil functions, such as maintaining habitat and gene pool, continue to be treated (for the models presented here) in an excessively simplified way. However, modelling theory such as energy conservation and flow balance through food webs offers the potential to translate more complex conceptual models of these soil functions into mathematical expressions that can be coupled more comprehensively to process models such as the CAST and ICZM codes described here.

The compilation of site data and parameter sets from a multiple CZOs and other field sites along gradients of change, in this study with a focus on land use intensity, is a step forward. Currently, the international community envisages networks of sites from many regions with the potential for experimental design along other gradients of change; e.g. including climate, vegetation cover, lithology, stages of urbanisations and others. Such efforts on cross-site programmes for observation and modelling are underway (Brantley et al., 2015). The experience obtained from jointly studying the range of sites presented by Panakoulia et al. (2016) can offer evidence for successful experimental design as well as hindsight for potential pitfalls to be avoided.

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