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Article:

Banwart, S.A., Bernasconi, S.M., Blum, W.E.H. et al. (19 more authors) (2017) Soil Functions in Earth's Critical Zone: Key Results and Conclusions. Advances in Agronomy, 142. pp. 119-142. ISSN 0065-2113

https://doi.org/10.1016/bs.agron.2016.11.001

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Table 1. Summary of Soil Characterisation, Experimental and Mathematical Modelling Studies

No.	Study Title	Summary Outcomes
1	Soil Water Characteristics of European SoilTrEC Critical Zone Observatories Rouseva et al. (2016)	Soil sampling and characterisation by horizon in soil profiles at the European CZO sites provides qualitative and quantitative data on soil texture, soil structure, water retention curves, particle size and porosity distribution, and permeability to evaluate soil state and provide parameter values for soil process models.
2	Linkages between aggregate formation, porosity and soil chemical properties Regelink et al. (2015)	Results from physical characterisation of dry- and wet-sieved aggregate size fractions quantified the distributions of micro- and meso-porosity as a function of aggregate mass fraction by size and demonstrate that formation of water stable aggregates correlated significantly with iron oxide content, suggesting that these oxides and their known role in forming organo-mineral complexes with soil organic matter may be important in soil structure development.
3	Reduced subsurface lateral flow in agroforestry system is balanced by increased water retention capacity: rainfall simulation and model validation Wang et al., (2016a)	Results from experimental rainfall simulations on soil planted with arable crops and trees are compared to elucidate the impact of plant roots to enhance vertical infiltration and reduce later flow, in order to provide mechanistic insights and quantitative data on soil water storage and transmission for agronomic benefit.
4	Interception of subsurface lateral flow through enhanced vertical preferential flow in an agroforestry system observed using dye tracing and rainfall simulation experiments Wang et al. (2016b)	Results from experimental rainfall simulations on soil planted with arable crops and trees, combined with flow balance calculations and digital imaging and image analysis of tracer transport with infiltrating water quantify vertical and lateral flow rates and provide evidence that soils with tree roots have enhanced vertical infiltration rates compared with soils in arable farming.
5	Effects of dry- and wet-sieving of soil on identification and interpretation of microbial community composition Blaud et al. (2016)	Quantitative results on gene copy number for selected functional guilds of organisms from the soil microbiome show that wet sieving and dry sieving result in significant differences in apparent microbial diversity by aggregate size class and by land use illustrating, the importance of the soil microphysical structure as habitat that exerts selection pressure on the microbiome and, that physical characterisation methods can influence measurements of microbial biodiversity
6	An ecosystem approach to assess soil quality in organically and conventionally managed farms in Iceland and Austria	Data on soil biodiversity combined with data on soil physical and chemical properties was used to compare soil functions on 2 pairs of farms, on in the sub-arctic and one in temperature central Europe, with each pair including a conventional farm and an organic farm. The food web structure in terms of trophic groups diversity was similar between the 4 sites but with generally greater

	Van Leeuwen et al. (2014)	microbial and nematode biomass and greater taxonomic diversity of microarthropods on organic farms.
7	Soil mineralogy changes with different agricultural practices during eight-year soil development from the parent material of a Mollisol Liu et al. (2016)	A manipulation experiment replaced the top 0.8m of soil from the China black soil region with bare parent material from > 2m depth, as an analogue to a degraded soil, and compared the role of different agricultural practices for arable farming to potentially restore soil functions on the parent material. Significant and rapid changes in clay mineralogy occurred during the 10-year experiment and were influenced significantly by the availability and cycling of potassium ion as an exchangeable cation mineral nutrient, and that the amount and mechanisms of organic matter association with mineral surfaces was substantially different for different clay mineral phases, and that there were substantial differences in clay mineral phases associated with different particle size classes.
8	A coupled carbon, aggregation, and structure turnover (CAST) model for topsoils Stamati et al. (2013)	Results are presented for a newly developed mathematical model of soil processes that describe the coupled dynamics of soil organic carbon and soil structure and quantify sequestration of soil organic matter. The study describes the underlying conceptual model and translation to a dynamic model of soil processes, the model code and equations, and includes parameter sets obtained from site-specific model calibration. The results demonstrate the soil processes responsible for the quantitative changes in soil carbon sequestration and/or loss during land use change from arable agriculture to set-aside. Rapid degradation of particulate organic matter in large aggregates results in release of plant available forms of N explains the soil function of nutrient transformation, and slow degradation of humified organic matter bound to mineral surfaces in the clay-silt sized mass fraction explains the soil function of carbon storage.
9	Modeling soil aggregation at the early pedogenesis stage from the parent material of a Mollisol under different agricultural practices Li et al. (2016)	Mathematical modelling was applied to a 2-year series of data on soil chemistry and structure under different practices of arable agriculture to restore degraded soils represented by parent material underlying mollisols of the China black soil region. Rapid development of soil structure and larger aggregates was observed particularly for practices with the highest organic matter input. The results demonstrate the potential for arable farming practices to influence, through beneficial intervention, the soil carbon stocks and soil structure on the time scale of the annual cropping cycle.
10	Quantifying the Incipient Development of Soil Structure and Functions within a Glacial Forefield Chronosequence Andrianaki et al. (2016)	Results of mathematical modelling of soil function development along a chronosequence of soil formation in the Damma Glacier forefield demonstrated that dynamic modelling of soil organic carbon inputs and soil structure dynamics could reproduce the time series of soil function development along the chronsequence, and that this development was sensitive to the time series input of biological productivity and associated inputs of particulate organic carbon to drive soil structure and soil function development.
11	Factors controlling soil structure dynamics and carbon sequestration	Mathematical modelling results for soil structure development and soil organic carbon dynamics quantified model parameter values and soil carbon flux balances for soil profiles at 20 plots within 7

	across different climatic and lithological conditions Panakoulia et al. (2016)	different field sites representing a wide range of soil conditions and land use in the USA, Europe and China. Model parameter values were combined with soil characterisation data for the plots and were analysed using principle component analysis which demonstrated the soils clustered discretely by sites along a hypothesised life cycle of soil function. Dominant factors in the clustering included carbon degradation rate constants, organic matter input, clay mineral content, microbial biomass and humic material content of aggregates, evapotranspiration and others.
12	Integrated Critical Zone Model (1D-ICZ): A Tool for Dynamic Simulation of Soil Functions and Soil Structure Giannakis et al. (2016)	Experimental time series data for a horticulture small plot experiment with mineral fertiliser addition to augment soil fertility, allowed calibration of the Integrated Critical Zone Model and testing of the model calculation of state variable values against measured values. The study describes the soil processes included in the simulation methodology and includes soil carbon and soil structure dynamics, soil nutrient transformations, vegetation dynamics, a simplified soil food web model, hydrological flow and transport and geochemical speciation and weathering kinetics. The study documents the mathematical structure and computational procedure for the model code, the parameter sets for the calibrated model, and demonstration of goodness-of-fit for state variables.
13	Modeling the impact of carbon amendments on soil ecosystem functions using the 1D-ICZ model Kotronakis et al. (2016)	Results from tomato horticulture plot manipulation experiments using different soil amendments with organic carbon provided data to apply the Integrated Critical Zone Model to assess the impact of different mineral fertiliser, compost and manure additions on soil functions. Biomass production, C and N storage, nutrient transformation and water transmission and filtration were evaluated. Soil structure, biomass production and carbon storage improved most with the organic matter amendments but the water filtration function was adversely affected with greater nitrate loss to drainage water compared to mineral fertiliser addition. The model application demonstrates the practical value in using computational simulation together with field observation to test soil management options, interpret field measurement and to scope and design potential innovations in soil management and agriculture.
14	Valuation of Soil Ecosystem Services Jónsson et al. (2016)	Biophysical flows and transformations that are quantified in field measurements and modelling studies of the Koiliaris CZO are translated into environmental service flows that quantitatively represent the soil functions of biomass production, water filtration and carbon storage. Spatial variability in environmental service flows arising from variable soil type, land cover and land use results in geospatial variation in economic value for soil functions that are mapped for the Koiliaris River watershed. Values are expressed in international dollars per hectare per year and include positive economic value for the soil functions of water filtration to remove nitrate from river discharge and biomass production from agriculture, and environmental costs for the soil function of carbon storage due to the ongoing loss of soil organic matter in the watershed.

Figure Captions

Figure 1. The architecture of Earth's Critical Zone (CZ) with soil functions described as flows and transformations of mass, energy and genetic information. Arrows show flow and transport pathways and classes of transformation processes that define soil functions which provide benefits to humans. Text boxes name the associated soil functions that are the focus of this study.

Figure 2. Earth's critical zone soil layer and its functions. Translation of soil functions into mathematical descriptions of flows and transformations applies flux balance equations across hypothetical horizontal planes that are defined by the top of the vegetation canopy, the land surface, the bottom of the soil profile, the water table, and considers water mass exchange with surface waters. Mass transfer and transport equations apply principles of physics from continuum mechanics that describe fluid flow and mass transport by advection, diffusion and dispersion in freshwaters and the atmosphere. Mass transformations are described by the thermodynamic law of mass action for reversible reactions and the kinetic law of mass action for irreversible reactions. Biodiversity is described by functional pools of organisms as producers, decomposers and consumers by applying food web theory to this highly simplified network of functional groups.

Figure 3. A schematic diagram of the modelling approach applied with the Integrated Critical Zone Model. Individual process models were applied using data from the CZOs sites in order to develop parameter sets and test model representations of site processes and rates. The individual modelling codes were integrated into the coupled 1-D ICZM for simulation of multiple soil functions and the 1-D ICZM was also embedded as a module within the SWAT code for simulation of soil functions and their geospatial variation with soil properties and land cover and land use at catchment scale.

Figure 4. Conceptual site models for the 4 European CZOs representing different stages of the life cycle for soil functions; (a) Damma Glacier CZO representing incipient soil formation from freshly

exposed parent material, (b) Lysina-Slavkov Forest CZO representing productive plantation forestry, (c) Fuchsenbigl/Marchfeld CZO representing productive agriculture grassland, arable agriculture land and forest, and (d) the Koiliaris CZO representing degraded soils undergoing desertification under land use pressures from long-term intensive agriculture.

Figure 5. A summary of climatic conditions (temperature, C; mean annual precipitation, mm), carbon flows (tonnes C ha^{-1} y^{-1}), plant available water capacity (PAWC, mm) and decomposition rate constants in soil for fresh particulate organic matter (k_{litter}, y^{-1}) at the 4 European Critical Zone Observatories. The Slavkov Forest CZO results are for the Lysina site; the Marchfeld results are for the M4 site, intensively farmed arable land; and the Koiliaris CZO results are for site K2, intensively managed horticulture land near sea level. The sites are placed along a gradient of climate from the alpine through temperate to Mediterranean, and along a gradient of increasing intensively managed land. The Koiliaris CZO has been under long-term (centuries) intensive land use for horticulture and livestock grazing. This conceptual model of a life cycle of soil functions is represented by the circle within the centre of the figure which illustrates the following stages of soil function development following exposure or deposition of regolith at the land surface; soil profile development, terrestrial ecosystem development, human development of land use, intensification of land use, and potential loss of soil functions with physical erosion of the soil profile to again expose fresh regolith.

Figure 6. (a) Results of model calibration for the Integrated Critical Zone Model applied to horticulture experiments at the Koiliaris CZO (Giannakis et al., 2016) for (a) soil organic carbon (SOC, tonnes C/ha) and (b) water stable aggregate mass fraction (%) over a 10-year period. The experimental treatment is application of mineral fertiliser. Parameter values for mathematical rate expressions that calculate carbon degradation and aggregate formation and loss are constrained by data obtained at the start of the experiment during year 5 of the simulation period.